IBM

Application Program

GH20-0205-4

System/360 Scientific Subroutine Package

Version III

Programmer's Manual

Program Number 360A-CM-03X

The Scientific Subroutine Package (SSP) is a collection of over 250 FORTRAN subroutines divided, for the sake of presentation, into two groups: statistics and mathematics. Also, over 200 subroutines are presented in both single and double precision mode. SSP is a collection of input/output-free computational building blocks that can be combined with a user's input, output, or computational routines to meet his needs. The package can be applied to the solution of many problems in industry, science, and engineering.

Version 3 of the Scientific Subroutine Package for System/360 incorporates and extends the capabilities of the original SSP/360. This version provides over 40 new mathematical and statistical subroutines 24 of which are in both single- and double-precision FORTRAN. Examples of the new capabilities are the use of the QR iteration for obtaining eigenvalues of a matrix, and the nonparametric test of Kolmogorov-Smirnov.

This manual contains sufficient information to permit the reader to understand and use all of the subroutines of the Scientific Subroutine Package.

Fifth Edition (August 1970)

This edition, GH20-0205-4, is a reprint of GH20-0205-3 incorporating TNL GN20-1994. It does not obsolete GH20-0205-3 as updated by that TNL.

This edition applies to Version 3, Modification Level 1, of System/360 Scientific Subroutine Package (360A-CM-03X) and to all subsequent versions and modifications until otherwise indicated in new editions or Technical Newsletters.

Changes are continually made to the information herein. Therefore, before using this publication, consult the latest System/360 SRL Newsletter (GN20-0360) for the editions that are applicable and current.

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This programming package has been developed with the cooperation and assistance of IBM Germany and IBM France.

PURPOSE AND OBJECTIVES OF THE PACKAGE

The Scientific Subroutine Package is a set of basic computational subroutines intended to aid the user in the development of his own FORTRAN subroutine library. While this package may provide many of the tools necessary to solve the more commonly encountered problems in engineering and science, there is no intent to imply that these subroutines represent the current state of the art in statistics or numerical analysis. As with all tools, the user should understand their capabilities and their application to his functional requirements before deciding to use them.

AREAS OF APPLICATION

Individual subroutines, or a combination of them, can be used to carry out the listed functions in the following areas:

Statistics

- Probit analysis
- Analysis of variance (factorial design)
- Correlation analysis
- Multiple linear regression
- Stepwise regression
- Polynomial regression
- Canonical correlation
- Factor analysis (principal components, varimax)
- Discriminant analysis (many groups)
- Time series analysis
- Data screening and analysis
- Nonparametric tests
- Random number generation (uniform, normal)
- Distribution functions

Mathematics

- Inversion
- Eigenvalues and eigenvectors
- Simultaneous linear algebraic equations
- Transpositions
- Matrix arithmetic (addition, product, etc.)
- Matrix partitioning
- Matrix tabulation and sorting of rows or columns
- Elementary operations on rows or columns of matrices
- Matrix factorization
- Integration and differentiation of given or tabulated functions
- Solution of systems of first-order differential equations
- Fourier analysis of given or tabulated functions
- Bessel and modified Bessel function evaluation
- Gamma function evaluation
- Jacobian elliptic functions
- Elliptic, exponential, sine cosine, Fresnel integrals
- Finding real roots of a given function
- Finding real and complex roots of a real polynomial
- Polynomial arithmetic (addition, division, etc.)
- Polynomial evaluation, integration, differentiation
- Chebyshev, Hermite, Laguerre, Legendre polynomials
- Minimum of a function
- Approximation, interpolation, and table construction

CHARACTERISTICS

Some of the characteristics of the Scientific Subroutine Package are:

- All subroutines are free of input/output statements.
- Subroutines do not contain fixed maximum dimensions for the data arrays named in their calling sequences.
- All subroutines are written in FORTRAN.
- Many matrix manipulation subroutines handle symmetric and diagonal matrices (stored in economical, compressed formats) as well as general matrices. This can result in considerable saving in data storage for large arrays.
- The use of the more complex subroutines (or groups of them) is illustrated in the program documentation by sample main programs with input/output.
- All subroutines are documented uniformly.

The subroutines in SSP have been programmed in the subset of the FORTRAN IV language, which is compatible with all of the FORTRAN processors announced for System/360. Many of the larger functions such as those in statistics have been programmed as a series or sequence of subroutines.

An example of the use of sequences of subroutines is the statistical function called factor analysis. Factor analysis is a method of analyzing the intercorrelations within a set of variables. It determines whether the variance in the original set of variables can be accounted for adequately by a

smaller number of basic categories; namely, factors. In the Scientific Subroutine Package, factor analysis is normally performed by calling the following five subroutines in sequence:

1. CORRE - to find means, standard deviations, and correlation matrix
2. EIGEN - to compute eigenvalues and associated eigenvectors of the correlation matrix
3. TRACE - to select the eigenvalues that are greater than or equal to the control value specified by the user
4. LOAD - to compute a factor matrix
5. VARMX - to perform varimax rotation of the factor matrix

The multiple use of subroutines is illustrated by the fact that subroutine CORRE is also utilized in the multiple linear regression and canonical correlation. Subroutine EIGEN is used in canonical correlation as a third-level subroutine.

OVERALL RULES OF USAGE

GENERAL RULES

All subroutines in the Scientific Subroutine Package (SSP) are entered by means of the standard FORTRAN CALL statement. These subroutines are purely computational in nature and do not contain any references to input/output devices. The user must therefore furnish, as part of his program, whatever input/output and other operations are necessary for the total solution of his problem. In addition, the user must define by DIMENSION statements all matrices to be operated on by SSP subroutines as well as those matrices utilized in his program. The subroutines contained in SSP are no different from any user-supplied subroutine. All of the normal rules of FORTRAN concerning subroutines must therefore be adhered to, with the exception that the dimensioned areas in the SSP subroutine are not required to be the same as those in the calling program.

The CALL statement transfers control to the subroutine and replaces the dummy variables in that subroutine with the value of the actual arguments that appear in the CALL statement if the argument is a constant or a variable. When the argument is an array or function subprogram name, the address of the array or subprogram is transmitted to the called subroutine.

The arguments in a CALL statement must agree in order, number, and type with the corresponding arguments in the subroutine. A number may be passed to a subroutine either as a variable name in the argument list or as a constant in the argument list. For example, if the programmer wishes to add matrix AR1 to matrix AR2 in order to form matrix AR3 using the SSP subroutine GMADD, and if AR1 and AR2 are both matrices with ten rows and twenty columns, either of the two following methods can be used:

Method 1

```
CALL GMADD(AR1, AR2, AR3, 10, 20)
```

Method 2

```
N = 10
M= 20
CALL GMADD(AR1, AR2, AR3, N, M)
```

Many of the subroutines in SSP require the name of a user function subprogram or a FORTRAN-supplied function name as part of the argument list in the CALL statement. If the user's program contains such a CALL, the function name appearing in the argument list must also appear in an EXTERNAL statement at the beginning of that program.

For example, the SSP subroutine RK2 integrates a function furnished by the user. The user must therefore program the function and give the name of the function to RK2 as a parameter in the CALL statement. If the user wishes to integrate the function $\frac{dy}{dx} = 3.0x + 2.0Y$, his main program may appear as:

```
EXTERNAL DERY
      .
      .
CALL RK2(DERY, .....)
      .
      .
RETURN
END
```

His function subprogram can be:

```
FUNCTION DERY (X, Y)
DERY= 3.0*X+2.0* Y
RETURN
END
```

The user's main program gives the name of the programmed function to RK2 by including that name in the CALL statement and in an EXTERNAL statement. RK2, in turn, goes to the function DERY each time it requires a value for the derivative. The subroutine RK2 is not modified by the programmer. The dummy function name FUN in subroutine RK2 is, in effect, replaced by the name appearing in the user's CALL statement during execution of the subroutine.

MATRIX OPERATIONS

Special consideration must be given to the subroutines that perform matrix operations. These subroutines have two characteristics that affect the format of the data in storage--variable dimensioning and data storage compression.

Variable Dimensioning

Those subroutines that deal with matrices can operate on any size array, limited in most cases only by the available core storage and numerical analysis considerations. The subroutines do not contain fixed maximum dimensions for data arrays named in their calling sequence. The variable dimension capability

has been implemented in SSP by using a vector storage approach. Under this approach, each column of a matrix is immediately followed in storage by the next column. Vector storage and two-dimensional storage result in the same layout of data in core, so long as the number of rows and columns in the matrix are the same as those in the user's dimension statement. If, however, the matrix is smaller than the dimensioned area, the two forms of storage are not compatible.

Consider the layout of data storage when operating on a 5 by 5 array of numbers in an area dimensioned as 10 by 10. If the programmer has been using double-subscripted variables in the normal FORTRAN sense, the 25 elements of data will appear as shown in Figure 1. FORTRAN stores double-subscripted data by column based on the column length specified in the DIMENSION statement. Thus, in the example, sequential core locations will contain data elements 1 to 5, five blank locations, data elements 6 to 10, five blank locations, and so on. The matrix subroutines take a vector approach in storing arrays by column, which means that they assume the data is stored as shown in Figure 2.

	Column									
	1	2	3	4	5	6	7	8	9	10
1	(1)	(6)	(11)	(16)	(21)					
2	(2)	(7)	(12)	(17)	(22)					
3	(3)	(8)	(13)	(18)	(23)					
4	(4)	(9)	(14)	(19)	(24)					
Row 5	(5)	(10)	(15)	(20)	(25)					
6										
7										
8										
9										
10										

Figure 1. Double-subscripted data storage

(1)	(11)	(21)
(2)	(12)	(22)
(3)	(13)	(23)
(4)	(14)	(24)
(5)	(15)	(25)
(6)	(16)	
(7)	(17)	
(8)	(18)	
(9)	(19)	
(10)	(20)	

Figure 2. Vector storage

As stated previously, if the dimensioned area is the same as the matrix size, the two approaches will have the same data storage layout, and the user can proceed in a regular double-subscripted fashion. If, however, he is operating in a mode where the dimensioned area is larger than the arrays, and if he wishes to use the SSP subroutines, he must be certain that his data is stored in the vector fashion illustrated by Figure 2. A subroutine called ARRAY is available in SSP to change from one form of storage to the other. In addition, a subroutine called LOC is available to assist in referencing elements in an array stored in the vector fashion.

Storage Compression

Many subroutines in SSP can operate on compressed forms of matrices as well as on the normal form. By using this capability, which is called "storage mode", considerable savings in data storage can be obtained for special forms of large arrays. The three modes of storage are termed general, symmetric, and diagonal. In this context, general mode is one in which all elements of the matrix are in storage. Symmetric mode is one in which only the upper triangular portion of the matrix is retained columnwise in sequential locations in storage. (The assumption is made that the corresponding elements in the lower triangle have the same value.) Diagonal mode is one in which only the diagonal elements of the matrix are retained in sequential locations in storage. (The off-diagonal elements are assumed to be zero.) This capability has been implemented using the vector storage approach.

Figure 3 illustrates the effect of the storage mode capability. A symmetric matrix is shown in Figure 3A. If this array is to be manipulated using the SSP matrix subroutines with storage mode capability, the array may be stored as shown in Figure 3B. This is the upper triangular portion of the array and corresponds to a storage mode code of 1. Symmetric matrices of order N may be stored in a vector of only N*(N+1)/2 locations rather than N*N locations. For larger matrices, this will be a saving of almost one half.

The effect of storage mode when dealing with diagonal matrices is even more pronounced. Diagonal matrices of order N may be stored in a vector only N locations long. Figure 3C shows a 3 by 3 diagonal matrix. If this array is to be manipulated using the SSP matrix subroutines with storage mode capability, only the diagonal elements of the array need be stored. This is shown in Figure 3D and corresponds to a storage mode code of 2.

General matrices of order N by M require a vector N*M long and use a storage mode code of 0.

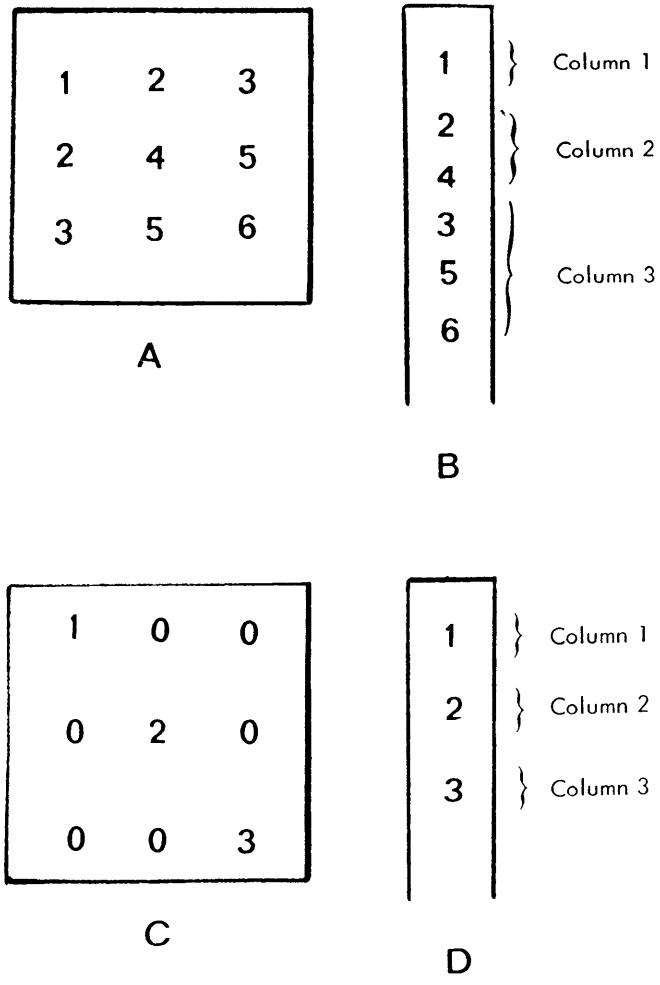

Figure 3. Storage mode

Thus, if the programmer wishes to use SSP subroutines on matrix A, which is general, matrix B, which is symmetric, and matrix C, which is diagonal, and all matrices are 10 by 10 or smaller, the dimension statement in his program can be:

```
DIMENSION A(100), B(55), C(10)
```

Matrix Element References

Subroutine LOC in the Scientific Subroutine Package may be used to reference elements within a matrix stored in a vector fashion, and may involve storage mode compression. The calling sequence for LOC is:

```
CALL LOC (I, J, IJ, N, M, MS)
```

The capabilities of subroutine LOC are as follows. If reference is required to the element at row I and column J of matrix A whose dimensions are N by M, and if the storage mode code is MS, a CALL to the LOC subroutine as shown above will result in the computation of the subscript IJ such that A(IJ) is the desired element. The parameters represented by I, J, N, M, MS can be either integer variables or integer constants. The parameter represented by IJ is an integer variable. Note that the user must dimension the array A as a single-subscripted variable to meet the restrictions of some FORTRAN systems. To illustrate the use of LOC, if reference is required to the element at row 2, column 2 of the 3 by 3 symmetric matrix illustrated in Figure 3A and stored as shown in Figure 3B (storage mode code 1), the sequence may be:

```
CALL LOC (2, 2, IJ, 3, 3, 1)
```

The value of IJ computed by LOC will be 3, meaning that the proper element is the third element in the specially stored symmetric matrix (Figure 3B). If the storage mode code is for a symmetric matrix where only the upper triangular portion is retained in storage, and if I and J refer to an element in the lower triangular portion, IJ will contain the subscript for the corresponding element in the retained upper triangle. Thus if the user wanted the element in row 3, column 1 of the matrix shown in Figure 3A, and the array was stored as in Figure 3B, the statement:

```
CALL LOC (3, 1, IJ, 3, 3, 1)
```

would result in IJ having the value of 4; that is, the fourth element in Figure 3B. If a matrix is stored as shown in Figure 3D (storage mode 2), and LOC is used to compute the subscript for an off-diagonal element (I not equal to J), the result in IJ will be zero. This is due to the fact that the element does not exist in storage. In this situation, the user must not utilize IJ as a subscript. Following is an illustration of how to take care of this condition and also handle the case where the current storage mode is unknown.

If the user wishes to set a variable X equal to the element in the third row and fourth column of a 10 by 10 array named A, for either a symmetric, diagonal, or general matrix, the required program can be implemented for any storage mode MS as follows:

```
      CALL LOC (3, 4, IJ, 10, 10, MS)
      X = 0.0
      IF(IJ)20, 30, 20
   20 X = A(IJ)
   30 --------
```

(MS is assumed to have been set at 0, 1, or 2 at some earlier point in the program.) This sequence will then set the proper value for X, given any storage mode that may be encountered. The second and third statements take care of the off-diagonal condition for a matrix with a storage mode of 2.

As a special case, LOC can be used to compute the total length of an array in storage with a statement such as:

```
CALL LOC (N, M, IJ, N, M, MS)
```

For example, if the user has a 3 by 3 matrix whose storage mode is 1 (Figure 3B), the statement:

```
CALL LOC (3, 3, IJ, 3, 3, 1)
```

will result in IJ being set to 6. This is not only the proper subscript to reference element 3, 3, but is also the actual length of the vector in storage.

The information contained in the fifth parameter (number of columns) in the calling sequence for LOC is not actually used in the calculations performed by LOC. It has been included in the calling sequence in case the user wishes to expand LOC to cover other forms of data storage.

ADVANCED FORTRAN FEATURES

The user may wish to take advantage of more advanced FORTRAN compiler features. For example, the larger FORTRAN systems include a subroutine multiple entry point capability. Some of the subroutines in SSP can be combined by using this feature. To illustrate this, GMADD and GMSUB (addition and subtraction of general matrices) can be combined as shown in Figure 4. This will in no way affect the programs using these subroutines but will reduce the total program storage requirements.

```
      SUBROUTINE GMADD (A,B,R,N,M)
      DIMENSION A(1),B(1),R(1)
      K=0
      GO TO 10
      ENTRY GMSUB (A,B,R,N,M)
      K=1
10    NM=N*M
      DO 40 I=1,NM
      IF(K) 20,20,30
20    R(I)=A(I)+B(I)
      GO TO 40
30    R(I)=A(I)-B(I)
40    CONTINUE
      RETURN
      END
```

Figure 4. Multiple entry point

OPTIMIZATION OF TIME

The subroutines in SSP are designed to conserve storage for data. If the user wishes to exchange space for time, there are several ways in which SSP may be modified to effect this end. For example, many of the subroutines in SSP make use of the LOC subroutine to handle vector storage and storage mode referencing. The execution time of these subroutines can be substantially reduced by implementing LOC in Assembler Language. (The distributed version of LOC is implemented in FORTRAN.) Another approach is to incorporate the function of LOC within each subroutine and thus avoid the "set-up" costs of repeated calls to LOC. This has the effect of reducing execution time but at some cost in subroutine storage and in the ease with which other modes of storage, such as triangular matrix storage or storage by row rather than by column, can be implemented. Figure 5 shows how matrix addition and the LOC capabilities can be implemented within the same subroutine.

```
      SUBROUTINE MACX(A,B,R,N,M,MSA,MSB)
      DIMENSION A(1),B(1),R(1)
C
C        TEST FOR SAME STORAGE MODE
C
      IF(MSA-MSB) 30,10,30
C
C        COMPUTE VECTOR LENGTH
C
   10 ND=N*M
      IF(MSA-1) 24,22,23
   22 ND=(ND+N)/2
      GO TO 24
   23 ND=N
C
C        ADD MATRICES OF SAME STORAGE MODE
C
   24 DO 25 I=1,ND
   25 R(I)=A(I)+B(I)
      RETURN
C
C        GET STORAGE MODE OF OUTPUT MATRIX
C
   30 MTEST=MSA*MSB
      MSR=0
      IF(MTEST) 35,35,32
   32 MSR=1
   35 DO 60 J=1,M
      DO 60 I=1,N
C
C        LOCATE ELEMENT IN OUTPUT MATRIX
C
      KX=-1
      MS=MSR
      GO TO 65
   40 IJR=IR
C
C        LOCATE ELEMENT IN MATRIX A
C
      KX=0
      MS=MSA
      GO TO 65
   45 IJA=IR
      AEL=0.0
      IF(IJA) 46,48,46
   46 AEL=A(IJA)
C
C        LOCATE ELEMENT IN MATRIX B
C
   48 KX=1
      MS=MSB
      GO TO 65
   50 IJB=IR
      BEL=0.0
      IF(IJB) 55,60,55
   55 BEL=B(IJB)
C
C        ADD MATRICES OF DIFFERENT STORAGE MODES
C
   60 R(IJR)=AEL+BEL
      RETURN
C
C        IN LINE LOC
C
   65 IF(MS-1) 70,75,90
   70 IR=N*(J-1)+I
      GO TO 95
   75 IF(I-J) 80,85,85
   80 IR=I+(J*J-J)/2
      GO TO 95
   85 IR=J+(I*I-I)/2
      GO TO 95
   90 IP=0
      IF(I-J) 95,92,95
   92 IR=I
   95 IF(KX) 40,45,50
      END
```

Figure 5. Inline LOC

DOUBLE PRECISION

The accuracy of the computations in many of the SSP subroutines is highly dependent upon the number of significant digits available for arithmetic operations. Matrix inversion, integration, and many of the statistical subroutines fall into this category. The user may, therefore, wish to use double-precision versions of these subroutines.

Many of the subroutines in SSP have been provided in both single- and double-precision versions. In others, instructions for converting to double precision are included as part of the subroutine description. FORTRAN double-precision statements have been included in each of these subroutines in the form of a comments card. In most cases, the double-precision version of the subroutine can be obtained merely by removing the C from column 1 of the double-precision statement card(s) before compilation. In a few cases, additional instructions are given for changing references to FORTRAN-furnished functions; for example, SQRT to DSQRT and ABS to DABS; in other cases, new constants are given.

The use of double-precision subroutines requires a detailed knowledge of the FORTRAN rules concerning double precision. A few of the more basic ones are as follows:

1. Any real variable, vector, or array name contained in the argument list of a CALL to a double-precision subroutine must be declared as double precision in the calling program. For example, if the SSP matrix inversion subroutine MINV has been modified for double precision, and if the user's program contains the statement:

```
CALL MINV (AR1, N, DET, MY1, MY2)
```

where:

AR1 is the array name (real, double-precision array)
N is the dimension (integer variable)
DET is the determinant (real, double-precision variable)
MY1 is a work vector (integer array)
MY2 is a work vector (integer array)

then the program must also have at its beginning the specification statement:

```
DOUBLE PRECISION AR1, DET
```

The other variables are integer variables and should not be included in the specification statement.

2. Any user-supplied function named in the CALL statement for a double-precision SSP subroutine must be programmed as a double-precision function. For example, the sample program for Runge-Kutta integration performs the integration on a sample function called FUN using subroutine RK2. This function is programmed as:

```
FUNCTION FUN (X, Y)

FUN = 1.1*X

RETURN

END
```

If a double-precision version of RK2 is used, the function must also be double precision. The sample function will then be:

```
DOUBLE PRECISION FUNCTION FUN (X, Y)

DOUBLE PRECISION X, Y

FUN = 1.1*X

RETURN

END
```

FORMAT OF THE DOCUMENTATION

The major portion of this manual consists of the documentation for the individual subroutines and the sample programs.

SUBROUTINE DESCRIPTIONS

Subroutine and sample program guides, both categorial and alphabetic, designed to aid in locating any particular subroutine are given in the pages that follow.

Each of the subroutine descriptions consists of a program listing and, in some cases, a mathematical description. The first part of the program listing is a set of comment cards containing the subroutine name, its calling sequence, description of parameters, remarks, names of other subroutines required, and method. References to books and periodicals will be found under the method section of the description. The mathematical description pages do not, in most cases, indicate the derivation of the mathematics. They are intended to indicate what mathematical operations are actually being performed in the subroutines. Some of the major statistical functions are performed by a sequence of SSP subroutines. An explanation of this sequence will be found just before the description of the first subroutine that is specific to this function.

SAMPLE PROGRAM DESCRIPTIONS

The sample program listings are given in Appendix B.

Each sample program consists of a detailed description including information on the problem, the program, input, output, program modification, operating instructions, error messages, timing and machine listings of the programs, input data and output results. The sample programs have been chosen to (1) illustrate a sequence of SSP subroutines, (2) illustrate the use of a complex subroutine, or (3) show the way in which one member (such as matrix addition) of a large set of simple subroutines might be used.

As part of the development of the sample programs, some special sample subroutines have been implemented that may prove useful to the programmer. These include:

HIST - print a histogram of frequencies

MATIN - read an input matrix into storage in vector form for use by SSP matrix subroutines

PLOT - plot several variables versus a base variable

MXOUT - print a matrix stored in the SSP vector format

Listings of the above subroutines are included after the sample program documentation in this manual. The source decks are part of the sample program source decks on the distributed magnetic tape.

The sample programs have been implemented for execution on a 32K byte (8K word) System/360 using Basic Programming Support FORTRAN (Tape). Instructions for modifying the sample programs for different data capacities are included in the documentation. In addition, those sample programs that illustrate potentially double-precision subroutines include double-precision statements in the form of comment cards. These comment cards are contained in the sample program source decks.

It is recommended that those SSP subroutines that will be frequently used in an installation be compiled and the relocatable decks placed on the FORTRAN system's residence device. In the case of Basic Programming Support FORTRAN (Tape), this will be the library portion of the system tape. Information on the method for updating the system to include user-supplied subroutines will be found in the appropriate FORTRAN programmer's guide. SSP subroutines are handled in the same manner as user-supplied subroutines. If the subroutines are not placed on the FORTRAN system's residence device. those required by a particular program will have to be included in that program each time it is run.

CATEGORIAL GUIDE TO SUBROUTINES AND SAMPLE PROGRAMS

(Subroutines added in Version III are marked with an asterisk)

STATISTICS

ALPHABETIC GUIDE TO SUBROUTINES WITH STORAGE REQUIREMENTS

The following table lists the number of characters of storage required by each of the subroutines in the Scientific Subroutine Package. The figures given were obtained by using Basic Programming Support FORTRAN (Tape), Version 3, Level 0. The use of other FORTRAN compilers on System/360 may cause deviations from these figures.

The double-precision version of the subroutines in the Scientific Subroutine Package are listed immediately following their alphabetized single-precision counterparts. Main line routines are asterisked.

Name	(Label)	Storage Required (Bytes)	Page
ABSNT	(ABSN)	428	28
ACFI	(ACFI)	1214	245
DACFI	(DACF)	1286	245
*ADSAM	(ADSA)	13244	443
AHI	(AHI)	1084	243
DAHI	(DAHI)	1116	243
ALI	(ALI)	760	241
DALI	(DALI)	784	241
*ANOVA	(ANOV)	14624	425
APCH	(APCH)	1492	263
DAPCH	(DAPC)	1548	263
APFS	(APFS)	1602	260
DAPFS	(DAPF)	1626	260
APLL	(APLL)	836	271
DAPLL	(DAPL)	860	271
APMM	(APMM)	4694	283
DAPMM	(DAPM)	4728	283
ARAT	(ARAT)	3004	265
DARAT	(DARA)	3090	265
ARRAY	(ARRA)	670	98
ATEIG	(ATEI)	4538	167

Name	(Label)	Storage Required (Bytes)	Page
ATSE	(ATSE)	1022	251
DATSE	(DTSE)	1050	251
ATSG	(ATSG)	852	248
DATSG	(DTSG)	892	248
ATSM	(ATSM)	1124	250
DATSM	(DTSM)	1148	250
AUTO	(AUTO)	624	59
AVCAL	(AVCA)	802	50
AVDAT	(AVDA)	926	49
BDTR	(BDTR)	3354	78
BESJ	(BESJ)	1466	363
BESK	(BESK)	2022	366
BESY	(BESY)	1968	364
BISER	(BISE)	1182	87
BOOL	(BOOL)	164	452
BOUND	(BOUN)	784	27
CADD	(CADD)	550	107
CANOR	(CANO)	2836	47
CCPY	(CCPY)	500	95
CCUT	(CCUT)	716	114
CDTR	(CDTR)	3390	81
CEL1	(CEL1)	544	374
DCEL1	(DCE1)	584	374
CEL2	(CEL2)	718	376
DCEL2	(DCE2)	774	376
CHISQ	(CHIS)	1220	68
CINT	(CINT)	364	109
CNP	(CNP)	340	198
DCNP	(DNP)	364	198
CNPS	(CNPS)	442	199
DCNPS	(DNPS)	482	199
CONVT	(CONV)	538	97
CORRE	(CORR)	2950	32
CROSS	(CROS)	750	60
CS	(CS)	906	372
CSP	(CSP)	352	201
DCSP	(DSP)	376	201
CSPS	(CSPS)	458	202
DCSPS	(DSPS)	506	202
CSRT	(CSRT)	978	113
CSUM	(CSUM)	502	110
CTAB	(CTAB)	826	112
CTIE	(CTIE)	746	115
*DASCR	(DASC)	6848	403
DATA	(DATA)	308	452
DBAR	(DBAR)	1252	327
DDBAR	(DDBA)	1354	327
DCAR	(DCAR)	1308	324
DDCAR	(DDCA)	1392	324
DCLA	(DCLA)	392	106
DCPY	(DCPY)	394	95
DET3	(DET3)	554	320
DDET3	(DDT3)	594	320

Name	(Label)	Storage Required (Bytes)	Page
DET5	(DET5)	752	322
DDET5	(DDT5)	832	322
DGT3	(DGT3)	738	319
DDGT3	(DDGT)	770	319
DISCR	(DISC)	2532	53
DLGAM	(DLGA)	826	362
DMATX	(DMAT)	1170	52
EIGEN	(EIGE)	2556	164
ELI1	(ELI1)	836	378
DELI1	(DEL1)	900	378
ELI2	(ELI2)	1254	380
DELI2	(DEL2)	1356	380
EXPI	(EXPI)	1032	368
*EXPON	(EXPO)	8952	440
EXSMO	(EXSM)	620	62
*FACTO	(FCTO)	11212	432
FACTR	(FCTR)	1586	126
FMCG	(FMCG)	2820	225
DFMCG	(DFMC)	2956	225
FMFP	(FMFP)	3580	221
DFMFP	(DFMF)	3702	221
FORIF	(FRIF)	990	274
FORIT	(FRIT)	946	275
FRAT	(FRAT)	912	269
DFRAT	(DFRA)	944	271
FUN	(FUN)	186	452
GAUSS	(GAUS)	430	77
GDATA	(GDAT)	1764	39
GELB	(GELB)	2640	137
DGELB	(DELB)	2674	137
GELG	(GELG)	1882	121
DGELG	(DELG)	1920	121
GELS	(GELS)	1990	133
DGELS	(DELS)	2028	133
GMADD	(GMAD)	288	98
GMMMA	(GMMM)	826	361
GMPRD	(GMPR)	570	99
GMSUB	(GMSU)	288	99
GMTRA	(GMTR)	358	100
GTPRD	(GTPR)	566	100
HARM	(HARM)	5988	276
DHARM	(DHAR)	6070	276
HEP	(HEP)	398	205
DHEP	(DHP)	422	205
HEPS	(HEPS)	454	206
DHEPS	(DHPS)	486	206
HIST	(HIST)	1778	452
HPCG	(HPCG)	5560	337
DHPCG	(DHCG)	5744	337
HPCL	(HPCL)	5606	343
DHPCL	(DHCL)	5798	343
HSBG	(HSBG)	1440	169
I0	(I0)	546	365
INUE	(INUE)	768	366
JELF	(JELF)	1254	382
DJELF	(DJEL)	1416	382

Name	(Label)	Storage Required (Bytes)	Page	Name	(Label)	Storage Required (Bytes)	Page
*KOLM	(KOLM)	7952	438	MFGR	(MFGR)	2092	127
KOLMO	(KLMO)	1704	63	DMFGR	(DMGR)	2120	127
KOLM2	(KLM2)	1514	65	MFSD	(MFSD)	904	158
KRANK	(KRAN)	1598	69	DMFSD	(DMSD)	906	158
LAP	(LAP)	408	208	MFSS	(MFSS)	2688	152
DLAP	(DAP)	432	208	DMFSS	(DMSS)	2664	152
LAPS	(LAPS)	472	209	MFUN	(MFUN)	446	117
DLAPS	(DAPS)	512	209	MINV	(MINV)	1874	118
LBVP	(LBVP)	8000	350	MISR	(MISR)	2856	33
DLBVP	(DLBV)	8256	350	MLSS	(MLSS)	2020	145
LEP	(LEP)	400	212	DMLSS	(DMLS)	2004	145
DLEP	(DEP)	424	212	MOMEN	(MOME)	1288	85
LEPS	(LEPS)	464	213	MPAIR	(MPAI)	1380	70
DLEPS	(DEPS)	496	213	MPRC	(MPRC)	810	115
LLSQ	(LLSQ)	2938	160	DMPRC	(DMPR)	822	115
DLLSQ	(DLLS)	2986	160	MPRD	(MPRD)	944	102
LOAD	(LOAD)	490	56	MSTR	(MSTR)	590	96
LOC	(LOC)	492	97	MSUB	(MSUB)	942	101
MADD	(MADD)	942	101	MTDS	(MTDS)	1436	142
MATA	(MATA)	790	103	DMTDS	(DMTD)	1428	142
MATIN	(MATI)	1180	453	MTRA	(MTRA)	552	102
*MCANO	(MCAN)	8196	421	MULTR	(MULT)	1356	37
MCHB	(MCHB)	2286	148	MXOUT	(MXOU)	1440	454
DMCHB	(DMCH)	2270	148	NDTR	(NDTR)	488	78
MCPY	(MCPY)	410	94	NDTRI	(NTRI)	758	83
*MDISC	(MDIS)	15368	428	NROOT	(NROO)	1940	166
MEANQ	(MEAN)	1708	51	ORDER	(ORDE)	682	36

Name	(Label)	Storage Required (Bytes)	Page
PADD	(PADD)	474	171
PADDM	(PDDM)	510	173
PCLA	(PCLA)	282	173
PCLD	(PCLD)	314	177
PDER	(PDER)	350	175
PDIV	(PDIV)	794	172
PECN	(PECN)	848	178
DPECN	(DPCN)	862	178
PECS	(PECS)	746	180
DPECS	(DPCS)	766	180
PERM	(PERM)	1024	232
PGCD	(PGCD)	566	177
PHI	(PHI)	1390	88
PILD	(PILD)	402	175
PINT	(PINT)	344	176
PLOT	(PLOT)	2500	452
PMPY	(PMPY)	506	172
PNORM	(PNOR)	258	178
POINT	(POIN)	1144	89
*POLRG	(PLRG)	9282	411
POLRT	(PLRT)	2086	181
PPRCN	(PPRC)	704	231
PQFB	(PQFB)	2252	193
DPQFB	(DPQF)	2384	193
PQSD	(PQSD)	382	176
PRBM	(PRBM)	2400	189
DPRBM	(DPRB)	2476	189
PROBT	(PROB)	2466	44
PRQD	(PRQD)	4572	183
DPRQD	(DPRQ)	4636	183
PSUB	(PSUB)	476	171
PVAL	(PVAL)	302	174
PVSUB	(PVSU)	714	174
QATR	(QATR)	1128	297
DQATR	(DQAT)	1190	297
QA2	(QA2)	330	314
QA3	(QA3)	376	314
QA4	(QA4)	422	314
DQA4	(DQA4)	462	315
QA5	(QA5)	468	315
QA6	(QA6)	514	315
QA7	(QA7)	560	315
QA8	(QA8)	606	316
DQA8	(DQA8)	678	316
QA9	(QA9)	652	316
QA10	(QA10)	698	316
DQA12	(DA12)	894	317
DQA16	(DA16)	1110	317
DQA24	(DA24)	1542	318
DQA32	(DA32)	1974	318
*QDINT	(QDIN)	2916	445
QG2	(QG2)	442	299
QG3	(QG3)	468	299
QG4	(QG4)	538	300

Name	(Label)	Storage Required (Bytes)	Page	Name	(Label)	Storage Required (Bytes)	Page
DQG4	(DQG4)	598	300	DQH8	(DQH8)	622	310
QG5	(QG5)	576	300	QH9	(QH9)	616	310
QG6	(QG6)	638	300	QH10	(QH10)	652	310
QG7	(QG7)	676	301	DQH16	(DH16)	982	311
QG8	(QG8)	738	301	DQH24	(DH24)	1342	311
DQG8	(DQG8)	814	301	DQH32	(DH32)	1702	312
QG9	(QG9)	776	301	DQH48	(DH48)	2422	312
QG10	(QG10)	838	302	DQH64	(DH64)	3142	313
DQG12	(DG12)	1030	302	QL2	(QL2)	330	303
DQG16	(DG16)	1246	302	QL3	(QL3)	376	304
DQG24	(DG24)	1678	302	QL4	(QL4)	422	304
DQG32	(DG32)	2110	303	DQL4	(DQL4)	462	304
QHFE	(QHFE)	434	294	QL5	(QL5)	468	304
DQHFE	(DQHE)	482	294	QL6	(QL6)	514	305
QHFG	(QHFG)	414	293	QL7	(QL7)	560	305
DQHFG	(DQHG)	454	293	QL8	(QL8)	606	305
QHSE	(QHSE)	478	296	DQL8	(DQL8)	678	305
DQHSE	(DQHS)	542	296	QL9	(QL9)	652	306
QHSG	(QHSG)	462	295	QL10	(QL10)	698	306
DQHSG	(DHSG)	514	295	DQL12	(DL12)	894	306
QH2	(QH2)	324	308	DQL16	(DL16)	1110	306
QH3	(QH3)	370	308	DQL24	(DL24)	1542	307
QH4	(QH4)	406	309	DQL32	(DL32)	1974	307
QH5	(QH5)	452	309	QSF	(QSF)	1286	291
QH6	(QH6)	488	309	DQSF	(DQSF)	1358	291
QH7	(QH7)	534	309	QTEST	(QTES)	710	71
QH8	(QH8)	570	310	QTFE	(QTFE)	382	290

Name	(Label)	Storage Required (Bytes)	Page	Name	(Label)	Storage Required (Bytes)	Page
DQTFE	(DTFE)	422	290	RTWI	(RTWI)	770	215
QTFG	(QTFG)	370	289	DRTWI	(DRTW)	804	215
DQTFG	(DTFG)	402	289	SADD	(SADD)	434	104
RADD	(RADD)	538	107	SCLA	(SCLA)	420	106
RANDU	(RAND)	310	77	SCMA	(SCMA)	430	108
RANK	(RANK)	672	71	SDIV	(SDIV)	470	105
RCPY	(RCPY)	500	94	SE13	(SE13)	460	255
RCUT	(RCUT)	716	113	DSE13	(DE13)	500	255
RECP	(RECP)	224	117	SE15	(SE15)	588	256
*REGRE	(REGR)	13736	407	DSE15	(DE15)	620	256
RHARM	(RHAR)	1660	281	SE35	(SE35)	564	258
DRHARM	(DRAR)	1762	281	DSE35	(DSE3)	604	258
RINT	(RINT)	376	109	SG13	(SG13)	648	253
RKGS	(RKGS)	2878	333	DSG13	(DSG1)	696	253
DRKGS	(DRKG)	3018	333	SICI	(SICI)	1192	370
*RKINT	(RKIN)	2704	446	SIGNT	(SIGN)	1170	72
RK1	(RK1)	1420	331	SIMQ	(SIMQ)	1286	120
RK2	(RK2)	770	332	SINV	(SINV)	1092	119
RSLMC	(RSLM)	1830	124	DSINV	(DSIN)	1080	119
RSRT	(RSRT)	1034	112	SMIRN	(SMIR)	700	66
RSUM	(RSUM)	502	110	SMO	(SMO)	542	61
RTAB	(RTAB)	826	111	*SMPRT	(SMPR)	1792	449
RTIE	(RTIE)	778	114	SMPY	(SMPY)	434	105
RTMI	(RTMI)	1510	217	*SOLN	(SOLN)	11754	451
DRTMI	(DRTM)	1582	217	SRANK	(SRAN)	1260	73
RTNI	(RTNI)	724	220	SRATE	(SRAT)	1534	92
DRTNI	(DRTN)	770	220	SRMA	(SRMA)	442	108

Name	(Label)	Storage Required (Bytes)	Page
SSUB	(SSUB)	434	104
*STEPR	(STEP)	11584	417
STOUT	(STOU)	1684	454
STPRG	(STPR)	3200	41
SUBMX	(SUBM)	512	31
SUBST	(SUBS)	888	28
TAB1	(TAB1)	1636	29
TAB2	(TAB2)	2806	30
TALLY	(TALL)	1206	27
TCNP	(TCNP)	678	200
DTCNP	(DTCN)	726	200
TCSP	(TCSP)	706	203
DTCSP	(DTCS)	754	203
TEAS	(TEAS)	2024	234
DTEAS	(DTEA)	2096	234
TETRA	(TETR)	2038	90
TEUL	(TEUL)	844	238
DTEUL	(DTEU)	924	238
THEP	(THEP)	712	207
DTHEP	(DTHE)	768	207
TIE	(TIE)	640	74
TLAP	(TLAP)	776	210
DTLAP	(DTLA)	820	210
TLEP	(TLEP)	716	214
DTLEP	(DTLE)	772	214
TPRD	(TPRD)	904	103
TRACE	(TRAC)	560	55
TTEST	(TTES)	1794	86
TWOAV	(TWOA)	1108	74
UTEST	(UTES)	1064	75
VARMX	(VARM)	2914	56
WTEST	(WTES)	1488	76
XCPY	(XCPY)	670	96

Listed below are the subroutines. A brief description precedes those subroutines that require further clarification.

STATISTICS

Data Screening

Subroutine TALLY

```
C                                                                       TALL  10
C     ..................................................................TALL  20
C                                                                       TALL  30
C        SUBROUTINE TALLY                                               TALL  40
C                                                                       TALL  50
C        PURPOSE                                                        TALL  60
C           CALCULATE TOTAL, MEAN, STANDARD DEVIATION, MINIMUM, MAXIMUM TALL  70
C           FOR EACH VARIABLE IN A SET (OR A SUBSET) OF OBSERVATIONS    TALL  80
C                                                                       TALL  90
C        USAGE                                                          TALL 100
C           CALL TALLY(A,S,TCTAL,AVER,SD,VMIN,VMAX,NO,NV,IER)           TALL 110
C                                                                       TALL 120
C        DESCRIPTION OF PARAMETERS                                      TALL 130
C           A     - OBSERVATION MATRIX, NO BY NV                        TALL 140
C           S     - INPUT VECTOR INDICATING SUBSET OF A. ONLY THOSE     TALL 150
C                   OBSERVATIONS WITH A NON-ZERO S(J) ARE CONSIDERED.   TALL 160
C                   VECTOR LENGTH IS NO.                                TALL 170
C           TCTAL - OUTPUT VECTOR OF TOTALS OF EACH VARIABLE. VECTOR    TALL 180
C                   LENGTH IS NV.                                       TALL 190
C           AVER  - OUTPUT VECTOR OF AVERAGES OF EACH VARIABLE. VECTOR  TALL 200
C                   LENGTH IS NV.                                       TALL 210
C           SD    - OUTPUT VECTOR OF STANDARD DEVIATIONS OF EACH        TALL 220
C                   VARIABLE. VECTOR LENGTH IS NV.                      TALL 230
C           VMIN  - OUTPUT VECTOR OF MINIMA OF EACH VARIABLE. VECTOR    TALL 240
C                   LENGTH IS NV.                                       TALL 250
C           VMAX  - OUTPUT VECTOR OF MAXIMA OF EACH VARIABLE. VECTOR    TALL 260
C                   LENGTH IS NV.                                       TALL 270
C           NO    - NUMBER OF OBSERVATIONS                              TALL 280
C           NV    - NUMBER OF VARIABLES FOR EACH OBSERVATION            TALL 290
C           IER   - ZERO, IF NO ERROR.                                  TALL 291
C                   - 1, IF S IS NULL.  VMIN=-1.E75, VMAX=SD=AVER=1.E75.TALL 292
C                   - 2, IF S HAS ONLY ONE NON-ZERO ELEMENT. VMIN=VMAX. TALL 293
C                     SD=0.0                                            TALL 294
C                                                                       TALL 300
C        REMARKS                                                        TALL 310
C           NONE                                                        TALL 320
C                                                                       TALL 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TALL 340
C           NONE                                                        TALL 350
C                                                                       TALL 360
C        METHOD                                                         TALL 370
C           ALL OBSERVATIONS CORRESPONDING TO A NON-ZERO ELEMENT IN S   TALL 380
C           VECTOR ARE ANALYZED FOR EACH VARIABLE IN MATRIX A.          TALL 390
C           TOTALS ARE ACCUMULATED AND MINIMUM AND MAXIMUM VALUES ARE   TALL 400
C           FOUND. FOLLOWING THIS, MEANS AND STANDARD DEVIATIONS ARE    TALL 410
C           CALCULATED.  THE DIVISOR FOR STANDARD DEVIATION IS ONE LESS TALL 420
C           THAN THE NUMBER OF OBSERVATIONS USED.                       TALL 430
C                                                                       TALL 440
C     ..................................................................TALL 450
C                                                                       TALL 460
      SUBROUTINE TALLY(A,S,TCTAL,AVER,SD,VMIN,VMAX,NO,NV)               TALL 470
      DIMENSION A(1),S(1),TOTAL(1),AVER(1),SD(1),VMIN(1),VMAX(1)        TALL 480
C                                                                       TALL 490
C        CLEAR OUTPUT VECTORS AND INITIALIZE VMIN,VMAX                  TALL 500
C                                                                       TALL 510
      IER=0                                                             TALL 511
      DO 1 K=1,NV                                                       TALL 520
      TOTAL(K)=0.0                                                      TALL 530
      AVER(K)=1.0E75                                                    TALL 540
      SD(K)=1.0E75                                                      TALL 550
      VMIN(K)=-1.0E75                                                   TALL 560
    1 VMAX(K)=1.0E75                                                    TALL 570
C                                                                       TALL 580
C        TEST SUBSET VECTOR                                             TALL 590
C                                                                       TALL 600
      SCNT=0.0                                                          TALL 610
      DO 7 J=1,NO                                                       TALL 620
      IJ=J-NO                                                           TALL 630
      IF(S(J)) 2,7,2                                                    TALL 640
    2 SCNT=SCNT+1.0                                                     TALL 650
C                                                                       TALL 660
C        CALCULATE TOTAL, MINIMA, MAXIMA                                TALL 670
C                                                                       TALL 680
      DO 6 I=1,NV                                                       TALL 690
      IJ=IJ+NO                                                          TALL 700
      TOTAL(I)=TOTAL(I)+A(IJ)                                           TALL 710
      IF(A(IJ)-VMIN(I)) 3,4,4                                           TALL 720
    3 VMIN(I)=A(IJ)                                                     TALL 730
    4 IF(A(IJ)-VMAX(I)) 6,6,5                                           TALL 740
    5 VMAX(I)=A(IJ)                                                     TALL 750
    6 SD(I)=SD(I)+A(IJ)*A(IJ)                                           TALL 760
    7 CONTINUE                                                          TALL 770
C                                                                       TALL 780
C        CALCULATE MEANS AND STANDARD DEVIATIONS                        TALL 790
C                                                                       TALL 800
      IF (SCNT)8,8,9                                                    TALL 801
    8 IER=1                                                             TALL 802
      GO TO 15                                                          TALL 803
    9 DO 10 I=1,NV                                                      TALL 810
   10 AVER(I)=TOTAL(I)/SCNT                                             TALL 820
      IF (SCNT-1.0) 13,11,13                                            TALL 821
   11 IER=2                                                             TALL 822
      DO 12 I=1,NV                                                      TALL 823
   12 SD(I)=0.0                                                         TALL 824
      GO TO 15                                                          TALL 825
   13 DO 14 I=1,NV                                                      TALL 826
   14 SD(I)=SQRT(ABS((SD(I)-TOTAL(I)*TOTAL(I)/SCNT)/(SCNT-1.0)))        TALL 830
   15 RETURN                                                            TALL 840
      END                                                               TALL 850
```

Subroutine BOUND

```
C                                                                       BOUN  10
C     ..................................................................BOUN  20
C                                                                       BOUN  30
C        SUBROUTINE BOUND                                               BOUN  40
C                                                                       BOUN  50
C        PURPOSE                                                        BOUN  60
C           SELECT FROM A SET (OR A SUBSET) OF OBSERVATIONS THE NUMBER  BOUN  70
C           OF OBSERVATIONS UNDER, BETWEEN AND OVER TWO GIVEN BOUNDS    BOUN  80
C           FOR EACH VARIABLE                                           BOUN  90
C                                                                       BOUN 100
C        USAGE                                                          BOUN 110
C           CALL BOUND (A,S,BLO,BHI,UNDER,BETW,OVER,NO,NV,IER)          BOUN 120
C                                                                       BOUN 130
C        DESCRIPTION OF PARAMETERS                                      BOUN 140
C           A     - OBSERVATION MATRIX, NO BY NV                        BOUN 150
C           S     - VECTOR INDICATING SUBSET OF A. ONLY THOSE           BOUN 160
C                   OBSERVATIONS WITH A NON-ZERO S(J) ARE CONSIDERED.   BOUN 170
C                   VECTOR LENGTH IS NO.                                BOUN 180
C           BLO   - INPUT VECTOR OF LOWER BOUNDS ON ALL VARIABLES.      BOUN 190
C                   VECTOR LENGTH IS NV.                                BOUN 200
C           BHI   - INPUT VECTOR OF UPPER BOUNDS ON ALL VARIABLES.      BOUN 210
C                   VECTOR LENGTH IS NV.                                BOUN 220
C           UNDER - OUTPUT VECTOR INDICATING, FOR EACH VARIABLE, NUMBER BOUN 230
C                   OF OBSERVATIONS UNDER LOWER BOUNDS. VECTOR LENGTH   BOUN 240
C                   IS NV.                                              BOUN 250
C           BETW  - OUTPUT VECTOR INDICATING, FOR EACH VARIABLE, NUMBER BOUN 260
C                   OF OBSERVATIONS EQUAL TO OR BETWEEN LOWER AND UPPER BOUN 270
C                   BOUNDS. VECTOR LENGTH IS NV.                        BOUN 280
C           OVER  - OUTPUT VECTOR INDICATING, FOR EACH VARIABLE, NUMBER BOUN 290
C                   OF OBSERVATIONS OVER UPPER BOUNDS. VECTOR LENGTH    BOUN 300
C                   IS NV.                                              BOUN 310
C           NO    - NUMBER OF OBSERVATIONS                              BOUN 320
C           NV    - NUMBER OF VARIABLES FOR EACH OBSERVATION            BOUN 330
C           IER   - ZERO, IF NO ERROR.                                  BOUN 331
C                   - 1, IF LOWER BOUND IS GREATER THAN THE UPPER BOUND BOUN 332
C                     FOR SOME VARIABLE                                 BOUN 333
C                                                                       BOUN 340
C        REMARKS                                                        BOUN 350
C           NONE                                                        BOUN 360
C                                                                       BOUN 370
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  BOUN 380
C           NONE                                                        BOUN 390
C                                                                       BOUN 400
C        METHOD                                                         BOUN 410
C           EACH ROW (OBSERVATION) OF MATRIX A WITH CORRESPONDING       BOUN 420
C           NON-ZERO ELEMENT IN S VECTOR IS TESTED. OBSERVATIONS ARE    BOUN 430
C           COMPARED WITH SPECIFIED LOWER AND UPPER VARIABLE BOUNDS AND BOUN 440
C           A COUNT IS KEPT IN VECTORS UNDER, BETWEEN, AND OVER.        BOUN 450
C                                                                       BOUN 460
C     ..................................................................BOUN 470
C                                                                       BOUN 480
      SUBROUTINE BOUND(A,S,BLO,BHI,UNDER,BETW,OVER,NO,NV)               BOUN 490
      DIMENSION A(1),S(1),BLO(1),BHI(1),UNDER(1),BETW(1),OVER(1)        BOUN 500
C                                                                       BOUN 510
C        CLEAR OUTPUT VECTORS.                                          BOUN 520
C                                                                       BOUN 530
      IER=0                                                             BOUN 531
      DO 10 I=1,NV                                                      BOUN 532
      IF (BLO(I)-BHI(I)) 10,10,11                                       BOUN 533
   11 IER=1                                                             BOUN 534
      GO TO 12                                                          BOUN 535
   10 CONTINUE                                                          BOUN 536
      DO 1 K=1,NV                                                       BOUN 540
      UNDER(K)=0.0                                                      BOUN 550
      BETW(K)=0.0                                                       BOUN 560
    1 OVER(K)=0.0                                                       BOUN 570
C                                                                       BOUN 580
C        TEST SUBSET VECTOR                                             BOUN 590
C                                                                       BOUN 600
      DO 8 J=1,NO                                                       BOUN 610
      IJ=J-NO                                                           BOUN 620
      IF(S(J)) 2,8,2                                                    BOUN 630
C                                                                       BOUN 640
C        COMPARE OBSERVATIONS WITH BOUNDS                               BOUN 650
C                                                                       BOUN 660
    2 DO 7 I=1,NV                                                       BOUN 670
      IJ=IJ+NO                                                          BOUN 680
      IF(A(IJ)-BLO(I)) 5,3,3                                            BOUN 690
    3 IF(A(IJ)-BHI(I)) 4,4,6                                            BOUN 700
C                                                                       BOUN 710
C        COUNT                                                          BOUN 720
C                                                                       BOUN 730
    4 BETW(I)=BETW(I)+1.0                                               BOUN 740
      GO TO 7                                                           BOUN 750
    5 UNDER(I)=UNDER(I)+1.0                                             BOUN 760
      GO TO 7                                                           BOUN 770
    6 OVER(I)=OVER(I)+1.0                                               BOUN 780
    7 CONTINUE                                                          BOUN 790
    8 CONTINUE                                                          BOUN 800
   12 RETURN                                                            BOUN 810
      END                                                               BOUN 820
```

Subroutine SUBST

```
C                                                                       SUBS  10
C     ..................................................................SUBS  20
C                                                                       SUBS  30
C     SUBROUTINE SUBST                                                  SUBS  40
C                                                                       SUBS  50
C     PURPOSE                                                           SUBS  60
C        DERIVE A SUBSET VECTOR INDICATING WHICH OBSERVATIONS IN A      SUBS  70
C        SET HAVE SATISFIED CERTAIN CONDITIONS ON THE VARIABLES.        SUBS  80
C                                                                       SUBS  90
C     USAGE                                                             SUBS 100
C        CALL SUBST (A,C,R,B,S,NC,NV,NC)                                SUBS 110
C        PARAMETER B MUST BE DEFINED BY AN EXTERNAL STATEMENT IN THE    SUBS 120
C        CALLING PROGRAM                                                SUBS 130
C                                                                       SUBS 140
C     DESCRIPTION OF PARAMETERS                                         SUBS 150
C        A  - OBSERVATION MATRIX, NC BY NV                              SUBS 160
C        C  - INPUT MATRIX, 3 BY NC, OF CONDITIONS TO BE CONSIDERED.    SUBS 170
C             THE FIRST ELEMENT OF EACH COLUMN OF C REPRESENTS THE      SUBS 180
C             NUMBER OF THE VARIABLE (COLUMN OF THE MATRIX A) TO BE     SUBS 190
C             TESTED, THE SECOND ELEMENT OF EACH COLUMN IS A            SUBS 200
C             RELATIONAL CODE AS FOLLOWS                                SUBS 210
C                  1. FOR LT (LESS THAN)                                SUBS 220
C                  2. FOR LE (LESS THAN OR EQUAL TO)                    SUBS 230
C                  3. FOR EQ (EQUAL TO)                                 SUBS 240
C                  4. FOR NE (NOT EQUAL TO)                             SUBS 250
C                  5. FOR GE (GREATER THAN OR EQUAL TO)                 SUBS 260
C                  6. FOR GT (GREATER THAN)                             SUBS 270
C             THE THIRD ELEMENT OF EACH COLUMN IS A QUANTITY TO BE      SUBS 280
C             USED FOR COMPARISON WITH THE OBSERVATION VALUES. FOR      SUBS 290
C             EXAMPLE, THE FOLLOWING COLUMN IN C                        SUBS 300
C                       2.                                              SUBS 310
C                       5.                                              SUBS 320
C                      92.5                                             SUBS 330
C             CAUSES THE SECOND VARIABLE TO BE TESTED FOR GREATER       SUBS 340
C             THAN OR EQUAL TO 92.5                                     SUBS 350
C        R  - WORKING VECTOR USED TO STORE INTERMEDIATE RESULTS OF      SUBS 360
C             ABOVE TESTS ON A SINGLE OBSERVATION. IF CONDITION IS      SUBS 370
C             SATISFIED, R(I) IS SET TO 1. IF IT IS NOT, R(I) IS SET    SUBS 380
C             TO 0. VECTOR LENGTH IS NC.                                SUBS 390
C        E  - NAME OF SUBROUTINE TO BE SUPPLIED BY THE USER. IT         SUBS 400
C             CONSISTS OF A BOOLEAN EXPRESSION LINKING THE              SUBS 410
C             INTERMEDIATE VALUES STORED IN VECTOR R. THE BOOLEAN       SUBS 420
C             OPERATORS ARE '*' FOR 'AND', '+' FOR 'OR'. EXAMPLE        SUBS 430
C                  SUBROUTINE BOOLER,T)                                 SUBS 440
C                  DIMENSION R(3)                                       SUBS 450
C                  T=R(1)*(R(2)+R(3))                                   SUBS 460
C                  RETURN                                               SUBS 470
C                  END                                                  SUBS 480
C             THE ABOVE EXPRESSION IS TESTED FOR                        SUBS 490
C                  R(1).AND.(R(2).OR.R(3))                              SUBS 500
C        S  - OUTPUT VECTOR INDICATING, FOR EACH OBSERVATION,           SUBS 510
C             WHETHER OR NOT PROPOSITION B IS SATISFIED. IF IT IS,      SUBS 520
C             S(I) IS NON-ZERO. IF IT IS NOT, S(I) IS ZERO. VECTOR      SUBS 530
C             LENGTH IS NC.                                             SUBS 540
C        NC - NUMBER OF OBSERVATIONS. NO MUST BE > OR = TO 1.           SUBS 550
C        NV - NUMBER OF VARIABLES. NV MUST BE > OR = TO 1.              SUBS 560
C        NC - NUMBER OF BASIC CONDITIONS TO BE SATISFIED. NC MUST BE    SUBS 570
C             GREATER THAN OR EQUAL TO 1.                               SUBS 571
C                                                                       SUBS 580
C     REMARKS                                                           SUBS 590
C        NONE                                                           SUBS 600
C                                                                       SUBS 610
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     SUBS 620
C        B  THE NAME OF ACTUAL SUBROUTINE SUPPLIED BY THE USER MAY      SUBS 630
C           BE DIFFERENT (E.G., BCOL), BUT SUBROUTINE SUBST ALWAYS      SUBS 640
C           CALLS IT AS B.  IN ORDER FOR SUBROUTINE SUBST TO DO THIS,   SUBS 650
C           THE NAME OF THE USER-SUPPLIED SUBROUTINE MUST BE            SUBS 660
C           DEFINED BY AN EXTERNAL STATEMENT IN THE CALLING PROGRAM.    SUBS 670
C           THE NAME MUST ALSO BE LISTED IN THE ''CALL SUBST''          SUBS 680
C           STATEMENT.  (SEE USAGE ABOVE)                               SUBS 690
C                                                                       SUBS 700
C     METHOD                                                            SUBS 710
C        THE FOLLOWING IS DONE FOR EACH OBSERVATION.                    SUBS 720
C        CONDITION MATRIX IS ANALYZED TO DETERMINE WHICH VARIABLES      SUBS 730
C        ARE TO BE EXAMINED. INTERMEDIATE VECTOR R IS FORMED. THE       SUBS 740
C        BOOLEAN EXPRESSION (IN SUBROUTINE B) IS THEN EVALUATED TO      SUBS 750
C        DERIVE THE ELEMENT IN SUBSET VECTOR S CORRESPONDING TO THE     SUBS 760
C        OBSERVATION.                                                   SUBS 770
C                                                                       SUBS 780
C     ..................................................................SUBS 790
C                                                                       SUBS 800
      SUBROUTINE SUBST(A,C,R,B,S,NC,NV,NC)                              SUBS 810
      DIMENSION A(1),C(1),R(1),S(1)                                     SUBS 820
C                                                                       SUBS 830
      DO 5 I=1,NC                                                       SUBS 840
      IC=I-NC                                                           SUBS 850
      K=-2                                                              SUBS 860
      DO 8 J=1,NC                                                       SUBS 870
C                                                                       SUBS 880
C        CLEAR R VECTOR                                                 SUBS 890
C                                                                       SUBS 900
      R(J)=0.0                                                          SUBS 910
C                                                                       SUBS 920
C        LOCATE ELEMENT IN OBSERVATION MATRIX AND RELATIONAL CODE       SUBS 930
C                                                                       SUBS 940
      K=K+3                                                             SUBS 950
      I2=C(K)                                                           SUBS 960
      IA=IC+I2*NC                                                       SUBS 970
      IGO=C(K+1)                                                        SUBS 980
C                                                                       SUBS 990
C        FORM R VECTOR                                                  SUBS1000
C                                                                       SUBS1010
      C=A(IA)-C(K+2)                                                    SUBS1020
      GO TO(1,2,3,4,5,6),IGO                                            SUBS1030
    1 IF(C) 7,8,8                                                       SUBS1040
    2 IF(C) 7,7,8                                                       SUBS1050
    3 IF(C) 8,7,8                                                       SUBS1060
    4 IF(C) 7,8,7                                                       SUBS1070
    5 IF(C) 8,7,7                                                       SUBS1080
    6 IF(C) 8,8,7                                                       SUBS1090
    7 R(J)=1.0                                                          SUBS1100
    8 CONTINUE                                                          SUBS1110
C                                                                       SUBS1120
C        CALCULATE S VECTOR                                             SUBS1130
C                                                                       SUBS1140
    5 CALL B(R,S(I))                                                    SUBS1150
      RETURN                                                            SUBS1160
      END                                                               SUBS1170
```

Subroutine ABSNT

```
C                                                                       ABSN  10
C     ..................................................................ABSN  20
C                                                                       ABSN  30
C     SUBROUTINE ABSNT                                                  ABSN  40
C                                                                       ABSN  50
C     PURPOSE                                                           ABSN  60
C        TEST MISSING OR ZERO VALUES FOR EACH OBSERVATION IN            ABSN  70
C        MATRIX A.                                                      ABSN  80
C                                                                       ABSN  90
C     USAGE                                                             ABSN 100
C        CALL ABSNT (A,S,NC,NV)                                         ABSN 110
C                                                                       ABSN 120
C     DESCRIPTION OF PARAMETERS                                         ABSN 130
C        A  - OBSERVATION MATRIX, NC BY NV                              ABSN 140
C        S  - OUTPUT VECTOR OF LENGTH NO INDICATING THE FOLLOWING       ABSN 150
C             CODES FOR EACH OBSERVATION.                               ABSN 160
C             1  THERE IS NOT A MISSING OR ZERO VALUE.                  ABSN 170
C             0  AT LEAST ONE VALUE IS MISSING OR ZERO.                 ABSN 180
C        NC - NUMBER OF OBSERVATIONS. NO MUST BE > OR = TO 1.           ABSN 190
C        NV - NUMBER OF VARIABLES FOR EACH OBSERVATION. NV MUST BE      ABSN 200
C             GREATER THAN OR EQUAL TO 1.                               ABSN 201
C                                                                       ABSN 210
C     REMARKS                                                           ABSN 220
C        NONE                                                           ABSN 230
C                                                                       ABSN 240
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     ABSN 250
C        NONE                                                           ABSN 260
C                                                                       ABSN 270
C     METHOD                                                            ABSN 280
C        A TEST IS MADE FOR EACH ROW (OBSERVATION) OF THE MATRIX A.     ABSN 290
C        IF THERE IS NOT A MISSING OR ZERO VALUE, 1 IS PLACED IN        ABSN 300
C        S(J). IF AT LEAST ONE VALUE IS MISSING OR ZERO, 0 IS PLACED    ABSN 310
C        IN S(J).                                                       ABSN 320
C                                                                       ABSN 330
C     ..................................................................ABSN 340
C                                                                       ABSN 350
      SUBROUTINE ABSNT(A,S,NC,NV)                                       ABSN 360
      DIMENSION A(1),S(1)                                               ABSN 370
C                                                                       ABSN 380
      DO 2C J=1,NC                                                      ABSN 390
      IJ=J-NC                                                           ABSN 400
      S(J)=1.0                                                          ABSN 410
      DO 1C I=1,NV                                                      ABSN 420
      IJ=IJ+NC                                                          ABSN 430
      IF(A(IJ)) 1C,5,1C                                                 ABSN 440
    5 S(J)=0                                                            ABSN 450
      GO TO 2C                                                          ABSN 460
   1C CONTINUE                                                          ABSN 470
   2C CONTINUE                                                          ABSN 480
      RETURN                                                            ABSN 490
      END                                                               ABSN 500
```

Subroutine TAB1

This subroutine tabulates, for a selected variable in an observation matrix, the frequencies and percent frequencies over class intervals. Interval size is computed as follows:

$$k = \frac{UBO_3 - UBO_1}{UBO_2 - 2} \qquad (1)$$

where UBO_1 = given lower bound

UBO_2 = given number of intervals

UBO_3 = given upper bound

If $UBO_1 = UBO_3$, the subroutine finds and uses the minimum and maximum values of the variable.

A table lookup is used to obtain the frequency of the i^{th} class interval for the variable, where i = 1, 2, ..., UBO_2. Then each frequency is divided by the number of observations, n, to obtain the percent frequency:

$$P_i = \frac{100F_i}{n} \qquad (2)$$

In addition, the following statistics are calculated for the variable:

$$\text{Total: } T = \sum_{i=1}^{n} X_{ij} \qquad (3)$$

where j = selected variable

$$\text{Mean: } \overline{X} = \frac{T}{n} \qquad (4)$$

Standard deviation:

$$s = \sqrt{\frac{\sum_{i=1}^{n} X_{ij}^2 - \left(\sum_{i=1}^{n} X_{ij}\right)^2 \Big/ n}{n-1}} \qquad (5)$$

```
C                                                                       TAB1  10
C     ...............................................................   TAB1  20
C                                                                       TAB1  30
C        SUBROUTINE TAB1                                                TAB1  40
C                                                                       TAB1  50
C        PURPOSE                                                        TAB1  60
C           TABULATE FOR ONE VARIABLE IN AN OBSERVATION MATRIX (OR A    TAB1  70
C           MATRIX SUBSET), THE FREQUENCY AND PERCENT FREQUENCY OVER    TAB1  80
C           GIVEN CLASS INTERVALS. IN ADDITION, CALCULATE FOR THE SAME  TAB1  90
C           VARIABLE THE TOTAL, AVERAGE, STANDARD DEVIATION, MINIMUM,   TAB1 100
C           AND MAXIMUM.                                                TAB1 110
C                                                                       TAB1 120
C                                                                       TAB1 130
C        USAGE                                                          TAB1 140
C           CALL TAB1(A,S,NOVAR,UBC,FREQ,PCT,STATS,NO,NV)               TAB1 150
C                                                                       TAB1 160
C        DESCRIPTION OF PARAMETERS                                      TAB1 170
C           A      - OBSERVATION MATRIX, NO BY NV                       TAB1 180
C           S      - INPUT VECTOR GIVING SUBSET OF A. ONLY THOSE        TAB1 190
C                    OBSERVATIONS WITH A CORRESPONDING NON-ZERO S(I) ARE TAB1 200
C                    CONSIDERED. VECTOR LENGTH IS NO.                   TAB1 210
C           NOVAR  - THE VARIABLE TO BE TABULATED. NOVAR MUST BE GREATER TAB1 220
C                    THAN OR EQUAL TO 1 AND LESS THAN OR EQUAL TO NV.   TAB1 230
C                    AND UPPER LIMIT OF VARIABLE TO BE TABULATED        TAB1 240
C                    IN UBC(1), UBC(2) AND UBC(3) RESPECTIVELY. IF      TAB1 250
C                    LOWER LIMIT IS EQUAL TO UPPER LIMIT, THE PROGRAM   TAB1 260
C                    USES THE MINIMUM AND MAXIMUM VALUES OF THE VARIABLE.TAB1 270
C                    NUMBER OF INTERVALS, UBC(2), MUST INCLUDE TWO CELLS TAB1 280
C                    FOR VALUES UNDER AND ABOVE LIMITS. VECTOR LENGTH   TAB1 290
C                    IS 3.                                              TAB1 300
C                    FREQ   - OUTPUT VECTOR OF FREQUENCIES. VECTOR LENGTH IS TAB1 310
C                             UBC(2).                                   TAB1 320
C                    PCT    - OUTPUT VECTOR OF RELATIVE FREQUENCIES. VECTOR TAB1 330
C                             LENGTH IS UBC(2).                         TAB1 340
C                    STATS  - OUTPUT VECTOR OF SUMMARY STATISTICS, I.E., TOTAL, TAB1 350
C                             AVERAGE, STANDARD DEVIATION, MINIMUM AND MAXIMUM. TAB1 360
C                             VECTOR LENGTH IS 5. IF S IS NULL, THEN TOTAL,AVERAGETAB1 361
C                             AND STANDARD DEVIATION = 0, MIN=1.E75 AND MAX=-1.E75TAB1 370
C                    NO     - NUMBER OF OBSERVATIONS. NO MUST BE > OR = TO 1   TAB1 380
C                    NV     - NUMBER OF VARIABLES FOR EACH OBSERVATION. NV MUST TAB1 381
C                             BE GREATER THAN OR EQUAL TO 1.                  TAB1 390
C                                                                             TAB1 400
C           REMARKS                                                           TAB1 410
C              NONE                                                           TAB1 420
C                                                                             TAB1 430
C           SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     TAB1 440
C              NONE                                                           TAB1 450
C                                                                             TAB1 460
C           METHOD                                                            TAB1 470
C              THE INTERVAL SIZE IS CALCULATED FROM THE GIVEN INFORMATION     TAB1 480
C              OR OPTIONALLY FROM THE MINIMUM AND MAXIMUM VALUES FOR          TAB1 490
C              VARIABLE NOVAR. THE FREQUENCIES AND PERCENT FREQUENCIES ARE    TAB1 500
C              THEN CALCULATED ALONG WITH SUMMARY STATISTICS.                 TAB1 510
C              THE DIVISOR FOR STANDARD DEVIATION IS ONE LESS THAN THE        TAB1 520
C              NUMBER OF OBSERVATIONS USED.                                   TAB1 530
C                                                                             TAB1 540
C     ...............................................................         TAB1 550
C                                                                             TAB1 560
      SUBROUTINE TAB1(A,S,NOVAR,UBC,FREQ,PCT,STATS,NO,NV)                     TAB1 570
      DIMENSION A(1),S(1),UBC(1),FREQ(1),PCT(1),STATS(1)                      TAB1 580
      DIMENSION XBC(3)                                                        TAB1 590
      DO 5 I=1,3                                                              TAB1 600
    5 XBC(I)=UBC(I)                                                           TAB1 610
C                                                                             TAB1 620
C        CALCULATE MIN AND MAX                                                TAB1 630
C                                                                             TAB1 640
      VMIN=1.0E75                                                             TAB1 650
      VMAX=-1.0E75                                                            TAB1 660
      IJ=NO*(NOVAR-1)                                                         TAB1 670
      DO 3C J=1,NO                                                            TAB1 680
      IJ=IJ+1                                                                 TAB1 690
      IF(S(J)) 1C,3C,1C                                                       TAB1 700
   1C IF(A(IJ)-VMIN) 15,2C,2C                                                 TAB1 710
   15 VMIN=A(IJ)                                                              TAB1 720
   2C IF(A(IJ)-VMAX) 3C,3C,25                                                 TAB1 730
   25 VMAX=A(IJ)                                                              TAB1 740
   3C CONTINUE                                                                TAB1 750
      STATS(4)=VMIN                                                           TAB1 760
      STATS(5)=VMAX                                                           TAB1 770
C                                                                             TAB1 780
C        DETERMINE LIMITS                                                     TAB1 790
C                                                                             TAB1 800
      IF(UBC(1)-UBC(3)) 4C,35,4C                                              TAB1 810
   35 UBC(1)=VMIN                                                             TAB1 820
      UBC(3)=VMAX                                                             TAB1 830
   4C IAA=UBC(2)                                                              TAB1 840
C                                                                             TAB1 850
C        CLEAR OUTPUT AREAS                                                   TAB1 860
C                                                                             TAB1 870
      DO 45 I=1,IAA                                                           TAB1 880
      FREQ(I)=0.0                                                             TAB1 890
   45 PCT(I)=0.0                                                              TAB1 900
      DO 5C I=1,3                                                             TAB1 910
   5C STATS(I)=0.0                                                            TAB1 920
C                                                                             TAB1 930
C        CALCULATE INTERVAL SIZE                                              TAB1 940
C                                                                             TAB1 950
      SIAT=ABS((UBC(3)-UBC(1))/(UBC(2)-2.0))                                  TAB1 960
C                                                                             TAB1 970
C        TEST SUBSET VECTOR                                                   TAB1 980
C                                                                             TAB1 990
      SCNT=0.0                                                                TAB11000
      IJ=NO*(NOVAR-1)                                                         TAB11010
      DO 75 J=1,NO                                                            TAB11020
      IJ=IJ+1                                                                 TAB11030
      IF(S(J)) 55,75,55                                                       TAB11040
   55 SCNT=SCNT+1.0                                                           TAB11050
C                                                                             TAB11060
C        DEVELOP TOTAL AND FREQUENCIES                                        TAB11070
C                                                                             TAB11080
      STATS(1)=STATS(1)+A(IJ)                                                 TAB11090
      STATS(3)=STATS(3)+A(IJ)*A(IJ)                                           TAB11100
      TEMP=UBC(1)-SIAT                                                        TAB11110
      IATX=IAA-1                                                              TAB11120
      DO 6C I=1,IATX                                                          TAB11130
      TEMP=TEMP+SIAT                                                          TAB11140
      IF(A(IJ)-TEMP) 7C,6C,6C                                                 TAB11150
   6C CONTINUE                                                                TAB11160
      IF(A(IJ)-TEMP) 75,65,65                                                 TAB11170
   65 FREQ(IAA)=FREQ(IAA)+1.0                                                 TAB11180
      GO TO 75                                                                TAB11190
   7C FREQ(I)=FREQ(I)+1.0                                                     TAB11200
   75 CONTINUE                                                                TAB11201
      IF (SCNT)79,1C5,79                                                      TAB11210
C                                                                             TAB11220
C        CALCULATE RELATIVE FREQUENCIES                                       TAB11230
C                                                                             TAB11240
   79 DO 8C I=1,IAA                                                           TAB11250
   8C PCT(I)=FREQ(I)*1CO.0/SCNT                                               TAB11260
C                                                                             TAB11270
C        CALCULATE MEAN AND STANDARD DEVIATION                                TAB11280
C                                                                             TAB11290
      IF(SCNT-1.0) 85,85,9C                                                   TAB11300
   85 STATS(2)=STATS(1)                                                       TAB11310
      STATS(3)=0.0                                                            TAB11320
      GO TO 95                                                                TAB11330
   9C STATS(2)=STATS(1)/SCNT                                                  TAB11340
      STATS(3)=SQRT(ABS((STATS(3)-STATS(1)*STATS(1)/SCNT)/(SCNT-1.0)))        TAB11349
   95 DO 1CC I=1,3                                                            TAB11350
  1CC UBC(I)=XBC(I)                                                           TAB11360
  105 RETURN                                                                  TAB11370
      END                                                                     TAB11380
```

Subroutine TAB2

This subroutine performs a two-way classification of the frequency, percent frequency, and other statistics over given class intervals, for two selected variables in an observation matrix.

Interval size for each variable is computed as follows:

$$k_j = \frac{UBO_{3j} - UBO_{1j}}{UBO_{2j} - 2} \quad (1)$$

where UBO_{1j} = given lower bound

UBO_{2j} = given number of intervals

UBO_{3j} = given upper bound

$j = 1, 2$

If $UBO_{1j} = UBO_{3j}$, the subroutine finds and uses the minimum and maximum values of the j^{th} variable.

A frequency tabulation is then made for each pair of observations in a two-way table as shown in Figure 6.

Symbols $\geq$ and $<$ in Figure 6 indicate that a count is classified into a particular interval if the data point is greater than or equal to the lower limit of that interval but less than the upper limit of the same interval.

Then, each entry in the frequency matrix, F_{ij}, is divided by the number of observations, N, to obtain the percent frequency:

$$P_{ij} = \frac{100F_{ij}}{N} \quad (2)$$

where $i = 1, 2, \ldots, UBO_{21}$

$j = 1, 2, \ldots, UBO_{22}$

As data are classified into the frequency matrix, the following intermediate results are accumulated for each class interval of both variables:

1. Number of data points, n
2. Sum of data points, $\sum_{i=1}^{n} X_i$
3. Sum of data points squared, $\sum_{i=1}^{n} X_i^2$

From these, the following statistics are calculated for each class interval:

Mean: $$\overline{X} = \frac{\sum_{i=1}^{n} X_i}{n} \quad (3)$$

Standard deviation:

$$s = \sqrt{\frac{\sum_{i=1}^{n} X_i^2 - \left(\sum_{i=1}^{n} X_i\right)^2 / n}{n - 1}} \quad (4)$$

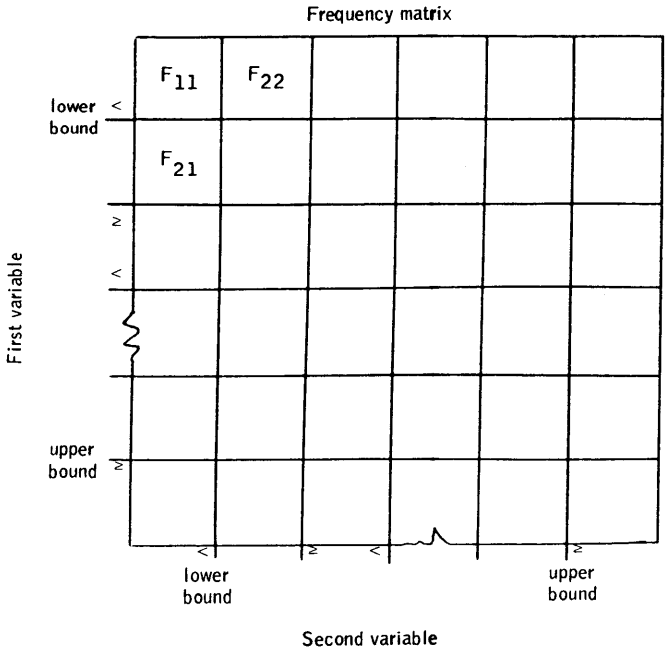

Figure 6. Frequency matrix

```
C                                                                       TAB2  10
C  .....TAB2  20
C                                                                       TAB2  30
C     SUBROUTINE TAB2                                                   TAB2  40
C                                                                       TAB2  50
C     PURPOSE                                                           TAB2  60
C        PERFORM A TWO-WAY CLASSIFICATION FOR TWO VARIABLES IN AN       TAB2  70
C        OBSERVATION MATRIX (OR A MATRIX SUBSET) OF THE FREQUENCY,      TAB2  80
C        PERCENT FREQUENCY, AND OTHER STATISTICS OVER GIVEN CLASS       TAB2  90
C        INTERVALS.                                                     TAB2 100
C                                                                       TAB2 110
C     USAGE                                                             TAB2 120
C        CALL TAB2(A,S,NDV,LBC,FREQ,PCT,STAT1,STAT2,NC,NV)              TAB2 130
C                                                                       TAB2 140
C     DESCRIPTION OF PARAMETERS                                         TAB2 150
C        A      - OBSERVATION MATRIX, NC BY NV                         TAB2 160
C        S      - INPUT VECTOR GIVING SUBSET OF A. ONLY THOSE          TAB2 170
C                 OBSERVATIONS WITH A CORRESPONDING NON-ZERO S(J) ARE  TAB2 180
C                 CONSIDERED. VECTOR LENGTH IS NC.                     TAB2 190
C        NDV    - VARIABLES TO BE CROSS-TABULATED. NDV(1) IS VARIABLE  TAB2 200
C                 1; NDV(2) IS VARIABLE 2. VECTOR LENGTH IS 2. NDV     TAB2 210
C                 MUST BE GREATER THAN OR EQUAL TO 1 AND LESS THAN     TAB2 211
C                 OR EQUAL TO NV.                                      TAB2 212
C        LBC    - 3 BY 2 MATRIX GIVING LOWER LIMIT, NUMBER OF          TAB2 220
C                 INTERVALS, AND UPPER LIMIT OF BOTH VARIABLES TO BE   TAB2 230
C                 TABULATED (FIRST COLUMN FOR VARIABLE 1, SECOND       TAB2 240
C                 COLUMN FOR VARIABLE 2). IF LOWER LIMIT IS EQUAL TO   TAB2 250
C                 UPPER LIMIT FOR VARIABLE 1, THE PROGRAM USES THE     TAB2 260
C                 MINIMUM AND MAXIMUM VALUES ON EACH VARIABLE. NUMBER  TAB2 270
C                 OF INTERVALS MUST INCLUDE TWO CELLS FOR UNDER AND    TAB2 280
C                 ABOVE LIMITS.                                        TAB2 290
C        FREQ   - OUTPUT MATRIX OF FREQUENCIES IN THE TWO-WAY          TAB2 300
C                 CLASSIFICATION. ORDER OF MATRIX IS INT1 BY INT2,     TAB2 310
C                 WHERE INT1 IS THE NUMBER OF INTERVALS OF VARIABLE 1  TAB2 320
C                 AND INT2 IS THE NUMBER OF INTERVALS OF VARIABLE 2.   TAB2 330
C                 INT1 AND INT2 MUST BE SPECIFIED IN THE SECOND        TAB2 340
C                 POSITION OF RESPECTIVE COLUMN OF LBC MATRIX.         TAB2 350
C        PCT    - OUTPUT MATRIX OF PERCENT FREQUENCIES, SAME ORDER     TAB2 360
C                 AS FREQ.                                             TAB2 370
C        STAT1  - OUTPUT MATRIX SUMMARIZING TOTALS, MEANS, AND         TAB2 380
C                 STANDARD DEVIATIONS FOR EACH CLASS INTERVAL OF       TAB2 390
C                 VARIABLE 1. ORDER OF MATRIX IS 3 BY INT1.            TAB2 400
C        STAT2  - SAME AS STAT1 BUT OVER VARIABLE 2. ORDER OF MATRIX   TAB2 410
C                 IS 3 BY INT2.                                        TAB2 420
C        NC     - NUMBER OF OBSERVATIONS. NC MUST BE GREATER THAN      TAB2 430
C                 OR EQUAL TO 1.                                       TAB2 431
C        NV     - NUMBER OF VARIABLES FOR EACH OBSERVATION. NV         TAB2 440
C                 MUST BE GREATER THAN OR EQUAL TO 1.                  TAB2 441
C                                                                       TAB2 450
C     REMARKS                                                           TAB2 460
C        IF S IS NULL, OUTPUT AREAS ARE SET TO ZERO                     TAB2 470
C                                                                       TAB2 480
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     TAB2 490
C        NONE                                                           TAB2 500
C                                                                       TAB2 510
C     METHOD                                                            TAB2 520
C        INTERVAL SIZES FOR BOTH VARIABLES ARE CALCULATED FROM THE      TAB2 530
C        GIVEN INFORMATION OR OPTIONALLY FROM THE MINIMUM AND MAXIMUM   TAB2 540
```

```
C          VALUES. THE FREQUENCY AND PERCENT FREQUENCY MATRICES ARE    TAB2 550
C          GENERATED. MATRICES STAT1 AND STAT2 SUMMARIZING TOTALS,     TAB2 560
C          MEANS, AND STANDARD DEVIATIONS ARE THEN CALCULATED.         TAB2 570
C          THE DIVISOR FOR STANDARD DEVIATION IS ONE LESS THAN THE     TAB2 580
C          NUMBER OF OBSERVATIONS USED IN EACH CLASS INTERVAL.         TAB2 590
C                                                                      TAB2 600
C     ******************************************************************TAB2 610
C                                                                      TAB2 620
      SUBROUTINE TAB2(A,S,NOV,LBC,FREQ,PCT,STAT1,STAT2,NC,NV) \        TAB2 630
      DIMENSION A(1),S(1),NOV(2),UBC(3,2),FREQ(1),PCT(1),STAT1(1),     TAB2 640
     1STAT2(2),SINT(2)                                                 TAB2 650
      DIMENSION UBC(3,2)                                               TAB2 660
      DO 5 I=1,3                                                       TAB2 670
      DO 5 J=1,2                                                       TAB2 680
    5 UBC(I,J)=LBC(I,J)                                                TAB2 690
C                                                                      TAB2 700
C        DETERMINE LIMITS                                              TAB2 710
C                                                                      TAB2 720
      DO 4C I=1,2                                                      TAB2 730
      IF(UBC(1,I)-UBC(3,I)) 4C, 1C, 4C                                 TAB2 740
   1C VMIN=1.0E75                                                      TAB2 750
      VMAX=-1.0E75                                                     TAB2 760
      IJ=NC*(NOV(I)-1)                                                 TAB2 770
      DO 35 J=1,NC                                                     TAB2 780
      IJ=IJ+1                                                          TAB2 790
      IF(S(IJ)) 15,35,15                                               TAB2 800
   15 IF(A(IJ)-VMIN) 2C,25,25                                          TAB2 810
   2C VMIN=A(IJ)                                                       TAB2 820
   25 IF(A(IJ)-VMAX) 35,35,30                                          TAB2 830
   3C VMAX=A(IJ)                                                       TAB2 840
   35 CONTINUE                                                         TAB2 850
      UBC(1,I)=VMIN                                                    TAB2 860
      LBC(3,I)=VMAX                                                    TAB2 870
   4C CONTINUE                                                         TAB2 880
C                                                                      TAB2 890
C        CALCULATE INTERVAL SIZE                                       TAB2 900
C                                                                      TAB2 910
      DO 5C I=1,2                                                      TAB2 920
   5C SINT(I)=ABS(UBC(3,I)-UBC(1,I))/(UBC(2,I)-2.0)                    TAB2 930
C                                                                      TAB2 940
C        CLEAR OUTPUT AREAS                                            TAB2 950
C                                                                      TAB2 960
      INT1=LBC(2,1)                                                    TAB2 970
      INT2=LBC(2,2)                                                    TAB2 980
      INTT=INT1*INT2                                                   TAB2 990
      DO 55 I=1,INTT                                                   TAB21000
      FREQ(I)=0.0                                                      TAB21010
   55 PCT(I)=0.0                                                       TAB21020
      INTY=3*INT1                                                      TAB21030
      DO 6C I=1,INTY                                                   TAB21040
   6C STAT1(I)=0.0                                                     TAB21050
      INTZ=3*INT2                                                      TAB21060
      DO 65 I=1,INTZ                                                   TAB21070
   65 STAT2(I)=0.0                                                     TAB21080
C                                                                      TAB21090
C        TEST SUBSET VECTOR                                            TAB21100
C                                                                      TAB21110
      SCNT=0.0                                                         TAB21120
      INTY=INT1-1                                                      TAB21130
      INTX=INT2-1                                                      TAB21140
      IJ=NC*(NOV(1)-1)                                                 TAB21150
      IJX=NC*(NOV(2)-1)                                                TAB21160
      DO 55 J=1,NC                                                     TAB21170
      IJ=IJ+1                                                          TAB21180
      IJX=IJX+1                                                        TAB21190
      IF(S(IJ)) 7C,55,7C                                               TAB21200
   7C SCNT=SCNT+1.0                                                    TAB21210
C                                                                      TAB21220
C        CALCULATE FREQUENCIES                                         TAB21230
C                                                                      TAB21240
      TEMP1=LBC(1,1)-SINT(1)                                           TAB21250
      DO 75 IY=1,INTY                                                  TAB21260
      TEMP1=TEMP1+SINT(1)                                              TAB21270
      IF(A(IJ)-TEMP1) 8Q,75,75                                         TAB21280
   75 CONTINUE                                                         TAB21290
      IY=INT1                                                          TAB21300
   8Q IYY=3*(IY-1)+1                                                   TAB21310
      STAT1(IYY)=STAT1(IYY)+A(IJ)                                      TAB21320
      IYY=IYY+1                                                        TAB21330
      STAT1(IYY)=STAT1(IYY)+1.0                                        TAB21340
      IYY=IYY+1                                                        TAB21350
      STAT1(IYY)=STAT1(IYY)+A(IJ)*A(IJ)                                TAB21360
      TEMP2=LBC(1,2)-SINT(2)                                           TAB21370
      DO 85 IX=1,INTX                                                  TAB21380
      TEMP2=TEMP2+SINT(2)                                              TAB21390
      IF(A(IJX)-TEMP2) 9C,85,85                                        TAB21400
   85 CONTINUE                                                         TAB21410
      IX=INT2                                                          TAB21420
   9C IJF=INT1*(IX-1)+IY                                               TAB21430
      FREQ(IJF)=FREQ(IJF)+1.0                                          TAB21440
      IX=3*(IX-1)+1                                                    TAB21450
      STAT2(IX)=STAT2(IX)+A(IJX)                                       TAB21460
      IX=IX+1                                                          TAB21470
      STAT2(IX)=STAT2(IX)+1.0                                          TAB21480
      IX=IX+1                                                          TAB21490
      STAT2(IX)=STAT2(IX)+A(IJX)*A(IJX)                                TAB21500
   95 CONTINUE                                                         TAB21510
      IF (SCNT)58,151,58                                               TAB21511
C                                                                      TAB21520
C        CALCULATE PERCENT FREQUENCIES                                 TAB21530
C                                                                      TAB21540
   58 DO 1CC I=1,INTT                                                  TAB21550
  1CC PCT(I)=FREQ(I)*100.0/SCNT                                        TAB21560
C                                                                      TAB21570
C        CALCULATE TOTALS, MEANS, STANDARD DEVIATIONS                  TAB21580
C                                                                      TAB21590
      IXY=-1                                                           TAB21600
      DO 12C I=1,INT1                                                  TAB21610
      IXY=IXY+2                                                        TAB21620
      ISC=IXY+1                                                        TAB21630
      TEMP1=STAT1(IXY)                                                 TAB21640
      SUM=STAT1(IXY-1)                                                 TAB21650
      IF(TEMP1-1.0) 12C,1C5,11C                                        TAB21660
  1C5 STAT1(ISC)=0.0                                                   TAB21670
      GO TO 115                                                        TAB21680
  11C STAT1(ISC)=SQRT(ABS((STAT1(ISC)-SUM*SUM/TEMP1)/(TEMP1-1.0)))     TAB21690
  115 STAT1(IXY)=SUM/TEMP1                                             TAB21700
  12C CONTINUE                                                         TAB21710
      IXX=-1                                                           TAB21720
      DO 14C I=1,INT2                                                  TAB21730
      IXX=IXX+2                                                        TAB21740
      ISC=IXX+1                                                        TAB21750
      TEMP2=STAT2(IXX)                                                 TAB21760
      SUM=STAT2(IXX-1)                                                 TAB21770
      IF(TEMP2-1.0) 14C,125,13C                                        TAB21780
  125 STAT2(ISC)=0.0                                                   TAB21790
      GO TO 135                                                        TAB21800
  13C STAT2(ISC)=SQRT(ABS((STAT2(ISC)-SUM*SUM/TEMP2)/(TEMP2-1.0)))     TAB21810
  135 STAT2(IXX)=SUM/TEMP2                                             TAB21820
  14C CONTINUE                                                         TAB21830
      DO 15C I=1,3                                                     TAB21840
      DO 15C J=1,2                                                     TAB21850
  15C UBC(I,J)=UBC(I,J)                                                TAB21860
  151 RETURN                                                           TAB21870
      END                                                              TAB21880
```

Subroutine SUBMX

```
C                                                                      SUBM  10
C     ******************************************************************SUBM  20
C                                                                      SUBM  30
C        SUBROUTINE SUBMX                                              SUBM  40
C                                                                      SUBM  50
C        PURPOSE                                                       SUBM  60
C           BASED ON VECTOR S DERIVED FROM SUBROUTINE SUBST OR ABSNT,  SUBM  70
C           THIS SUBROUTINE COPIES FROM A LARGER MATRIX OF OBSERVATION SUBM  80
C           DATA A SUBSET MATRIX OF THOSE OBSERVATIONS WHICH HAVE      SUBM  90
C           SATISFIED CERTAIN CONDITION.  THIS SUBROUTINE IS NORMALLY  SUBM 100
C           USED PRIOR TO STATISTICAL ANALYSES (E.G., MULTIPLE REGRES- SUBM 110
C           SION, FACTOR ANALYSIS).                                    SUBM 120
C                                                                      SUBM 130
C        USAGE                                                         SUBM 140
C           CALL SUBMX (A,C,S,NC,NV,N)                                 SUBM 150
C                                                                      SUBM 160
C        DESCRIPTION OF PARAMETERS                                     SUBM 170
C           A  - INPUT MATRIX OF OBSERVATIONS, NO BY NV.               SUBM 180
C           C  - OUTPUT MATRIX OF OBSERVATIONS, N BY NV.               SUBM 190
C           S  - INPUT VECTOR OF LENGTH NO CONTAINING THE CODES DERIVED SUBM 200
C                FROM SUBROUTINE SUBST OR ABSNT.                       SUBM 210
C           NC - NUMBER OF OBSERVATIONS. NC MUST BE > OR = TO 1.       SUBM 220
C           NV - NUMBER OF VARIABLES. NV MUST BE > OR = TO 1.          SUBM 230
C           N  - OUTPUT VARIABLE CONTAINING THE NUMBER OF NON-ZERO CODESSUBM 240
C                IN VECTOR S.                                          SUBM 250
C                                                                      SUBM 260
C        REMARKS                                                       SUBM 270
C           MATRIX C CAN BE IN THE SAME LOCATION AS MATRIX A.          SUBM 280
C                                                                      SUBM 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 SUBM 300
C           NONE                                                       SUBM 310
C                                                                      SUBM 320
C        METHOD                                                        SUBM 330
C           IF S(I) CONTAINS A NON-ZERO CODE, I-TH OBSERVATION IS      SUBM 340
C           COPIED FROM THE INPUT MATRIX TO THE OUTPUT MATRIX.         SUBM 350
C                                                                      SUBM 360
C     ******************************************************************SUBM 370
C                                                                      SUBM 380
      SUBROUTINE SUBMX (A,C,S,NO,NV,N)                                 SUBM 390
      DIMENSION A(1),C(1),S(1)                                         SUBM 400
C                                                                      SUBM 410
      L=0                                                              SUBM 420
      LL=0                                                             SUBM 430
      DO 2C J=1,NV                                                     SUBM 440
      DO 15 I=1,NC                                                     SUBM 450
      L=L+1                                                            SUBM 460
      IF(S(I)) 15, 15, 1C                                              SUBM 470
   1C LL=LL+1                                                          SUBM 480
      C(LL)=A(L)                                                       SUBM 490
   15 CONTINUE                                                         SUBM 500
   2C CONTINUE                                                         SUBM 510
C                                                                      SUBM 520
C        COUNT NON-ZERO CODES IN VECTOR S                              SUBM 530
C                                                                      SUBM 540
      N=0                                                              SUBM 550
      DO 3C I=1,NC                                                     SUBM 560
      IF(S(I)) 3C, 3C, 25                                              SUBM 570
   25 N=N+1                                                            SUBM 580
   3C CONTINUE                                                         SUBM 590
C                                                                      SUBM 600
      RETURN                                                           SUBM 610
      END                                                              SUBM 620
```

Correlation and Regression (see Smoothing, Factorization)

Subroutine CORRE

This subroutine calculates means, standard deviations, sums of cross-products of deviations from means, and product moment correlation coefficients from input data X_{ij}, where i = 1, 2, ..., n implies observations and j = 1, 2, ..., m implies variables.

The following equations are used to calculate these statistics.

Sums of cross-products of deviations:

$$S_{jk} = \sum_{i=1}^{n} \left(X_{ij} - T_j \right) \left(X_{ik} - T_k \right) - \frac{\sum_{i=1}^{n} \left(X_{ij} - T_j \right) \sum_{i=1}^{n} \left(X_{ik} - T_k \right)}{n} \quad (1)$$

where j = 1, 2, ..., m; k = 1, 2, ..., m

$$T_j = \frac{\sum_{i=1}^{m} X_{ij}}{m} \quad (2)$$

(These temporary means T_j are subtracted from the data in equation (1) to obtain computational accuracy.)

Means: $$\overline{X}_j = \frac{\sum_{i=1}^{n} X_{ij}}{n} \quad (3)$$

where j = 1, 2, ..., m

Correlation coefficients:

$$r_{jk} = \frac{S_{jk}}{\sqrt{S_{jj}} \sqrt{S_{kk}}} \quad (4)$$

where j = 1, 2, ..., m; k = 1, 2, ..., m

Standard deviations:

$$s_j = \frac{\sqrt{S_{jj}}}{\sqrt{n-1}} \quad (5)$$

where j = 1, 2, ..., m

```
C                                                                       CORR  10
C     ..................................................................CORR  20
C                                                                       CORR  30
C        SUBROUTINE CORRE                                               CORR  40
C                                                                       CORR  50
C        PURPOSE                                                        CORR  60
C           COMPUTE MEANS, STANDARD DEVIATIONS, SUMS OF CROSS-PRODUCTS  CORR  70
C           OF DEVIATIONS, AND CORRELATION COEFFICIENTS.                CORR  80
C                                                                       CORR  90
C        USAGE                                                          CORR 100
C           CALL CORRE (N,M,IC,X,XBAR,STD,RX,R,B,D,T)                   CORR 110
C                                                                       CORR 120
C        DESCRIPTION OF PARAMETERS                                      CORR 130
C           N     - NUMBER OF OBSERVATIONS. N MUST BE > OR = TO 2.      CORR 140
C           M     - NUMBER OF VARIABLES. M MUST BE > OR = TO 1.         CORR 150
C           IC    - OPTION CODE FOR INPUT DATA                          CORR 160
C                   0 IF DATA ARE TO BE READ IN FROM INPUT DEVICE IN THCORR 170
C                     SPECIAL SUBROUTINE NAMED DATA.  (SEE SUBROUTINES  CORR 180
C                     USED BY THIS SUBROUTINE BELOW.)                   CORR 190
C                   1 IF ALL DATA ARE ALREADY IN CORE.                  CORR 200
C           X     - IF IC=0, THE VALUE OF X IS 0.0.                     CORR 210
C                   IF IC=1, X IS THE INPUT MATRIX (N BY M) CONTAINING  CORR 220
C                            DATA.                                      CORR 230
C           XBAR  - OUTPUT VECTOR OF LENGTH M CONTAINING MEANS.         CORR 240
C           STD   - OUTPUT VECTOR OF LENGTH M CONTAINING STANDARD       CORR 250
C                   DEVIATIONS.                                         CORR 260
C           RX    - OUTPUT MATRIX (M X M) CONTAINING SUMS OF CROSS-     CORR 270
C                   PRODUCTS OF DEVIATIONS FROM MEANS.                  CORR 280
C           R     - OUTPUT MATRIX (ONLY UPPER TRIANGULAR PORTION OF THE CORR 290
C                   SYMMETRIC MATRIX OF M BY M) CONTAINING CORRELATION  CORR 300
C                   COEFFICIENTS.  (STORAGE MODE OF 1)                  CORR 310
C           B     - OUTPUT VECTOR OF LENGTH M CONTAINING THE DIAGONAL   CORR 320
C                   OF THE MATRIX OF SUMS OF CROSS-PRODUCTS OF          CORR 330
C                   DEVIATIONS FROM MEANS.                              CORR 340
C           C     - WORKING VECTOR OF LENGTH M.                         CORR 350
C           T     - WORKING VECTOR OF LENGTH M.                         CORR 360
C                                                                       CORR 370
C        REMARKS                                                        CORR 380
C           CORRE WILL NOT ACCEPT A CONSTANT VECTOR.                    CORR 390
C                                                                       CORR 400
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CORR 410
C           DATA(M,C) - THIS SUBROUTINE MUST BE PROVIDED BY THE USER.   CORR 420
C                       (1) IF IC=0, THIS SUBROUTINE IS EXPECTED TO     CORR 430
C                           FURNISH AN OBSERVATION IN VECTOR D FROM AN  CORR 440
C                           EXTERNAL INPUT DEVICE.                      CORR 450
C                       (2) IF IC=1, THIS SUBROUTINE IS NOT USED BY     CORR 460
C                           CORRE BUT MUST EXIST IN JOB DECK. IF USER   CORR 470
C                           HAS NOT SUPPLIED A SUBROUTINE NAMED DATA,   CORR 480
C                           THE FOLLOWING IS SUGGESTED.                 CORR 490
C                                SUBROUTINE DATA                        CORR 500
C                                RETURN                                 CORR 510
C                                END                                    CORR 520
C                                                                       CORR 530
C        METHOD                                                         CORR 540
C           PRODUCT-MOMENT CORRELATION COEFFICIENTS ARE COMPUTED.       CORR 550
C                                                                       CORR 560
C     ..................................................................CORR 570
C                                                                       CORR 580
      SUBROUTINE CORRE (N,M,IC,X,XBAR,STD,RX,R,B,D,T)                   CORR 590
      DIMENSION X(1),XBAR(1),STD(1),RX(1),R(1),B(1),D(1),T(1)           CORR 600
C                                                                       CORR 610
C     ..................................................................CORR 620
C                                                                       CORR 630
C     IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE     CORR 640
C     C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION         CORR 650
C     STATEMENT WHICH FOLLOWS.                                          CORR 660
C                                                                       CORR 670
C     DOUBLE PRECISION XBAR,STD,RX,R,B,T                                CORR 680
C                                                                       CORR 690
C     THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS       CORR 700
C     APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS         CORR 710
C     ROUTINE.                                                          CORR 720
C                                                                       CORR 730
C     THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO         CORR 740
C     CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT AND ABS IN      CORR 750
C     STATEMENT 220 MUST BE CHANGED TO DSQRT AND DABS.                  CORR 760
C                                                                       CORR 770
C     ..................................................................CORR 780
C                                                                       CORR 790
C     INITIALIZATION                                                    CORR 800
C                                                                       CORR 810
      DO 100 J=1,M                                                      CORR 820
      B(J)=0.0                                                          CORR 830
  100 T(J)=0.0                                                          CORR 840
      K=(M*M+M)/2                                                       CORR 850
      DO 102 I=1,K                                                      CORR 860
  102 R(I)=0.0                                                          CORR 870
      FN=N                                                              CORR 880
      L=0                                                               CORR 890
C                                                                       CORR 900
      IF(IC) 105, 127, 105                                              CORR 910
C                                                                       CORR 920
C     DATA ARE ALREADY IN CORE                                          CORR 930
C                                                                       CORR 940
  105 DO 108 J=1,M                                                      CORR 950
      DO 107 I=1,N                                                      CORR 960
      L=L+1                                                             CORR 970
  107 T(J)=T(J)+X(L)                                                    CORR 980
      XBAR(J)=T(J)                                                      CORR 990
  108 T(J)=T(J)/FN                                                      CORR1000
C                                                                       CORR1010
      DO 115 I=1,N                                                      CORR1020
      JK=0                                                              CORR1030
      L=I-N                                                             CORR1040
      DO 110 J=1,M                                                      CORR1050
      L=L+N                                                             CORR1060
      D(J)=X(L)-T(J)                                                    CORR1070
  110 B(J)=B(J)+D(J)                                                    CORR1080
      DO 115 J=1,M                                                      CORR1090
      DO 115 K=1,J                                                      CORR1100
      JK=JK+1                                                           CORR1110
  115 R(JK)=R(JK)+D(J)*D(K)                                             CORR1120
      GO TO 205                                                         CORR1130
C                                                                       CORR1140
C     READ OBSERVATIONS AND CALCULATE TEMPORARY                         CORR1150
C     MEANS FROM THESE DATA IN T(J)                                     CORR1160
C                                                                       CORR1170
  127 IF(N-M) 130, 130, 135                                             CORR1180
  130 KK=N                                                              CORR1190
      GO TO 137                                                         CORR1200
  135 KK=M                                                              CORR1210
  137 DO 140 I=1,KK                                                     CORR1220
      CALL DATA (M,D)                                                   CORR1230
      DO 140 J=1,M                                                      CORR1240
      T(J)=T(J)+D(J)                                                    CORR1250
      L=L+1                                                             CORR1260
  140 RX(L)=D(J)                                                        CORR1270
      FKK=KK                                                            CORR1280
      DO 150 J=1,M                                                      CORR1290
      XBAR(J)=T(J)                                                      CORR1300
  150 T(J)=T(J)/FKK                                                     CORR1310
```

```
C
C     CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS
C     FROM TEMPORARY MEANS FOR M OBSERVATIONS
C
      L=0                                                          CORR1320
      DO 180 I=1,KK                                                CORR1330
      JK=0                                                         CORR1340
      DO 170 J=1,M                                                 CORR1350
      L=L+1                                                        CORR1360
  170 C(J)=RX(L)-T(J)                                              CORR1370
      DO 180 J=1,M                                                 CORR1380
      B(J)=B(J)+C(J)                                               CORR1390
      DO 180 K=1,J                                                 CORR1400
      JK=JK+1                                                      CORR1410
  180 R(JK)=R(JK)+C(J)*C(K)                                        CORR1420
C                                                                  CORR1430
      IF(N-KK) 205, 205, 185                                       CORR1440
C                                                                  CORR1450
C     READ THE REST OF OBSERVATIONS ONE AT A TIME, SUB             CORR1460
C     THE OBSERVATION, AND CALCULATE SUMS OF CROSS-                CORR1470
C     PRODUCTS OF DEVIATIONS FROM TEMPORARY MEANS                  CORR1480
C                                                                  CORR1490
  185 KK=N-KK                                                      CORR1500
      DO 200 I=1,KK                                                CORR1510
      JK=0                                                         CORR1520
      CALL DATA (M,C)                                              CORR1530
      DO 190 J=1,M                                                 CORR1540
      XBAR(J)=XBAR(J)+C(J)                                         CORR1550
      C(J)=C(J)-T(J)                                               CORR1560
  190 B(J)=B(J)+C(J)                                               CORR1570
      DO 200 J=1,M                                                 CORR1580
      DO 200 K=1,J                                                 CORR1590
      JK=JK+1                                                      CORR1600
  200 R(JK)=R(JK)+C(J)*C(K)                                        CORR1610
C                                                                  CORR1620
C     CALCULATE MEANS                                              CORR1630
C                                                                  CORR1640
  205 JK=0                                                         CORR1650
      DO 210 J=1,M                                                 CORR1660
      XBAR(J)=XBAR(J)/FN                                           CORR1670
C                                                                  CORR1680
C     ADJUST SUMS OF CROSS-PRODUCTS OF DEVIATIONS                  CORR1690
C     FROM TEMPORARY MEANS                                         CORR1700
C                                                                  CORR1710
      DO 210 K=1,J                                                 CORR1720
      JK=JK+1                                                      CORR1730
  210 R(JK)=R(JK)-B(J)*B(K)/FN                                     CORR1740
C                                                                  CORR1750
C     CALCULATE CORRELATION COEFFICIENTS                           CORR1760
C                                                                  CORR1770
      JK=0                                                         CORR1780
      DO 220 J=1,M                                                 CORR1790
      JK=JK+J                                                      CORR1800
  220 STD(J)= SQRT( ABS(R(JK)))                                    CORR1810
      DO 230 J=1,M                                                 CORR1820
      DO 230 K=J,M                                                 CORR1830
      JK=J+(K*K-K)/2                                               CORR1840
      L=M*(J-1)+K                                                  CORR1850
      RX(L)=R(JK)                                                  CORR1860
      L=M*(K-1)+J                                                  CORR1870
      RX(L)=R(JK)                                                  CORR1880
      IF(STD(J)*STD(K)) 225, 222, 225                              CORR1890
  222 R(JK)=0.0                                                    CORR1900
      GO TO 230                                                    CORR1910
  225 R(JK)=R(JK)/(STD(J)*STD(K))                                  CORR1920
  230 CONTINUE                                                     CORR1930
C                                                                  CORR1940
C     CALCULATE STANDARD DEVIATIONS                                CORR1950
C                                                                  CORR1960
      FN=SQRT(FN-1.0)                                              CORR1970
      DO 240 J=1,M                                                 CORR1980
  240 STD(J)=STD(J)/FN                                             CORR1990
C                                                                  CORR2000
C     COPY THE DIAGONAL OF THE MATRIX OF SUMS OF CROSS-PRODUCTS OF CORR2010
C     DEVIATIONS FROM MEANS.                                       CORR2020
C                                                                  CORR2030
      L=-M                                                         CORR2040
      DO 250 I=1,M                                                 CORR2050
      L=L+M+1                                                      CORR2060
  250 B(I)=RX(L)                                                   CORR2070
      RETURN                                                       CORR2080
      END                                                          CORR2090
                                                                   CORR2100
                                                                   CORR2110
                                                                   CORR2120
                                                                   CORR2130
```

Subroutine MISR

This subroutine computes means, standard deviations, third and fourth moments, correlation coefficients, regression coefficients, and standard errors of regression coefficients when there is missing data. Effective sample sizes are also provided. Missing observations or certain values of the data can be skipped at the user's option. The computational steps are as follows:

1. Compute means:

$$\bar{x}_j = \frac{\sum_{\alpha=1}^{n} x_{\alpha j}}{n} \qquad (1)$$

where j = 1, 2, . . . , m implies variables
n = number of nonmissing values for the jth variable

2. Compute sums of cross-products of deviations from means for complete sets of ith and jth variables:

$$S_{ij} = \sum_{\alpha=1}^{n'} (x_{\alpha i} - \bar{x}_i)(x_{\alpha j} - \bar{x}_j) - \frac{\sum_{\alpha=1}^{n'} (x_{\alpha i} - \bar{x}_i) \sum_{\alpha=1}^{n'} (x_{\alpha j} - \bar{x}_j)}{n'} \qquad (2)$$

where $\bar{x}_i$, $\bar{x}_j$ = means of ith and jth variables computed as above
n' = number of sets where the ith and jth variables are both present

3. Compute product-moment correlations:

$$r_{ij} = \frac{S_{ij}}{\sqrt{S_{ii}}\sqrt{S_{jj}}} \qquad (3)$$

4. Compute regression coefficients, intercepts, and standard errors of regression coefficients:

a. ith variable as independent and jth variable as dependent:

Regression coefficient: $b_{ij} = \frac{S_{ij}}{S_{ii}}$ (4)

Intercept: $a_{ij} = \bar{x}'_j - b_{ij}\bar{x}_i'$ (5)

Standard error regression coefficient:

$$s_{b_{ij}} = \frac{S_{jj} - r_{ij}^2 \, S_{jj}}{(n' - 2) \, S_{ii}} \qquad (6)$$

b. jth variable as independent and ith variable as dependent:

Regression coefficient: $b_{ji} = \frac{S_{ij}}{S_{jj}}$ (7)

Intercept: $a_{ji} = \bar{x}_i' - b_{ji} \bar{x}_j'$ (8)

Standard error of regression coefficient:

$$s_{b_{ji}} = \frac{S_{ii} - r_{ij}^2 \, S_{ii}}{(n' - 2) \, S_{jj}} \qquad (9)$$

5. Compute standard deviations:

$$s_j = \sqrt{\frac{S_{jj}}{n - 1}} \qquad (10)$$

where n = number of nonmissing values for jth variable

6. Compute skewness and kurtosis, s and k:

Let $\mu_{i_j} = \sum_{\alpha=1}^{n} (x_{\alpha_j} - \bar{x}_j)^{i} / n$

Then $s_j = \mu_{3_j} / (\mu_{2_j})^{3/2}$ (11)

and $k_j = (\mu_{4_j} / \mu_{2_j}^2) - 3$ (12)

Note: This subroutine cannot distinguish between a blank and a zero. Therefore, if a blank is specified as a missing data code in input cards, it will be treated as 0 (zero).

For reference see B. Ostle, Statistics in Research. The Iowa State College Press, 1954, chapter 6.

```
C                                                                       MISR  10
C     ..................................................................MISR  20
C                                                                       MISR  30
C        SUBROUTINE MISR                                                MISR  40
C                                                                       MISR  50
C        PURPOSE                                                        MISR  60
C           COMPUTE MEANS, STANDARD DEVIATIONS, SKEWNESS AND KURTOSIS.  MISR  70
C           CORRELATION COEFFICIENTS, REGRESSION COEFFICIENTS, AND      MISR  80
C           STANDARD ERRORS OF REGRESSION COEFFICIENTS WHEN THERE ARE    MISR  90
C           MISSING DATA POINTS.  THE USER IDENTIFIES THE MISSING DATA  MISR 100
C           BY MEANS OF A NUMERIC CODE.  THOSE VALUES HAVING THIS CODE  MISR 110
C           ARE SKIPPED IN COMPUTING THE STATISTICS.  IN THE CASE OF THEMISR 120
C           CORRELATION COEFFICIENTS, ANY PAIR OF VALUES ARE SKIPPED IF MISR 130
C           EITHER ONE OF THEM ARE MISSING.                             MISR 140
C                                                                       MISR 150
C        USAGE                                                          MISR 160
C           CALL MISR (NO,M,X,CODE,XBAR,STD,SKEW,CURT,R,N,A,B,S,IER)    MISR 170
C                                                                       MISR 180
C        DESCRIPTION OF PARAMETERS                                      MISR 190
C           NO   - NUMBER OF OBSERVATIONS                               MISR 200
C           M    - NUMBER OF VARIABLES                                  MISR 210
C           X    - INPUT DATA MATRIX OF SIZE NO X M.                    MISR 220
C           CODE - INPUT VECTOR OF LENGTH M, WHICH CONTAINS A NUMERIC   MISR 230
C                  MISSING DATA CODE FOR EACH VARIABLE. ANY OBSERVATION MISR 240
C                  FOR A GIVEN VARIABLE HAVING A VALUE EQUAL TO THE CODEMISR 250
C                  WILL BE DROPPED FOR THE COMPUTATIONS.                MISR 260
C           XBAR - OUTPUT VECTOR OF LENGTH M CONTAINING MEANS           MISR 270
C           STD  - OUTPUT VECTOR OF LENGTH M CONTAINING STANDARD DEVI-  MISR 280
C                  ATIONS                                               MISR 290
C           SKEW - OUTPUT VECTOR OF LENGTH M CONTAINING SKEWNESS        MISR 300
C           CURT - OUTPUT VECTOR OF LENGTH M CONTAINING KURTOSIS        MISR 310
C           R    - OUTPUT MATRIX OF PRODUCT-MOMENT CORRELATION          MISR 320
C                  COEFFICIENTS.  THIS WILL BE THE UPPER TRIANGULAR     MISR 330
C                  MATRIX ONLY, SINCE THE M X M MATRIX OF COEFFICIENTS  MISR 340
C                  IS SYMMETRIC. (STORAGE MODE 1)                       MISR 350
C           N    - OUTPUT MATRIX OF NUMBER OF PAIRS OF OBSERVATIONS USEDMISR 360
C                  IN COMPUTING THE CORRELATION COEFFICIENTS.  ONLY THE MISR 370
C                  UPPER TRIANGULAR PORTION OF THE MATRIX IS GIVEN.     MISR 380
C                  (STORAGE MODE 1)                                     MISR 390
C           A    - OUTPUT MATRIX (M BY M)  CONTAINING INTERCEPTS OF     MISR 400
C                  REGRESSION LINES (A) OF THE FORM Y=A+BX.  THE FIRST  MISR 410
C                  SUBSCRIPT OF THIS MATRIX REFERS TO THE INDEPENDENT   MISR 420
C                  VARIABLE AND THE SECOND TO THE DEPENDENT VARIABLE.   MISR 430
C                  FOR EXAMPLE, A(1,3) CONTAINS THE INTERCEPT OF THE    MISR 440
C                  REGRESSION LINE FOR TWO VARIABLES WHERE VARIABLE 1   MISR 450
C                  IS INDEPENDENT AND VARIABLE 3 IS DEPENDENT.  NOTE    MISR 460
C                  THAT MATRIX A IS STORED IN A VECTOR FORM.            MISR 470
C           B    - OUTPUT MATRIX (M BY M)  CONTAINING REGRESSION        MISR 480
C                  COEFFICIENTS (B) CORRESPONDING TO THE VALUES OF      MISR 490
C                  INTERCEPTS CONTAINED IN THE OUTPUT MATRIX A.         MISR 500
C           S    - OUTPUT MATRIX (M BY M)  CONTAINING STANDARD ERRORS   MISR 510
C                  OF REGRESSION COEFFICIENTS CORRESPONDING TO THE      MISR 520
C                  COEFFICIENTS CONTAINED IN THE OUTPUT MATRIX B.       MISR 530
C           IER  - 0, NO ERROR.                                         MISR 540
C                  1, IF NUMBER OF NON-MISSING DATA ELEMENTS FOR J-TH    MISR 550
C                     VARIABLE IS TWO OR LESS.  IN THIS CASE, STD(J),   MISR 560
C                     SKEW(J), AND CURT(J) ARE SET TO 10**75.  ALL      MISR 570
C                     VALUES OF R, A, B, AND S RELATED TO THIS VARIABLE MISR 580
C                     ARE ALSO SET TO 10**75.                           MISR 590
C                  2, IF VARIANCE OF J-TH VARIABLE IS LESS THAN         MISR 600
C                     10**(-20).  IN THIS CASE, STD(J), SKEW(J), AND    MISR 610
C                     CURT(J) ARE SET TO 10**75.  ALL VALUES OF R, A,   MISR 620
C                     B, AND S RELATED TO THIS VARIABLE ARE ALSO SET TO MISR 630
C                     10**75.                                           MISR 640
C                                                                       MISR 650
C        REMARKS                                                        MISR 660
C           THIS SUBROUTINE CANNOT DISTINGUISH A BLANK AND A ZERO.      MISR 670
C           THEREFORE, IF A BLANK IS SPECIFIED AS A MISSING DATA CODE INMISR 680
C           INPUT CARDS, IT WILL BE TREATED AS 0 (ZERO).                MISR 690
C                                                                       MISR 700
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MISR 710
C           NONE                                                        MISR 720
C                                                                       MISR 730
C        METHOD                                                         MISR 740
C           LEAST SQUARES REGRESSION LINES AND PRODUCT-MOMENT CORRE-     MISR 750
C           LATION COEFFICIENTS ARE COMPUTED.                           MISR 760
C                                                                       MISR 770
C     ..................................................................MISR 780
C                                                                       MISR 790
      SUBROUTINE MISR (NO,M,X,CODE,XBAR,STD,SKEW,CURT,R,N,A,B,S,IER)    MISR 800
C                                                                       MISR 810
      DIMENSION X(1),CODE(1),XBAR(1),STD(1),SKEW(1),CURT(1),R(1),N(1)   MISR 820
      DIMENSION A(1),B(1),S(1)                                          MISR 830
C                                                                       MISR 840
C        COMPUTE MEANS                                                  MISR 850
C                                                                       MISR 860
      IER=0                                                             MISR 870
      L=0                                                               MISR 880
      DO 20 J=1,M                                                       MISR 890
      FN=0.0                                                            MISR 900
      XBAR(J)=0.0                                                       MISR 910
      DO 15 I=1,NO                                                      MISR 920
      L=L+1                                                             MISR 930
      IF(X(L)-CODE(J)) 12, 15, 12                                       MISR 940
   12 FN=FN+1.0                                                         MISR 950
      XBAR(J)=XBAR(J)+X(L)                                              MISR 960
   15 CONTINUE                                                          MISR 970
      IF(FN) 16, 16, 17                                                 MISR 980
   16 XBAR(J)=0.0                                                       MISR 990
      GO TO 20                                                          MISR1000
   17 XBAR(J)=XBAR(J)/FN                                                MISR1010
   20 CONTINUE                                                          MISR1020
C                                                                       MISR1030
C        SET-UP WORK AREAS AND TEST WHETHER DATA IS MISSING             MISR1040
C                                                                       MISR1050
      L=0                                                               MISR1060
      DO 55 J=1,M                                                       MISR1070
      LJJ=NO*(J-1)                                                      MISR1080
      SKEW(J)=0.0                                                       MISR1090
      CURT(J)=0.0                                                       MISR1100
      KI=M*(J-1)                                                        MISR1110
      KJ=J-M                                                            MISR1120
      DO 54 I=1,J                                                       MISR1130
      KI=KI+1                                                           MISR1140
      KJ=KJ+M                                                           MISR1150
      SUMX=0.0                                                          MISR1160
      SUMY=0.0                                                          MISR1170
      TI=0.0                                                            MISR1180
      TJ=0.0                                                            MISR1190
      TII=0.0                                                           MISR1200
      TJJ=0.0                                                           MISR1210
      TIJ=0.0                                                           MISR1220
      NIJ=0                                                             MISR1230
      LI=NO*(I-1)                                                       MISR1240
      LJ=LJJ                                                            MISR1250
      L=L+1                                                             MISR1260
      DO 38 K=1,NO                                                      MISR1270
      LI=LI+1                                                           MISR1280
      LJ=LJ+1                                                           MISR1290
      IF(X(LI)-CODE(I)) 30, 38, 30                                      MISR1300
   30 IF(X(LJ)-CODE(J)) 35, 38, 35                                      MISR1310
```

```
C
C         BOTH DATA ARE PRESENT
C
   35 XX=X(LI)-XBAR(I)
      YY=X(LJ)-XBAR(J)
      TI=TI+XX
      TII=TII+XX**2
      TJ=TJ+YY
      TJJ=TJJ+YY**2
      TIJ=TIJ+XX*YY
      NIJ=NIJ+1
      SUMX=SUMX+X(LI)
      SUMY=SUMY+X(LJ)
      IF(I-J) 38, 37, 37
   37 SKEW(J)=SKEW(J)+YY**3
      CURT(J)=CURT(J)+YY**4
   38 CONTINUE
C
C         COMPUTE SUM OF CROSS-PRODUCTS OF DEVIATIONS
C
      IF(NIJ) 40, 40, 39
   39 FN=NIJ
      R(L)=TIJ-TI*TJ/FN
      N(L)=NIJ
      TII=TII-TI*TI/FN
      TJJ=TJJ-TJ*TJ/FN
C
C         COMPUTE STANDARD DEVIATION, SKEWNESS, AND KURTOSIS
C
   40 IF(I-J) 47, 41, 47
   41 IF(NIJ-2) 42,42,43
   42 IER=1
      R(L)=1.0E75
      A(KI)=1.0E75
      B(KI)=1.0E75
      S(KI)=1.0E75
      GO TO 45
C
   43 STD(J)=R(L)
      R(L)=1.0
      A(KI)=0.0
      B(KI)=1.0
      S(KI)=0.0
C
      IF(STD(J)-(1.0E-20)) 44,44,46
   44 IER=2
   45 STD(J)=1.0E75
      SKEW(J)=1.0E75
      CURT(J)=1.0E75
      GO TO 55
C
   46 WORK=STD(J)/FN
      SKEW(J)=(SKEW(J)/FN)/(WORK*SQRT(WORK))
      CURT(J)=((CURT(J)/FN)/WORK**2)-3.0
      STD(J)=SQRT(STD(J)/(FN-1.0))
      GO TO 55
C
C         COMPUTE REGRESSION COEFFICIENTS
C
   47 IF(NIJ-2) 48,48,50
   48 IER=1
   49 R(L)=1.0E75
      A(KI)=1.0E75
      B(KI)=1.0E75
      S(KI)=1.0E75
      A(KJ)=1.0E75
      B(KJ)=1.0E75
      S(KJ)=1.0E75
      GO TO 54
C
   50 IF(TII-(1.0E-20)) 52,52,51
   51 IF(TJJ-(1.0E-20)) 52,52,53
   52 IER=2
      GO TO 49
C
   53 SUMX=SUMX/FN
      SUMY=SUMY/FN
      B(KI)=R(L)/TII
      A(KI)=SUMY-B(KI)*SUMX
      B(KJ)=R(L)/TJJ
      A(KJ)=SUMX-B(KJ)*SUMY
C
C         COMPUTE CORRELATION COEFFICIENTS
C
      R(L)=R(L)/(SQRT(TII)*SQRT(TJJ))
C
C         COMPUTE STANDARD ERRORS OF REGRESSION COEFFICIENTS
C
      RR=R(L)**2
      SUMX=(TJJ-TJJ*RR)/(FN-2)
      S(KI)=SQRT(SUMX/TII)
      SUMY=(TII-TII*RR)/(FN-2)
      S(KJ)=SQRT(SUMY/TJJ)
C
   54 CONTINUE
   55 CONTINUE
C
      RETURN
      END
```

In the Scientific Subroutine Package, multiple linear regression is normally performed by calling four subroutines in sequence.

1. CORRE - to find means, standard deviations, and correlation matrix

2. ORDER - to choose a dependent variable and a subset of independent variables from a larger set of variables

3. MINV - to invert the correlation matrix of the subset selected by ORDER

4. MULTR - to compute the regression coefficients b_0, b_1, b_2, ..., b_m, and various confidence measures

The subroutine CORRE works in either of two ways: (1) it expects all observations in core, or (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines Required" in the comment cards description of subroutine CORRE).

Subroutine ORDER

```
C                                                                       ORDE  10
C     ...................................................................ORDE  20
C                                                                       ORDE  30
C        SUBROUTINE ORDER                                               ORDE  40
C                                                                       ORDE  50
C        PURPOSE                                                        ORDE  60
C           CONSTRUCT FROM A LARGER MATRIX OF CORRELATION COEFFICIENTS  ORDE  70
C           A SUBSET MATRIX OF INTERCORRELATIONS AMONG INDEPENDENT      ORDE  80
C           VARIABLES AND A VECTOR OF INTERCORRELATIONS OF INDEPENDENT  ORDE  90
C           VARIABLES WITH DEPENDENT VARIABLE.  THIS SUBROUTINE IS      ORDE 100
C           NORMALLY USED IN THE PERFORMANCE OF MULTIPLE AND POLYNOMIAL ORDE 110
C           REGRESSION ANALYSES.                                        ORDE 120
C                                                                       ORDE 130
C        USAGE                                                          ORDE 140
C           CALL ORDER (M,R,NDEP,K,ISAVE,RX,RY)                         ORDE 150
C                                                                       ORDE 160
C        DESCRIPTION OF PARAMETERS                                      ORDE 170
C           M     - NUMBER OF VARIABLES AND ORDER OF MATRIX R.          ORDE 180
C           R     - INPUT MATRIX CONTAINING CORRELATION COEFFICIENTS.   ORDE 190
C                   THIS SUBROUTINE EXPECTS ONLY UPPER TRIANGULAR       ORDE 200
C                   PORTION OF THE SYMMETRIC MATRIX TO BE STORED (BY    ORDE 210
C                   COLUMN) IN R.  (STORAGE MODE OF 1)                  ORDE 220
C           NDEP  - THE SUBSCRIPT NUMBER OF THE DEPENDENT VARIABLE.     ORDE 230
C           K     - NUMBER OF INDEPENDENT VARIABLES TO BE INCLUDED      ORDE 240
C                   IN THE FORTHCOMING REGRESSION. K MUST BE GREATER    ORDE 250
C                   THAN OR EQUAL TO 1.                                 ORDE 251
C           ISAVE - INPUT VECTOR OF LENGTH K+1 CONTAINING, IN ASCENDING ORDE 260
C                   ORDER, THE SUBSCRIPT NUMBERS OF K INDEPENDENT       ORDE 270
C                   VARIABLES TO BE INCLUDED IN THE FORTHCOMING REGRES- ORDE 280
C                   SION.                                               ORDE 290
C                   UPON RETURNING TO THE CALLING ROUTINE, THIS VECTOR  ORDE 300
C                   CONTAINS, IN ADDITION, THE SUBSCRIPT NUMBER OF      ORDE 310
C                   THE DEPENDENT VARIABLE IN K+1 POSITION.             ORDE 320
C           RX    - OUTPUT MATRIX (K X K) CONTAINING INTERCORRELATIONS  ORDE 330
C                   AMONG INDEPENDENT VARIABLES TO BE USED IN FORTH-    ORDE 340
C                   COMING REGRESSION.                                  ORDE 350
C           RY    - OUTPUT VECTOR OF LENGTH K CONTAINING INTERCORRELA-  ORDE 360
C                   TIONS OF INDEPENDENT VARIABLES WITH DEPENDENT        ORDE 370
C                   VARIABLES.                                          ORDE 380
C                                                                       ORDE 390
C        REMARKS                                                        ORDE 400
C           NONE                                                        ORDE 410
C                                                                       ORDE 420
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ORDE 430
C           NONE                                                        ORDE 440
C                                                                       ORDE 450
C        METHOD                                                         ORDE 460
C           FROM THE SUBSCRIPT NUMBERS OF THE VARIABLES TO BE INCLUDED  ORDE 470
C           IN THE FORTHCOMING REGRESSION, THE SUBROUTINE CONSTRUCTS THEORDE 480
C           MATRIX RX AND THE VECTOR RY.                                ORDE 490
C                                                                       ORDE 500
C     ...................................................................ORDE 510
G                                                                       ORDE 520
      SUBROUTINE ORDER (M,R,NDEP,K,ISAVE,RX,RY)                         ORDE 530
      DIMENSION R(1),ISAVE(1),RX(1),RY(1)                               ORDE 540
C                                                                       ORDE 550
C        .................................................................ORDE 560
C                                                                       ORDE 570
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  ORDE 580
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      ORDE 590
C        STATEMENT WHICH FOLLOWS.                                       ORDE 600
C                                                                       ORDE 610
C     DOUBLE PRECISION R,RX,RY                                          ORDE 620
C                                                                       ORDE 630
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    ORDE 640
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      ORDE 650
C        ROUTINE.                                                       ORDE 660
C                                                                       ORDE 670
C        .................................................................ORDE 680
C                                                                       ORDE 690
C     COPY INTERCORRELATIONS OF INDEPENDENT VARIABLES                   ORDE 700
C    -WITH DEPENDENT VARIABLE                                           ORDE 710
C                                                                       ORDE 720
      MM=0                                                              ORDE 730
      DO 130 J=1,K                                                      ORDE 740
      L2=ISAVE(J)                                                       ORDE 750
      IF(NDEP-L2) 122, 123, 123                                         ORDE 760
  122 L=NDEP+(L2*L2-L2)/2                                               ORDE 770
      GO TO 125                                                         ORDE 780
  123 L=L2+(NDEP*NDEP-NDEP)/2                                           ORDE 790
  125 RY(J)=R(L)                                                        ORDE 800
C                                                                       ORDE 810
C     COPY A SUBSET MATRIX OF INTERCORRELATIONS AMONG                   ORDE 820
C     INDEPENDENT VARIABLES                                             ORDE 830
C                                                                       ORDE 840
      DO 130 I=1,K                                                      ORDE 850
      L1=ISAVE(I)                                                       ORDE 860
      IF(L1-L2) 127, 128, 128                                           ORDE 870
  127 L=L1+(L2*L2-L2)/2                                                 ORDE 880
      GO TO 129                                                         ORDE 890
  128 L=L2+(L1*L1-L1)/2                                                 ORDE 900
  129 MM=MM+1                                                           ORDE 910
  130 RX(MM)=R(L)                                                       ORDE 920
C                                                                       ORDE 930
C     PLACE THE SUBSCRIPT NUMBER OF THE DEPENDENT                       ORDE 940
C     VARIABLE IN ISAVE(K+1)                                            ORDE 950
C                                                                       ORDE 960
      ISAVE(K+1)=NDEP                                                   ORDE 970
      RETURN                                                            ORDE 980
      END                                                               ORDE 990
```

Subroutine MULTR

This subroutine performs a multiple regression analysis for a dependent variable and a set of independent variables.

Beta weights are calculated using the following equation:

$$\beta_j = \sum_{i=1}^{k} r_{iy} \cdot r_{ij}^{-1} \quad (1)$$

where r_{iy} = intercorrelation of i^{th} independent variable with dependent variable

r_{ij}^{-1} = the inverse of intercorrelation r_{ij}

$i, j = 1, 2, \ldots, k$ imply independent variables

r_{iy} and r_{ij}^{-1} are input to this subroutine.

Then, the regression coefficients are calculated as follows:

$$b_j = \beta_j \cdot \frac{s_y}{s_j} \quad (2)$$

where s_y = standard deviation of dependent variable

s_j = standard deviation of j^{th} independent variable

$j = 1, 2, \ldots, k$

s_y and s_j are input to this subroutine.

The intercept is found by the following equation:

$$b_0 = \overline{Y} - \sum_{j=1}^{k} b_j \cdot \overline{X}_j \quad (3)$$

where $\overline{Y}$ = mean of dependent variable

$\overline{X}_j$ = mean of j^{th} independent variable

$\overline{Y}$ and $\overline{X}_j$ are input to this subroutine.

Multiple correlation coefficient, R, is found first by calculating the coefficient of determination by the following equation:

$$R^2 = \sum_{i=1}^{k} \beta_i r_{iy} \quad (4)$$

and taking the square root of R^2:

$$R = \sqrt{R^2} \quad (5)$$

The sum of squares attributable to the regression is found by:

$$SSAR = R^2 \cdot D_{yy} \quad (6)$$

where D_{yy} = sum of squares of deviations from mean for dependent variable

D_{yy} is input to this subroutine.

The sum of squares of deviations from the regression is obtained by:

$$SSDR = D_{yy} - SSAR \quad (7)$$

Then, the F-value for the analysis of variance is calculated as follows:

$$F = \frac{SSAR/k}{SSDR/(n-k-1)} = \frac{SSAR(n-k-1)}{SSDR(k)} \quad (8)$$

Certain other statistics are calculated as follows:

Variance and standard error of estimate:

$$S^2_{y.12\ldots k} = \frac{SSDR}{n-k-1} \quad (9)$$

where n = number of observations

$$S_{y.12\ldots k} = \sqrt{S^2_{y.12\ldots k}} \quad (10)$$

Standard deviations of regression coefficients:

$$S_{b_j} = \sqrt{\frac{r_{jj}^{-1}}{D_{jj}} \cdot S^2_{y.12\ldots k}} \quad (11)$$

where D_{jj} = sum of squares of deviations from mean for j^{th} independent variable. D_{jj} is input to this subroutine.

$j = 1, 2, \ldots, k$

Computed t:

$$t_j = \frac{b_j}{S_{b_j}} \quad (12)$$

$j = 1, 2, \ldots, k$

```
C                                                                       MULT  10
C  ...................................................................  MULT  20
C                                                                       MULT  30
C      SUBROUTINE MULTR                                                 MULT  40
C                                                                       MULT  50
C      PURPOSE                                                          MULT  60
C         PERFORM A MULTIPLE LINEAR REGRESSION ANALYSIS FOR A           MULT  70
C         DEPENDENT VARIABLE AND A SET OF INDEPENDENT VARIABLES.  THIS  MULT  80
C         SUBROUTINE IS NORMALLY USED IN THE PERFORMANCE OF MULTIPLE    MULT  90
C         AND POLYNOMIAL REGRESSION ANALYSES.                           MULT 100
C                                                                       MULT 110
C      USAGE                                                            MULT 120
C         CALL MULTR (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,ANS)            MULT 130
C                                                                       MULT 140
C      DESCRIPTION OF PARAMETERS                                        MULT 150
C         N      - NUMBER OF OBSERVATIONS.                              MULT 160
C         K      - NUMBER OF INDEPENDENT VARIABLES IN THIS REGRESSION.  MULT 170
C         XBAR   - INPUT VECTOR OF LENGTH M CONTAINING MEANS OF ALL     MULT 180
C                  VARIABLES. M IS NUMBER OF VARIABLES IN OBSERVATIONS. MULT 190
C         STD    - INPUT VECTOR OF LENGTH M CONTAINING STANDARD DEVI-   MULT 200
C                  ATIONS OF ALL VARIABLES.                             MULT 210
C         D      - INPUT VECTOR OF LENGTH M CONTAINING THE DIAGONAL OF  MULT 220
C                  THE MATRIX OF SUMS OF CROSS-PRODUCTS OF DEVIATIONS   MULT 230
C                  FROM MEANS FOR ALL VARIABLES.                        MULT 240
C         RX     - INPUT MATRIX (K X K) CONTAINING THE INVERSE OF       MULT 250
C                  INTERCORRELATIONS AMONG INDEPENDENT VARIABLES.       MULT 260
C         RY     - INPUT VECTOR OF LENGTH K CONTAINING INTERCORRELA-    MULT 270
C                  TIONS OF INDEPENDENT VARIABLES WITH DEPENDENT         MULT 280
C                  VARIABLE.                                            MULT 290
C         ISAVE  - INPUT VECTOR OF LENGTH K+1 CONTAINING SUBSCRIPTS OF  MULT 300
C                  INDEPENDENT VARIABLES IN ASCENDING ORDER.  THE       MULT 310
C                  SUBSCRIPT OF THE DEPENDENT VARIABLE IS STORED IN     MULT 320
C                  THE LAST, K+1, POSITION.                             MULT 330
C         B      - OUTPUT VECTOR OF LENGTH K CONTAINING REGRESSION      MULT 340
C                  COEFFICIENTS.                                        MULT 350
C         SB     - OUTPUT VECTOR OF LENGTH K CONTAINING STANDARD        MULT 360
C                  DEVIATIONS OF REGRESSION COEFFICIENTS.               MULT 370
C         T      - OUTPUT VECTOR OF LENGTH K CONTAINING T-VALUES.       MULT 380
C         ANS    - OUTPUT VECTOR OF LENGTH 10 CONTAINING THE FOLLOWING  MULT 390
C                  INFORMATION..                                        MULT 400
C                  ANS(1)  INTERCEPT                                    MULT 410
C                  ANS(2)  MULTIPLE CORRELATION COEFFICIENT             MULT 420
C                  ANS(3)  STANDARD ERROR OF ESTIMATE                   MULT 430
C                  ANS(4)  SUM OF SQUARES ATTRIBUTABLE TO REGRES-       MULT 440
C                          SION (SSAR)                                  MULT 450
C                  ANS(5)  DEGREES OF FREEDOM ASSOCIATED WITH SSAR      MULT 460
C                  ANS(6)  MEAN SQUARE OF SSAR                          MULT 470
C                  ANS(7)  SUM OF SQUARES OF DEVIATIONS FROM REGRES-    MULT 480
C                          SION (SSDR)                                  MULT 490
C                  ANS(8)  DEGREES OF FREEDOM ASSOCIATED WITH SSDR      MULT 500
C                  ANS(9)  MEAN SQUARE OF SSDR                          MULT 510
C                  ANS(10) F-VALUE                                      MULT 520
C                                                                       MULT 530
C      REMARKS                                                          MULT 540
C         N MUST BE GREATER THAN K+1.                                   MULT 550
C                                                                       MULT 560
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                    MULT 570
C         NONE                                                          MULT 580
C                                                                       MULT 590
C      METHOD                                                           MULT 600
C         THE GAUSS-JORDAN METHOD IS USED IN THE SOLUTION OF THE        MULT 610
C         NORMAL EQUATIONS.  REFER TO W. W. COOLEY AND P. R. LOHNES,    MULT 620
C         'MULTIVARIATE PROCEDURES FOR THE BEHAVIORAL SCIENCES',        MULT 630
C         JOHN WILEY AND SONS, 1962, CHAPTER 3; AND B. OSTLE,           MULT 640
C         'STATISTICS IN RESEARCH', THE IOWA STATE COLLEGE PRESS,       MULT 650
C         1954, CHAPTER 8.                                              MULT 660
C                                                                       MULT 670
C  ...................................................................  MULT 680
C                                                                       MULT 690
      SUBROUTINE MULTR (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SE,T,ANS)          MULT 700
      DIMENSION XBAR(1),STD(1),D(1),RX(1),RY(1),ISAVE(1),B(1),SB(1),    MULT 710
     1          T(1),ANS(1)                                             MULT 720
C                                                                       MULT 730
C     ..................................................................MULT 740
C                                                                       MULT 750
C     IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE     MULT 760
C     C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION         MULT 770
C     STATEMENT WHICH FOLLOWS.                                          MULT 780
C                                                                       MULT 790
C     DOUBLE PRECISION XBAR,STD,D,RX,RY,B,SB,T,ANS,RM,BO,SSAR,SSDR,SY,  MULT 800
C    1                 FN,FK,SSARM,SSDRM,F                            MULT 810
C                                                                       MULT 820
C     THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS       MULT 830
C     APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS         MULT 840
C     ROUTINE.                                                          MULT 850
C                                                                       MULT 860
C     THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO         MULT 870
C     CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT AND ABS IN      MULT 880
C     STATEMENTS 122, 125, AND 135 MUST BE CHANGED TO DSQRT AND DABS.   MULT 890
C                                                                       MULT 900
C     ..................................................................MULT 910
C                                                                       MULT 920
      MM=K+1                                                            MULT 930
C                                                                       MULT 940
C     BETA WEIGHTS                                                      MULT 950
C                                                                       MULT 960
      DO 100 J=1,K                                                      MULT 970
  100 B(J)=0.0                                                          MULT 980
      DO 110 J=1,K                                                      MULT 990
      L1=K*(J-1)                                                        MULT1000
      DO 110 I=1,K                                                      MULT1010
      L=L1+I                                                            MULT1020
  110 B(J)=B(J)+RY(I)*RX(L)                                             MULT1030
      RM=0.0                                                            MULT1040
      BO=0.0                                                            MULT1050
      L1=ISAVE(MM)                                                      MULT1060
C                                                                       MULT1070
C     COEFFICIENT OF DETERMINATION                                      MULT1080
C                                                                       MULT1090
      DO 120 I=1,K                                                      MULT1100
      RM=RM+B(I)*RY(I)                                                  MULT1110
C                                                                       MULT1120
C     REGRESSION COEFFICIENTS                                           MULT1130
C                                                                       MULT1140
      L=ISAVE(I)                                                        MULT1150
      B(I)=B(I)*(STD(L1)/STD(L))                                        MULT1160
C                                                                       MULT1170
C     INTERCEPT                                                         MULT1180
C                                                                       MULT1190
  120 BO=BO+B(I)*XBAR(L)                                                MULT1200
      BO=XBAR(L1)-BO                                                    MULT1210
C                                                                       MULT1220
C     SUM OF SQUARES ATTRIBUTABLE TO REGRESSION                         MULT1230
C                                                                       MULT1240
      SSAR=RM*D(L1)                                                     MULT1250
C                                                                       MULT1260
C     MULTIPLE CORRELATION COEFFICIENT                                  MULT1270
C                                                                       MULT1280
  122 RM= SQRT( ABS(RM))                                                MULT1290
C                                                                       MULT1300
C     SUM OF SQUARES OF DEVIATIONS FROM REGRESSION                      MULT1310
C                                                                       MULT1320
      SSDR=D(L1)-SSAR                                                   MULT1330
C                                                                       MULT1340
C     VARIANCE OF ESTIMATE                                              MULT1350
C                                                                       MULT1360
      FN=N-K-1                                                          MULT1370
      SY=SSDR/FN                                                        MULT1380
C                                                                       MULT1390
C     STANDARD DEVIATIONS OF REGRESSION COEFFICIENTS                    MULT1400
C                                                                       MULT1410
      DO 130 J=1,K                                                      MULT1420
      L1=K*(J-1)+J                                                      MULT1430
      L=ISAVE(J)                                                        MULT1440
  125 SB(J)= SQRT( ABS((RX(L1)/D(L))*SY))                               MULT1450
C                                                                       MULT1460
C     COMPUTED T-VALUES                                                 MULT1470
C                                                                       MULT1480
  130 T(J)=B(J)/SB(J)                                                   MULT1490
C                                                                       MULT1500
C     STANDARD ERROR OF ESTIMATE                                        MULT1510
C                                                                       MULT1520
  135 SY= SQRT( ABS(SY))                                                MULT1530
C                                                                       MULT1540
C     F VALUE                                                           MULT1550
C                                                                       MULT1560
      FK=K                                                              MULT1570
      SSARM=SSAR/FK                                                     MULT1580
      SSDRM=SSDR/FN                                                     MULT1590
      F=SSARM/SSDRM                                                     MULT1600
C                                                                       MULT1610
      ANS(1)=BO                                                         MULT1620
      ANS(2)=RM                                                         MULT1630
      ANS(3)=SY                                                         MULT1640
      ANS(4)=SSAR                                                       MULT1650
      ANS(5)=FK                                                         MULT1660
      ANS(6)=SSARM                                                      MULT1670
      ANS(7)=SSDR                                                       MULT1680
      ANS(8)=FN                                                         MULT1690
      ANS(9)=SSDRM                                                      MULT1700
      ANS(10)=F                                                         MULT1710
      RETURN                                                            MULT1720
      END                                                               MULT1730
```

Polynomial Regression

In the Scientific Subroutine Package, polynomial regression is normally performed by calling the following four subroutines in sequence:

1. GDATA - to generate the powers of the independent variable and find means, standard deviations, and correlation matrix
2. ORDER - to choose a dependent variable and subset of independent variables from a larger set of variables
3. MINV - to invert the correlation coefficient matrix
4. MULTR - to compute the regression coefficients $b_0, b_1, b_2, \ldots, b_m$, and various confidence measures

Subroutine GDATA

This subroutine generates independent variables up to the m^{th} power (the highest degree polynomial specified) and calculates means, standard deviations, sums of cross-products of deviations from means, and product moment correlation coefficients.

X_{il} denotes the i^{th} case of the independent variable;

X_{ip} denotes the i^{th} case of the dependent variable,

where $i = 1, 2, \ldots, n$

n = number of cases (observations)

$p = m + 1$

m = highest degree polynomial specified

The subroutine GDATA generates powers of the independent variable as follows:

$$\begin{aligned} X_{i2} &= X_{i1} \cdot X_{i1} \\ X_{i3} &= X_{i2} \cdot X_{i1} \\ X_{i4} &= X_{i3} \cdot X_{i1} \\ &\vdots \\ X_{im} &= X_{i,m-1} \cdot X_{i1} \end{aligned} \qquad (1)$$

where i and m are as defined as above.

Then, the following are calculated.

Means:

$$\bar{X}_j = \frac{\sum_{i=1}^{n} X_{ij}}{n} \qquad (2)$$

where $j = 1, 2, \ldots, p$

Sums of cross-products of deviations from means:

$$D_{jk} = \sum_{i=1}^{n}\left(X_{ij} - \bar{X}_j\right)\left(X_{ik} - \bar{X}_k\right) - \frac{\sum_{i=1}^{n}\left(X_{ij} - \bar{X}_j\right)\sum_{i=1}^{n}\left(X_{ik} - \bar{X}_k\right)}{n} \qquad (3)$$

where $j = 1, 2, \ldots, p$; $k = 1, 2, \ldots, p$.

Correlation coefficients:

$$r_{ij} = \frac{D_{ij}}{\sqrt{D_{ii}}\ \sqrt{D_{jj}}} \qquad (4)$$

where $i = 1, 2, \ldots, p$; $j = 1, 2, \ldots, p$.

Standard deviations:

$$s_j = \frac{\sqrt{D_{jj}}}{\sqrt{n-1}} \qquad (5)$$

where $j = 1, 2, \ldots, p$

```
C                                                                       GDAT  10
C     .................................................................GDAT  20
C                                                                       GDAT  30
C        SUBROUTINE GDATA                                               GDAT  40
C                                                                       GDAT  50
C        PURPOSE                                                        GDAT  60
C           GENERATE INDEPENDENT VARIABLES UP TO THE M-TH POWER (THE    GDAT  70
C           HIGHEST DEGREE POLYNOMIAL SPECIFIED) AND COMPUTE MEANS,     GDAT  80
C           STANDARD DEVIATIONS, AND CORRELATION COEFFICIENTS.  THIS    GDAT  90
C           SUBROUTINE IS NORMALLY CALLED BEFORE SUBROUTINES ORDER,     GDAT 100
C           MINV AND MULTR IN THE PERFORMANCE OF A POLYNOMIAL           GDAT 110
C           REGRESSION.                                                 GDAT 120
C                                                                       GDAT 130
C        USAGE                                                          GDAT 140
C           CALL GDATA (N,M,X,XBAR,STD,D,SUMSQ)                         GDAT 150
C                                                                       GDAT 160
C        DESCRIPTION OF PARAMETERS                                      GDAT 170
C           N      - NUMBER OF OBSERVATIONS.                            GDAT 180
C           M      - THE HIGHEST DEGREE POLYNOMIAL TO BE FITTED.        GDAT 190
C           X      - INPUT MATRIX (N BY M+1) .  WHEN THE SUBROUTINE IS  GDAT 200
C                    CALLED, DATA FOR THE INDEPENDENT VARIABLE ARE      GDAT 210
C                    STORED IN THE FIRST COLUMN OF MATRIX X, AND DATA FORGDAT 220
C                    THE DEPENDENT VARIABLE ARE STORED IN THE LAST      GDAT 230
C                    COLUMN OF THE MATRIX.  UPON RETURNING TO THE       GDAT 240
C                    CALLING ROUTINE, GENERATED POWERS OF THE INDEPENDENTGDAT 250
C                    VARIABLE ARE STORED IN COLUMNS 2 THROUGH M.        GDAT 260
C           XBAR   - OUTPUT VECTOR OF LENGTH M+1 CONTAINING MEANS OF    GDAT 270
C                    INDEPENDENT AND DEPENDENT VARIABLES.               GDAT 280
C           STD    - OUTPUT VECTOR OF LENGTH M+1 CONTAINING STANDARD    GDAT 290
C                    DEVIATIONS OF INDEPENDENT AND DEPENDENT VARIABLES. GDAT 300
C           D      - OUTPUT MATRIX (ONLY UPPER TRIANGULAR PORTION OF THE GDAT 310
C                    SYMETRIC MATRIX OF M+1 BY M+1) CONTAINING CORRELA- GDAT 320
C                    TION COEFFICIENTS.  (STORAGE MODE OF 1)            GDAT 330
C           SUMSQ  - OUTPUT VECTOR OF LENGTH M+1 CONTAINING SUMS OF     GDAT 340
C                    PRODUCTS OF DEVIATIONS FROM MEANS OF INDEPENDENT   GDAT 350
C                    AND DEPENDENT VARIABLES.                           GDAT 360
C                                                                       GDAT 370
C        REMARKS                                                        GDAT 380
C           N MUST BE GREATER THAN M+1.                                 GDAT 390
C           IF M IS EQUAL TO 5 OR GREATER, SINGLE PRECISION MAY NOT BE  GDAT 400
C           SUFFICIENT TO GIVE SATISFACTORY COMPUTATIONAL RESULTS.      GDAT 410
```

```
C                                                                       GDAT 420
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   GDAT 430
C          NONE                                                         GDAT 440
C                                                                       GDAT 450
C       METHOD                                                          GDAT 460
C          REFER TO B. DALE, 'STATISTICS IN RESEARCH', THE IOWA STATE   GDAT 470
C          COLLEGE PRESS, 1954, CHAPTER 6.                              GDAT 480
C                                                                       GDAT 490
C     ..................................................................GDAT 500
C                                                                       GDAT 510
      SUBROUTINE GDATA (N,M,X,XBAR,STD,D,SUMSQ)                         GDAT 520
      DIMENSION X(1),XBAR(1),STD(1),D(1),SUMSQ(1)                       GDAT 530
C                                                                       GDAT 540
C     ..................................................................GDAT 550
C                                                                       GDAT 560
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  GDAT 570
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      GDAT 580
C        STATEMENT WHICH FOLLOWS.                                       GDAT 590
C                                                                       GDAT 600
C     DOUBLE PRECISION X,XBAR,STD,D,SUMSQ,T1,T2                         GDAT 610
C                                                                       GDAT 620
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    GDAT 630
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      GDAT 640
C        ROUTINE.                                                       GDAT 650
C                                                                       GDAT 660
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      GDAT 670
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT AND ABS IN   GDAT 680
C        STATEMENT 180 MUST BE CHANGED TO DSQRT AND DABS.               GDAT 690
C                                                                       GDAT 700
C     ..................................................................GDAT 710
C                                                                       GDAT 720
C     GENERATE INDEPENDENT VARIABLES                                    GDAT 730
C                                                                       GDAT 740
      IF(M-1) 105, 105, 90                                              GDAT 750
   90 L1=0                                                              GDAT 760
      DO 100 I=2,M                                                      GDAT 770
      L1=L1+N                                                           GDAT 780
      DO 100 J=1,N                                                      GDAT 790
      L=L1+J                                                            GDAT 800
      K=L-N                                                             GDAT 810
  100 X(L)=X(K)*X(J)                                                    GDAT 820
C                                                                       GDAT 830
C     CALCULATE MEANS                                                   GDAT 840
C                                                                       GDAT 850
  105 MM=M+1                                                            GDAT 860
      DF=N                                                              GDAT 870
      L=0                                                               GDAT 880
      DO 115 I=1,MM                                                     GDAT 890
      XBAR(I)=0.0                                                       GDAT 900
      DO 110 J=1,N                                                      GDAT 910
      L=L+1                                                             GDAT 920
  110 XBAR(I)=XBAR(I)+X(L)                                              GDAT 930
  115 XBAR(I)=XBAR(I)/DF                                                GDAT 940
C                                                                       GDAT 950
      DO 130 I=1,MM                                                     GDAT 960
  130 STD(I)=0.0                                                        GDAT 970
C                                                                       GDAT 980
C     CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS                    GDAT 990
C                                                                       GDAT1000
      L=((MM+1)*MM)/2                                                   GDAT1010
      DO 150 I=1,L                                                      GDAT1020
  150 D(I)=0.0                                                          GDAT1030
      DO 170 K=1,N                                                      GDAT1040
      L=0                                                               GDAT1050
      DO 170 J=1,MM                                                     GDAT1060
      L2=N*(J-1)+K                                                      GDAT1070
      T2=X(L2)-XBAR(J)                                                  GDAT1080
      STD(J)=STD(J)+T2                                                  GDAT1090
      DO 170 I=1,J                                                      GDAT1100
      L1=N*(I-1)+K                                                      GDAT1110
      T1=X(L1)-XBAR(I)                                                  GDAT1120
      L=L+1                                                             GDAT1130
  170 D(L)=D(L)+T1*T2                                                   GDAT1140
      L=0                                                               GDAT1150
      DO 175 J=1,MM                                                     GDAT1160
      DO 175 I=1,J                                                      GDAT1170
      L=L+1                                                             GDAT1180
  175 D(L)=D(L)-STD(I)*STD(J)/DF                                        GDAT1190
      L=0                                                               GDAT1200
      DO 180 I=1,MM                                                     GDAT1210
      L=L+1                                                             GDAT1220
      SUMSQ(I)=D(L)                                                     GDAT1230
  180 STD(I)= SQRT( ABS(D(L)))                                          GDAT1240
C                                                                       GDAT1250
C     CALCULATE CORRELATION COEFFICIENTS                                GDAT1260
C                                                                       GDAT1270
      L=0                                                               GDAT1280
      DO 190 J=1,MM                                                     GDAT1290
      DO 190 I=1,J                                                      GDAT1300
      L=L+1                                                             GDAT1310
  190 D(L)=D(L)/(STD(I)*STD(J))                                         GDAT1320
C                                                                       GDAT1330
C     CALCULATE STANDARD DEVIATIONS                                     GDAT1340
C                                                                       GDAT1350
      DF=SQRT(DF-1.0)                                                   GDAT1360
      DO 200 I=1,MM                                                     GDAT1370
  200 STD(I)=STD(I)/DF                                                  GDAT1380
      RETURN                                                            GDAT1390
      END                                                               GDAT1400
```

Stepwise Multiple Regression

In the Scientific Subroutine Package, stepwise multiple regression is normally performed by calling the following subroutines:

1. CORRE - to find means, standard deviations, sums of cross-products of deviation matrix, and correlation matrix
2. MSTR - to save the matrix of sums of cross-products of deviations and to copy it to a working matrix for the purpose of using the same data repeatedly
3. LOC - to compute a vector subscript for an element in general and symmetric matrices. This subroutine is called by the subroutine MSTR
4. STPRG - to compute regression coefficients and other statistics for each step of regression

The subroutine CORRE works in either of two ways: (1) it expects all observations in core, or (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines and Function Subprograms Required" in the comment cards description of the subroutine CORRE).

The subroutine STPRG calls an output subroutine, STOUT, in order to print various statistics computed for each step of regression. The subroutine STOUT must also be provided by the user.

Subroutine STPRG

This subroutine performs a stepwise multiple regression analysis for a dependent variable and a set of independent variables. In each step of the regression $i=1,2,\ldots,q$, where q is the number of independent variables, the abbreviated Doolittle method is used to calculate the following statistics:

The independent variable entering in the regression is selected, first, by computing the amount of reduction of sum of squares for each variable:

$$C_j = \frac{a_{jy}^2}{a_{jj}} \tag{1}$$

where a_{jj} is initially an element in the sums of cross-products of deviations matrix which will be modified in successive steps.

$j = 1,2,\ldots,q$ are independent variables ($j \neq$ variables deleted and variables entered before the i^{th} step)

$y =$ dependent variable

and, second, by finding the maximum (over j) of C.

Set $S_i = C_j$ to indicate the sum of squares that will be reduced in the i^{th} step.

The proportion of S_i to the total is obtained by:

$$p = \frac{S_i}{D} \tag{2}$$

where $D = \sum_{j=1}^{n} (y_j - \bar{y})^2$

n = number of observations

If p is less than the constant specified by the user to limit independent variables, the analysis will be terminated without entering the last variable selected; otherwise, the following calculations are continued:

The cumulative sum of squares reduced is obtained by

$$S_{cum} = S_{cum} + S_i \tag{3}$$

and the cumulative proportion reduced by

$$P_{cum} = P_{cum} + p \tag{4}$$

The multiple correlation coefficient is computed by

$$R = \sqrt{P_{cum}} \tag{5}$$

and adjusted for degrees of freedom by

$$R_c = \sqrt{1 - (1-R^2) \quad (n-1) / (n-k)}$$

where there are k independent variables in the regression.

The F-value for analysis of variance is given by

$$F = \frac{S_{cum} / k}{(D-S_{cum}) / (n-k-1)} \tag{6}$$

The standard error of the estimated y is obtained by the use of the formula

$$s_{y.12\ldots i} = \sqrt{\frac{D - S_{cum}}{n - k - 1}} \tag{7}$$

and adjusted by

$$s_c = s \sqrt{(n-1) / (n-k)}$$

Then, the following is computed:

$$a_{jj} = a_{jj} + \frac{a_{ij}^2}{a_{ii}} \tag{8}$$

where i = variable entered in the ith step

$j = v_1, v_2, \ldots, v_{i-1}$ are the variables entered in the regression before the ith step, and

$$g_{ik} = \frac{a_{ik}}{a_{ii}} \tag{9}$$

where $k = 1,2,\ldots,m$ are variables including y ($k \neq$ variables deleted and the variable entered in the ith step).

Regression coefficients are computed by:

$$\begin{aligned} b_i &= g_{iy} \\ b_{i-1} &= g_{(i-1)y} - b_i g_{(i-1)i} \\ b_{i-2} &= g_{(i-2)y} - b_i g_{(i-2)i} - b_{i-1} g_{(i-2)(i-1)} \\ &\text{etc.,} \end{aligned} \tag{10}$$

and the value of the intercept as

$$b_0 = \bar{y} - \sum_{j=1}^{k} b_j \bar{x}_j \tag{11}$$

where k = number of independent variables in the regression.

Standard errors of regression coefficients are given by

$$s_{b_j} = \sqrt{a_{jj}}\, s_{y.12\ldots i} \qquad (12)$$

where j = $v_1, v_2, \ldots, v_i$ are variables in the regression, and t-values as

$$t_j = \frac{b_j}{s_{b_j}} \qquad (13)$$

Perform the reduction to eliminate the variable entered in the ith step:

$$a_{jk} = a_{jk} - a_{ji} g_{ik} \qquad (14)$$

where i = variable entered in the ith step

j = 1,2,...,m (j ≠ variables deleted or variables in the regression)

k = 1,2,...,m (k ≠ variables deleted and the variable entered in the ith step)

$$a_{ji} = \frac{a_{ji}}{-a_{ii}} \qquad (15)$$

$$a_{ii} = \frac{1}{a_{ii}} \qquad (16)$$

For reference see C. A. Bennett and N. L. Franklin, Statistical Analysis in Chemistry and the Chemical Industry. John Wiley and Sons, 1954, Appendix 6A.

```
C                                                                       STPR  10
C     ..................................................................STPR  20
C                                                                       STPR  30
C        SUBROUTINE STPRC                                               STPR  40
C                                                                       STPR  50
C        PURPOSE                                                        STPR  60
C           TO PERFORM A STEPWISE MULTIPLE REGRESSION ANALYSIS FOR A    STPR  70
C           DEPENDENT VARIABLE AND A SET OF INDEPENDENT VARIABLES.  AT  STPR  80
C           EACH STEP, THE VARIABLE ENTERED INTO THE REGRESSION EQUATIONSTPR  90
C           IS THAT WHICH EXPLAINS THE GREATEST AMOUNT OF VARIANCE      STPR 100
C           BETWEEN IT AND THE DEPENDENT VARIABLE (I.E. THE VARIABLE    STPR 110
C           WITH THE HIGHEST PARTIAL CORRELATION WITH THE DEPENDENT     STPR 120
C           VARIABLE).  ANY VARIABLE CAN BE DESIGNATED AS THE DEPENDENT STPR 130
C           VARIABLE.  ANY INDEPENDENT VARIABLE CAN BE FORCED INTO OR   STPR 140
C           DELETED FROM THE REGRESSION EQUATION, IRRESPECTIVE OF ITS   STPR 150
C           CONTRIBUTION TO THE EQUATION.                               STPR 160
C                                                                       STPR 170
C        USAGE                                                          STPR 180
C           CALL STPRC (M,A,C,XBAR,ICX,PCT,NSTEP,ANS,L,B,S,T,LL,IER)    STPR 190
C                                                                       STPR 200
C        DESCRIPTION OF PARAMETERS                                      STPR 210
C           M   - TOTAL NUMBER OF VARIABLES IN DATA MATRIX              STPR 220
C           N   - NUMBER OF OBSERVATIONS                                STPR 230
C           C   - INPUT MATRIX (M X M) OF SUMS OF CROSS-PRODUCTS OF     STPR 240
C                 DEVIATIONS FROM MEAN.  THIS MATRIX WILL BE DESTROYED. STPR 250
C           XBAR - INPUT VECTOR OF LENGTH M OF MEANS                    STPR 260
C           ICX  - INPUT VECTOR OF LENGTH M HAVING ONE OF THE FOLLOWING STPR 270
C                  CODES FOR EACH VARIABLE.                             STPR 280
C                    0 - INDEPENDENT VARIABLE AVAILABLE FOR SELECTION    STPR 290
C                    1 - INDEPENDENT VARIABLE TO BE FORCED INTO THE      STPR 300
C                        REGRESSION EQUATION                            STPR 310
C                    2 - VARIABLE NOT TO BE CONSIDERED IN THE EQUATION  STPR 320
C                    3 - DEPENDENT VARIABLE                             STPR 330
C                  THIS VECTOR WILL BE DESTROYED                        STPR 340
C           PCT  - A CONSTANT VALUE INDICATING THE PROPORTION OF THE    STPR 350
C                  TOTAL VARIANCE TO BE EXPLAINED BY ANY INDEPENDENT    STPR 360
C                  VARIABLE.  THOSE INDEPENDENT VARIABLES WHICH FALL    STPR 370
C                  BELOW THIS PROPORTION WILL NOT ENTER THE REGRESSION  STPR 380
C                  EQUATION.  TO ENSURE THAT ALL VARIABLES ENTER THE    STPR 390
C                  EQUATION, SET PCT = 0.0.                             STPR 400
C           NSTEP- OUTPUT VECTOR OF LENGTH 5 CONTAINING THE FOLLOWING   STPR 410
C                  INFORMATION                                          STPR 420
C                    NSTEP(1)- THE NUMBER OF THE DEPENDENT VARIABLE     STPR 430
C                    NSTEP(2)- NUMBER OF VARIABLES FORCED INTO THE      STPR 440
C                              REGRESSION EQUATION                      STPR 450
C                    NSTEP(3)- NUMBER OF VARIABLE DELETED FROM THE      STPR 460
C                              EQUATION                                 STPR 470
C                    NSTEP(4)- THE NUMBER OF THE LAST STEP              STPR 480
C                    NSTEP(5)- THE NUMBER OF THE LAST VARIABLE ENTERED  STPR 490
C           ANS  - OUTPUT VECTOR OF LENGTH 11 CONTAINING THE FOLLOWING  STPR 500
C                  INFORMATION FOR THE LAST STEP                        STPR 510
C                    ANS(1)- SUM OF SQUARES REDUCED BY THIS STEP        STPR 520
C                    ANS(2)- PROPORTION OF TOTAL SUM OF SQUARES REDUCED STPR 530
C                    ANS(3)- CUMULATIVE SUM OF SQUARES REDUCED UP TO    STPR 540
C                            THIS STEP                                  STPR 550
C                    ANS(4)- CUMULATIVE PROPORTION OF TOTAL SUM OF      STPR 560
C                            SQUARES REDUCED                            STPR 570
C                    ANS(5)- SUM OF SQUARES OF THE DEPENDENT VARIABLE   STPR 580
C                    ANS(6)- MULTIPLE CORRELATION COEFFICIENT           STPR 590
C                    ANS(7)- F RATIO FOR SUM OF SQUARES DUE TO          STPR 600
C                            REGRESSION                                 STPR 610
C                    ANS(8)- STANDARD ERROR OF THE ESTIMATE (RESIDUAL   STPR 620
C                            MEAN SQUARE)                               STPR 630
C                    ANS(9)- INTERCEPT CONSTANT                         STPR 640
C                    ANS(10)-MULTIPLE CORRELATION COEFFICIENT ADJUSTED  STPR 650
C                            FOR DEGREES OF FREEDOM.                    STPR 660
C                    ANS(11)-STANDARD ERROR OF THE ESTIMATE ADJUSTED    STPR 670
C                            FOR DEGREES OF FREEDOM.                    STPR 680
C           L    - OUTPUT VECTOR OF LENGTH K, WHERE K IS THE NUMBER OF  STPR 690
C                  INDEPENDENT VARIABLES IN THE REGRESSION EQUATION.    STPR 700
C                  THIS VECTOR CONTAINS THE NUMBERS OF THE INDEPENDENT  STPR 710
C                  VARIABLES IN THE EQUATION.                           STPR 720
C           B    - OUTPUT VECTOR OF LENGTH K, CONTAINING THE PARTIAL     STPR 730
C                  REGRESSION COEFFICIENTS CORRESPONDING TO THE         STPR 740
C                  VARIABLES IN VECTOR L.                               STPR 750
C           S    - OUTPUT VECTOR OF LENGTH K, CONTAINING THE STANDARD   STPR 760
C                  ERRORS OF THE PARTIAL REGRESSION COEFFICIENTS,       STPR 770
C                  CORRESPONDING TO THE VARIABLES IN VECTOR L.          STPR 780
C           T    - OUTPUT VECTOR OF LENGTH K, CONTAINING THE COMPUTED    STPR 790
C                  T-VALUES CORRESPONDING TO THE VARIABLES IN VECTOR L.  STPR 800
C           LL   - WORKING VECTOR OF LENGTH M                           STPR 810
C           IER  - 0, IF THERE IS NO ERROR.                             STPR 820
C                  1, IF RESIDUAL SUM OF SQUARES IS NEGATIVE OR IF THE  STPR 830
C                  PIVOTAL ELEMENT IN THE STEPWISE INVERSION PROCESS IS STPR 840
C                  ZERO.  IN THIS CASE, THE VARIABLE WHICH CAUSES THIS  STPR 850
C                  ERROR IS NOT ENTERED IN THE REGRESSION, THE RESULT   STPR 860
C                  PRIOR TO THIS STEP IS RETAINED, AND THE CURRENT      STPR 870
C                  SELECTION IS TERMINATED.                             STPR 880
C                                                                       STPR 890
C        REMARKS                                                        STPR 900
C           THE NUMBER OF DATA POINTS MUST BE AT LEAST GREATER THAN THE STPR 910
C           NUMBER OF INDEPENDENT VARIABLES PLUS ONE.  FORCED VARIABLES STPR 920
C           ARE ENTERED INTO THE REGRESSION EQUATION BEFORE ALL OTHER   STPR 930
C           INDEPENDENT VARIABLES.  WITHIN THE SET OF FORCED VARIABLES, STPR 940
C           THE ONE TO BE CHOSEN FIRST WILL BE THAT ONE WHICH EXPLAINS  STPR 950
C           THE GREATEST AMOUNT OF VARIANCE.                            STPR 960
C           INSTEAD OF USING, AS A STOPPING CRITERION, A PROPORTION OF  STPR 970
C           THE TOTAL VARIANCE, SOME OTHER CRITERION MAY BE ADDED TO    STPR 980
C           SUBROUTINE STCLT.                                           STPR 990
C                                                                       STPR1000
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  STPR1010
C           STCLT(NSTEP,ANS,L,B,S,T,NSTOP)                              STPR1020
C           THIS SUBROUTINE MUST BE PROVIDED BY THE USER.  IT IS AN     STPR1030
C           OUTPUT ROUTINE WHICH WILL PRINT THE RESULTS OF EACH STEP OF STPR1040
C           THE REGRESSION ANALYSIS.  NSTOP IS AN OPTION CODE WHICH IS  STPR1050
C           ONE IF THE STEPWISE REGRESSION IS TO BE TERMINATED, AND IS  STPR1060
C           ZERO IF IT IS TO CONTINUE.  THE USER MUST CONSIDER THIS IF  STPR1070
C           SOME OTHER STOPPING CRITERION THAN VARIANCE PROPORTION IS TOSTPR1080
C           BE USED.                                                    STPR1090
C                                                                       STPR1100
C        METHOD                                                         STPR1110
C           THE ABBREVIATED DOOLITTLE METHOD IS USED TO (1) DECIDE VARI-STPR1120
C           ABLES ENTERING IN THE REGRESSION AND (2) COMPUTE REGRESSION STPR1130
C           COEFFICIENTS.  REFER TO C. A. BENNETT AND N. L. FRANKLIN,   STPR1140
C           'STATISTICAL ANALYSIS IN CHEMISTRY AND THE CHEMICAL INDUS-  STPR1150
C           TRY', JOHN WILEY AND SONS, 1954, APPENDIX 6A.               STPR1160
C                                                                       STPR1170
C     ..................................................................STPR1180
C                                                                       STPR1190
      SUBROUTINE STPRC (M,N,C,XBAR,ICX,PCT,NSTEP,ANS,L,B,S,T,LL,IER)    STPR1200
C                                                                       STPR1210
      DIMENSION C(1),XBAR(1),ICX(1),NSTEP(1),ANS(1),L(1),B(1),S(1),T(1),STPR1220
     1LL(1)                                                             STPR1230
C                                                                       STPR1240
C     ..................................................................STPR1250
C                                                                       STPR1260
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  STPR1270
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      STPR1280
C        STATEMENT WHICH FOLLOWS.                                       STPR1290
C                                                                       STPR1300
C     DOUBLE PRECISION C,XBAR,ANS,B,S,T,RC,RE                           STPR1310
C                                                                       STPR1320
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    STPR1330
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      STPR1340
C        ROUTINE.                                                       STPR1350
C                                                                       STPR1360
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      STPR1370
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENTSSTPR1380
C        85,90,114,132,AND 134, MUST BE CHANGED TO DSQRT.               STPR1390
C                                                                       STPR1400
C     ..................................................................STPR1410
C                                                                       STPR1420
C        INITIALIZATION                                                 STPR1430
C                                                                       STPR1440
      IER=0                                                             STPR1450
      CNP=N-1                                                           STPR1460
      AFC=0                                                             STPR1470
      NSTEP(3)=0                                                        STPR1480
      ANS(3)=0.0                                                        STPR1490
      ANS(4)=0.0                                                        STPR1500
      NSTEP=0                                                           STPR1510
C                                                                       STPR1520
C        FIND DEPENDENT VARIABLE, NUMBER OF VARIABLES TO BE FORCED TO   STPR1530
C        ENTER IN THE REGRESSION, AND NUMBER OF VARIABLES TO BE DELETED STPR1540
C                                                                       STPR1550
      DO 30 I=1,M                                                       STPR1560
      LL(I)=1                                                           STPR1570
      IF(ICX(I)) 30, 30, 10                                             STPR1580
   10 IF(ICX(I)-2) 15, 20, 25                                           STPR1590
   15 AFC=AFC+1.                                                        STPR1600
      ICX(AFC)=I                                                        STPR1610
      GO TO 30                                                          STPR1620
   20 NSTEP(3)=NSTEP(3)+1                                               STPR1630
      LL(I)=-1                                                          STPR1640
      GO TO 30                                                          STPR1650
   25 PY=I                                                              STPR1660
```

```
      ASTEP(1)=PY                                                       STPR1670
      LY=P*(PY-1)                                                       STPR1680
      LYP=LY+PY                                                         STPR1690
      ANS(5)=C(LYP)                                                     STPR1700
   3C CONTINUE                                                          STPR1710
      ASTEP(2)=AFC                                                      STPR1720
C                                                                       STPR1730
C        FIND THE MAXIMUM NUMBER OF STEPS                               STPR1740
C                                                                       STPR1750
      PX=P-ASTEP(3)-1                                                   STPR1760
C                                                                       STPR1770
C        START SELECTION OF VARIABLES                                   STPR1780
C                                                                       STPR1790
      CC 14C NL=1,PX                                                    STPR1800
      RC=C                                                              STPR1810
      IF(NL-AFC) 35, 35, 55                                             STPR1820
C                                                                       STPR1830
C        SELECT NEXT VARIABLE TO ENTER AMONG FORCED VARIABLES           STPR1840
C                                                                       STPR1850
   35 CC 5C I=1,AFC                                                     STPR1860
      K=IX(I)                                                           STPR1870
      IF(LL(K)) 5C, 5C, 4C                                              STPR1880
   4C LYF=LY+K                                                          STPR1890
      IF=P*(K-1)+K                                                      STPR1900
      RE=C(LYF)*C(LYF)/C(IF)                                            STPR1910
      IF(RC-RE) 45, 5C, 5C                                              STPR1920
   45 RC=RE                                                             STPR1930
      NEW=K                                                             STPR1940
   5C CONTINUE                                                          STPR1950
      GO TO 75                                                          STPR1960
C                                                                       STPR1970
C        SELECT NEXT VARIABLE TO ENTER AMONG NON-FORCED VARIABLES       STPR1980
C                                                                       STPR1990
   55 CC 7C I=1,P                                                       STPR2000
      IF(I-PY) 6C, 7C, 6C                                               STPR2010
   6C IF(LL(I)) 7C, 7C, 62                                              STPR2020
   62 LYF=LY+I                                                          STPR2030
      IF=P*(I-1)+I                                                      STPR2040
      RE=C(LYF)*C(LYF)/C(IF)                                            STPR2050
      IF(RC-RE) 64, 7C, 7C                                              STPR2060
   64 RC=RE                                                             STPR2070
      NEW=I                                                             STPR2080
   7C CONTINUE                                                          STPR2090
C                                                                       STPR2100
C        TEST WHETHER THE PROPORTION OF THE SUM OF SQUARES REDUCED BY   STPR2110
C        THE LAST VARIABLE ENTERED IS GREATER THAN OR EQUAL TO THE      STPR2120
C        SPECIFIED PROPORTION                                           STPR2130
C                                                                       STPR2140
      IF(RC) 77,77,7E                                                   STPR2150
   7E IF(ANS(5)-(ANS(3)*RC))77,77,7E                                    STPR2160
   77 IER=1                                                             STPR2170
      GO TO 15C                                                         STPR2180
   7E RE=RC/ANS(5)                                                      STPR2190
      IF(RE-FCT) 15C, EC, EC                                            STPR2200
C                                                                       STPR2210
C        IT IS GREATER THAN OR EQUAL                                    STPR2220
C                                                                       STPR2230
   EC LL(NEW)=C                                                         STPR2240
      L(NL)=NEW                                                         STPR2250
      ANS(1)=RE                                                         STPR2260
      ANS(2)=RE                                                         STPR2270
      ANS(3)=ANS(3)*RC                                                  STPR2280
      ANS(4)=ANS(4)*RE                                                  STPR2290
      ASTEP(4)=NL                                                       STPR2300
      ASTEP(5)=NEW                                                      STPR2310
C                                                                       STPR2320
C        COMPUTE MULTIPLE CORRELATION, F-VALUE FOR ANALYSIS OF          STPR2330
C        VARIANCE, AND STANDARD ERROR OF ESTIMATE                       STPR2340
C                                                                       STPR2350
   85 ANS(6)= SQRT(ANS(4))                                              STPR2360
      RC=NL                                                             STPR2370
      RE=CAP-RC                                                         STPR2380
      RE=(ANS(5)-ANS(3))/RE                                             STPR2390
      ANS(7)=(ANS(3)/RC)/RE                                             STPR2400
   9C ANS(8)= SQRT(RE)                                                  STPR2410
C                                                                       STPR2420
C        DIVIDE BY THE PIVOTAL ELEMENT                                  STPR2430
C                                                                       STPR2440
      IF=P*(NEW-1)+NEW                                                  STPR2450
      RC=C(IF)                                                          STPR2460
      LYF=NEW-P                                                         STPR2470
      CC 1CC J=1,P                                                      STPR2480
      LYF=LYF+P                                                         STPR2490
      IF(LL(J)) 1CC, 94, 97                                             STPR2500
   94 IF(J-NEW) 9E, 98, 9E                                              STPR2510
   9E IJ=P*(J-1)+J                                                      STPR2520
      C(IJ)=C(IJ)*C(LYP)*C(LYP)/RC                                      STPR2530
   97 C(LYF)=C(LYF)/RC                                                  STPR2540
      GO TO 1CC                                                         STPR2550
   9E C(IF)=1.C/RC                                                      STPR2560
  1CC CONTINUE                                                          STPR2570
C                                                                       STPR2580
C        COMPUTE REGRESSION COEFFICIENTS                                STPR2590
C                                                                       STPR2600
      LYF=LY+NEW                                                        STPR2610
      E(NL)=C(LYP)                                                      STPR2620
      IF(NL-1) 112, 112, 1C5                                            STPR2630
  1C5 IC=NL-1                                                           STPR2640
      CC 11C J=1,IC                                                     STPR2650
      IJ=NL-J                                                           STPR2660
      KK=L(IJ)                                                          STPR2670
      LYF=LY+KK                                                         STPR2680
      E(IJ)=C(LYP)                                                      STPR2690
      CC 11C K=1,J                                                      STPR2700
      IK=NL-K+1                                                         STPR2710
      PK=L(IK)                                                          STPR2720
      LYF=P*(PK-1)+KK                                                   STPR2730
  11C E(IJ)=E(IJ)-C(LYF)*E(IK)                                          STPR2740
C                                                                       STPR2750
C        COMPUTE INTERCEPT                                              STPR2760
C                                                                       STPR2770
  112 ANS(5)=XBAR(PY)                                                   STPR2780
      CC 115 I=1,NL                                                     STPR2790
      KK=L(I)                                                           STPR2800
      ANS(5)=ANS(5)-E(I)*XBAR(KK)                                       STPR2810
      IJ=P*(KK-1)+KK                                                    STPR2820
  114 S(I)=ANS(8)* SQRT(C(IJ))                                          STPR2830
  115 T(I)=E(I)/S(I)                                                    STPR2840
C                                                                       STPR2850
C        PERFORM A REDUCTION TO ELIMINATE THE LAST VARIABLE ENTERED     STPR2860
C                                                                       STPR2870
      IF=P*(NEW-1)                                                      STPR2880
      CC 13C I=1,P                                                      STPR2890
      IJ=I-P                                                            STPR2900
      IK=NEW-P                                                          STPR2910
      IF=IF+1                                                           STPR2920
      IF(LL(I)) 13C, 13C, 12C                                           STPR2930
  12C CC 12E J=1,P                                                      STPR2940
      IJ=IJ+P                                                           STPR2950
      IK=IK+P                                                           STPR2960
      IF(LL(J)) 12E, 122, 122                                           STPR2970
  122 IF(J-NEW) 124, 126, 124                                           STPR2980
  124 C(IJ)=C(IJ)-C(IP)*C(IK)                                           STPR2990
  12E CONTINUE                                                          STPR3000
      C(IF)=C(IF)/(-RC)                                                 STPR3010
  13C CONTINUE                                                          STPR3020
C                                                                       STPR3030
C        ADJUST STANDARD ERROR OF THE ESTIMATE AND MULTIPLE CORRELATION STPR3040
C        COEFFICIENT                                                    STPR3050
C                                                                       STPR3060
      RC=A-ASTEP(4)                                                     STPR3070
      RC=CAP/RC                                                         STPR3080
  132 ANS(1C)=SQRT(1.C-(1.C-ANS(6)*ANS(6))*RC)                          STPR3090
  134 ANS(11)=ANS(8)*SQRT(RC)                                           STPR3100
C                                                                       STPR3110
C        CALL THE OUTPUT SUBROUTINE                                     STPR3120
      CALL STOUT (ASTEP,ANS,L,B,S,T,ASTOP)                              STPR3130
C                                                                       STPR3140
C        TEST WHETHER THE STEP-WISE REGRESSION WAS TERMINATED IN        STPR3150
C        SUBROUTINE STOUT                                               STPR3160
C                                                                       STPR3170
      IF(ASTOP) 14C, 14C, 15C                                           STPR3180
C                                                                       STPR3190
  14C CONTINUE                                                          STPR3200
C                                                                       STPR3210
  15C RETURN                                                            STPR3220
      END                                                               STPR3230
```

Subroutine PROBT

This subroutine obtains maximum likelihood estimates of a and b for the probit equation $Y = a+bX$. An iterative scheme is used. The input to the subroutine consists of k different levels $X_1, X_2, \ldots, X_k$ of a stimulus applied to $N_1, N_2, \ldots, N_k$ objects with $R_1, R_2, \ldots, R_k$ responses respectively. The procedures described here assume that the distribution of critical values is normal. The computational steps are as follows:

1. Compute the proportions of objects responding to various levels of a stimulus:

$$p_i = \frac{R_i}{N_i} \tag{1}$$

where $i = 1, 2, \ldots, k$ are levels of a stimulus.

2. Compute the initial estimates of a and b for the probit equation, $Y = a+bX$, as follows:

$$b = \frac{\sum_{i=1}^{m} X_i Z_i - \frac{\left(\sum_{i=1}^{m} X_i\right)\left(\sum_{i=1}^{m} Z_i\right)}{m}}{\sum_{i=1}^{m} X^2_i - \frac{\left(\sum_{i=1}^{m} X_i\right)^2}{m}} \tag{2}$$

$$a = \bar{Z} - b\bar{X} \tag{3}$$

where X_i = ith level of a stimulus

Z_i = 5 plus the standard normal variable corresponding to p_i

m = number of p values which are not equal to 0.0 and 1.0

3. Compute values of expected probit using the initial estimates of a and b:

$$Y_i = a + bX_i \tag{4}$$

where $i = 1, 2, \ldots, k$

4. Corresponding to each value of Y, compute the following:

a. Weighting coefficient for probit analysis:

$$W_i = \frac{D^2_i}{P_i Q_i} \tag{5}$$

where D_i = density of the normal curve corresponding to the standard normal variable $Y_i - 5$

P_i = cumulative normal distribution value corresponding to $Y_i - 5$

$Q_i = 1 - P_i$

b. Working probit:

For $Y_i \leq 5.0$

$$y_i = Y_i - \frac{P_i}{D_i} + p_i \frac{1}{D_i} \tag{6}$$

For $Y_i > 5.0$

$$y_i = Y_i + \frac{Q_i}{D_i} - (1-p_i)\frac{1}{D_i} \tag{7}$$

5. Compute:

$$S_1 = \sum_{i=1}^{k} N_i W_i X^2_i - \frac{\left(\sum_{i=1}^{k} N_i W_i X_i\right)^2}{\sum_{i=1}^{k} N_i W_i} \tag{8}$$

$$S_2 = \sum_{i=1}^{k} N_i W_i X_i y_i - \frac{\left(\sum_{i=1}^{k} N_i W_i X_i\right)\left(\sum_{i=1}^{k} N_i W_i y_i\right)}{\sum_{i=1}^{k} N_i W_i} \tag{9}$$

$$S_3 = \sum_{i=1}^{k} N_i W_i y^2_i - \frac{\left(\sum_{i=1}^{k} N_i W_i y_i\right)^2}{\sum_{i=1}^{k} N_i W_i} \tag{10}$$

6. Compute new estimates of a and b for the probit equation:

$$b = \frac{S_2}{S_1} \tag{11}$$

$$a = \frac{\sum_{i=1}^{k} N_i W_i y_i}{\sum_{i=1}^{k} N_i W_i} - b \cdot \frac{\sum_{i=1}^{k} N_i W_i X_i}{\sum_{i=1}^{k} N_i W_i} \tag{12}$$

7. Compute new values of expected probit and compare them against the values computed in the previous iteration:

$$Y'_i = a + bX_i \tag{13}$$

$$DSQ = \sum_{i=1}^{k} (Y_i - Y')^2 \tag{14}$$

If the difference between two consecutive values of DSQ is less than or equal to 10^{-7}, go to step 8 and compute χ^2. Otherwise, set $Y_i = Y_i'$, where $i = 1, 2, \ldots, k$, and go back to step 4 for another iteration.

8. Compute χ^2 for the test of the final probit equation:

$$\chi^2 = \sum_{i=1}^{k} \frac{(R_i - N_i P_i)^2}{N_i P_i (1-P_i)} \tag{15}$$

where P_i = cumulative normal distribution value corresponding to z_i

$z_i = (a+bX_i) - 5$

a and b are computed for the final probit equation.

9. Degrees of freedom for χ^2:

$$d.f. = k - 2 \tag{16}$$

For reference see:

(1) M.G. Natrella, Experimental Statistics - NBS Handbook 91. National Bureau of Standards, 1963, chapter 10.

(2) D.J. Finney, Probit Analysis (2nd ed.). Cambridge University Press, 1952.

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C                                                                       PROB  10
C  .....................................................................PROB  20
C                                                                       PROB  30
C     SUBROUTINE PROBT                                                  PROB  40
C                                                                       PROB  50
C     PURPOSE                                                           PROB  60
C        TO OBTAIN MAXIMUM LIKELIHOOD ESTIMATES FOR THE PARAMETERS A    PROB  70
C        AND B IN THE PROBIT EQUATION  Y = A + BX.  AN ITERATIVE        PROB  80
C        SCHEME IS USED.  THE INPUT TO THE SUBROUTINE CONSISTS OF K     PROB  90
C        DIFFERENT DOSAGE LEVELS APPLIED TO K GROUPS OF SUBJECTS, ANDPROB 100
C        THE NUMBER OF SUBJECTS IN EACH GROUP RESPONDING TO THE         PROB 110
C        RESPECTIVE DOSAGE OF THE DRUG.                                 PROB 120
C                                                                       PROB 130
C     USAGE                                                             PROB 140
C        CALL PROBT (K,X,S,R,LOG,ANS,W1,W2,IER)                         PROB 150
C                                                                       PROB 160
C     DESCRIPTION OF PARAMETERS                                         PROB 170
C        K   - NUMBER OF DIFFERENT DOSE LEVELS OF THE DRUG.  K SHOULDPROB 180
C              BE GREATER THAN 2.                                       PROB 190
C        X   - INPUT VECTOR OF LENGTH K CONTAINING THE DOSE LEVEL OF PROB 200
C              THE DRUG TESTED.  X MUST BE NON-NEGATIVE.                PROB 210
C        S   - INPUT VECTOR OF LENGTH K CONTAINING THE NUMBER OF        PROB 220
C              SUBJECTS TESTED AT EACH DOSE LEVEL                       PROB 230
C        R   - INPUT VECTOR OF LENGTH K CONTAINING THE NUMBER OF        PROB 240
C              SUBJECTS AT EACH LEVEL RESPONDING TO THE DRUG            PROB 250
C        LOG - INPUT OPTION CODE                                        PROB 260
C              1- IF IT IS DESIRED TO CONVERT THE DOSE LEVELS TO        PROB 270
C                 COMMON LOGARITHMS.  THE DOSAGE LEVELS SHOULD BE       PROB 280
C                 NON-NULL IN THIS CASE.                                PROB 290
C              0- IF NO CONVERSION IS DESIRED                           PROB 300
C        ANS - OUTPUT VECTOR OF LENGTH 4 CONTAINING THE FOLLOWING       PROB 310
C              RESULTS                                                  PROB 320
C              ANS(1)- ESTIMATE OF THE INTERCEPT CONSTANT A             PROB 330
C              ANS(2)- ESTIMATE OF THE PROBIT REGRESSION COEFFICIENT    PROB 340
C                      B                                                PROB 350
C              ANS(3)- CHI-SQUARED VALUE FOR A TEST OF SIGNIFICANCE     PROB 360
C                      OF THE FINAL PROBIT EQUATION                     PROB 370
C              ANS(4)- DEGREES OF FREEDOM FOR THE CHI-SQUARE            PROB 380
C                      STATISTIC                                        PROB 390
C        W1  - OUTPUT VECTOR OF LENGTH K CONTAINING THE PROPORTIONS     PROB 400
C              OF SUBJECTS RESPONDING TO THE VARIOUS DOSE LEVELS OF     PROB 410
C              THE DRUG                                                 PROB 420
C        W2  - OUTPUT VECTOR OF LENGTH K CONTAINING THE VALUES OF THEPROB 430
C              EXPECTED PROBIT FOR THE VARIOUS LEVELS OF A DRUG         PROB 440
C        IER - 1 IF K IS NOT GREATER THAN 2.                            PROB 450
C              2 IF SOME DOSAGE LEVEL IS NEGATIVE, OR IF THE INPUT      PROB 460
C                OPTION CODE LOG IS 1 AND SOME DOSAGE LEVEL IS ZERO.    PROB 470
C              3 IF SOME ELEMENT OF S IS NOT POSITIVE.                  PROB 480
C              4 IF NUMBER OF SUBJECTS RESPONDING IS GREATER THAN       PROB 490
C                NUMBER OF SUBJECTS TESTED.                             PROB 500
C              ONLY IF IER IS ZERO IS A PROBIT ANALYSIS PERFORMED.      PROB 510
C              OTHERWISE, ANS, W1, AND W2 ARE SET TO ZERO.              PROB 520
C                                                                       PROB 530
C     REMARKS                                                           PROB 540
C        THE PROGRAM WILL ITERATE ON THE PROBIT EQUATION UNTIL TWO      PROB 550
C        SUCCESSIVE SOLUTIONS PRODUCE CHANGES OF LESS THAN 10**(-7).    PROB 560
C                                                                       PROB 570
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     PROB 580
C        NDTF                                                           PROB 590
C        NDTRI                                                          PROB 600
C                                                                       PROB 610
C     METHOD                                                            PROB 620
C        REFER TO D. J. FINNEY, PROBIT ANALYSIS. 2ND ED. (CAMBRIDGE,    PROB 630
C        1952)                                                          PROB 640
C                                                                       PROB 650
C  .....................................................................PROB 660
C                                                                       PROB 670
      SUBROUTINE PROBT (K,X,S,R,LOG,ANS,W1,W2,IER)                      PROB 680
C                                                                       PROB 690
      DIMENSION X(1),S(1),R(1),ANS(1),W1(1),W2(1)                       PROB 700
C                                                                       PROB 710
C        TEST WHETHER LOG CONVERSION IS NEEDED                          PROB 720
C                                                                       PROB 730
      IEP=0                                                             PROB 740
      IF(K-2)5,5,7                                                      PROB 750
    5 IER = 1                                                           PROB 760
      GO TO 90                                                          PROB 770
    7 DO 8 I=1,K                                                        PROB 780
      IF(X(I))12,8,8                                                    PROB 790
    8 CONTINUE                                                          PROB 800
      IF(LOG-1) 16,10,16                                                PROB 810
   10 DO 15 I=1,K                                                       PROB 820
      IF(X(I))12,12,14                                                  PROB 830
   12 IER=2                                                             PROB 840
      GO TO 90                                                          PROB 850
   14 X(I)= ALOG10(X(I))                                                PROB 860
   15 CONTINUE                                                          PROB 870
```

```
C                                                                       PROB 880
C       COMPUTE PROPORTIONS OF OBJECTS RESPONDING                       PROB 890
C                                                                       PROB 900
   16 DO 18 I=1,K                                                       PROB 910
      IF(S(I)-R(I)) 17,18,18                                            PROB 920
   17 IER=4                                                             PROB 930
      GO TO 90                                                          PROB 940
   18 CONTINUE                                                          PROB 950
   20 DO 23 I=1,K                                                       PROB 960
      IF(S(I))21,21,22                                                  PROB 970
   21 IER=3                                                             PROB 980
      GO TO 90                                                          PROB 990
   22 W1(I)=R(I)/S(I)                                                   PROB1000
   23 CONTINUE                                                          PROB1010
C                                                                       PROB1020
C       COMPUTE INITIAL ESTIMATES OF INTERCEPT AND PROBIT REGRESSION    PROB1030
C       COEFFICIENT                                                     PROB1040
C                                                                       PROB1050
      WN=0.0                                                            PROB1060
      XBAR=0.0                                                          PROB1070
      SNWY=0.0                                                          PROB1080
      SXX=0.0                                                           PROB1090
      SXY=0.0                                                           PROB1100
C                                                                       PROB1110
      DO 30 I=1,K                                                       PROB1120
      P=W1(I)                                                           PROB1130
      IF(P) 30, 30, 24                                                  PROB1140
   24 IF(P-1.0) 25, 30, 30                                              PROB1150
   25 WN=WN+1.0                                                         PROB1160
C                                                                       PROB1170
      CALL NDTRI (P,Z,D,IER)                                            PROB1180
C                                                                       PROB1190
      Z=Z+5.0                                                           PROB1200
      XBAR=XBAR+X(I)                                                    PROB1210
      SNWY=SNWY+Z                                                       PROB1220
      SXX=SXX+X(I)**2                                                   PROB1230
      SXY=SXY+X(I)*Z                                                    PROB1240
   30 CONTINUE                                                          PROB1250
C                                                                       PROB1260
      B=(SXY-(XBAR*SNWY)/WN)/(SXX-(XBAR*XBAR)/WN)                       PROB1270
      XBAR=XBAR/WN                                                      PROB1280
      SNWY=SNWY/WN                                                      PROB1290
      A=SNWY-B*XBAR                                                     PROB1300
      DD=0.0                                                            PROB1310
C                                                                       PROB1320
C       COMPUTE EXPECTED PROBIT                                         PROB1330
C                                                                       PROB1340
      DO 31 I=1,K                                                       PROB1350
   31 W2(I)=A+B*X(I)                                                    PROB1360
C                                                                       PROB1370
   33 SNW=0.0                                                           PROB1380
      SNWX=0.0                                                          PROB1390
      SNWY=0.0                                                          PROB1400
      SNWXX=0.0                                                         PROB1410
      SNWXY=0.0                                                         PROB1420
      DO 50 I=1,K                                                       PROB1430
      Y=W2(I)                                                           PROB1440
C                                                                       PROB1450
C       FIND A WEIGHTING COEFFICIENT FOR PROBIT ANALYSIS                PROB1460
C                                                                       PROB1470
      D=Y-5.0                                                           PROB1480
C                                                                       PROB1490
      CALL NDTF (D,P,Z)                                                 PROB1500
C                                                                       PROB1510
      Q=1.0-P                                                           PROB1520
      W=(Z*Z)/(P*Q)                                                     PROB1530
C                                                                       PROB1540
C       COMPUTE WORKING PROBIT                                          PROB1550
C                                                                       PROB1560
      IF(Y-5.0) 35, 35, 40                                              PROB1570
   35 WP=(Y-P/Z)+W1(I)/Z                                                PROB1580
      GO TO 45                                                          PROB1590
   40 WP=(Y+Q/Z)-(1.0-W1(I))/Z                                          PROB1600
C                                                                       PROB1610
C       SUM INTERMEDIATE RESULTS                                        PROB1620
C                                                                       PROB1630
   45 WN=W*S(I)                                                         PROB1640
      SNW=SNW+WN                                                        PROB1650
      SNWX=SNWX+WN*X(I)                                                 PROB1660
      SNWY=SNWY+WN*WP                                                   PROB1670
      SNWXX=SNWXX+WN*X(I)**2                                            PROB1680
   50 SNWXY=SNWXY+WN*X(I)*WP                                            PROB1690
C                                                                       PROB1700
C       COMPUTE NEW ESTIMATES OF INTERCEPT AND COEFFICIENT              PROB1710
C                                                                       PROB1720
      XBAR=SNWX/SNW                                                     PROB1730
C                                                                       PROB1740
      SXX=SNWXX-(SNWX)*(SNWX)/SNW                                       PROB1750
      SXY=SNWXY-(SNWX)*(SNWY)/SNW                                       PROB1760
      B=SXY/SXX                                                         PROB1770
C                                                                       PROB1780
      A=SNWY/SNW-B*XBAR                                                 PROB1790
C                                                                       PROB1800
C       EXAMINE THE CHANGES IN Y                                        PROB1810
C                                                                       PROB1820
      SXX=0.0                                                           PROB1830
      DO 60 I=1,K                                                       PROB1840
      Y=A+B*X(I)                                                        PROB1850
      D=W2(I)-Y                                                         PROB1860
      SXX=SXX+D*D                                                       PROB1870
   60 W2(I)=Y                                                           PROB1880
      IF(( ABS(DD-SXX))-(1.0E-7)) 65, 65, 63                            PROB1890
   63 DD=SXX                                                            PROB1900
      GO TO 33                                                          PROB1910
C                                                                       PROB1920
C       STORE INTERCEPT AND COEFFICIENT                                 PROB1930
C                                                                       PROB1940
   65 ANS(1)=A                                                          PROB1950
      ANS(2)=B                                                          PROB1960
C                                                                       PROB1970
C       COMPUTE CHI-SQUARE                                              PROB1980
C                                                                       PROB1990
      ANS(3)=0.0                                                        PROB2000
      DO 70 I=1,K                                                       PROB2010
      Y=W2(I)-5.0                                                       PROB2020
C                                                                       PROB2030
      CALL NDTR (Y,P,D)                                                 PROB2040
C                                                                       PROB2050
      AA=P(I)-S(I)*P                                                    PROB2060
      DD=S(I)*P*(1.0-P)                                                 PROB2070
   70 ANS(3)=ANS(3)+AA*AA/DD                                            PROB2080
C                                                                       PROB2090
C       DEGREES OF FREEDOM FOR CHI-SQUARE                               PROB2100
C                                                                       PROB2110
      ANS(4)=K-2                                                        PROB2120
C                                                                       PROB2130
   80 RETURN                                                            PROB2140
   90 DO 100 I=1,K                                                      PROB2150
      W1(I)=0.0                                                         PROB2160
  100 W2(I)=0.0                                                         PROB2170
      DO 110 I=1,4                                                      PROB2180
  110 ANS(I)=0.0                                                        PROB2190
      GO TO 80                                                          PROB2200
      END                                                               PROB2210
```

Canonical Correlation

In the Scientific Subroutine Package, canonical correlation analysis is normally performed by calling the following five subroutines:

1. CORRE - to compute means, standard deviations, and correlation matrix
2. MINV - to invert a part of the correlation matrix
3. EIGEN - to compute eigenvalues and eigenvectors
4. NROOT - to compute eigenvalues and eigenvectors of real nonsymmetric matrix of the form $B^{-1}A$
5. CANOR - to compute canonical correlations and coefficients

The subroutine CORRE works in either of two ways: (1) it expects all observations in core, or (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines Required" in the comment cards description of subroutine CORRE).

Subroutine CANOR

This subroutine performs a canonical correlation analysis between two sets of variables.

The matrix of intercorrelations, R, is partitioned into four submatrices:

$$R = \left[\begin{array}{c|c} R_{11} & R_{12} \\ \hline R_{21} & R_{22} \end{array}\right] \qquad (1)$$

R_{11} = intercorrelations among p variables in the first set (that is, left-hand variables)

R_{12} = intercorrelations between the variables in the first and second sets

R_{21} = the transpose of R_{12}

R_{22} = intercorrelations among q variables in the second set (that is, right-hand variables)

The equation:

$$\left| R_{22}^{-1} R_{21} R_{11}^{-1} R_{12} - \lambda I \right| = 0 \qquad (2)$$

is then solved for all values of λ, eigenvalues, in the following matrix operation:

$$T = R_{11}^{-1} R_{12} \qquad (3)$$

$$A = R_{21} T \qquad (4)$$

The subroutine NROOT calculates eigenvalues (λ_i), with associated eigenvectors, of $R_{22}^{-1} A$, where i = 1, 2, ..., q.

For each subscript i = 1, 2, . . ., q, the following statistics are calculated:

Canonical correlation:

$$CANR = \sqrt{\lambda_i} \qquad (5)$$

where λ_i = i^{th} eigenvalue

Chi-square:

$$\chi^2 = -\left[n - 0.5\,(p + q + 1)\right] \log_e \Lambda \qquad (6)$$

where n = number of observations

$$\Lambda = \prod_{j=i}^{q} (1 - \lambda_j);$$

Degrees of freedom for χ^2:

$$DF = \left[p - (i-1)\right]\left[q - (i-1)\right] \qquad (7)$$

i^{th} set of right-hand coefficients:

$$b_k = v_{ki} \qquad (8)$$

where v_{ki} = eigenvector associated with λ_i

k = 1, 2, . . ., q;

i^{th} set of left-hand coefficients:

$$a_j = \frac{\sum_{k=1}^{q} t_{jk}\, b_k}{CANR} \qquad (9)$$

where $\left\{ t_{jk} \right\} = T = R_{11}^{-1} R_{12}$

j = 1, 2, ..., p

```
C                                                                       CANO  10
C     ...................................................................CANO  20
C                                                                       CANO  30
C        SUBROUTINE CANOR                                               CANO  40
C                                                                       CANO  50
C        PURPOSE                                                        CANO  60
C           COMPUTE THE CANONICAL CORRELATIONS BETWEEN TWO SETS OF      CANO  70
C           VARIABLES.  CANOR IS NORMALLY PRECEDED BY A CALL TO SUBROU- CANO  80
C           TINE CORRE.                                                 CANO  90
C                                                                       CANO 100
C        USAGE                                                          CANO 110
C           CALL CANOR (N,MP,MQ,RR,ROOTS,WLAM,CANR,CHISQ,NDF,COEFR,     CANO 120
C                       COEFL,R)                                        CANO 130
C                                                                       CANO 140
C        DESCRIPTION OF PARAMETERS                                      CANO 150
C           N     - NUMBER OF OBSERVATIONS                              CANO 160
C           MP    - NUMBER OF LEFT HAND VARIABLES                       CANO 170
C           MQ    - NUMBER OF RIGHT HAND VARIABLES                      CANO 180
C           RR    - INPUT MATRIX (ONLY UPPER TRIANGULAR PORTION OF THE  CANO 190
C                   SYMMETRIC MATRIX OF M X M, WHERE M = MP + MQ)       CANO 200
C                   CONTAINING CORRELATION COEFFICIENTS.  (STORAGE MODE CANO 210
C                   OF 1)                                               CANO 220
C           ROOTS - OUTPUT VECTOR OF LENGTH MQ CONTAINING EIGENVALUES   CANO 230
C                   COMPUTED IN THE NROOT SUBROUTINE.                   CANO 240
C           WLAM  - OUTPUT VECTOR OF LENGTH MQ CONTAINING LAMBDA.       CANO 250
C           CANR  - OUTPUT VECTOR OF LENGTH MQ CONTAINING CANONICAL     CANO 260
C                   CORRELATIONS.                                       CANO 270
C           CHISQ - OUTPUT VECTOR OF LENGTH MQ CONTAINING THE           CANO 280
C                   VALUES OF CHI-SQUARES.                              CANO 290
C           NDF   - OUTPUT VECTOR OF LENGTH MQ CONTAINING THE DEGREES   CANO 300
C                   OF FREEDOM ASSOCIATED WITH CHI-SQUARES.             CANO 310
C           COEFR - OUTPUT MATRIX (MQ X MQ) CONTAINING MQ SETS OF       CANO 320
C                   RIGHT HAND COEFFICIENTS COLUMNWISE.                 CANO 330
C           COEFL - OUTPUT MATRIX (MP X MQ) CONTAINING MQ SETS OF       CANO 340
C                   LEFT HAND COEFFICIENTS COLUMNWISE.                  CANO 350
C           R     - WORK MATRIX (M X M)                                 CANO 360
C                                                                       CANO 370
C        REMARKS                                                        CANO 380
C           THE NUMBER OF LEFT HAND VARIABLES (MP) SHOULD BE GREATER    CANO 390
C           THAN OR EQUAL TO THE NUMBER OF RIGHT HAND VARIABLES (MQ).   CANO 400
C           THE VALUES OF CANONICAL CORRELATION, LAMBDA, CHI-SQUARE,    CANO 410
C           DEGREES OF FREEDOM, AND CANONICAL COEFFICIENTS ARE COMPUTED CANO 420
C           ONLY FOR THOSE EIGENVALUES IN ROOTS WHICH ARE GREATER THAN  CANO 430
C           ZERO.                                                       CANO 440
C                                                                       CANO 450
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CANO 460
C           MINV                                                        CANO 470
C           NROOT  (WHICH, IN TURN, CALLS THE SUBROUTINE EIGEN.)        CANO 480
C                                                                       CANO 490
C        METHOD                                                         CANO 500
C           REFER TO W. W. COOLEY AND P. R. LOHNES, 'MULTIVARIATE PRO-  CANO 510
C           CEDURES FOR THE BEHAVIORAL SCIENCES', JOHN WILEY AND SONS,  CANO 520
C           1962, CHAPTER 3.                                            CANO 530
C                                                                       CANO 540
C     ...................................................................CANO 550
C                                                                       CANO 560
      SUBROUTINE CANOR (N,MP,MQ,RR,ROOTS,WLAM,CANR,CHISQ,NDF,COEFR,     CANO 570
     1                  COEFL,R)                                        CANO 580
      DIMENSION RR(1),ROOTS(1),WLAM(1),CANR(1),CHISQ(1),NDF(1),COEFR(1),CANO 590
     1          COEFL(1),R(1)                                           CANO 600
C                                                                       CANO 610
C     ...................................................................CANO 620
C                                                                       CANO 630
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  CANO 640
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      CANO 650
C        STATEMENT WHICH FOLLOWS.                                       CANO 660
C                                                                       CANO 670
C     DOUBLE PRECISION RR,ROOTS,WLAM,CANR,CHISQ,COEFR,COEFL,R,DET,SUM   CANO 680
C                                                                       CANO 690
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    CANO 700
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      CANO 710
C        ROUTINE.                                                       CANO 720
C                                                                       CANO 730
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      CANO 740
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENT CANO 750
C        165 MUST BE CHANGED TO DSQRT.  ALOG IN STATEMENT 175 MUST BE   CANO 760
C        CHANGED TO DLOG.                                               CANO 770
C                                                                       CANO 780
C     ...................................................................CANO 790
C                                                                       CANO 800
C     PARTITION INTERCORRELATIONS AMONG LEFT HAND VARIABLES, BETWEEN    CANO 810
C     LEFT AND RIGHT HAND VARIABLES, AND AMONG RIGHT HAND VARIABLES.    CANO 820
C                                                                       CANO 830
      M=MP+MQ                                                           CANO 840
      N1=0                                                              CANO 850
      DO 105 I=1,M                                                      CANO 860
      DO 105 J=1,M                                                      CANO 870
      IF(I-J) 102, 103, 103                                             CANO 880
  102 L=I+(J*J-J)/2                                                     CANO 890
      GO TO 104                                                         CANO 900
  103 L=J+(I*I-I)/2                                                     CANO 910
  104 N1=N1+1                                                           CANO 920
  105 R(N1)=RR(L)                                                       CANO 930
      L=MP                                                              CANO 940
      DO 108 J=2,MP                                                     CANO 950
      N1=M*(J-1)                                                        CANO 960
      DO 108 I=1,MP                                                     CANO 970
      L=L+1                                                             CANO 980
      N1=N1+1                                                           CANO 990
  108 R(L)=R(N1)                                                        CANO1000
      N2=MP+1                                                           CANO1010
      L=0                                                               CANO1020
      DO 110 J=N2,M                                                     CANO1030
      N1=M*(J-1)                                                        CANO1040
      DO 110 I=1,MP                                                     CANO1050
      L=L+1                                                             CANO1060
      N1=N1+1                                                           CANO1070
  110 COEFL(L)=R(N1)                                                    CANO1080
      L=0                                                               CANO1090
      DO 120 J=N2,M                                                     CANO1100
      N1=M*(J-1)+MP                                                     CANO1110
      DO 120 I=N2,M                                                     CANO1120
      L=L+1                                                             CANO1130
      N1=N1+1                                                           CANO1140
  120 COEFR(L)=R(N1)                                                    CANO1150
C                                                                       CANO1160
C     SOLVE THE CANONICAL EQUATION                                      CANO1170
C                                                                       CANO1180
      L=MP*MP+1                                                         CANO1190
      K=L+MP                                                            CANO1200
      CALL MINV (R,MP,DET,R(L),R(K))                                    CANO1210
C                                                                       CANO1220
C        CALCULATE T = INVERSE OF R11 * R12                             CANO1230
C                                                                       CANO1240
      DO 140 I=1,MP                                                     CANO1250
      N2=0                                                              CANO1260
      DO 135 J=1,MQ                                                     CANO1270
      N1=I-MP                                                           CANO1280
      ROOTS(J)=0.0                                                      CANO1290
      DO 130 K=1,MP                                                     CANO1300
      N1=N1+MP                                                          CANO1310
      N2=N2+1                                                           CANO1320
  130 ROOTS(J)=ROOTS(J)+R(N1)*COEFL(N2)                                 CANO1330
      L=I-MP                                                            CANO1340
      DO 140 J=1,MQ                                                     CANO1350
      L=L+MP                                                            CANO1360
  140 R(L)=ROOTS(J)                                                     CANO1370
C                                                                       CANO1380
C        CALCULATE A = R21 * T                                          CANO1390
C                                                                       CANO1400
      L=MP*MQ                                                           CANO1410
      N3=L+1                                                            CANO1420
      DO 165 J=1,MQ                                                     CANO1430
      N1=0                                                              CANO1440
      DO 160 I=1,MQ                                                     CANO1450
      N2=MP*(J-1)                                                       CANO1460
      SUM=0.0                                                           CANO1470
      DO 150 K=1,MP                                                     CANO1480
      N1=N1+1                                                           CANO1490
      N2=N2+1                                                           CANO1500
  150 SUM=SUM+COEFL(N1)*R(N2)                                           CANO1510
      L=L+1                                                             CANO1520
  160 R(L)=SUM                                                          CANO1530
C                                                                       CANO1540
C        CALCULATE EIGENVALUES WITH ASSOCIATED EIGENVECTORS OF THE      CANO1550
C        INVERSE OF R22 * A                                             CANO1560
C                                                                       CANO1570
      L=L+1                                                             CANO1580
      CALL NROOT (MQ,R(N3),COEFR,ROOTS,R(L))                            CANO1590
C                                                                       CANO1600
C     FOR EACH VALUE OF I = 1, 2, ..., MQ, CALCULATE THE FOLLOWING      CANO1610
C     STATISTICS                                                        CANO1620
C                                                                       CANO1630
      DO 210 I=1,MQ                                                     CANO1640
C                                                                       CANO1650
C        TEST WHETHER EIGENVALUE IS GREATER THAN ZERO                   CANO1660
C                                                                       CANO1670
      IF(ROOTS(I)) 220, 220, 165                                        CANO1680
C                                                                       CANO1690
C        CANONICAL CORRELATION                                          CANO1700
C                                                                       CANO1710
  165 CANR(I)= SQRT(ROOTS(I))                                           CANO1720
C                                                                       CANO1730
C        CHI-SQUARE                                                     CANO1740
C                                                                       CANO1750
      WLAM(I)=1.0                                                       CANO1760
      DO 170 J=I,MQ                                                     CANO1770
  170 WLAM(I)=WLAM(I)*(1.0-ROOTS(J))                                    CANO1780
      FN=N                                                              CANO1790
      FMP=MP                                                            CANO1800
      FMQ=MQ                                                            CANO1810
  175 CHISQ(I)=-(FN-0.5*(FMP+FMQ+1.0))*ALOG(WLAM(I))                    CANO1820
C                                                                       CANO1830
C        DEGREES OF FREEDOM FOR CHI-SQUARE                              CANO1840
C                                                                       CANO1850
      N1=I-1                                                            CANO1860
      NDF(I)=(MP-N1)*(MQ-N1)                                            CANO1870
C                                                                       CANO1880
C        I-TH SET OF RIGHT HAND COEFFICIENTS                            CANO1890
C                                                                       CANO1900
      N1=MQ*(I-1)                                                       CANO1910
      N2=MQ*(I-1)+L-1                                                   CANO1920
      DO 180 J=1,MQ                                                     CANO1930
      N1=N1+1                                                           CANO1940
      N2=N2+1                                                           CANO1950
  180 COEFR(N1)=R(N2)                                                   CANO1960
C                                                                       CANO1970
C        I-TH SET OF LEFT HAND COEFFICIENTS                             CANO1980
C                                                                       CANO1990
      DO 200 J=1,MP                                                     CANO2000
      N1=J-MP                                                           CANO2010
      N2=MQ*(I-1)                                                       CANO2020
      K=MP*(I-1)+J                                                      CANO2030
      COEFL(K)=0.0                                                      CANO2040
      DO 190 JJ=1,MQ                                                    CANO2050
      N1=N1+MP                                                          CANO2060
      N2=N2+1                                                           CANO2070
  190 COEFL(K)=COEFL(K)+R(N1)*COEFR(N2)                                 CANO2080
  200 COEFL(K)=COEFL(K)/CANR(I)                                         CANO2090
  210 CONTINUE                                                          CANO2100
  220 RETURN                                                            CANO2110
      END                                                               CANO2120
```

Design Analysis (see Smoothing, Regression, Factorization)

In the Scientific Subroutine Package, analysis of variance is normally performed by calling the following three subroutines in sequence:

1. AVDAT - to place data in properly distributed positions of storage
2. AVCAL - to apply the operators sigma and delta in order to compute deviates for analysis of variance
3. MEANQ - to pool the deviates and compute sums of squares, degrees of freedom, and mean squares

Subroutine AVDAT

This subroutine places data for analysis of variance in properly distributed positions of storage.

The size of data array X required for an analysis-of-variance problem is calculated as follows:

$$n = \prod_{i=1}^{k} (L_i + 1) \qquad (1)$$

where L_i = number of levels of i^{th} factor

k = number of factors

The input data placed in the lower part of the array X are moved temporarily to the upper part of the array. From there, the data are redistributed according to the equation (4) below. Prior to that, multipliers, s_j, to be used in finding proper positions of storage, are calculated as follows:

$$s_1 = 1 \qquad (2)$$

$$s_j = \prod_{i=1}^{j-1} (L_i + 1) \qquad (3)$$

where $j = 2, 3, \ldots, k$

Then a position for each data point is calculated by the following equation:

$$S = KOUNT_1 + \sum_{j=2}^{k} s_j \cdot (KOUNT_j - 1) \qquad (4)$$

where $KOUNT_j$ = value of j^{th} subscript of the data to be stored.

The subroutine increments the value(s) of subscript(s) after each data point is stored.

```
C                                                                       AVDA  10
C  ....................................................................AVDA  20
C                                                                       AVDA  30
C     SUBROUTINE AVDAT                                                  AVDA  40
C                                                                       AVDA  50
C     PURPOSE                                                           AVDA  60
C        PLACE DATA FOR ANALYSIS OF VARIANCE IN PROPERLY DISTRIBUTED    AVDA  70
C        POSITIONS OF STORAGE.  THIS SUBROUTINE IS NORMALLY FOLLOWED    AVDA  80
C        BY CALLS TO AVCAL AND MEANQ SUBROUTINES IN THE PERFORMANCE     AVDA  90
C        OF ANALYSIS OF VARIANCE FOR A COMPLETE FACTORIAL DESIGN.       AVDA 100
C                                                                       AVDA 110
C     USAGE                                                             AVDA 120
C        CALL AVDAT (K,LEVEL,N,X,L,ISTEP,KOUNT)                         AVDA 130
C                                                                       AVDA 140
C     DESCRIPTION OF PARAMETERS                                         AVDA 150
C        K      - NUMBER OF VARIABLES (FACTORS). K MUST BE .GT. ONE.    AVDA 160
C        LEVEL  - INPUT VECTOR OF LENGTH K CONTAINING LEVELS (CATE-     AVDA 170
C                 GORIES) WITHIN EACH VARIABLE.                         AVDA 180
C        N      - TOTAL NUMBER OF DATA POINTS READ IN.                  AVDA 190
C        X      - WHEN THE SUBROUTINE IS CALLED, THIS VECTOR CONTAINS   AVDA 200
C                 DATA IN LOCATIONS X(1) THROUGH X(N).  UPON RETURNING AVDA 210
C                 TO THE CALLING ROUTINE, THE VECTOR CONTAINS THE DATA AVDA 220
C                 IN PROPERLY REDISTRIBUTED LOCATIONS OF VECTOR X.      AVDA 230
C                 THE LENGTH OF VECTOR X IS CALCULATED BY (1) ADDING    AVDA 240
C                 ONE TO EACH LEVEL OF VARIABLE AND (2) OBTAINING THE   AVDA 250
C                 CUMULATIVE PRODUCT OF ALL LEVELS.  (THE LENGTH OF     AVDA 260
C                 X = (LEVEL(1)+1)*(LEVEL(2)+1)*...*(LEVEL(K)+1).)     AVDA 270
C        L      - OUTPUT VARIABLE CONTAINING THE POSITION IN VECTOR X  AVDA 280
C                 WHERE THE LAST INPUT DATA IS STORED.                  AVDA 290
C        ISTEP  - OUTPUT VECTOR OF LENGTH K CONTAINING CONTROL STEPS   AVDA 300
C                 WHICH ARE USED TO LOCATE DATA IN PROPER POSITIONS     AVDA 310
C                 OF VECTOR X.                                          AVDA 320
C        KOUNT  - WORKING VECTOR OF LENGTH K.                           AVDA 330
C                                                                       AVDA 340
C                                                                       AVDA 350
C     REMARKS                                                           AVDA 360
C        INPUT DATA MUST BE ARRANGED IN THE FOLLOWING MANNER.           AVDA 370
C        CONSIDER THE 3-VARIABLE ANALYSIS OF VARIANCE DESIGN, WHERE     AVDA 380
C        ONE VARIABLE HAS 3 LEVELS AND THE OTHER TWO VARIABLES HAVE     AVDA 390
C        2 LEVELS.  THE DATA MAY BE REPRESENTED IN THE FORM X(I,J,K),   AVDA 400
C        I=1,2,3  J=1,2  K=1,2.  IN ARRANGING DATA, THE INNER           AVDA 410
C        SUBSCRIPT, NAMELY I, CHANGES FIRST.  WHEN I=3, THE NEXT        AVDA 420
C        INNER SUBSCRIPT, J, CHANGES AND SO ON UNTIL I=3, J=2, AND      AVDA 430
C        K=2.                                                           AVDA 440
C                                                                       AVDA 450
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     AVDA 460
C        NONE                                                           AVDA 470
C                                                                       AVDA 480
C     METHOD                                                            AVDA 490
C        THE METHOD IS BASED ON THE TECHNIQUE DISCUSSED BY H. O.        AVDA 500
C        HARTLEY IN 'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS',       AVDA 510
C        EDITED BY A. RALSTON AND H. WILF, JOHN WILEY AND SONS,         AVDA 520
C        1962, CHAPTER 20.                                              AVDA 530
C                                                                       AVDA 540
C  ....................................................................AVDA 550
      SUBROUTINE AVDAT (K,LEVEL,N,X,L,ISTEP,KOUNT)                      AVDA 560
      DIMENSION LEVEL(1),X(1),ISTEP(1),KOUNT(1)                         AVDA 570
C                                                                       AVDA 580
C     ..................................................................AVDA 590
C                                                                       AVDA 600
C     IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE     AVDA 610
C     C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION         AVDA 620
C     STATEMENT WHICH FOLLOWS.                                          AVDA 630
C                                                                       AVDA 640
C     DOUBLE PRECISION X                                                AVDA 650
C                                                                       AVDA 660
C     THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS       AVDA 670
C     APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS         AVDA 680
C     ROUTINE.                                                          AVDA 690
C                                                                       AVDA 700
C     ..................................................................AVDA 710
C                                                                       AVDA 720
C     CALCULATE TOTAL DATA AREA REQUIRED                                AVDA 730
C                                                                       AVDA 740
      M=LEVEL(1)+1                                                      AVDA 750
      DO 105 I=2,K                                                      AVDA 760
  105 M=M*(LEVEL(I)+1)                                                  AVDA 770
C                                                                       AVDA 780
C     MOVE DATA TO THE UPPER PART OF THE ARRAY X                        AVDA 790
C     FOR THE PURPOSE OF REARRANGEMENT                                  AVDA 800
C                                                                       AVDA 810
      N1=M+1                                                            AVDA 820
      N2=N+1                                                            AVDA 830
      DO 107 I=1,N                                                      AVDA 840
      N1=N1-1                                                           AVDA 850
      N2=N2-1                                                           AVDA 860
  107 X(N1)=X(N2)                                                       AVDA 870
C                                                                       AVDA 880
C     CALCULATE MULTIPLIERS TO BE USED IN FINDING STORAGE LOCATIONS FOR  AVDA 890
C     INPUT DATA                                                        AVDA 900
C                                                                       AVDA 910
      ISTEP(1)=1                                                        AVDA 920
      DO 110 I=2,K                                                      AVDA 930
  110 ISTEP(I)=ISTEP(I-1)*(LEVEL(I-1)+1)                                AVDA 940
      DO 115 I=1,K                                                      AVDA 950
  115 KOUNT(I)=1                                                        AVDA 960
C                                                                       AVDA 970
C     PLACE DATA IN PROPER LOCATIONS                                    AVDA 980
C                                                                       AVDA 990
      N1=N1-1                                                           AVDA1000
      DO 135 I=1,N                                                      AVDA1010
      L=KOUNT(1)                                                        AVDA1020
      DO 120 J=2,K                                                      AVDA1030
  120 L=L+ISTEP(J)*(KOUNT(J)-1)                                         AVDA1040
      N1=N1+1                                                           AVDA1050
      X(L)=X(N1)                                                        AVDA1060
      DO 130 J=1,K                                                      AVDA1070
      IF(KOUNT(J)-LEVEL(J)) 124, 125, 124                               AVDA1080
  124 KOUNT(J)=KOUNT(J)+1                                               AVDA1090
      GO TO 135                                                         AVDA1100
  125 KOUNT(J)=1                                                        AVDA1110
  130 CONTINUE                                                          AVDA1120
  135 CONTINUE                                                          AVDA1130
      RETURN                                                            AVDA1140
      END                                                               AVDA1150
```

Subroutine AVCAL

This subroutine performs the calculus for the general k-factor experiment: operator Σ and operator Δ. An example is presented in terms of k = 3 to illustrate these operators.

Let x_{abc} denote the experimental reading from the a^{th} level of factor A, the b^{th} level of factor B, and the c^{th} level of factor C. The symbols A, B, and C will also denote the number of levels for each factor so that a = 1, 2, ..., A; b = 1, 2, ..., B; and c = 1, 2, ..., C.

With regard to the first factor A:

operator $\sum_a \equiv$ sum over all levels a = 1, 2, ..., A, holding the other subscripts at constant levels, and

operator $\underset{a}{\triangle} \equiv$ multiply all items by A and subtract the result of $\sum_a$ from all items

In mathematical notation, these operators are defined as follows:

$$\sum_a x_{abc} \equiv X_{.bc} \equiv \sum_{a=1}^{A} x_{abc} \qquad (1)$$

$$\underset{a}{\triangle} x_{abc} \equiv A\, x_{abc} - X_{.bc} \qquad (2)$$

The operators Σ and Δ will be applied sequentially to all factors A, B, and C. Upon the completion of these operations, the storage array X contains deviates to be used for analysis-of-variance components in the subroutine MEANQ.

```
C                                                                       AVCA  10
C     ..................................................................AVCA  20
C                                                                       AVCA  30
C        SUBROUTINE AVCAL                                               AVCA  40
C                                                                       AVCA  50
C        PURPOSE                                                        AVCA  60
C           PERFORM THE CALCULUS OF A FACTORIAL EXPERIMENT USING        AVCA  70
C           OPERATOR SIGMA AND OPERATOR DELTA.  THIS SUBROUTINE IS      AVCA  80
C           PRECEDED BY SUBROUTINE AVDAT AND FOLLOWED BY SUBROUTINE     AVCA  90
C           MEANQ IN THE PERFORMANCE OF ANALYSIS OF VARIANCE FOR A      AVCA 100
C           COMPLETE FACTORIAL DESIGN.                                  AVCA 110
C                                                                       AVCA 120
C        USAGE                                                          AVCA 130
C           CALL AVCAL (K,LEVEL,X,L,ISTEP,LASTS)                        AVCA 140
C                                                                       AVCA 150
C        DESCRIPTION OF PARAMETERS                                      AVCA 160
C           K      - NUMBER OF VARIABLES (FACTORS). K MUST BE .GT. ONE. AVCA 170
C           LEVEL  - INPUT VECTOR OF LENGTH K CONTAINING LEVELS (CATE- AVCA 180
C                    GORIES) WITHIN EACH VARIABLE.                      AVCA 190
C           X      - INPUT VECTOR CONTAINING DATA.  DATA HAVE BEEN PLACEDAVCA 200
C                    IN VECTOR X BY SUBROUTINE AVDAT.  THE LENGTH OF X  AVCA 210
C                    IS (LEVEL(1)+1)*(LEVEL(2)+1)*...*(LEVEL(K)+1).    AVCA 220
C           L      - THE POSITION IN VECTOR X WHERE THE LAST INPUT DATA AVCA 230
C                    IS LOCATED.  L HAS BEEN CALCULATED BY SUBROUTINE   AVCA 240
C                    AVDAT.                                             AVCA 250
C           ISTEP  - INPUT VECTOR OF LENGTH K CONTAINING STORAGE CONTROL AVCA 260
C                    STEPS WHICH HAVE BEEN CALCULATED BY SUBROUTINE     AVCA 270
C                    AVDAT.                                             AVCA 280
C           LASTS  - WORKING VECTOR OF LENGTH K.                        AVCA 290
C                                                                       AVCA 300
C        REMARKS                                                        AVCA 310
C           THIS SUBROUTINE MUST FOLLOW SUBROUTINE AVDAT.               AVCA 320
C                                                                       AVCA 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  AVCA 340
C           NONE                                                        AVCA 350
C                                                                       AVCA 360
C        METHOD                                                         AVCA 370
C           THE METHOD IS BASED ON THE TECHNIQUE DISCUSSED BY H. O.     AVCA 380
C           HARTLEY IN 'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS',    AVCA 390
C           EDITED BY A. RALSTON AND H. WILF, JOHN WILEY AND SONS,      AVCA 400
C           1962, CHAPTER 20.                                           AVCA 410
C                                                                       AVCA 420
C     ..................................................................AVCA 430
C                                                                       AVCA 440
      SUBROUTINE AVCAL (K,LEVEL,X,L,ISTEP,LASTS)                        AVCA 450
      DIMENSION LEVEL(1),X(1),ISTEP(1),LASTS(1)                         AVCA 460
C                                                                       AVCA 470
C     ..................................................................AVCA 480
C                                                                       AVCA 490
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  AVCA 500
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      AVCA 510
C        STATEMENT WHICH FOLLOWS.                                       AVCA 520
C                                                                       AVCA 530
C     DOUBLE PRECISION X,SUM                                            AVCA 540
C                                                                       AVCA 550
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    AVCA 560
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      AVCA 570
C        ROUTINE.                                                       AVCA 580
C                                                                       AVCA 590
C     ..................................................................AVCA 600
C                                                                       AVCA 610
C     CALCULATE THE LAST DATA POSITION OF EACH FACTOR                   AVCA 620
C                                                                       AVCA 630
      LASTS(1)=L+1                                                      AVCA 640
      DO 145 I=2,K                                                      AVCA 650
  145 LASTS(I)=LASTS(I-1)*ISTEP(I)                                      AVCA 660
C                                                                       AVCA 670
C     PERFORM CALCULUS OF OPERATION                                     AVCA 680
C                                                                       AVCA 690
  150 DO 175 I=1,K                                                      AVCA 700
      L=1                                                               AVCA 710
      LL=1                                                              AVCA 720
      SUM=0.0                                                           AVCA 730
      NN=LEVEL(I)                                                       AVCA 740
      FN=NN                                                             AVCA 750
      INCRE=ISTEP(I)                                                    AVCA 760
      LAST=LASTS(I)                                                     AVCA 770
C                                                                       AVCA 780
C     SIGMA OPERATION                                                   AVCA 790
C                                                                       AVCA 800
  155 DO 160 J=1,NN                                                     AVCA 810
      SUM=SUM+X(L)                                                      AVCA 820
  160 L=L+INCRE                                                         AVCA 830
      X(L)=SUM                                                          AVCA 840
C                                                                       AVCA 850
C     DELTA OPERATION                                                   AVCA 860
C                                                                       AVCA 870
      DO 165 J=1,NN                                                     AVCA 880
      X(LL)=FN*X(LL)-SUM                                                AVCA 890
  165 LL=LL+INCRE                                                       AVCA 900
      SUM=0.0                                                           AVCA 910
      IF(L-LAST) 167, 175, 175                                          AVCA 920
  167 IF(L-LAST+INCRE) 168, 168, 170                                    AVCA 930
  168 L=L+INCRE                                                         AVCA 940
      LL=LL+INCRE                                                       AVCA 950
      GO TO 155                                                         AVCA 960
  170 L=L+INCRE+1-LAST                                                  AVCA 970
      LL=LL+INCRE+1-LAST                                                AVCA 980
      GO TO 155                                                         AVCA 990
  175 CONTINUE                                                          AVCA1000
      RETURN                                                            AVCA1010
      END                                                               AVCA1020
```

Subroutine MEANQ

This subroutine performs the mean square operation for the general k-factor experiment in the following two steps:

1. Square each value of deviates for analysis of variance stored in the array X (the result of the operators Σ and Δ applied in the subroutine AVCAL).

2. Add the squared value into summation storage. In a three-factor experiment, for example, the squared value is added into one of seven storages ($7 = 2^3 - 1$) as shown in the first column of Table 1. The symbols A, B, and C in the first column denote factor A, factor B, and factor C.

After the mean square operation is completed for all values in the storage array X, the subroutine forms sums of squares of analysis of variance by dividing the totals of squared values by proper divisors. These divisors for the three-factor experiment mentioned above are shown in the second column of Table 1. The symbols A, B, and C in the second column denote the number of levels for each factor.

The subroutine, then, forms mean squares by dividing sums of squares by degrees of freedom. The third column of the summary table shows the degrees of freedom. The symbols A, B, and C denote the number of levels for each factor.

Table 1. Table Showing Summation Storages, Divisors to Form Sum of Squares, and Degrees of Freedom (Subroutine MEANQ)

Designation of Store and of Quantity Contained in it	Divisor Required to Form Sum of Squares of Analysis of Variance	Degrees of Freedom Required to Form Mean Squares
$(A)^2$	ABC·A	(A-1)
$(B)^2$	ABC·B	(B-1)
$(AB)^2$	ABC·AB	(A-1) (B-1)
$(C)^2$	ABC·C	(C-1)
$(AC)^2$	ABC·AC	(A-1) (C-1)
$(BC)^2$	ABC·BC	(B-1) (C-1)
$(ABC)^2$	ABC·ABC	(A-1) (B-1) (C-1)

```
C                                                                       MEAN  10
C     ...................................................................MEAN  20
C                                                                       MEAN  30
C        SUBROUTINE MEANQ                                               MEAN  40
C                                                                       MEAN  50
C        PURPOSE                                                        MEAN  60
C           COMPUTE SUM OF SQUARES, DEGREES OF FREEDOM, AND MEAN SQUARE MEAN  70
C           USING THE MEAN SQUARE OPERATOR.  THIS SUBROUTINE NORMALLY   MEAN  80
C           FOLLOWS CALLS TO AVDAT AND AVCAL SUBROUTINES IN THE PER-    MEAN  90
C           FORMANCE OF ANALYSIS OF VARIANCE FOR A COMPLETE FACTORIAL   MEAN 100
C           DESIGN.                                                     MEAN 110
C                                                                       MEAN 120
C        USAGE                                                          MEAN 130
C           CALL MEANQ (K,LEVEL,X,GMEAN,SUMSQ,NDF,SMEAN,MSTEP,KOUNT,   MEAN 140
C                       LASTS)                                          MEAN 150
C                                                                       MEAN 160
C        DESCRIPTION OF PARAMETERS                                      MEAN 170
C           K      - NUMBER OF VARIABLES (FACTORS). K MUST BE .GT. ONE. MEAN 180
C           LEVEL  - INPUT VECTOR OF LENGTH K CONTAINING LEVELS (CATE- MEAN 190
C                    GORIES) WITHIN EACH VARIABLE.                      MEAN 200
C           X      - INPUT VECTOR CONTAINING THE RESULT OF THE SIGMA AND MEAN 210
C                    DELTA OPERATIONS. THE LENGTH OF X IS               MEAN 220
C                    (LEVEL(1)+1)*(LEVEL(2)+1)*...*(LEVEL(K)+1).       MEAN 230
C           GMEAN  - OUTPUT VARIABLE CONTAINING GRAND MEAN.             MEAN 240
C           SUMSQ  - OUTPUT VECTOR CONTAINING SUMS OF SQUARES.  THE     MEAN 250
C                    LENGTH OF SUMSQ IS 2 TO THE K-TH POWER MINUS ONE,  MEAN 260
C                    (2**K)-1.                                          MEAN 270
C           NDF    - OUTPUT VECTOR CONTAINING DEGREES OF FREEDOM.  THE  MEAN 280
C                    LENGTH OF NDF IS 2 TO THE K-TH POWER MINUS ONE,    MEAN 290
C                    (2**K)-1.                                          MEAN 300
C           SMEAN  - OUTPUT VECTOR CONTAINING MEAN SQUARES.  THE        MEAN 310
C                    LENGTH OF SMEAN IS 2 TO THE K-TH POWER MINUS ONE,  MEAN 320
C                    (2**K)-1.                                          MEAN 330
C           MSTEP  - WORKING VECTOR OF LENGTH K.                        MEAN 340
C           KOUNT  - WORKING VECTOR OF LENGTH K.                        MEAN 350
C           LASTS  - WORKING VECTOR OF LENGTH K.                        MEAN 360
C                                                                       MEAN 370
C        REMARKS                                                        MEAN 380
C           THIS SUBROUTINE MUST FOLLOW SUBROUTINE AVCAL                MEAN 390
C                                                                       MEAN 400
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MEAN 410
C           NONE                                                        MEAN 420
C                                                                       MEAN 430
C        METHOD                                                         MEAN 440
C           THE METHOD IS BASED ON THE TECHNIQUE DISCUSSED BY H. O.     MEAN 450
C           HARTLEY IN 'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS',    MEAN 460
C           EDITED BY A. RALSTON AND H. WILF, JOHN WILEY AND SONS,      MEAN 470
C           1962, CHAPTER 20.                                           MEAN 480
C                                                                       MEAN 490
C     ...................................................................MEAN 500
C                                                                       MEAN 510
      SUBROUTINE MEANQ (K,LEVEL,X,GMEAN,SUMSQ,NDF,SMEAN,MSTEP,KOUNT,   MEAN 520
     1                  LASTS)                                          MEAN 530
      DIMENSION LEVEL(1),X(1),SUMSQ(1),NDF(1),SMEAN(1),MSTEP(1),       MEAN 540
     1          KOUNT(1),LASTS(1)                                       MEAN 550
C                                                                       MEAN 560
C     ...................................................................MEAN 570
C                                                                       MEAN 580
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  MEAN 590
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      MEAN 600
C        STATEMENT WHICH FOLLOWS.                                       MEAN 610
C                                                                       MEAN 620
C     DOUBLE PRECISION X,GMEAN,SUMSQ,SMEAN,FN1                          MEAN 630
C                                                                       MEAN 640
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    MEAN 650
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      MEAN 660
C        ROUTINE.                                                       MEAN 670
C                                                                       MEAN 680
C     ...................................................................MEAN 690
C                                                                       MEAN 700
C     CALCULATE TOTAL NUMBER OF DATA                                    MEAN 710
C                                                                       MEAN 720
      N=LEVEL(1)                                                        MEAN 730
      DO 150 I=2,K                                                      MEAN 740
  150 N=N*LEVEL(I)                                                      MEAN 750
C                                                                       MEAN 760
C     SET UP CONTROL FOR MEAN SQUARE OPERATOR                           MEAN 770
C                                                                       MEAN 780
      LASTS(1)=LEVEL(1)                                                 MEAN 790
      DO 170 I=2,K                                                      MEAN 800
  170 LASTS(I)=LEVEL(I)+1                                               MEAN 810
      NN=1                                                              MEAN 820
C                                                                       MEAN 830
C     CLEAR THE AREA TO STORE SUMS OF SQUARES                           MEAN 840
C                                                                       MEAN 850
      LL=(2**K)-1                                                       MEAN 860
      MSTEP(1)=1                                                        MEAN 870
      DO 180 I=2,K                                                      MEAN 880
  180 MSTEP(I)=MSTEP(I-1)*2                                             MEAN 890
      DO 185 I=1,LL                                                     MEAN 900
  185 SUMSQ(I)=0.0                                                      MEAN 910
C                                                                       MEAN 920
C     PERFORM MEAN SQUARE OPERATOR                                      MEAN 930
C                                                                       MEAN 940
      DO 190 I=1,K                                                      MEAN 950
  190 KOUNT(I)=0                                                        MEAN 960
  200 L=0                                                               MEAN 970
      DO 260 I=1,K                                                      MEAN 980
      IF(KOUNT(I)-LASTS(I)) 210, 250, 210                               MEAN 990
  210 IF(L) 220, 220, 240                                               MEAN1000
  220 KOUNT(I)=KOUNT(I)+1                                               MEAN1010
      IF(KOUNT(I)-LEVEL(I)) 230, 230, 250                               MEAN1020
  230 L=L+MSTEP(I)                                                      MEAN1030
      GO TO 260                                                         MEAN1040
  240 IF(KOUNT(I)-LEVEL(I)) 230, 260, 230                               MEAN1050
  250 KOUNT(I)=0                                                        MEAN1060
  260 CONTINUE                                                          MEAN1070
      IF(L) 285, 285, 270                                               MEAN1080
  270 SUMSQ(L)=SUMSQ(L)+X(NN)*X(NN)                                     MEAN1090
      NN=NN+1                                                           MEAN1100
      GO TO 200                                                         MEAN1110
C                                                                       MEAN1120
C     CALCULATE THE GRAND MEAN                                          MEAN1130
C                                                                       MEAN1140
  285 FN=N                                                              MEAN1150
      GMEAN=X(NN)/FN                                                    MEAN1160
C                                                                       MEAN1170
C     CALCULATE FIRST DIVISOR REQUIRED TO FORM SUM OF SQUARES AND SECOND MEAN1180
C     DIVISOR, WHICH IS EQUAL TO DEGREES OF FREEDOM, REQUIRED TO FORM   MEAN1190
C     MEAN SQUARES                                                      MEAN1200
C                                                                       MEAN1210
      DO 310 I=2,K                                                      MEAN1220
  310 MSTEP(I)=0                                                        MEAN1230
      NN=0                                                              MEAN1240
      MSTEP(1)=1                                                        MEAN1250
  320 ND1=1                                                             MEAN1260
      ND2=1                                                             MEAN1270
      DO 340 I=1,K                                                      MEAN1280
      IF(MSTEP(I)) 330, 340, 330                                        MEAN1290
```

```
330 ND1=ND1*LEVEL(I)                                    MEANI300
    ND2=ND2*(LEVEL(I)-1)                                MEANI310
340 CONTINUE                                            MEANI320
    FN1=N*ND1                                           MEANI330
    FN2=ND2                                             MEANI340
    NN=NN+1                                             MEANI350
    SUMSQ(NN)=SUMSQ(NN)/FN1                             MEANI360
    NDF(NN)=ND2                                         MEANI370
    SMEAN(NN)=SUMSQ(NN)/FN2                             MEANI380
    IF(NN-LL) 345, 370, 370                             MEANI390
345 DO 360 I=1,K                                        MEANI400
    IF(MSTEP(I)) 347, 350, 347                          MEANI410
347 MSTEP(I)=0                                          MEANI420
    GO TO 360                                           MEANI430
350 MSTEP(I)=1                                          MEANI440
    GO TO 320                                           MEANI450
360 CONTINUE                                            MEANI460
370 RETURN                                              MEANI470
    END                                                 MEANI480
```

Discriminant Analysis

In the Scientific Subroutine Package, discriminant analysis is normally performed by calling the following three subroutines in sequence:

1. DMATX - to compute means of variables in each group and a pooled dispersion matrix
2. MINV - to invert the pooled dispersion matrix
3. DISCR - to compute coefficients of discriminant functions and evaluate the functions for each observation (individual)

Subroutine DMATX

This subroutine calculates means of variables in each group and a pooled dispersion matrix for the set of groups in a discriminant analysis.

For each group k = 1, 2, ..., g, the subroutine calculates means and sums of cross-products of deviations from means as shown below.

Means:

$$\bar{x}_{jk} = \frac{\sum_{i=1}^{n_k} x_{ijk}}{n_k} \qquad (1)$$

where n_k = sample size in the k^{th} group

$j = 1, 2, \ldots, m$ are variables

Sum of cross-products of deviations from means:

$$S_k = \left\{ s_{j\ell}^{k} \right\} = \sum (x_{ijk} - \bar{x}_{jk})\ (x_{i\ell k} - \bar{x}_{\ell k}) \qquad (2)$$

where $j = 1, 2, \ldots, m$

$\ell = 1, 2, \ldots, m$

The pooled dispersion matrix is calculated as follows:

$$D = \frac{\sum_{k=1}^{g} S_k}{\sum_{k=1}^{g} n_k - g} \qquad (3)$$

where g = number of groups

```
C                                                                       DMAT  10
C     ...................................................................DMAT  20
C                                                                       DMAT  30
C        SUBROUTINE DMATX                                               DMAT  40
C                                                                       DMAT  50
C        PURPOSE                                                        DMAT  60
C           COMPUTE MEANS OF VARIABLES IN EACH GROUP AND A POOLED       DMAT  70
C           DISPERSION MATRIX FOR ALL THE GROUPS. NORMALLY THIS SUB-    DMAT  80
C           ROUTINE IS USED IN THE PERFORMANCE OF DISCRIMINANT ANALYSIS.DMAT  90
C                                                                       DMAT 100
C        USAGE                                                          DMAT 110
C           CALL DMATX (K,M,N,X,XBAR,D,CMEAN)                           DMAT 120
C                                                                       DMAT 130
C        DESCRIPTION OF PARAMETERS                                      DMAT 140
C           K     - NUMBER OF GROUPS                                    DMAT 150
C           M     - NUMBER OF VARIABLES (MUST BE THE SAME FOR ALL       DMAT 160
C                   GROUPS).                                            DMAT 170
C           N     - INPUT VECTOR OF LENGTH K CONTAINING SAMPLE SIZES OF DMAT 180
C                   GROUPS.                                             DMAT 190
C           X     - INPUT VECTOR CONTAINING DATA IN THE MANNER EQUIVA-  DMAT 200
C                   LENT TO A 3-DIMENSIONAL FORTRAN ARRAY, X(1,1,1),    DMAT 210
C                   X(2,1,1), X(3,1,1), ETC.  THE FIRST SUBSCRIPT IS    DMAT 220
C                   CASE NUMBER, THE SECOND SUBSCRIPT IS VARIABLE NUMBERDMAT 230
C                   AND THE THIRD SUBSCRIPT IS GROUP NUMBER.  THE       DMAT 240
C                   LENGTH OF VECTOR X IS EQUAL TO THE TOTAL NUMBER OF  DMAT 250
C                   DATA POINTS, T=M, WHERE T = N(1)+N(2)+...+N(K).     DMAT 260
C           XBAR  - OUTPUT MATRIX (M X K) CONTAINING MEANS OF VARIABLES DMAT 270
C                   IN K GROUPS.                                        DMAT 280
C           D     - OUTPUT MATRIX (M X M) CONTAINING POOLED DISPERSION. DMAT 290
C           CMEAN - WORKING VECTOR OF LENGTH M.                         DMAT 300
C                                                                       DMAT 310
C        REMARKS                                                        DMAT 320
C           THE NUMBER OF VARIABLES MUST BE GREATER THAN OR EQUAL TO    DMAT 330
C           THE NUMBER OF GROUPS.                                       DMAT 340
C                                                                       DMAT 350
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DMAT 360
C           NONE                                                        DMAT 370
C                                                                       DMAT 380
C        METHOD                                                         DMAT 390
C           REFER TO 'BMD COMPUTER PROGRAMS MANUAL', EDITED BY W. J.    DMAT 400
C           DIXON, UCLA, 1964, AND T. W. ANDERSON, 'INTRODUCTION TO     DMAT 410
C           MULTIVARIATE STATISTICAL ANALYSIS', JOHN WILEY AND SONS,    DMAT 420
C           1958, SECTION 6.6-6.8.                                      DMAT 430
C                                                                       DMAT 440
C     ...................................................................DMAT 450
C                                                                       DMAT 460
      SUBROUTINE DMATX (K,M,N,X,XBAR,D,CMEAN)                           DMAT 470
      DIMENSION N(1),X(1),XBAR(1),D(1),CMEAN(1)                         DMAT 480
C                                                                       DMAT 490
C     ...................................................................DMAT 500
C                                                                       DMAT 510
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  DMAT 520
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      DMAT 530
C        STATEMENT WHICH FOLLOWS.                                       DMAT 540
C                                                                       DMAT 550
C     DOUBLE PRECISION XBAR,D,CMEAN                                     DMAT 560
C                                                                       DMAT 570
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    DMAT 580
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      DMAT 590
C        ROUTINE.                                                       DMAT 600
C                                                                       DMAT 610
C     ...................................................................DMAT 620
C                                                                       DMAT 630
C     INITIALIZATION                                                    DMAT 640
C                                                                       DMAT 650
      MM=M*M                                                            DMAT 660
      DO 100 I=1,MM                                                     DMAT 670
  100 D(I)=0.0                                                          DMAT 680
C                                                                       DMAT 690
C     CALCULATE MEANS                                                   DMAT 700
C                                                                       DMAT 710
      N4=0                                                              DMAT 720
      L=0                                                               DMAT 730
      LM=0                                                              DMAT 740
      DO 160 NG=1,K                                                     DMAT 750
      N1=N(NG)                                                          DMAT 760
      FN=N1                                                             DMAT 770
      DO 130 J=1,M                                                      DMAT 780
      LM=LM+1                                                           DMAT 790
      XBAR(LM)=0.0                                                      DMAT 800
      DO 120 I=1,N1                                                     DMAT 810
      L=L+1                                                             DMAT 820
  120 XBAR(LM)=XBAR(LM)+X(L)                                            DMAT 830
  130 XBAR(LM)=XBAR(LM)/FN                                              DMAT 840
C                                                                       DMAT 850
C     CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS                    DMAT 860
C                                                                       DMAT 870
      LMEAN=LM-M                                                        DMAT 880
      DO 150 I=1,N1                                                     DMAT 890
      LL=N4+I-N1                                                        DMAT 900
      DO 140 J=1,M                                                      DMAT 910
      LL=LL+N1                                                          DMAT 920
      N2=LMEAN+J                                                        DMAT 930
  140 CMEAN(J)=X(LL)-XBAR(N2)                                           DMAT 940
      LL=0                                                              DMAT 950
      DO 150 JJ=1,M                                                     DMAT 960
      DO 150 J=1,M                                                      DMAT 970
      LL=LL+1                                                           DMAT 980
  150 D(LL)=D(LL)+CMEAN(J)*CMEAN(JJ)                                    DMAT 990
  160 N4=N4+N1*M                                                        DMAT1000
C                                                                       DMAT1010
C     CALCULATE THE POOLED DISPERSION MATRIX                            DMAT1020
C                                                                       DMAT1030
      LL=-K                                                             DMAT1040
      DO 170 I=1,K                                                      DMAT1050
  170 LL=LL+N(I)                                                        DMAT1060
      FN=LL                                                             DMAT1070
      DO 180 I=1,MM                                                     DMAT1080
  180 D(I)=D(I)/FN                                                      DMAT1090
C                                                                       DMAT1100
      RETURN                                                            DMAT1110
      END                                                               DMAT1120
```

Subroutine DISCR

This subroutine performs a discriminant analysis by calculating a set of linear functions that serve as indices for classifying an individual into one of K groups.

For all groups combined, the following are obtained.

Common means:

$$\bar{X}_j = \frac{\sum_{k=1}^{g} n_k \bar{x}_{jk}}{\sum_{k=1}^{g} n_k} \qquad (1)$$

where g = number of groups

j = 1, 2, ..., m are variables

n_k = sample size in the k^{th} group

$\bar{x}_{jk}$ = mean of j^{th} variable in k^{th} group

Generalized Mahalanobis D^2 statistics, V:

$$V = \sum_{i=1}^{m} \sum_{j=1}^{m} d_{ij} \sum_{k=1}^{g} n_k (\bar{x}_{ik} - \bar{X}_i)(\bar{x}_{jk} - \bar{X}_j) \qquad (2)$$

where d_{ij} = the inverse element of the pooled dispersion matrix D

V can be used as chi-square (under assumption of normality) with m(g-1) degrees of freedom, to test the hypothesis that the mean values are the same in all the g groups for these m variables. For each discriminant function $k_* = 1, 2, \ldots, g$, the following statistics are calculated.

Coefficients:

$$C_{ik*} = \sum_{j=1}^{m} d_{ij} \bar{x}_{jk} \qquad (3)$$

where $i = 1, 2, \ldots, m$

$k = k*$

Constant:

$$C_{ok*} = -1/2 \sum_{j=1}^{m} \sum_{l=1}^{m} d_{jl} \bar{x}_{jk} \bar{x}_{lk} \qquad (4)$$

For each i^{th} case in each k^{th} group, the following calculations are performed.

Discriminant functions:

$$f_{k*} = \sum_{j=1}^{m} C_{jk} x_{ijk} + C_{ok*} \qquad (5)$$

where $k* = 1, 2, \ldots, g$

Probability associated with largest discriminant function:

$$P_L = \frac{1}{\sum_{k*=1}^{g} e^{(f_{k*} - f_L)}} \qquad (6)$$

where f_L = the value of the largest discriminant function

L = the subscript of the largest discriminant function

```
C
C
C     ..................................................................DISC  10
C                                                                       DISC  20
C       SUBROUTINE DISCR                                                DISC  30
C                                                                       DISC  40
C       PURPOSE                                                         DISC  50
C          COMPUTE A SET OF LINEAR FUNCTIONS WHICH SERVE AS INDICES     DISC  60
C          FOR CLASSIFYING AN INDIVIDUAL INTO ONE OF SEVERAL GROUPS.    DISC  70
C          NORMALLY THIS SUBROUTINE IS USED IN THE PERFORMANCE OF       DISC  80
C          DISCRIMINANT ANALYSIS.                                       DISC  90
C                                                                       DISC 100
C       USAGE                                                           DISC 110
C          CALL DISCR (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG)                   DISC 120
C                                                                       DISC 130
C       DESCRIPTION OF PARAMETERS                                       DISC 140
C          K     - NUMBER OF GROUPS. K MUST BE GREATER THAN ONE.        DISC 150
C          M     - NUMBER OF VARIABLES                                  DISC 160
C          N     - INPUT VECTOR OF LENGTH K CONTAINING SAMPLE SIZES OF  DISC 170
C                  GROUPS.                                              DISC 180
C          X     - INPUT VECTOR CONTAINING DATA IN THE MANNER EQUIVA-   DISC 190
C                  LENT TO A 3-DIMENSIONAL FORTRAN ARRAY, X(1,1,1),     DISC 200
C                  X(2,1,1), X(3,1,1), ETC.  THE FIRST SUBSCRIPT IS     DISC 210
C                  CASE NUMBER, THE SECOND SUBSCRIPT IS VARIABLE NUMBER DISC 220
C                  AND THE THIRD SUBSCRIPT IS GROUP NUMBER.  THE        DISC 230
C                  LENGTH OF VECTOR X IS EQUAL TO THE TOTAL NUMBER OF   DISC 240
C                  DATA POINTS, T*M, WHERE T = N(1)+N(2)+...+N(K).      DISC 250
C          XBAR  - INPUT MATRIX (M X K) CONTAINING MEANS OF M VARIABLES DISC 260
C                  IN K GROUPS                                          DISC 270
C          D     - INPUT MATRIX (M X M) CONTAINING THE INVERSE OF       DISC 280
C                  POOLED DISPERSION MATRIX.                            DISC 290
C          CMEAN - OUTPUT VECTOR OF LENGTH M CONTAINING COMMON MEANS.   DISC 300
C          V     - OUTPUT VARIABLE CONTAINING GENERALIZED MAHALANOBIS   DISC 310
C                  D-SQUARE.                                            DISC 320
C          C     - OUTPUT MATRIX (M+1 X K) CONTAINING THE COEFFICIENTS  DISC 330
C                  OF DISCRIMINANT FUNCTIONS.  THE FIRST POSITION OF    DISC 340
C                  EACH COLUMN (FUNCTION) CONTAINS THE VALUE OF THE     DISC 350
C                  CONSTANT FOR THAT FUNCTION.                          DISC 360
C          P     - OUTPUT VECTOR CONTAINING THE PROBABILITY ASSOCIATED  DISC 370
C                  WITH THE LARGEST DISCRIMINANT FUNCTIONS OF ALL CASES DISC 380
C                  IN ALL GROUPS.  CALCULATED RESULTS ARE STORED IN THE DISC 390
C                  MANNER EQUIVALENT TO A 2-DIMENSIONAL AREA (THE       DISC 400
C                  FIRST SUBSCRIPT IS CASE NUMBER, AND THE SECOND       DISC 410
C                  SUBSCRIPT IS GROUP NUMBER).  VECTOR P HAS LENGTH     DISC 420
C                  EQUAL TO THE TOTAL NUMBER OF CASES, T (T = N(1)+N(2) DISC 430
C                  +...+N(K)).                                          DISC 440
C          LG    - OUTPUT VECTOR CONTAINING THE SUBSCRIPTS OF THE       DISC 450
C                  LARGEST DISCRIMINANT FUNCTIONS STORED IN VECTOR P.    DISC 460
C                  THE LENGTH OF VECTOR LG IS THE SAME AS THE LENGTH    DISC 470
C                  OF VECTOR P.                                         DISC 480
C                                                                       DISC 490
C       REMARKS                                                         DISC 500
C          THE NUMBER OF VARIABLES MUST BE GREATER THAN OR EQUAL TO     DISC 510
C          THE NUMBER OF GROUPS.                                        DISC 520
C                                                                       DISC 530
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DISC 540
C          NONE                                                         DISC 550
C                                                                       DISC 560
C       METHOD                                                          DISC 570
C          REFER TO *BMD COMPUTER PROGRAMS MANUAL*, EDITED BY W. J.     DISC 580
C          DIXON, UCLA, 1964, AND T. W. ANDERSON, *INTRODUCTION TO      DISC 590
C          MULTIVARIATE STATISTICAL ANALYSIS*, JOHN WILEY AND SONS,     DISC 600
C          1958, SECTION 6.6-6.6.                                       DISC 610
C                                                                       DISC 620
C     ..................................................................DISC 630
C                                                                       DISC 640
      SUBROUTINE DISCR (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG)                  DISC 650
      DIMENSION N(1),X(1),XBAR(1),D(1),CMEAN(1),C(1),P(1),LG(1)         DISC 660
C                                                                       DISC 670
C     ..................................................................DISC 680
C                                                                       DISC 690
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  DISC 700
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      DISC 710
C        STATEMENT WHICH FOLLOWS.                                       DISC 720
C                                                                       DISC 730
C     DOUBLE PRECISION XBAR,D,CMEAN,V,C,SUM,P,PL                        DISC 740
C                                                                       DISC 750
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    DISC 760
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      DISC 770
C        ROUTINE.                                                       DISC 780
C                                                                       DISC 790
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      DISC 800
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  EXP IN STATEMENT  DISC 810
C        250 MUST BE CHANGED TO DEXP.                                   DISC 820
C                                                                       DISC 830
C     ..................................................................DISC 840
C                                                                       DISC 850
C     CALCULATE COMMON MEANS                                            DISC 860
C                                                                       DISC 870
      N1=N(1)                                                           DISC 880
      DO 100 I=2,K                                                      DISC 890
  100 N1=N1+N(I)                                                        DISC 900
      ENT=N1                                                            DISC 910
      DO 110 I=1,K                                                      DISC 920
  110 P(I)=N(I)                                                         DISC 930
      DO 130 I=1,M                                                      DISC 940
      CMEAN(I)=0                                                        DISC 950
      N1=I-M                                                            DISC 960
      DO 120 J=1,K                                                      DISC 970
      N1=N1+M                                                           DISC 980
  120 CMEAN(I)=CMEAN(I)+P(J)*XBAR(N1)                                   DISC 990
  130 CMEAN(I)=CMEAN(I)/ENT                                             DISC1000
C                                                                       DISC1010
C     CALCULATE GENERALIZED MAHALANOBIS D SQUARE                        DISC1020
C                                                                       DISC1030
      L=0                                                               DISC1040
      DO 140 I=1,K                                                      DISC1050
      DO 140 J=1,M                                                      DISC1060
      L=L+1                                                             DISC1070
  140 C(L)=XBAR(L)-CMEAN(J)                                             DISC1080
      V=0.0                                                             DISC1090
      L=0                                                               DISC1100
      DO 160 J=1,M                                                      DISC1110
      DO 160 I=1,M                                                      DISC1120
      N1=I-M                                                            DISC1130
      N2=J-M                                                            DISC1140
      SUM=0.0                                                           DISC1150
      DO 150 IJ=1,K                                                     DISC1160
      N1=N1+M                                                           DISC1170
      N2=N2+M                                                           DISC1180
  150 SUM=SUM+P(IJ)*C(N1)*C(N2)                                         DISC1190
      L=L+1                                                             DISC1200
  160 V=V+D(L)*SUM                                                      DISC1210
C                                                                       DISC1220
C     CALCULATE THE COEFFICIENTS OF DISCRIMINANT FUNCTIONS              DISC1230
C                                                                       DISC1240
      N2=0                                                              DISC1250
      DO 190 KA=1,K                                                     DISC1260
      DO 170 I=1,M                                                      DISC1270
      N2=N2+1                                                           DISC1280
  170 P(I)=XBAR(N2)                                                     DISC1290
      IQ=(M+1)*(KA-1)+1                                                 DISC1300
      SUM=0.0                                                           DISC1310
      DO 180 J=1,M                                                      DISC1320
      N1=J-M                                                            DISC1330
      DO 180 L=1,M                                                      DISC1340
      N1=N1+M                                                           DISC1350
  180 SUM=SUM+D(N1)*P(J)*P(L)                                           DISC1360
      C(IQ)=-(SUM/2.0)                                                  DISC1370
      DO 190 I=1,M                                                      DISC1380
      N1=I-M                                                            DISC1390
      IQ=IQ+1                                                           DISC1400
      C(IQ)=0.0                                                         DISC1410
      DO 190 J=1,M                                                      DISC1420
      N1=N1+M                                                           DISC1430
  190 C(IQ)=C(IQ)+D(N1)*P(J)                                            DISC1440
C                                                                       DISC1450
C     FOR EACH CASE IN EACH GROUP, CALCULATE..                          DISC1460
C                                                                       DISC1470
C        DISCRIMINANT FUNCTIONS                                         DISC1480
C                                                                       DISC1490
      LBASE=0                                                           DISC1500
      N1=0                                                              DISC1510
      DO 270 KG=1,K                                                     DISC1520
      NN=N(KG)                                                          DISC1530
      DO 260 I=1,NN                                                     DISC1540
      L=I-NN+LBASE                                                      DISC1550
      DO 200 J=1,M                                                      DISC1560
      L=L+NN                                                            DISC1570
  200 D(J)=X(L)                                                         DISC1580
      N2=0                                                              DISC1590
      DO 220 KA=1,K                                                     DISC1600
      A2=N2+1                                                           DISC1610
      SUM=C(N2)                                                         DISC1620
      DO 210 J=1,M                                                      DISC1630
      N2=N2+1                                                           DISC1640
  210 SUM=SUM+C(N2)*D(J)                                                DISC1650
  220 XBAR(KA)=SUM                                                      DISC1660
C                                                                       DISC1670
C        THE LARGEST DISCRIMINANT FUNCTION                              DISC1680
C                                                                       DISC1690
      L=1                                                               DISC1700
      SUM=XBAR(1)                                                       DISC1710
      DO 240 J=2,K                                                      DISC1720
      IF(SUM-XBAR(J)) 230, 240, 240                                     DISC1730
  230 L=J                                                               DISC1740
      SUM=XBAR(J)                                                       DISC1750
  240 CONTINUE                                                          DISC1760
C                                                                       DISC1770
C        PROBABILITY ASSOCIATED WITH THE LARGEST DISCRIMINANT FUNCTION  DISC1780
C                                                                       DISC1790
      PL=0.0                                                            DISC1800
      DO 250 J=1,K                                                      DISC1810
  250 PL=PL+ EXP(XBAR(J)-SUM)                                           DISC1820
      N1=N1+1                                                           DISC1830
      LG(N1)=L                                                          DISC1840
  260 P(N1)=1.0/PL                                                      DISC1850
  270 LBASE=LBASE+NN                                                    DISC1860
C                                                                       DISC1870
      RETURN                                                            DISC1880
      END                                                               DISC1890
                                                                        DISC1900
```

Factor Analysis (see Eigenanalysis)

In the Scientific Subroutine Package, factor analysis is normally performed by calling the following five subroutines in sequence:

1. CORRE - to find means, standard deviations, and correlation matrix
2. EIGEN - to compute eigenvalues and associated eigenvectors of the correlation matrix
3. TRACE - to select the eigenvalues that are greater than or equal to the control value specified by the user
4. LOAD - to compute a factor matrix
5. VARMX - to perform varimax rotation of the factor matrix

The subroutine CORRE works in either of two ways: (1) it expects all observations in core, or (2) it triggers a user-provided input subroutine, DATA, to read one observation at a time into a work area. In either case, the user must provide a subroutine named DATA (see "Subroutines Required" in the comment cards designation of subroutine CORRE).

Subroutine TRACE

This subroutine finds k, the number of eigenvalues that are greater than or equal to the value of a specified constant. The given eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_m$ must be arranged in descending order.

Cumulative percentages for these k eigenvalues are:

$$d_j = \sum_{i=1}^{j} \frac{\lambda_i}{m} \qquad (1)$$

where $j = 1, 2, \ldots, k$

m = number of eigenvalues (or variables)

$k \leq m$

```
C                                                                       TRAC  10
C     ...................................................................TRAC  20
C                                                                       TRAC  30
C        SUBROUTINE TRACE                                               TRAC  40
C                                                                       TRAC  50
C        PURPOSE                                                        TRAC  60
C           COMPUTE CUMULATIVE PERCENTAGE OF EIGENVALUES GREATER THAN   TRAC  70
C           OR EQUAL TO A CONSTANT SPECIFIED BY THE USER.  THIS SUB-    TRAC  80
C           ROUTINE NORMALLY OCCURS IN A SEQUENCE OF CALLS TO SUB-      TRAC  90
C           ROUTINES CORRE, EIGEN, TRACE, LOAD, AND VARMX IN THE PER-   TRAC 100
C           FORMANCE OF A FACTOR ANALYSIS.                              TRAC 110
C                                                                       TRAC 120
C        USAGE                                                          TRAC 130
C           CALL TRACE (M,R,CCR,K,C)                                    TRAC 140
C                                                                       TRAC 150
C        DESCRIPTION OF PARAMETERS                                      TRAC 160
C           M     - NUMBER OF VARIABLES. M MUST BE > OR = TO 1          TRAC 170
C           R     - INPUT MATRIX (SYMMETRIC AND STORED IN COMPRESSED    TRAC 180
C                   FORM WITH ONLY LOWER TRIANGLE BY COLUMN IN CORE)    TRAC 190
C                   CONTAINING EIGENVALUES IN DIAGONAL.  EIGENVALUES ARETRAC 200
C                   ARRANGED IN DESCENDING ORDER.  THE ORDER OF MATRIX RTRAC 210
C                   IS M BY M.  ONLY M*(M+1)/2 ELEMENTS ARE IN STORAGE. TRAC 220
C                   (STORAGE MODE OF 1)                                 TRAC 230
C           CCR   - A CONSTANT USED TO DECIDE HOW MANY EIGENVALUES TO   TRAC 240
C                   RETAIN.  CUMULATIVE PERCENTAGE OF EIGENVALUES       TRAC 250
C                   WHICH ARE GREATER THAN OR EQUAL TO THIS VALUE IS    TRAC 260
C                   CALCULATED.                                         TRAC 270
C           K     - OUTPUT VARIABLE CONTAINING THE NUMBER OF EIGENVALUESTRAC 280
C                   GREATER THAN OR EQUAL TO CCR.  (K IS THE NUMBER OF  TRAC 290
C                   FACTORS.)                                           TRAC 300
C           C     - OUTPUT VECTOR OF LENGTH M CONTAINING CUMULATIVE     TRAC 310
C                   PERCENTAGE OF EIGENVALUES WHICH ARE GREATER THAN    TRAC 320
C                   OR EQUAL TO CCR.                                    TRAC 330
C                                                                       TRAC 340
C        REMARKS                                                        TRAC 350
C           NONE                                                        TRAC 360
C                                                                       TRAC 370
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TRAC 380
C           NONE                                                        TRAC 390
C                                                                       TRAC 400
C        METHOD                                                         TRAC 410
C           EACH EIGENVALUE GREATER THAN OR EQUAL TO CCR IS DIVIDED BY MTRAC 420
C           AND THE RESULT IS ADDED TO THE PREVIOUS TOTAL TO OBTAIN     TRAC 430
C           THE CUMULATIVE PERCENTAGE FOR EACH EIGENVALUE.              TRAC 440
C                                                                       TRAC 450
C     ...................................................................TRAC 460
C                                                                       TRAC 470
      SUBROUTINE TRACE (M,R,CCR,K,C)                                    TRAC 480
      DIMENSION R(1),C(1)                                               TRAC 490
C     ...................................................................TRAC 500
C                                                                       TRAC 510
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  TRAC 520
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      TRAC 530
C        STATEMENT WHICH FOLLOWS.                                       TRAC 540
C                                                                       TRAC 550
C     DOUBLE PRECISION R,C                                              TRAC 560
C                                                                       TRAC 570
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    TRAC 580
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      TRAC 590
C        ROUTINE.                                                       TRAC 600
C                                                                       TRAC 610
C     ...................................................................TRAC 620
C                                                                       TRAC 630
      FM=M                                                              TRAC 640
      L=0                                                               TRAC 650
      DO 100 I=1,M                                                      TRAC 660
      L=L+I                                                             TRAC 670
  100 C(I)=R(L)                                                         TRAC 680
      K=0                                                               TRAC 690
C                                                                       TRAC 700
C     TEST WHETHER I-TH EIGENVALUE IS GREATER                           TRAC 710
C     THAN OR EQUAL TO THE CONSTANT                                     TRAC 720
C                                                                       TRAC 730
      DO 110 I=1,M                                                      TRAC 740
      IF(C(I)-CCR) 120, 105, 105                                        TRAC 750
  105 K=K+1                                                             TRAC 760
  110 C(I)=C(I)/FM                                                      TRAC 770
C                                                                       TRAC 780
C     COMPUTE CUMULATIVE PERCENTAGE OF EIGENVALUES                      TRAC 790
C                                                                       TRAC 800
  120 DO 130 I=2,M                                                      TRAC 810
  130 C(I)=C(I)+C(I-1)                                                  TRAC 820
      RETURN                                                            TRAC 830
      END                                                               TRAC 840
```

Subroutine LOAD

This subroutine calculates the coefficients of each factor by multiplying the elements of each normalized eigenvector by the square root of the corresponding eigenvalue.

$$a_{ij} = v_{ij} \cdot \sqrt{\lambda_j} \qquad (1)$$

where i = 1, 2, ..., m are variables

j = 1, 2, ..., k are eigenvalues retained (see the subroutine TRACE)

k ≤ m

```
C                                                                       LOAD  10
C     ...................................................................LOAD  20
C                                                                       LOAD  30
C        SUBROUTINE LOAD                                                LOAD  40
C                                                                       LOAD  50
C        PURPOSE                                                        LOAD  60
C           COMPUTE A FACTOR MATRIX (LOADING) FROM EIGENVALUES AND      LOAD  70
C           ASSOCIATED EIGENVECTORS.  THIS SUBROUTINE NORMALLY OCCURS   LOAD  80
C           IN A SEQUENCE OF CALLS TO SUBROUTINES CORRE, EIGEN, TRACE,  LOAD  90
C           LOAD, AND VARMX IN THE PERFORMANCE OF A FACTOR ANALYSIS.    LOAD 100
C                                                                       LOAD 110
C        USAGE                                                          LOAD 120
C           CALL LOAD (M,K,R,V)                                         LOAD 130
C                                                                       LOAD 140
C        DESCRIPTION OF PARAMETERS                                      LOAD 150
C           M      - NUMBER OF VARIABLES.                               LOAD 160
C           K      - NUMBER OF FACTORS. K MUST BE GREATER THAN OR EQUAL LOAD 170
C                    TO 1 AND LESS THAN OR EQUAL TO M.                  LOAD 171
C           R      - A MATRIX (SYMMETRIC AND STORED IN COMPRESSED FORM  LOAD 180
C                    WITH ONLY UPPER TRIANGLE BY COLUMN IN CORE) CON-   LOAD 190
C                    TAINING EIGENVALUES IN DIAGONAL.  EIGENVALUES ARE  LOAD 200
C                    ARRANGED IN DESCENDING ORDER, AND FIRST K          LOAD 210
C                    EIGENVALUES ARE USED BY THIS SUBROUTINE.  THE ORDER LOAD 220
C                    OF MATRIX R IS M BY M.  ONLY M*(M+1)/2 ELEMENTS ARE LOAD 230
C                    IN STORAGE.  (STORAGE MODE OF 1)                   LOAD 240
C           V      - WHEN THIS SUBROUTINE IS CALLED, MATRIX V (M X M)   LOAD 250
C                    CONTAINS EIGENVECTORS COLUMNWISE.  UPON RETURNING TOLOAD 260
C                    THE CALLING PROGRAM, MATRIX V CONTAINS A FACTOR    LOAD 270
C                    MATRIX (M X K).                                    LOAD 280
C                                                                       LOAD 290
C        REMARKS                                                        LOAD 300
C           NONE                                                        LOAD 310
C                                                                       LOAD 320
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  LOAD 330
C           NONE                                                        LOAD 340
C                                                                       LOAD 350
C        METHOD                                                         LOAD 360
C           NORMALIZED EIGENVECTORS ARE CONVERTED TO THE FACTOR PATTERN LOAD 370
C           BY MULTIPLYING THE ELEMENTS OF EACH VECTOR BY THE SQUARE    LOAD 380
C           ROOT OF THE CORRESPONDING EIGENVALUE.                       LOAD 390
C                                                                       LOAD 400
C     ...................................................................LOAD 410
C                                                                       LOAD 420
      SUBROUTINE LOAD (M,K,R,V)                                         LOAD 430
      DIMENSION R(1),V(1)                                               LOAD 440
C                                                                       LOAD 450
C     ...................................................................LOAD 460
C                                                                       LOAD 470
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  LOAD 480
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      LOAD 490
C        STATEMENT WHICH FOLLOWS.                                       LOAD 500
C                                                                       LOAD 510
C     DOUBLE PRECISION R,V,SC                                           LOAD 520
C                                                                       LOAD 530
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    LOAD 540
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      LOAD 550
C        ROUTINE.                                                       LOAD 560
C                                                                       LOAD 570
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      LOAD 580
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENT LOAD 590
C        150 MUST BE CHANGED TO DSQRT.                                  LOAD 600
C                                                                       LOAD 610
C     ...................................................................LOAD 620
C                                                                       LOAD 630
      L=0                                                               LOAD 640
      JJ=0                                                              LOAD 650
      DO 160 J=1,K                                                      LOAD 660
      JJ=JJ+J                                                           LOAD 670
  150 SC= SQRT(R(JJ))                                                   LOAD 680
      DO 160 I=1,M                                                      LOAD 690
      L=L+1                                                             LOAD 700
  160 V(L)=SC*V(L)                                                      LOAD 710
      RETURN                                                            LOAD 720
      END                                                               LOAD 730
```

Subroutine VARMX

This subroutine performs orthogonal rotations on an m by k factor matrix such that:

$$\sum_j \left\{ m \sum_i \left(a_{ij}^2 / h_i^2 \right)^2 - \left[\sum_i \left(a_{ij}^2 / h_i^2 \right) \right]^2 \right\} \qquad (1)$$

is a maximum, where i = 1, 2, ..., m are variables, j = 1, 2, ..., k are factors, a_{ij} is the loading for the i^{th} variable on the j^{th} factor, and h_i^2 is the communality of the i^{th} variable defined below.

Communalities:

$$h_i^2 = \sum_{j=1}^{k} a_{ij}^2 \qquad (2)$$

where i = 1, 2, ..., m

Normalized factor matrix:

$$b_{ij} = a_{ij} / \sqrt{h_i^2} \qquad (3)$$

where i = 1, 2, ..., m

j = 1, 2, ..., k

Variance for factor matrix:

$$V_c = \sum_j \left\{ \left[m \sum_i \left(b_{ij}^2 \right)^2 - \left(\sum_i b_{ij}^2 \right)^2 \right] / m^2 \right\} \qquad (4)$$

where c = 1, 2, ... (iteration cycle)

Convergence test:

$$\text{If } V_c - V_{c-1} \leq 10^{-7} \qquad (5)$$

four successive times, the program stops rotation and performs the equation (28). Otherwise, the program repeats rotation of factors until the convergence test is satisfied.

Rotation of two factors:

The subroutine rotates two normalized factors (b_{ij}) at a time. 1 with 2, 1 with 3, ..., 1 with k, 2 with 3, ..., 2 with k, ..., k - 1 with k. This constitutes one iteration cycle.

Assuming that x and y are factors to be rotated, where x is the lower-numbered or left-hand factor, the following notation for rotating these two factors is used:

$$\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ . & . \\ . & . \\ . & . \\ x_m & y_m \end{bmatrix} \cdot \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} = \begin{bmatrix} X_1 & Y_1 \\ X_2 & Y_2 \\ . & . \\ . & . \\ . & . \\ X_m & Y_m \end{bmatrix} \quad (6)$$

where x_i and y_i are presently available normalized loadings, and X_i and Y_i, the desired normalized loadings, are functions of ϕ, the angle of rotation. The computational steps are (a) through (e) below.

(a) Calculation of NUM and DEN:

$$A = \sum_i (x_i + y_i)\ (x_i - y_i)$$

$$B = 2 \sum_i x_i\, y_i$$

$$C = \sum_i \left[(x_i+y_i)\ (x_i-y_i) + 2x_i\, y_i \right] \left[(x_i + y_i)\ (x_i - y_i) - 2x_i\, y_i \right]$$

$$D = 4 \sum_i (x_i + y_i)\ (x_i - y_i)\ x_i\, y_i \quad (7)$$

$$NUM = D - 2AB/m$$

$$DEN = C - [\,(A + B)\ (A - B)\,]/m$$

(b) Comparison of NUM and DEN:

The following four cases may arise.

NUM < DEN, go to (b1) below

NUM > DEN, go to (b2) below

(NUM + DEN) $\geq \epsilon$*, go to (b3) below

(NUM + DEN) $< \epsilon$, skip to the next rotation

* ϵ is a small tolerance factor.

(b1) $$\tan 4\theta = |NUM|/|DEN| \quad (8)$$

If $\tan 4\theta < \epsilon$ and

(i) DEN is positive, skip to the next rotation.

(ii) DEN is negative, set $\cos\phi = \sin\phi = (\sqrt{2})/2$ and go to (e) below.

If $\tan 4\theta \geq \epsilon$, calculate:

$$\cos 4\theta = 1/\sqrt{1 + \tan^2 4\theta} \quad (9)$$

$$\sin 4\theta = \tan 4\theta \cdot \cos 4\theta \quad (10)$$

and go to (c) below.

(b2) $$\text{ctn}\,4\theta = |NUM|/|DEN| \quad (11)$$

If $\text{ctn}4\theta < \epsilon$, set $\cos 4\theta = 0$ and $\sin 4\theta = 1$. Go to (c) below.

If $\text{ctn}4\theta \geq \epsilon$, calculate:

$$\sin 4\theta = 1/\sqrt{1 + \text{ctn}^2 4\theta} \quad (12)$$

$$\cos 4\theta = \text{ctn}4\theta \cdot \sin 4\theta \quad (13)$$

and go to (c) below.

(b3) Set $\cos 4\theta = \sin 4\theta = (\sqrt{2})/2$ and go to (c) below.

(c) Determining $\cos\theta$ and $\sin\theta$:

$$\cos 2\theta = \sqrt{(1 + \cos 4\theta)/2} \quad (14)$$

$$\sin 2\theta = \sin 4\theta / 2\cos 2\theta \quad (15)$$

$$\cos\theta = \sqrt{(1 + \cos 2\theta)/2} \quad (16)$$

$$\sin\theta = \sin 2\theta / 2\cos\theta \quad (17)$$

(d) Determining $\cos\phi$ and $\sin\phi$:

(d1) If DEN is positive, set

$$\cos\phi = \cos\theta \quad (18)$$

$$\sin\phi = \sin\theta \quad (19)$$

and go to (d2) below.

If DEN is negative, calculate

$$\cos\phi = \frac{\sqrt{2}}{2}\cos\theta + \frac{\sqrt{2}}{2}\sin\theta \quad (20)$$

$$\sin\phi = \left| \frac{\sqrt{2}}{2} \cos\theta - \frac{\sqrt{2}}{2} \sin\theta \right| \quad (21)$$

and go to (d2) below.

(d2) If NUM is positive, set

$$\cos\phi = |\cos\phi| \quad (22)$$

$$\sin\phi = |\sin\phi| \quad (23)$$

and go to (e) below.

If NUM is negative, set

$$\cos\phi = |\cos\phi| \quad (24)$$

$$\sin\phi = -|\sin\phi| \quad (25)$$

(e) Rotation:

$$X_i = x_i \cos\phi + y_i \sin\phi \quad (26)$$

$$Y_i = x_i \sin\phi + y_i \cos\phi \quad (27)$$

where $i = 1, 2, \ldots, m$

After one cycle of $k(k-1)/2$ rotations is completed, the subroutine goes back to calculate the variance for the factor matrix by equation (4).

Denormalization:

$$a_{ij} = b_{ij} \cdot h_i \quad (28)$$

where $i = 1, 2, \ldots, m$

$j = 1, 2, \ldots, k$

Check on communalities:

Final communalities $$f_i^2 = \sum_{j=1}^{k} a_{ij}^2 \quad (29)$$

Difference $$d_i = h_i^2 - f_i^2 \quad (30)$$

where $i = 1, 2, \ldots, m$

```
C     ..................................................................VARM  10
C                                                                       VARM  20
C        SUBROUTINE VARMX                                               VARM  30
C                                                                       VARM  40
C        PURPOSE                                                        VARM  50
C           PERFORM ORTHOGONAL ROTATIONS OF A FACTOR MATRIX.  THIS      VARM  60
C           SUBROUTINE NORMALLY OCCURS IN A SEQUENCE OF CALLS TO SUB-   VARM  70
C           ROUTINES CORR, EIGEN, TRACE, LOAD, VARMX IN THE PERFORMANCE VARM  80
C           OF A FACTOR ANALYSIS.                                       VARM  90
C                                                                       VARM 100
C        USAGE                                                          VARM 110
C           CALL VARMX (P,R,A,NC,TV,F,G,C,IER)                          VARM 120
C                                                                       VARM 130
C        DESCRIPTION OF PARAMETERS                                      VARM 140
C           P   - NUMBER OF VARIABLES AND NUMBER OF ROWS OF MATRIX A.   VARM 150
C           K   - NUMBER OF FACTORS.                                    VARM 160
C           A   - INPUT IS THE ORIGINAL FACTOR MATRIX, AND OUTPUT IS    VARM 170
C                 THE ROTATED FACTOR MATRIX.  THE ORDER OF MATRIX A     VARM 180
C                 IS P X K.                                             VARM 190
C           NC  - OUTPUT VARIABLE CONTAINING THE NUMBER OF ITERATION    VARM 200
C                 CYCLES PERFORMED.                                     VARM 210
C           TV  - OUTPUT VECTOR CONTAINING THE VARIANCE OF THE FACTOR   VARM 220
C                 MATRIX FOR EACH ITERATION CYCLE.  THE VARIANCE PRIOR  VARM 230
C                 TO THE FIRST ITERATION CYCLE IS ALSO CALCULATED.      VARM 240
C                 THIS MEANS THAT NC+1 VARIANCES ARE STORED IN VECTOR   VARM 250
C                 TV.  MAXIMUM NUMBER OF ITERATION CYCLES ALLOWED IN    VARM 260
C                 THIS SUBROUTINE IS 50.  THEREFORE, THE LENGTH OF      VARM 270
C                 VECTOR TV IS 51.                                      VARM 280
C           F   - OUTPUT VECTOR OF LENGTH P CONTAINING THE ORIGINAL     VARM 290
C                 COMMUNALITIES.                                        VARM 300
C           G   - OUTPUT VECTOR OF LENGTH P CONTAINING THE FINAL        VARM 310
C                 COMMUNALITIES.                                        VARM 320
C           C   - OUTPUT VECTOR OF LENGTH P CONTAINING THE DIFFERENCES  VARM 330
C                 BETWEEN THE ORIGINAL AND FINAL COMMUNALITIES.         VARM 340
C           IER - ERROR INDICATOR                                       VARM 350
C                 IER=0 - NO ERROR                                      VARM 351
C                 IER=1 - CONVERGENCE WAS NOT ACHIEVED IN 50 CYCLES     VARM 352
C                         OF ROTATION                                   VARM 353
C                                                                       VARM 354
C        REMARKS                                                        VARM 360
C           IF VARIANCE COMPUTED AFTER EACH ITERATION CYCLE DOES NOT    VARM 370
C           INCREASE FOR FOUR SUCCESSIVE TIMES, THE SUBROUTINE STOPS    VARM 380
C           ROTATION.                                                   VARM 390
C                                                                       VARM 400
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  VARM 410
C           NONE                                                        VARM 420
C                                                                       VARM 430
C        METHOD                                                         VARM 440
C           KAISER'S VARIMAX ROTATION AS DESCRIBED IN 'COMPUTER PROGRAM VARM 450
C           FOR VARIMAX ROTATION IN FACTOR ANALYSIS' BY THE SAME AUTHOR,VARM 460
C           EDUCATIONAL AND PSYCHOLOGICAL MEASUREMENT, VOL XIX, NO. 3,  VARM 470
C           1959.                                                       VARM 480
C                                                                       VARM 490
C     ..................................................................VARM 500
C                                                                       VARM 510
      SUBROUTINE VARMX (P,R,A,NC,TV,F,G,D,IER)                          VARM 520
      DIMENSION A(1),TV(1),H(1),F(1),C(1)                               VARM 530
C                                                                       VARM 540
C     ..................................................................VARM 550
C                                                                       VARM 560
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  VARM 570
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      VARM 580
C        STATEMENT WHICH FOLLOWS.                                       VARM 590
C                                                                       VARM 600
C     DOUBLE PRECISION A,TV,H,F,G,TVLT,CONS,AA,BB,CC,DD,U,T,B,COS4T,    VARM 610
C    1                 SIN4T,TAN4T,SINP,COSP,CTN4T,COS2T,SIN2T,COST,SINTVARM 620
C                                                                       VARM 630
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    VARM 640
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      VARM 650
C        ROUTINE.                                                       VARM 660
C                                                                       VARM 670
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      VARM 680
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENTSVARM 690
C        115, 290, 330, 350, AND 355 MUST BE CHANGED TO DSQRT.  ABS IN  VARM 700
C        STATEMENTS 280, 320, AND 375 MUST BE CHANGED TO DABS.          VARM 710
C                                                                       VARM 720
C     ..................................................................VARM 730
C                                                                       VARM 740
C     INITIALIZATION                                                    VARM 750
C                                                                       VARM 760
      IER=0                                                             VARM 761
      EPS=0.00116                                                       VARM 770
      TVLT=0.0                                                          VARM 780
      LL=K-1                                                            VARM 790
      NV=1                                                              VARM 800
      NC=0                                                              VARM 810
      FN=P                                                              VARM 820
      FN=FN*FN                                                          VARM 830
      CONS=0.7071068                                                    VARM 840
C                                                                       VARM 850
C     CALCULATE ORIGINAL COMMUNALITIES                                  VARM 860
C                                                                       VARM 870
      DO 110 I=1,P                                                      VARM 880
      H(I)=0.0                                                          VARM 890
      DO 110 J=1,K                                                      VARM 900
      L=P*(J-1)+I                                                       VARM 910
  110 H(I)=H(I)+A(L)*A(L)                                               VARM 920
C                                                                       VARM 930
C     CALCULATE NORMALIZED FACTOR MATRIX                                VARM 940
C                                                                       VARM 950
      DO 120 I=1,P                                                      VARM 960
  115 F(I)= SQRT(H(I))                                                  VARM 970
      DO 120 J=1,K                                                      VARM 980
      L=P*(J-1)+I                                                       VARM 990
  120 A(L)=A(L)/F(I)                                                    VARM1000
      GO TO 132                                                         VARM1010
C                                                                       VARM1020
C     CALCULATE VARIANCE FOR FACTOR MATRIX                              VARM1030
C                                                                       VARM1040
  130 NV=NV+1                                                           VARM1050
      TVLT=TV(NV-1)                                                     VARM1060
  132 TV(NV)=0.0                                                        VARM1070
      DO 150 J=1,K                                                      VARM1080
      AA=0.0                                                            VARM1090
      BB=0.0                                                            VARM1090
      LP=P*(J-1)                                                        VARM1100
      DO 140 I=1,P                                                      VARM1110
      L=LP+I                                                            VARM1120
      CC=A(L)*A(L)                                                      VARM1130
      AA=AA+CC                                                          VARM1140
  140 BB=BB+CC*CC                                                       VARM1150
  150 TV(NV)=TV(NV)+(FN*BB-AA*AA)/FN                                    VARM1160
      IF(NV-51)130,160,155                                              VARM1170
  155 IER=1                                                             VARM1180
      GO TO 430                                                         VARM1181
C                                                                       VARM1182
C     PERFORM CONVERGENCE TEST                                          VARM1190
C                                                                       VARM1200
                                                                        VARM1210
```

```
  16C IF(ETA(KK)-ETA(I)-E1.E-7)) 17C, 17C, 150
  17C KC=KC+1
      IF(KC-3) 15C, 15C, 42C
C
C     ROTATION OF THE FACTORS CONTAINED UP TO
C     THE STATEMENT 42C.
C
  15C DO 42C J=1,LL
      L1=P*(J-1)
      II=J+1
C
C        CALCULATE ALP AND GEN
C
      DO 42C K1=II,K
      L2=P*(K1-1)
      AA=C.C
      BB=C.C
      CC=C.C
      DD=C.C
      DO 23C I=1,P
      L3=L1+I
      L4=L2+I
      C=(A(L3)+A(L4))*(A(L3)-A(L4))
      T=A(L3)*A(L4)
      T=T+T
      CC=CC+(L+1)*(L-T)
      DD=DD+2.C*L*T
      AA=AA+C
  23C BB=BB+T
      T=DD-2.C*AA*BB/FN
      B=CC-(AA*AA-BB*BB)/FN
C
C        COMPARISON OF ALP AND GEN
C
      IF(T-B) 26C, 24C, 32C
  24C IF((T+B)-EPS) 42C, 25C, 25C
C
C        ALP + GEN IS GREATER THAN OR EQUAL TO THE
C        TOLERANCE FACTOR
C
  25C CCS4T=CCNS
      SIN4T=CCNS
      GO TO 35C
C
C        ALP IS LESS THAN GEN
C
  26C TAN4T= ABS(T)/ ABS(B)
      IF(TAN4T-EPS) 3CC, 29C, 29C
  29C CCS4T=1.C/ SQRT(1.C+TAN4T*TAN4T)
      SIN4T=TAN4T*CCS4T
      GO TO 35C
  3CC IF(B) 31C, 42C, 42C
  31C SINF=CCNS
      CCSF=CCNS
      GO TO 4CC
C
C        ALP IS GREATER THAN GEN
C
  32C CTN4T= ABS(T/B)
      IF(CTN4T-EPS) 34C, 33C, 33C
  33C SIN4T=1.C/ SQRT(1.C+CTN4T*CTN4T)
      CCS4T=CTN4T*SIN4T
      GO TO 35C
  34C CCS4T=C.C
      SIN4T=1.C
C
C        DETERMINE COS THETA AND SIN THETA
C
  35C CCS2T= SQRT((1.C+CCS4T)/2.C)
      SIN2T=SIN4T/(2.C*CCS2T)
  355 CCST= SQRT((1.C+CCS2T)/2.0)
      SINT=SIN2T/(2.0*CCST)
C
C        DETERMINE COS PHI AND SIN PHI
C
      IF(B) 37C, 37C, 36C
  36C CCSF=CCST
      SINF=SINT
      GO TO 38C
  37C CCSF=CCNS*CCST+CCNS*SINT
  375 SINF= ABS(CCNS*CCST-CCNS*SINT)
  38C IF(T) 35C, 35C, 4CC
  39C SINF=-SINF
C
C        PERFORM ROTATION
C
  4CC DO 41C I=1,P
      L3=L1+I
      L4=L2+I
      AA=A(L3)*CCSF+A(L4)*SINF
      A(L4)=-A(L3)*SINF+A(L4)*COSF
  41C A(L3)=AA
  42C CONTINUE
      GO TO 13C
C
C     GENERALIZE VARIMAX LOADINGS
C
  43C DO 44C I=1,P
      DO 44C J=1,K
      L=P*(J-1)+I
  44C A(L)=A(L)*F(I)
C
C     CHECK ON COMMUNALITIES
C
      NC=NV-1
      DO 45C I=1,P
  45C F(I)=F(I)*F(I)
      DO 47C I=1,P
      F(I)=C.C
      DO 46C J=1,K
      L=P*(J-1)+I
  46C F(I)=F(I)+A(L)*A(L)
  47C C(I)=F(I)-F(I)
      RETURN
      END
```

```
VARM1220
VARM1230
VARM1240
VARM1250
VARM1260
VARM1270
VARM1280
VARM1290
VARM1300
VARM1310
VARM1320
VARM1330
VARM1340
VARM1350
VARM1360
VARM1370
VARM1380
VARM1390
VARM1400
VARM1410
VARM1420
VARM1430
VARM1440
VARM1450
VARM1460
VARM1470
VARM1480
VARM1490
VARM1500
VARM1510
VARM1520
VARM1530
VARM1540
VARM1550
VARM1560
VARM1570
VARM1580
VARM1590
VARM1600
VARM1610
VARM1620
VARM1630
VARM1640
VARM1650
VARM1660
VARM1670
VARM1680
VARM1690
VARM1700
VARM1710
VARM1720
VARM1730
VARM1740
VARM1750
VARM1760
VARM1770
VARM1780
VARM1790
VARM1800
VARM1810
VARM1820
VARM1830
VARM1840
VARM1850
VARM1860
VARM1870
VARM1880
VARM1890
VARM1900
VARM1910
VARM1920
VARM1930
VARM1940
VARM1950
VARM1960
VARM1970
VARM1980
VARM1990
VARM2000
VARM2010
VARM2020
VARM2030
VARM2040
VARM2050
VARM2060
VARM2070
VARM2080
VARM2090
VARM2100
VARM2110
VARM2120
VARM2130
VARM2140
VARM2150
VARM2160
VARM2170
VARM2180
VARM2190
VARM2200
VARM2210
VARM2220
VARM2230
VARM2240
VARM2250
VARM2260
VARM2270
VARM2280
VARM2290
VARM2300
VARM2310
VARM2320
VARM2330
VARM2340
VARM2350
VARM2360
```

Time Series (see Smoothing)

Subroutine AUTO

This subroutine calculates the autocovariances for lags 0, 1, 2, ..., (L-1), given a time series of observations A_1, A_2, ..., A_n and a number L.

$$R_j = \frac{1}{n-j+1} \sum_{i=1}^{n-j+1} (A_i - AVER)\,(A_{i+j-1} - AVER) \quad (1)$$

where $AVER = \frac{1}{n} \sum_{i=1}^{n} A_i$

n = number of observations in time series A

j = 1, 2, 3, ..., L represent time lags 0, 1, 2, ..., (L-1)

```
C     ..................................................................
C
C        SUBROUTINE AUTO
C
C        PURPOSE
C           TO FIND AUTOCOVARIANCES OF SERIES A FOR LAGS 0 TO L-1.
C
C        USAGE
C           CALL AUTO (A,N,L,R)
C
C        DESCRIPTION OF PARAMETERS
C           A    - INPUT VECTOR OF LENGTH N CONTAINING THE TIME SERIES
C                  WHOSE AUTOCOVARIANCE IS DESIRED.
C           N    - LENGTH OF THE VECTOR A.
C           L    - AUTOCOVARIANCE IS CALCULATED FOR LAGS OF 0, 1, 2,...,
C                  L-1.
C           R    - OUTPUT VECTOR OF LENGTH L CONTAINING AUTOCOVARIANCES
C                  OF SERIES A.
C
C        REMARKS
C           THE LENGTH OF R IS DIFFERENT FROM THE LENGTH OF A.  N MUST
C           BE GREATER THAN L.  IF NOT, R(1) IS SET TO ZERO AND RETURN
C           IS MADE TO THE CALLING PROGRAM.
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           DESCRIBED IN R.B. BLACKMAN AND J.W. TUKEY, 'THE MEASURMENT
C        OF POWER SPECTRA', DOVER PUBLICATIONS INC., NEW YORK, 1959.
C
C     ..................................................................
C
      SUBROUTINE AUTO (A,N,L,R)
      DIMENSION A(1),R(1)
C
C     CALCULATE AVERAGE OF TIME SERIES A
C
      AVER=C.0
      IF(N-L) 50,5C,100
   50 R(1)=0.0
      RETURN
  100 DO 110 I=1,N
  110 AVER=AVER+A(I)
      FN=N
      AVER=AVER/FN
C
C     CALCULATE AUTOCOVARIANCES
C
      DO 130 J=1,L
      NJ=N-J+1
      SUM=0.0
      DO 120 I=1,NJ
      IJ=I+J-1
  120 SUM=SUM+(A(I)-AVER)*(A(IJ)-AVER)
      FNJ=NJ
  130 R(J)=SUM/FNJ
      RETURN
      END
```

```
AUTO  10
AUTO  20
AUTO  30
AUTO  40
AUTO  50
AUTO  60
AUTO  70
AUTO  80
AUTO  90
AUTO 100
AUTO 110
AUTO 120
AUTO 130
AUTO 140
AUTO 150
AUTO 160
AUTO 170
AUTO 180
AUTO 190
AUTO 200
AUTO 210
AUTO 220
AUTO 230
AUTO 240
AUTO 250
AUTO 260
AUTO 270
AUTO 280
AUTO 290
AUTO 300
AUTO 310
AUTO 320
AUTO 330
AUTO 340
AUTO 350
AUTO 360
AUTO 370
AUTO 380
AUTO 390
AUTO 400
AUTO 410
AUTO 420
AUTO 430
AUTO 440
AUTO 450
AUTO 460
AUTO 470
AUTO 480
AUTO 490
AUTO 500
AUTO 510
AUTO 520
AUTO 530
AUTO 540
AUTO 550
AUTO 560
AUTO 570
AUTO 580
AUTO 590
AUTO 600
```

Subroutine CROSS

This subroutine calculates the cross covariances of series B lagging and leading A, given two time series $A_1, A_2, \ldots, A_n$ and $B_1, B_2, \ldots, B_n$ and given a number L.

(a) B lags A:

$$R_j = \frac{1}{n-j+1} \sum_{i=1}^{n-j+1} (A_i - \text{AVERA})\,(B_{i+j-1} - \text{AVERB}) \qquad (1)$$

(b) B leads A:

$$S_j = \frac{1}{n-j+1} \sum_{i=1}^{n-j+1} (A_{i+j-1} - \text{AVERA})\,(B_i - \text{AVERB}) \qquad (2)$$

where $$\text{AVERA} = \frac{1}{n} \sum_{i=1}^{n} A_i$$

$$\text{AVERB} = \frac{1}{n} \sum_{i=1}^{n} B_i$$

n = number of observations in each series

j = 1, 2, ..., L represent time lags (or leads) of 0, 1, 2, ..., (L-1)

```
C                                                                       CROS  10
C     ..................................................................CROS  20
C                                                                       CROS  30
C        SUBROUTINE CROSS                                               CROS  40
C                                                                       CROS  50
C        PURPOSE                                                        CROS  60
C           TO FIND THE CROSSCOVARIANCES OF SERIES A WITH SERIES B      CROS  70
C           (WHICH LEADS AND LAGS A).                                   CROS  80
C                                                                       CROS  90
C        USAGE                                                          CROS 100
C           CALL CROSS (A,B,N,L,R,S)                                    CROS 110
C                                                                       CROS 120
C        DESCRIPTION OF PARAMETERS                                      CROS 130
C           A     - INPUT VECTOR OF LENGTH N CONTAINING FIRST TIME      CROS 140
C                   SERIES.                                             CROS 150
C           B     - INPUT VECTOR OF LENGTH N CONTAINING SECOND TIME     CROS 160
C                   SERIES.                                             CROS 170
C           N     - LENGTH OF SERIES A AND B.                           CROS 180
C           L     - CROSSCOVARIANCE IS CALCULATED FOR LAGS AND LEADS OF CROS 190
C                   0, 1, 2,..., L-1.                                   CROS 200
C           R     - OUTPUT VECTOR OF LENGTH L CONTAINING CROSSCOVARI-   CROS 210
C                   ANCES OF A WITH B, WHERE B LAGS A.                  CROS 220
C           S     - OUTPUT VECTOR OF LENGTH L CONTAINING CROSSCOVARI-   CROS 230
C                   ANCES OF A WITH B, WHERE B LEADS A.                 CROS 240
C                                                                       CROS 250
C        REMARKS                                                        CROS 260
C           N MUST BE GREATER THAN L.  IF NOT, R(1) AND S(1) ARE SET TO CROS 270
C           ZERO AND RETURN IS MADE TO THE CALLING PROGRAM.             CROS 280
C                                                                       CROS 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CROS 300
C           NONE                                                        CROS 310
C                                                                       CROS 320
C        METHOD                                                         CROS 330
C           DESCRIBED IN R.B. BLACKMAN AND J.W. TUKEY, 'THE MEASURMENT  CROS 340
C        OF POWER SPECTRA', DOVER PUBLICATIONS INC., NEW YORK, 1959.    CROS 350
C                                                                       CROS 360
C     ..................................................................CROS 370
C                                                                       CROS 380
      SUBROUTINE CROSS (A,B,N,L,R,S)                                    CROS 390
      DIMENSION A(1),B(1),R(1),S(1)                                     CROS 400
C                                                                       CROS 410
C     CALCULATE AVERAGES OF SERIES A AND B                              CROS 420
C                                                                       CROS 430
      FN=N                                                              CROS 440
      AVERA=0.0                                                         CROS 450
      AVERB=0.0                                                         CROS 460
      IF(N-L)50,50,100                                                  CROS 470
   50 R(1)=0.0                                                          CROS 480
      S(1)=0.0                                                          CROS 490
      RETURN                                                            CROS 500
  100 DO 110 I=1,N                                                      CROS 510
      AVERA=AVERA+A(I)                                                  CROS 520
  110 AVERB=AVERB+B(I)                                                  CROS 530
      AVERA=AVERA/FN                                                    CROS 540
      AVERB=AVERB/FN                                                    CROS 550
C                                                                       CROS 560
C     CALCULATE CROSSCOVARIANCES OF SERIES A AND B                      CROS 570
C                                                                       CROS 580
      DO 130 J=1,L                                                      CROS 590
      NJ=N-J+1                                                          CROS 600
      SUMR=0.0                                                          CROS 610
      SUMS=0.0                                                          CROS 620
      DO 120 I=1,NJ                                                     CROS 630
      IJ=I+J-1                                                          CROS 640
      SUMR=SUMR+(A(I)-AVERA)*(B(IJ)-AVERB)                              CROS 650
  120 SUMS=SUMS+(A(IJ)-AVERA)*(B(I)-AVERB)                              CROS 660
      FNJ=NJ                                                            CROS 670
      R(J)=SUMR/FNJ                                                     CROS 680
  130 S(J)=SUMS/FNJ                                                     CROS 690
      RETURN                                                            CROS 700
      END                                                               CROS 710
```

Subroutine SMO

This subroutine calculates the smoothed or filtered series, given a time series A_1, A_2, ..., A_n, a selection integer L, and a weighting series W_1, W_2, ..., W_m.

$$R_i = \sum_{j=1}^{m} A_p \cdot W_j \qquad (1)$$

where $p = j \cdot L - L + k$

$k = i - IL + 1$

$i = IL$ to IH

$$IL = \frac{L(m-1)}{2} + 1 \qquad (2)$$

$$IH = n - \frac{L(m-1)}{2} \qquad (3)$$

L = a given selection integer. For example, L = 4 applies weights to every 4th item of the time series.

m = number of weights. Must be an odd integer. (If m is an even integer, any fraction resulting from the calculation of $\frac{L(m-1)}{2}$ in (2) and (3) above will be truncated.)

n = number of items in the time series

From IL to IH elements of the vector R are filled with the smoothed series, and other elements with zeros.

```
C                                                                       SMO  10
C     ...................................................................SMO  20
C                                                                       SMO  30
C        SUBROUTINE SMO                                                 SMO  40
C                                                                       SMO  50
C        PURPOSE                                                        SMO  60
C           TO SMOOTH OR FILTER SERIES A BY WEIGHTS W.                  SMO  70
C                                                                       SMO  80
C        USAGE                                                          SMO  90
C           CALL SMO (A,N,W,M,L,R)                                      SMO 100
C                                                                       SMO 110
C        DESCRIPTION OF PARAMETERS                                      SMO 120
C           A - INPUT VECTOR OF LENGTH N CONTAINING TIME SERIES DATA.   SMO 130
C           N - LENGTH OF SERIES A.                                     SMO 140
C           W - INPUT VECTOR OF LENGTH M CONTAINING WEIGHTS.            SMO 150
C           M - NUMBER OF ITEMS IN WEIGHT VECTOR.  M MUST BE AN ODD     SMO 160
C               INTEGER.  (IF M IS AN EVEN INTEGER, ANY FRACTION        SMO 170
C               RESULTING FROM THE CALCULATION OF (L*(M-1))/2 IN (1)    SMO 180
C               AND (2) BELOW WILL BE TRUNCATED.)                       SMO 190
C           L - SELECTION INTEGER.  FOR EXAMPLE, L=12 MEANS THAT WEIGHTSSMO 200
C               ARE APPLIED TO EVERY 12-TH ITEM OF A.  L=1 APPLIES      SMO 210
C               WEIGHTS TO SUCCESSIVE ITEMS OF A.  FOR MONTHLY DATA,    SMO 220
C               L=12 GIVES YEAR-TO-YEAR AVERAGES AND L=1 GIVES MONTH-TO-SMO 230
C               MONTH AVERAGES.                                         SMO 240
C           R - OUTPUT VECTOR OF LENGTH N.  FROM IL TO IH ELEMENTS OF   SMO 250
C               THE VECTOR R ARE FILLED WITH THE SMOOTHED SERIES AND    SMO 260
C               OTHER ELEMENTS WITH ZERO, WHERE                         SMO 270
C                    IL=(L*(M-1))/2+1  ................. (1)           SMO 280
C                    IH=N-(L*(M-1))/2  ................. (2)           SMO 290
C                                                                       SMO 300
C        REMARKS                                                        SMO 310
C           N MUST BE GREATER THAN OR EQUAL TO THE PRODUCT OF L*M.      SMO 320
C                                                                       SMO 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SMO 340
C           NONE                                                        SMO 350
C                                                                       SMO 360
C        METHOD                                                         SMO 370
C           REFER TO THE ARTICLE 'FORTRAN SUBROUTINES FOR TIME SERIES   SMO 380
C           ANALYSIS', BY J. R. HEALY AND B. P. BOGERT, COMMUNICATIONS  SMO 390
C           OF ACM, V.6, NO.1, JANUARY, 1963.                           SMO 400
C                                                                       SMO 410
C     ...................................................................SMO 420
C                                                                       SMO 430
      SUBROUTINE SMO (A,N,W,M,L,R)                                      SMO 440
      DIMENSION A(1),W(1),R(1)                                          SMO 450
C                                                                       SMO 460
C     INITIALIZATION                                                    SMO 470
C                                                                       SMO 480
      DO 110 I=1,N                                                      SMO 490
  110 R(I)=0.0                                                          SMO 500
      IL=(L*(M-1))/2+1                                                  SMO 510
      IH=N-(L*(M-1))/2                                                  SMO 520
C                                                                       SMO 530
C     SMOOTH SERIES A BY WEIGHTS W                                      SMO 540
C                                                                       SMO 550
      DO 120 I=IL,IH                                                    SMO 560
      K=I-IL+1                                                          SMO 570
      DO 120 J=1,M                                                      SMO 580
      IP=(J*L)-L+K                                                      SMO 590
  120 R(I)=R(I)+A(IP)*W(J)                                              SMO 600
      RETURN                                                            SMO 610
      END                                                               SMO 620
```

Subroutine EXSMO

This subroutine calculates a smoothed series S_1, S_2, ..., S_{NX}, given time series X_1, X_2, ..., X_{NX} and a smoothing constant α. Also, at the end of the computation, the coefficients A, B, and C are given for the expression $A + B(T) + C(T)^2/2$. This expression can be used to find estimates of the smoothed series for a given number of time periods, T, ahead.

The subroutine has the following two stages for i = 1, 2, ..., NX, starting with A, B, and C either given by the user or provided automatically by the subroutine (see below).

(a) Find S_i for one period ahead:

$$S_i = A + B + 0.5C \tag{1}$$

(b) Update coefficients A, B, and C:

$$A = X_i + (1 - \alpha)^3 (S_i - X_i) \tag{2}$$

$$B = B + C - 1.5 (\alpha^2) (2 - \alpha) (S_i - X_i) \tag{3}$$

$$C = C - (\alpha^3) (S_i - X_i) \tag{4}$$

where α = smoothing constant specified by the user

$(0.0 < \alpha < 1.0)$

If coefficients A, B, and C are not all zero (0.0), take given values as initial values. However, if A = B = C = 0.0, generate initial values of A, B, and C as follows:

$$C = X_1 - 2X_2 + X_3 \tag{5}$$

$$B = X_2 - X_1 - 1.5C \tag{6}$$

$$A = X_1 - B - 0.5C \tag{7}$$

```
C                                                                       EXSM  10
C     ...................................................................EXSM  20
C                                                                       EXSM  30
C        SUBROUTINE EXSMO                                               EXSM  40
C                                                                       EXSM  50
C        PURPOSE                                                        EXSM  60
C           TO FIND THE TRIPLE EXPONENTIAL SMOOTHED SERIES S OF THE     EXSM  70
C           GIVEN SERIES X.                                             EXSM  80
C                                                                       EXSM  90
C        USAGE                                                          EXSM 100
C           CALL EXSMO (X,NX,AL,A,B,C,S)                                EXSM 110
C                                                                       EXSM 120
C        DESCRIPTION OF PARAMETERS                                      EXSM 130
C           X      - INPUT VECTOR OF LENGTH NX CONTAINING TIME SERIES   EXSM 140
C                    DATA WHICH IS TO BE EXPONENTIALLY SMOOTHED.        EXSM 150
C           NX     - THE NUMBER OF ELEMENTS IN X.                       EXSM 160
C           AL     - SMOOTHING CONSTANT, ALPHA.  AL MUST BE GREATER THAN EXSM 170
C                    ZERO AND LESS THAN ONE.                            EXSM 180
C           A,B,C  - COEFFICIENTS OF THE PREDICTION EQUATION WHERE S IS EXSM 190
C                    PREDICTED T PERIODS HENCE BY                       EXSM 200
C                                A + B*T + C*T*T/2.                     EXSM 210
C                    AS INPUT-- IF A=B=C=0, PROGRAM WILL PROVIDE INITIAL EXSM 220
C                    VALUES.  IF AT LEAST ONE OF A,B,C IS NOT ZERO,     EXSM 230
C                    PROGRAM WILL TAKE GIVEN VALUES AS INITIAL VALUES.  EXSM 240
C                    AS OUTPUT-- A,B,C CONTAIN LATEST, UPDATED COEFFI-  EXSM 250
C                    CIENTS OF PREDICTION.                              EXSM 260
C           S      - OUTPUT VECTOR OF LENGTH NX CONTAINING TRIPLE       EXSM 270
C                    EXPONENTIALLY SMOOTHED TIME SERIES.                EXSM 280
C                                                                       EXSM 290
C        REMARKS                                                        EXSM 300
C           NONE                                                        EXSM 310
C                                                                       EXSM 320
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  EXSM 330
C           NONE                                                        EXSM 340
C                                                                       EXSM 350
C        METHOD                                                         EXSM 360
C           REFER TO R. G. BROWN, 'SMOOTHING, FORECASTING AND PREDICTION EXSM 370
C           OF DISCRETE TIME SERIES', PRENTICE-HALL, N.J., 1963,        EXSM 380
C           PP. 140 TO 144.                                             EXSM 390
C                                                                       EXSM 400
C     ...................................................................EXSM 410
C                                                                       EXSM 420
      SUBROUTINE EXSMO (X,NX,AL,A,B,C,S)                                EXSM 430
      DIMENSION X(1),S(1)                                               EXSM 440
C                                                                       EXSM 450
C     IF A=B=C=0.0, GENERATE INITIAL VALUES OF A, B, AND C              EXSM 460
C                                                                       EXSM 470
      IF(A) 140, 110, 140                                               EXSM 480
  110 IF(B) 140, 120, 140                                               EXSM 490
  120 IF(C) 140, 130, 140                                               EXSM 500
  130 C=X(1)-2.0*X(2)+X(3)                                              EXSM 510
      B=X(2)-X(1)-1.5*C                                                 EXSM 520
      A=X(1)-B-0.5*C                                                    EXSM 530
C                                                                       EXSM 540
  140 BE=1.0-AL                                                         EXSM 550
      BECUB=BE*BE*BE                                                    EXSM 560
      ALCUB=AL*AL*AL                                                    EXSM 570
C                                                                       EXSM 580
C     DO THE FOLLOWING FOR I=1 TO NX                                    EXSM 590
C                                                                       EXSM 600
      DO 150 I=1,NX                                                     EXSM 610
C                                                                       EXSM 620
C        FIND S(I) FOR ONE PERIOD AHEAD                                 EXSM 630
C                                                                       EXSM 640
      S(I)=A+B+0.5*C                                                    EXSM 650
C                                                                       EXSM 660
C        UPDATE COEFFICIENTS A, B, AND C                                EXSM 670
C                                                                       EXSM 680
      DIF=S(I)-X(I)                                                     EXSM 690
      A=X(I)+BECUB*DIF                                                  EXSM 700
      B=B+C-1.5*AL*AL*(2.0-AL)*DIF                                      EXSM 710
  150 C=C-ALCUB*DIF                                                     EXSM 720
      RETURN                                                            EXSM 730
      END                                                               EXSM 740
```

Nonparametric Statistics

Subroutine KOLMO

Given a sample of n independent and identically distributed random variables $X_1, X_2, \ldots, X_n$ with continuous cumulative distribution function F(x), this subroutine tests the difference in absolute value between the empirical distribution $F_n(x)$ and theoretical distribution F(x), using Kolmogorov-Smirnov's limiting distribution.

For this purpose:

1. The order statistics $\{x_{(i)}\}$ are determined from the set $\{x_i\}$ by sorting $\{x_i\}$ into a nondecreasing sequence.
2. The empirical cumulative distribution function $F_n(x)$ is computed. This is the following step-function:

$$F_n(x) = \begin{cases} 0 & x < x_{(1)} \\ k/n & x_{(k)} \leq x < x_{(k+1)}; \; k=1,\ldots,n-1 \\ 1 & x_{(n)} \leq x \end{cases}$$

3. The maximum deviation D_n in absolute value between the empirical and theoretical distribution is computed:

$$D_n = \max_{-\infty<x<\infty} |F_n(x) - F(x)|$$

Since $F_n(x)$ and F(x) are nondecreasing functions, the result is:

$$D_n = \max_{1\leq k\leq n} \left| F_n\left[x_{(k)}\right] - F\left[x_{(k)}\right] \right|$$

D_n is a random variable, and L(z) is the limiting cumulative distribution function of $n^{1/2} D_n$:

$$\lim_{n\to\infty} \text{Prob}\{n^{1/2} D_n < z\} = L(z)$$

4. Finally,

$$z = n^{1/2} D_n$$

and the probability of being greater than or equal to the computed value of $n^{1/2} D_n$

$$P = 1 - L(z)$$

are computed.

Generally, theoretical distribution functions are to be included by the user, as specified in the program. However, four functions are evaluated in KOLMO, as follows:

$$\int_{-\infty}^{x} dF(t) = F(x) \qquad (1)$$

is evaluated at the points of the set $\{X_{(i)}\}$, where F(x) is one of the following:

- The normal pdf with mean u and variance s^2
- The exponential pdf with mean u and variance s^2
- The Cauchy pdf with median u, and first quartile s - u
- The uniform pdf with endpoints u and s

Any user-written pdf should evaluate (1) above, using the parameters u and s at his convenience. Instructions given in the program KOLMO should be followed.

Lilliefors (1967) notes that critical values determined by this test are not correct when one or more parameters are estimated from the sample. The user should refer to his article for notes on approximations which may be considered if such estimates are used.

For references see:

(1) W. Feller, "On the Kolmogorov - Smirnov limit theorems for empirical distributions", Annals of Math. Stat., 19, pp. 177-189.

(2) N. Smirnov, "Table for estimating the goodness of fit of empirical distributions", Annals of Math. Stat., 19, pp. 279-281.

(3) R. Von Mises, Mathematical Theory of Probability and Statistics. Academic Press, New York, 1964, pp. 490-493.

(4) B. V. Gnedenko, The Theory of Probability. Chelsea Publishing Co., New York, 1962, pp. 384-401.

(5) H. W. Lilliefors, "On the Kolmogorov-Smirnov test for normality with mean and variance unknown", J. A. S. A., 62 (1967), pp. 399-402.

```
C                                                                       KLMO  10
C  ...................................................................  KLMO  20
C                                                                       KLMO  30
C       SUBROUTINE KOLMO                                                KLMO  40
C                                                                       KLMO  50
C       PURPOSE                                                         KLMO  60
C          TESTS THE DIFFERENCE BETWEEN EMPIRICAL AND THEORETICAL       KLMO  70
C          DISTRIBUTIONS  USING THE KOLMOGOROV-SMIRNOV TEST             KLMO  80
C                                                                       KLMO  90
C       USAGE                                                           KLMO 100
C          CALL KOLMO(X,N,Z,PROB,IFCOD,U,S,IER)                         KLMO 110
C                                                                       KLMO 120
C       DESCRIPTION OF PARAMETERS                                       KLMO 130
C          X    - INPUT VECTOR OF N INDEPENDENT OBSERVATIONS.  ON       KLMO 140
C                 RETURN FROM KOLMO, X HAS BEEN SORTED INTO A           KLMO 150
C                 MONOTONIC NON-DECREASING SEQUENCE.                    KLMO 160
C          N    - NUMBER OF OBSERVATIONS IN X                           KLMO 170
C          Z    - OUTPUT VARIABLE CONTAINING THE GREATEST VALUE WITH    KLMO 180
C                 RESPECT TO X OF  SQRT(N)*ABS(FN(X)-F(X)) WHERE        KLMO 190
C                 F(X) IS A  THEORETICAL DISTRIBUTION FUNCTION AND      KLMO 200
C                 FN(X) AN EMPIRICAL DISTRIBUTION FUNCTION.             KLMO 210
C          PROB - OUTPUT VARIABLE CONTAINING THE PROBABILITY OF         KLMO 220
C                 THE STATISTIC BEING GREATER THAN OR EQUAL TO Z IF     KLMO 230
C                 THE HYPOTHESIS THAT X IS FROM THE DENSITY UNDER       KLMO 240
C                 CONSIDERATION IS TRUE.  E.G., PROB = 0.05 IMPLIES     KLMO 250
C                 THAT ONE CAN REJECT THE NULL HYPOTHESIS THAT THE SET  KLMO 260
C                 X IS FROM THE DENSITY UNDER CONSIDERATION WITH 5 PER  KLMO 270
C                 CENT PROBABILITY OF BEING INCORRECT.  PROB = 1. -     KLMO 280
C                 SMIRN(Z).                                             KLMO 290
C          IFCOD- A CODE DENOTING THE PARTICULAR THEORETICAL             KLMO 300
C                 PROBABILITY DISTRIBUTION FUNCTION BEING CONSIDERED.   KLMO 310
C                 = 1---F(X) IS THE NORMAL PDF.                         KLMO 320
C                 = 2---F(X) IS THE EXPONENTIAL PDF.                    KLMO 330
C                 = 3---F(X) IS THE CAUCHY PDF.                         KLMO 340
C                 = 4---F(X) IS THE UNIFORM PDF.                        KLMO 350
C                 = 5---F(X) IS USER SUPPLIED.                          KLMO 360
C          U    - WHEN IFCOD IS 1 OR 2, U IS THE MEAN OF THE DENSITY    KLMO 370
C                 GIVEN ABOVE.                                          KLMO 380
C                 WHEN IFCOD IS 3, U IS THE MEDIAN OF THE CAUCHY        KLMO 390
C                 DENSITY.                                              KLMO 400
C                 WHEN IFCOD IS 4, U IS THE LEFT ENDPOINT OF THE        KLMO 410
C                 UNIFORM DENSITY.                                      KLMO 420
C                 WHEN IFCOD IS 5, U IS USER SPECIFIED.                 KLMO 430
C          S    - WHEN IFCOD IS 1 OR 2, S IS THE STANDARD DEVIATION OF  KLMO 440
C                 DENSITY GIVEN ABOVE, AND SHOULD BE POSITIVE.          KLMO 450
C                 WHEN IFCOD IS 3, U - S SPECIFIES THE FIRST QUARTILE   KLMO 460
C                 OF THE CAUCHY DENSITY.  S SHOULD BE NON-ZERO.         KLMO 470
C                 IF IFCOD IS 4, S IS THE RIGHT ENDPOINT OF THE UNIFORM KLMO 480
C                 DENSITY.  S SHOULD BE GREATER THAN U.                 KLMO 490
C                 IF IFCOD IS 5, S IS USER SPECIFIED.                   KLMO 500
C          IER  - ERROR INDICATOR WHICH IS NON-ZERO IF S VIOLATES ABOVE KLMO 510
C                 CONVENTIONS.  ON RETURN NO TEST HAS BEEN MADE, AND X  KLMO 520
C                 AND Y HAVE BEEN SORTED INTO MONOTONIC NON-DECREASING  KLMO 530
C                 SEQUENCES.  IER IS SET TO ZERO ON ENTRY TO KOLMO.     KLMO 540
C                 IER IS CURRENTLY SET TO ONE IF THE USER-SUPPLIED PDF  KLMO 550
C                 IS REQUESTED FOR TESTING.  THIS SHOULD BE CHANGED     KLMO 560
C                 (SEE REMARKS) WHEN SOME PDF IS SUPPLIED BY THE USER.  KLMO 570
C                                                                       KLMO 580
C       REMARKS                                                         KLMO 590
C          N SHOULD BE GREATER THAN OR EQUAL TO 100.  (SEE THE          KLMO 600
C          MATHEMATICAL DESCRIPTION GIVEN FOR THE PROGRAM SMIRN.        KLMO 610
C          CONCERNING ASYMPTOTIC FORMULAE)  ALSO, PROBABILITY LEVELS    KLMO 620
C          DETERMINED BY THIS PROGRAM WILL NOT BE CORRECT IF THE        KLMO 630
C          SAME SAMPLES ARE USED TO ESTIMATE PARAMETERS FOR THE         KLMO 640
C          CONTINUOUS DISTRIBUTIONS WHICH ARE USED IN THIS TEST.        KLMO 650
C          (SEE THE MATHEMATICAL DESCRIPTION FOR THIS PROGRAM)          KLMO 660
C          F(X) SHOULD BE A CONTINUOUS FUNCTION.                        KLMO 670
C          ANY USER SUPPLIED CUMULATIVE PROBABILITY DISTRIBUTION        KLMO 680
C          FUNCTION SHOULD BE CODED BEGINNING WITH STATEMENT 26 BELOW,  KLMO 690
C          AND SHOULD RETURN TO STATEMENT 27.                           KLMO 700
C                                                                       KLMO 710
C          DOUBLE PRECISION USAGE---IT IS DOUBTFUL THAT THE USER WILL   KLMO 720
C          WISH TO PERFORM THIS TEST USING DOUBLE PRECISION ACCURACY.   KLMO 730
C          IF ONE WISHES TO COMMUNICATE WITH KOLMO IN A DOUBLE          KLMO 740
C          PRECISION PROGRAM, HE SHOULD CALL THE FORTRAN SUPPLIED       KLMO 750
C          PROGRAM SNGL(X) PRIOR TO CALLING KOLMO, AND CALL THE         KLMO 760
C          FORTRAN SUPPLIED PROGRAM DBLE(X) AFTER EXITING FROM KOLMO.   KLMO 770
C          (NOTE THAT SUBROUTINE SMIRN DOES HAVE DOUBLE PRECISION       KLMO 780
C          CAPABILITY AS SUPPLIED BY THIS PACKAGE.)                     KLMO 790
C                                                                       KLMO 800
C                                                                       KLMO 810
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   KLMO 820
C          SMIRN, NDTR, AND ANY USER SUPPLIED SUBROUTINES REQUIRED.     KLMO 830
C                                                                       KLMO 840
C       METHOD                                                          KLMO 850
C          FOR REFERENCE, SEE (1) W. FELLER--ON THE KOLMOGOROV-SMIRNOV  KLMO 860
C          LIMIT THEOREMS FOR EMPIRICAL DISTRIBUTIONS--                 KLMO 870
C          ANNALS OF MATH. STAT., 19, 1948.  177-189,                   KLMO 880
C          (2) N. SMIRNOV--TABLE FOR ESTIMATING THE GOODNESS OF FIT     KLMO 890
C          OF EMPIRICAL DISTRIBUTIONS--ANNALS OF MATH. STAT., 19,       KLMO 900
C          1948.  279-281.                                              KLMO 910
C          (3) R. VON MISES--MATHEMATICAL THEORY OF PROBABILITY AND      KLMO 920
C          STATISTICS--ACADEMIC PRESS, NEW YORK, 1964.  490-493,        KLMO 930
C          (4) B.V. GNEDENKO--THE THEORY OF PROBABILITY--CHELSEA        KLMO 940
C          PUBLISHING COMPANY, NEW YORK, 1962.  384-401.                KLMO 950
C                                                                       KLMO 960
C  ...................................................................  KLMO 970
C                                                                       KLMO 980
      SUBROUTINE KOLMO(X,N,Z,PROB,IFCOD,U,S,IER)                        KLMO 990
      DIMENSION X(1)                                                    KLM01000
C                                                                       KLM01010
C           NON DECREASING ORDERING OF X(I)'S  (DUBY METHOD)            KLM01020
C                                                                       KLM01030
      IER=0                                                             KLM01040
      DO 5 I=2,N                                                        KLM01050
      IF(X(I)-X(I-1))1,5,5                                              KLM01060
    1 TEMP=X(I)                                                         KLM01070
      IM=I-1                                                            KLM01080
      DO 3 J=1,IM                                                       KLM01090
      L=I-J                                                             KLM01100
      IF(TEMP-X(L))2,4,4                                                KLM01110
    2 X(L+1)=X(L)                                                       KLM01120
    3 CONTINUE                                                          KLM01130
      X(1)=TEMP                                                         KLM01140
      GO TO 5                                                           KLM01150
    4 X(L+1)=TEMP                                                       KLM01160
    5 CONTINUE                                                          KLM01170
C                                                                       KLM01180
C           COMPUTES MAXIMUM DEVIATION DN IN ABSOLUTE VALUE BETWEEN     KLM01190
C           EMPIRICAL AND THEORETICAL DISTRIBUTIONS                     KLM01200
C                                                                       KLM01210
      NM1=N-1                                                           KLM01220
      XN=N                                                              KLM01230
      DN=0.0                                                            KLM01240
      FS=0.0                                                            KLM01250
      IL=1                                                              KLM01260
      DO 7  I=IL,NM1                                                    KLM01270
      J=I                                                               KLM01280
      IF(X(J)-X(J+1))8,7,8                                              KLM01290
    7 CONTINUE                                                          KLM01300
    8 J=N                                                               KLM01310
    9 IL=J+1                                                            KLM01320
      FI=FS                                                             KLM01330
      FS=FLOAT(J)/XN                                                    KLM01340
      IF(IFCOD-2)10,13,17                                               KLM01350
   10 IF(S)11,11,12                                                     KLM01360
   11 IER=1                                                             KLM01370
      GO TO 29                                                          KLM01380
   12 Z =(X(J)-U)/S                                                     KLM01390
      CALL NDTR(Z,Y,D)                                                  KLM01400
      GO TO 27                                                          KLM01410
   13 IF(S)11,11,14                                                     KLM01420
   14 Z=(X(J)-U)/S+1.0                                                  KLM01430
      IF(Z)15,15,16                                                     KLM01440
   15 Y=0.0                                                             KLM01450
      GO TO 27                                                          KLM01460
   16 Y=1.-EXP(-Z)                                                      KLM01470
      GO TO 27                                                          KLM01480
   17 IF(IFCOD-4)18,20,26                                               KLM01490
   18 IF(S)19,11,19                                                     KLM01500
   19 Y=ATAN((X(J)-U)/S)*0.3183099+0.5                                  KLM01510
      GO TO 27                                                          KLM01520
   20 IF(S-U)11,11,21                                                   KLM01530
   21 IF(X(J)-U)22,22,23                                                KLM01540
   22 Y=0.0                                                             KLM01550
      GO TO 27                                                          KLM01560
   23 IF(X(J)-S)25,25,24                                                KLM01570
   24 Y=1.0                                                             KLM01580
      GO TO 27                                                          KLM01590
   25 Y=(X(J)-U)/(S-U)                                                  KLM01600
      GO TO 27                                                          KLM01610
   26 IER=1                                                             KLM01620
      GO TO 29                                                          KLM01630
   27 EI=ABS(Y-FI)                                                      KLM01640
      ES=ABS(Y-FS)                                                      KLM01650
      DN=AMAX1(DN,EI,ES)                                                KLM01660
      IF(IL-N)6,8,28                                                    KLM01670
C                                                                       KLM01680
C           COMPUTES Z=DN*SQRT(N)  AND  PROBABILITY                     KLM01690
C                                                                       KLM01700
   28 Z=DN*SQRT(XN)                                                     KLM01710
      CALL SMIRN(Z,PROB)                                                KLM01720
      PROB=1.0-PROB                                                     KLM01730
   29 RETURN                                                            KLM01740
      END                                                               KLM01750
```

Subroutine KOLM2

Given a sample of n i.i.d. (independent and identically distributed) random variables X, and a sample of m i.i.d. random variables Y, this subroutine tests the difference between the two empirical distribution functions $F_n(x)$ and $G_m(y)$ using Kolmogorov-Smirnov's limiting distribution. For this purpose:

1. The sets X and Y are sorted into the ordered sets $\{X_{(i)}\}$ and $\{Y_{(i)}\}$, which are nondecreasing sequences.

2. The empirical cumulative distribution functions $F_n(x)$ for the set X, and $G_m(y)$ for the set Y are computed. For example,

$$F_n(x) = \begin{cases} 0 & x < x_{(1)} \\ k/n & x_{(k)} \le x < x_{(k+1)} ; \; k=1,..,n-1 \\ 1 & x_{(n)} \le x \end{cases}$$

3. The maximum difference in absolute value between the two sample distribution functions is computed:

$$D_{m,n} = \max_{x,\,y} \left| F_n(x) - G_m(y) \right|$$

The statistic $\sqrt{\frac{mn}{m+n}}\, D_{m,n}$ is a random variable with limiting cumulative distribution function L(z), which is described under "Subroutine SMIRN" in this manual. That is,

$$\lim_{m,n \to \infty,\,\infty} \text{Prob}\left\{ \sqrt{\frac{mn}{m+n}}\, D_{m,n} < z \right\} = L(z)$$

4. Finally, the probability (asymptotic) of the statistic $\sqrt{\frac{mn}{m+n}}\, D_{m,n}$ being not less than its computed value, under the assumption of equality of the two theoretical distribution functions from which X and Y were taken, is computed:

$$P = 1 - L(z)$$

For reference see:

(1) W. Feller, "On the Kolmogorov-Smirnov limit theorems for empirical distributions", Annals of Math. Stat., 19, pp. 177-189.

(2) N. Smirnov, "Table for estimating the goodness of fit of empirical distributions", Annals of Math. Stat., 19, pp. 279-281.

(3) B. V. Gnedenko, The Theory of Probability. Chelsea Publishing Co. New York, 1962, pp. 384-401.


```
C                                                                       KLM2  10
C     ..................................................................KLM2  20
C                                                                       KLM2  30
C        SUBROUTINE KOLM2                                               KLM2  40
C                                                                       KLM2  50
C        PURPOSE                                                        KLM2  60
C                                                                       KLM2  70
C           TESTS THE DIFFERENCE BETWEEN TWO SAMPLE DISTRIBUTION        KLM2  80
C           FUNCTIONS USING THE KOLMOGOROV-SMIRNOV TEST                 KLM2  90
C                                                                       KLM2 100
C        USAGE                                                          KLM2 110
C           CALL KOLM2(X,Y,N,M,Z,PROB)                                  KLM2 120
C                                                                       KLM2 130
C        DESCRIPTION OF PARAMETERS                                      KLM2 140
C           X    - INPUT VECTOR OF N INDEPENDENT OBSERVATIONS.  ON      KLM2 150
C                  RETURN FROM KOLM2, X HAS BEEN SORTED INTO A          KLM2 160
C                  MONOTONIC NON-DECREASING SEQUENCE.                   KLM2 170
C           Y    - INPUT VECTOR OF M INDEPENDENT OBSERVATIONS.  ON      KLM2 180
C                  RETURN FROM KOLM2, Y HAS BEEN SORTED INTO A          KLM2 190
C                  MONOTONIC NON-DECREASING SEQUENCE.                   KLM2 200
C           N    - NUMBER OF OBSERVATIONS IN X                          KLM2 210
C           M    - NUMBER OF OBSERVATIONS IN Y                          KLM2 220
C           Z    - OUTPUT VARIABLE CONTAINING THE GREATEST VALUE WITH   KLM2 230
C                  RESPECT TO THE SPECTRUM OF X AND Y OF                KLM2 240
C                  SQRT((M*N)/(M+N))*ABS(FN(X)-GM(Y)) WHERE             KLM2 250
C                  FN(X) IS THE EMPIRICAL DISTRIBUTION FUNCTION OF THE  KLM2 260
C                  SET (X) AND GM(Y) IS THE EMPIRICAL DISTRIBUTION      KLM2 270
C                  FUNCTION OF THE SET (Y).                             KLM2 280
C           PROB - OUTPUT VARIABLE CONTAINING THE PROBABILITY OF        KLM2 290
C                  THE STATISTIC BEING GREATER THAN OR EQUAL TO Z IF    KLM2 300
C                  THE HYPOTHESIS THAT X AND Y ARE FROM THE SAME PDF IS KLM2 310
C                  TRUE.  E.G., PROB= 0.05 IMPLIES THAT ONE CAN REJECT  KLM2 320
C                  THE NULL HYPOTHESIS THAT THE SETS X AND Y ARE FROM   KLM2 330
C                  THE SAME DENSITY WITH 5 PER CENT PROBABILITY OF BEINGKLM2 340
C                  INCORRECT.  PROB = 1. - SMIRN(Z).                    KLM2 350
C                                                                       KLM2 360
C        REMARKS                                                        KLM2 370
C           N AND M SHOULD BE GREATER THAN OR EQUAL TO 100.  (SEE THE   KLM2 380
C           MATHEMATICAL DESCRIPTION FOR THIS SUBROUTINE AND FOR THE    KLM2 390
C           SUBROUTINE SMIRN, CONCERNING ASYMPTOTIC FORMULAE).          KLM2 400
C                                                                       KLM2 410
C           DOUBLE PRECISION USAGE---IT IS DOUBTFUL THAT THE USER WILL  KLM2 420
C           WISH TO PERFORM THIS TEST USING DOUBLE PRECISION ACCURACY.  KLM2 430
C           IF ONE WISHES TO COMMUNICATE WITH KOLM2 IN A DOUBLE         KLM2 440
C           PRECISION PROGRAM, HE SHOULD CALL THE FORTRAN SUPPLIED      KLM2 450
C           PROGRAM SNGL(X) PRIOR TO CALLING KOLM2, AND CALL THE        KLM2 460
C           FORTRAN SUPPLIED PROGRAM DBLE(X) AFTER EXITING FROM KOLM2.  KLM2 470
C           (NOTE THAT SUBROUTINE SMIRN DOES HAVE DOUBLE PRECISION      KLM2 480
C           CAPABILITY AS SUPPLIED BY THIS PACKAGE.)                    KLM2 490
C                                                                       KLM2 500
C                                                                       KLM2 510
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  KLM2 520
C           SMIRN                                                       KLM2 530
C                                                                       KLM2 540
C        METHOD                                                         KLM2 550
C           FOR REFERENCE, SEE (1) W. FELLER--ON THE KOLMOGOROV-SMIRNOV KLM2 560
C           LIMIT THEOREMS FOR EMPIRICAL DISTRIBUTIONS--                KLM2 570
C           ANNALS OF MATH. STAT., 19, 1948.  177-189,                  KLM2 580
C           (2) N. SMIRNOV--TABLE FOR ESTIMATING THE GOODNESS OF FIT    KLM2 590
C           OF EMPIRICAL DISTRIBUTIONS--ANNALS OF MATH. STAT., 19,      KLM2 600
C           1948.  279-281.                                             KLM2 610
C           (3) R. VON MISES--MATHEMATICAL THEORY OF PROBABILITY AND     KLM2 620
C           STATISTICS--ACADEMIC PRESS, NEW YORK, 1964.  490-493.        KLM2 630
C           (4) B.V. GNEDENKO--THE THEORY OF PROBABILITY--CHELSEA        KLM2 640
C           PUBLISHING COMPANY, NEW YORK, 1962.  384-401.                KLM2 650
C                                                                       KLM2 660
C     ..................................................................KLM2 670
C                                                                       KLM2 680
      SUBROUTINE KOLM2(X,Y,N,M,Z,PROB)                                  KLM2 690
      DIMENSION X(1),Y(1)                                               KLM2 700
C                                                                       KLM2 710
C        SORT X INTO ASCENDING SEQUENCE                                 KLM2 720
C                                                                       KLM2 730
      DO 5 I=2,N                                                        KLM2 740
      IF(X(I)-X(I-1))1,5,5                                              KLM2 750
    1 TEMP=X(I)                                                         KLM2 760
      IM=I-1                                                            KLM2 770
      DO 3 J=1,IM                                                       KLM2 780
      L=I-J                                                             KLM2 790
      IF(TEMP-X(L))2,4,4                                                KLM2 800
    2 X(L+1)=X(L)                                                       KLM2 810
    3 CONTINUE                                                          KLM2 820
      X(1)=TEMP                                                         KLM2 830
      GO TO 5                                                           KLM2 840
    4 X(L+1)=TEMP                                                       KLM2 850
    5 CONTINUE                                                          KLM2 860
C                                                                       KLM2 870
C        SORT Y INTO ASCENDING SEQUENCE                                 KLM2 880
C                                                                       KLM2 890
      DO 10 I=2,M                                                       KLM2 900
      IF(Y(I)-Y(I-1))6,10,10                                            KLM2 910
    6 TEMP=Y(I)                                                         KLM2 920
      IM=I-1                                                            KLM2 930
      DO 8  J=1,IM                                                      KLM2 940
      L=I-J                                                             KLM2 950
      IF(TEMP-Y(L))7,9,9                                                KLM2 960
    7 Y(L+1)=Y(L)                                                       KLM2 970
    8 CONTINUE                                                          KLM2 980
      Y(1)=TEMP                                                         KLM2 990
      GO TO 10                                                          KLM21000
    9 Y(L+1)=TEMP                                                       KLM21010
   10 CONTINUE                                                          KLM21020
C                                                                       KLM21030
C        CALCULATE D = ABS(FN-GM) OVER THE SPECTRUM OF X AND Y          KLM21040
C                                                                       KLM21050
      XN=FLOAT(N)                                                       KLM21060
      XNI=1./XN                                                         KLM21070
      XM=FLOAT(M)                                                       KLM21080
      XMI=1./XM                                                         KLM21090
      D=0.0                                                             KLM21100
      I=0                                                               KLM21110
```

```
      J=0                                                               KLM21120
      K=0                                                               KLM21130
      I=0                                                               KLM21140
   11 IF(X(I+1)-Y(J+1))12,13,18                                         KLM21150
   12 K=1                                                               KLM21160
      GO TO 14                                                          KLM21170
   13 K=0                                                               KLM21180
   14 I=I+1                                                             KLM21190
      IF(I-N)15,21,21                                                   KLM21200
   15 IF(X(I+1)-X(I))14,14,16                                           KLM21210
   16 IF(K)17,18,17                                                     KLM21220
C                                                                       KLM21230
C        CHOOSE THE MAXIMUM DIFFERENCE, D                               KLM21240
C                                                                       KLM21250
   17 D=AMAX1(D,ABS(FLOAT(I)*XN1-FLOAT(J)*XM1))                         KLM21260
      IF(L)22,11,22                                                     KLM21270
   18 J=J+1                                                             KLM21280
      IF(J-M)19,20,20                                                   KLM21290
   19 IF(Y(J+1)-Y(J))19,18,17                                           KLM21300
   20 L=1                                                               KLM21310
      GO TO 17                                                          KLM21320
   21 L=1                                                               KLM21330
      GO TO 16                                                          KLM21340
C                                                                       KLM21350
C        CALCULATE THE STATISTIC Z                                      KLM21360
C                                                                       KLM21370
   22 Z=D*SQRT((XN*XM)/(XN+XM))                                         KLM21380
C                                                                       KLM21390
C        CALCULATE THE PROBABILITY ASSOCIATED WITH Z                    KLM21400
C                                                                       KLM21410
      CALL SMIRN(Z,PROB)                                                KLM21420
      PROB=1.0-PROB                                                     KLM21430
      RETURN                                                            KLM21440
      END                                                               KLM21450
```

Subroutine SMIRN

This subroutine computes the values of Kolmogorov-Smirnov's limiting distribution for a given argument x.

$$L(x) = \begin{cases} 0 & x \le 0 \\ 1 - 2 \sum_{k=1}^{\infty} (-1)^{k-1} \exp(-2k^2x^2) & x > 0 \end{cases} \quad (1)$$

L(x) is the limit (Kolmogorov) of the cumulative distribution function of $\sqrt{n}\, D_n$, and of (Smirnov) $[mn/(m+n)]^{1/2} D_{m,n}$ where:

D_n is the maximum, over all x, of the difference $|F_n(x) - F(x)|$ between the sample distribution function $F_n(x)$ and the continuous theoretical distribution function F(x), and

$D_{m,n}$ is the maximum, over all x, of the difference between the two sample distribution functions $F_m(x)$ and $G_n(x)$, from two independent samples of sizes m and n.

When x is very small, the series (1) converges slowly, but, using Jacobi's Theta-functions $\theta_2(u,t)$ and $\theta_4(u,t)$:

$$\theta_2(u,t) = 2 \sum_{k=0}^{\infty} \exp[i\pi(k+1/2)^2 t] \cos[(2k+1)u]$$

$$\theta_4(u,t) = 1 - 2 \sum_{k=0}^{\infty} (-1)^{k-1} \exp(i\pi k^2 t) \cos(2ku)$$

and using the Jacobi imaginary transformation

$$\theta_4(0,t) = (-it)^{-1/2} \theta_2(0, -1/t)$$

it follows that:

$$L(x) = \theta_4(0, 2ix^2/\pi)$$

$$= (\sqrt{2\pi}/x) \sum_{k=1}^{\infty} \exp[-(2k-1)^2 \pi^2/8x^2]$$

which converges quickly when x is small. The computation here uses, with errors $E_i(x)$, i = 1, 2:

$$L(x) = \begin{cases} 0 & x \le 0.27 \\ (\sqrt{2\pi}/x) \sum_{k=1}^{3} \exp\left[-(2k-1)^2 \pi^2 / 8x^2\right] + E_1(x); & 0.27 < x < 1.0 \\ 1 - 2 \sum_{k=1}^{4} (-1)^{k-1} \exp(-2k^2 x^2) + E_2(x) & 1.0 \le x < 3.1 \\ 1 & 3.1 \le x < \infty \end{cases}$$

where:

$$E_1(x) \le 6\,(10^{-15}) \quad \text{when } x < 1$$

$$E_2(x) < 10^{-20} \quad \text{when } x \ge 1$$

For reference see:

(1) E. T. Whittaker and G. N. Watson, A Course of Modern Analysis. Cambridge University Press, Cambridge, England, 1952, pp. 462-476.

(2) W. Feller, "On the Kolmogorov-Smirnov limit theorems for empirical distributions", Annals of Math. Stat. 19, pp. 177-189.

(3) N. Smirnov, "Table for estimating the goodness of fit of empirical distributions", Annals of Math. Stat. 19, pp. 279-281.


```
C                                                                       SMIR  10
C  .....................................................................SMIR  20
C                                                                       SMIR  30
C     SUBROUTINE SMIRN                                                  SMIR  40
C                                                                       SMIR  50
C     PURPOSE                                                           SMIR  60
C        COMPUTES VALUES OF THE LIMITING DISTRIBUTION FUNCTION FOR      SMIR  70
C        THE KOLMOGOROV-SMIRNOV STATISTIC.                              SMIR  80
C                                                                       SMIR  90
C     USAGE                                                             SMIR 100
C        CALL SMIRN(X,Y)                                                SMIR 110
C                                                                       SMIR 120
C     DESCRIPTION OF PARAMETERS                                         SMIR 130
C        X    - THE ARGUMENT OF THE SMIRN FUNCTION                      SMIR 140
C        Y    - THE RESULTANT SMIRN FUNCTION VALUE                      SMIR 150
C                                                                       SMIR 160
C     REMARKS                                                           SMIR 170
C        Y IS SET TO ZERO IF X IS NOT GREATER THAN 0.27, AND IS SET     SMIR 180
C        TO ONE IF X IS NOT LESS THAN 3.1.  ACCURACY TESTS WERE MADE    SMIR 190
C        REFERRING TO THE TABLE GIVEN IN THE REFERENCE BELOW.           SMIR 200
C        TWO ARGUMENTS, X= 0.42, AND X = 1.87 GAVE RESULTS WHICH        SMIR 210
C        DIFFER FROM THE SMIRNOV TABLES BY 2.5 AND 1.9 IN THE 5TH       SMIR 220
C        DECIMAL PLACE.  ALL OTHER RESULTS SHOWED SMALLER ERRORS,       SMIR 230
C        AND ERROR SPECIFICATIONS ARE GIVEN IN THE ACCURACY TABLES      SMIR 240
C        IN THIS MANUAL.  IN DOUBLE PRECISION MODE, THESE SAME          SMIR 250
C        ARGUMENTS RESULTED IN DIFFERENCES FROM TABLED VALUES BY 3      SMIR 260
C        AND 2 IN THE 5TH  DECIMAL PLACE.  IT IS NOTED IN               SMIR 270
C        LINDGREN (REFERENCE BELOW) THAT FOR HIGH SIGNIFICANCE LEVELS   SMIR 280
C        (SAY, .01 AND .05) ASYMPTOTIC FORMULAS GIVE VALUES WHICH ARE   SMIR 290
C        TOO HIGH ( BY 1.5 PER CENT WHEN N = 80).  THAT IS, AT HIGH     SMIR 300
C        SIGNIFICANCE LEVELS, THE HYPOTHESIS OF NO DIFFERENCE WILL BE   SMIR 310
C        REJECTED TOO SELDOM USING ASYMPTOTIC FORMULAS.                 SMIR 320
C                                                                       SMIR 330
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     SMIR 340
C        NONE                                                           SMIR 350
C                                                                       SMIR 360
C     METHOD                                                            SMIR 370
C        THE METHOD IS DESCRIBED BY W. FELLER-ON THE KOLMOGOROV-        SMIR 380
C        SMIRNOV LIMIT THEOREMS FOR EMPIRICAL DISTRIBUTIONS- ANNALS     SMIR 390
C        OF MATH. STAT., 19, 1948, 177-189, BY N. SMIRNOV--TABLE        SMIR 400
C        FOR ESTIMATING THE GOODNESS OF FIT OF EMPIRICAL                SMIR 410
C        DISTRIBUTIONS- ANNALS OF MATH. STAT., 19, 1948, 279-281,       SMIR 420
C        AND GIVEN IN LINDGREN, STATISTICAL THEORY, THE MACMILLAN       SMIR 430
C        COMPANY, N. Y., 1962.                                          SMIR 440
C                                                                       SMIR 450
C  .....................................................................SMIR 460
C                                                                       SMIR 470
      SUBROUTINE SMIRN(X,Y)                                             SMIR 480
C     DOUBLE PRECISION X,G1,G2,G4,G8,Y                                  SMIR 490
C                                                                       SMIR 500
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  SMIR 510
C        IN COLUMN ONE OF THE DOUBLE PRECISION CARD ABOVE SHOULD BE     SMIR 520
C        REMOVED. AND THE C IN COLUMN ONE OF THE STATEMENTS NUMBERED    SMIR 530
C        C   3, C   5, AND C   8 SHOULD BE REMOVED, AND THESE CARDS     SMIR 540
C        SHOULD REPLACE THE STATEMENTS NUMBERED 3, 5, AND 8,            SMIR 550
C        RESPECTIVELY.  ALL ROUTINES CALLING THIS ROUTINE MUST ALSO     SMIR 560
C        PROVIDE DOUBLE PRECISION ARGUMENTS TO THIS ROUTINE.            SMIR 570
C                                                                       SMIR 580
C  .....................................................................SMIR 590
C                                                                       SMIR 600
      IF(X-.27)1,1,2                                                    SMIR 610
    1 Y=0.0                                                             SMIR 620
      GO TO 9                                                           SMIR 630
    2 IF(X-1.0)3,6,6                                                    SMIR 640
    3 G1=EXP(-1.2337*0.1/X**2)                                          SMIR 650
C   3 G1=DEXP(-1.2337D0*0.1/X**2)                                       SMIR 660
      G2=G1*G1                                                          SMIR 670
      G4=G2*G2                                                          SMIR 680
      G8=G4*G4                                                          SMIR 690
      IF(G8-1.0E-25)4,5,5                                               SMIR 700
    4 G8=0.0                                                            SMIR 710
    5 Y=(2.5066283/X)*G1*(1.0+G8*(1.0+G8*(1.0+G8*0.8)))                 SMIR 720
C   5 Y=(2.5066282746310D0/X)*G1*(1.0D0+G8*(1.0D0+G8*(1.0D0+G8*0.8D0))) SMIR 730
      GO TO 9                                                           SMIR 740
    6 IF(X-3.1)8,7,7                                                    SMIR 750
    7 Y=1.0                                                             SMIR 760
      GO TO 9                                                           SMIR 770
    8 G1=EXP(-2.0*X*X)                                                  SMIR 780
C   8 G1=DEXP(-2.0D0*X*X)                                               SMIR 790
      G2=G1*G1                                                          SMIR 800
      G4=G2*G2                                                          SMIR 810
      G8=G4*G4                                                          SMIR 820
      Y=1.0-2.0*(G1-G4+G8*(G1-G8))                                      SMIR 830
    9 RETURN                                                            SMIR 840
      END                                                               SMIR 850
```

Subroutine CHISQ

This subroutine calculates degrees of freedom and chi-square for a given contingency table A of observed frequencies with n rows (conditions) and m columns (groups). The degrees of freedom are:

$$d.f. = (n - 1)(m - 1) \quad (1)$$

If one or more cells contain an expected value less than 1.0, chi-square will be computed, but the error code will be set to one.

The following totals are computed:

$$T_i = \sum_{j=1}^{m} A_{ij}; \quad i = 1, 2, \ldots, n \text{ (row totals)} \quad (2)$$

$$T_j = \sum_{i=1}^{n} A_{ij}; \quad j = 1, 2, \ldots, m \text{ (column totals)} \quad (3)$$

$$GT = \sum_{i=1}^{n} T_i \quad \text{(grand total)} \quad (4)$$

Chi-square is obtained for two cases.

(a) For 2 x 2 table:

$$\chi^2 = \frac{GT\left(\left|A_{11}A_{22} - A_{12}A_{21}\right| - \frac{GT}{2}\right)^2}{(A_{11}+A_{12})(A_{21}+A_{22})(A_{11}+A_{21})(A_{12}+A_{22})} \quad (5)$$

(b) For other contingency tables:

$$\chi^2 = \sum_{i=1}^{n}\sum_{j=1}^{m} \frac{\left(A_{ij} - E_{ij}\right)^2}{E_{ij}} \quad (6)$$

where $E_{ij} = \frac{T_i T_j}{GT}$

$i = 1, 2, \ldots, n$

$j = 1, 2, \ldots, m$

```
C                                                                       CHIS  10
C     ...................................................................CHIS  20
C                                                                       CHIS  30
C        SUBROUTINE CHISQ                                               CHIS  40
C                                                                       CHIS  50
C        PURPOSE                                                        CHIS  60
C           COMPUTE CHI-SQUARE FROM A CONTINGENCY TABLE                 CHIS  70
C                                                                       CHIS  80
C        USAGE                                                          CHIS  90
C           CALL CHISQ(A,N,M,CS,NDF,IERR,TR,TC)                         CHIS 100
C                                                                       CHIS 110
C        DESCRIPTION OF PARAMETERS                                      CHIS 120
C           A    - INPUT MATRIX, N BY M, CONTAINING CONTINGENCY TABLE   CHIS 130
C           N    - NUMBER OF ROWS IN A                                  CHIS 140
C           M    - NUMBER OF COLUMNS IN A                               CHIS 150
C           CS   - CHI-SQUARE (OUTPUT)                                  CHIS 160
C           NDF  - NUMBER OF DEGREES OF FREEDOM (OUTPUT)                CHIS 170
C           IERR - ERROR CODE (OUTPUT)                                  CHIS 180
C                  0 - NORMAL CASE                                      CHIS 190
C                  1 - EXPECTED VALUE IS LESS THAN 1.0 IN ONE OR        CHIS 200
C                      MORE CELLS                                       CHIS 210
C                  3 - NUMBER OF DEGREES OF FREEDOM IS ZERO             CHIS 220
C           TR   - WORK VECTOR OF LENGTH N                              CHIS 230
C           TC   - WORK VECTOR OF LENGTH M                              CHIS 240
C                                                                       CHIS 250
C        REMARKS                                                        CHIS 260
C           IF ONE OR MORE CELLS CONTAIN AN EXPECTED VALUE (I.E.,       CHIS 270
C           THEORETICAL VALUE) LESS THAN 1.0, CHI-SQUARE WILL BE        CHIS 280
C           COMPUTED, BUT ERROR CODE WILL BE SET TO 1.                  CHIS 290
C           SEE REFERENCE GIVEN BELOW.                                  CHIS 300
C           CHI-SQUARE IS SET TO ZERO IF EITHER N OR M IS ONE (ERROR    CHIS 310
C           CODE 3).                                                    CHIS 320
C                                                                       CHIS 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CHIS 340
C           NONE                                                        CHIS 350
C                                                                       CHIS 360
C        METHOD                                                         CHIS 370
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   CHIS 380
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          CHIS 390
C           CHAPTER 6 AND CHAPTER 8.                                    CHIS 400
C                                                                       CHIS 410
C     ...................................................................CHIS 420
C                                                                       CHIS 430
      SUBROUTINE CHISQ(A,N,M,CS,NDF,IERR,TR,TC)                         CHIS 440
      DIMENSION A(1),TR(1),TC(1)                                        CHIS 450
C                                                                       CHIS 460
      NM=N*M                                                            CHIS 470
      IERR=0                                                            CHIS 480
      CS=0.0                                                            CHIS 490
C                                                                       CHIS 500
C        FIND DEGREES OF FREEDOM                                        CHIS 510
C                                                                       CHIS 520
      NDF=(N-1)*(M-1)                                                   CHIS 530
      IF(NDF) 5,5,10                                                    CHIS 540
    5 IERR=3                                                            CHIS 550
      RETURN                                                            CHIS 560
C                                                                       CHIS 570
C        COMPUTE TOTALS OF ROWS                                         CHIS 580
C                                                                       CHIS 590
   10 DO 90 I=1,N                                                       CHIS 600
      TR(I)=0.0                                                         CHIS 610
      IJ=I-N                                                            CHIS 620
      DO 90 J=1,M                                                       CHIS 630
      IJ=IJ+N                                                           CHIS 640
   90 TR(I)=TR(I)+A(IJ)                                                 CHIS 650
C                                                                       CHIS 660
C        COMPUTE TOTALS OF COLUMNS                                      CHIS 670
C                                                                       CHIS 680
      IJ=0                                                              CHIS 690
      DO 100 J=1,M                                                      CHIS 700
      TC(J)=0.0                                                         CHIS 710
      DO 100 I=1,N                                                      CHIS 720
      IJ=IJ+1                                                           CHIS 730
  100 TC(J)=TC(J)+A(IJ)                                                 CHIS 740
C                                                                       CHIS 750
C        COMPUTE GRAND TOTAL                                            CHIS 760
C                                                                       CHIS 770
      GT=0.0                                                            CHIS 780
      DO 110 I=1,N                                                      CHIS 790
  110 GT=GT+TR(I)                                                       CHIS 800
C                                                                       CHIS 810
C        COMPUTE CHI SQUARE FOR 2 BY 2 TABLE (SPECIAL CASE)             CHIS 820
C                                                                       CHIS 830
      IF(NM-4) 130,120,130                                              CHIS 840
  120 CS=GT*(ABS(A(1)*A(4)-A(2)*A(3))-GT/2.0)**2  /(TC(1)*TC(2)*TR(1)   CHIS 850
     1*TR(2))                                                           CHIS 860
      RETURN                                                            CHIS 870
C                                                                       CHIS 880
C        COMPUTE CHI SQUARE FOR OTHER CONTINGENCY TABLES                CHIS 890
C                                                                       CHIS 900
  130 IJ=0                                                              CHIS 910
      DO 140 J=1,M                                                      CHIS 920
      DO 140 I=1,N                                                      CHIS 930
      IJ=IJ+1                                                           CHIS 940
      E=TR(I)*TC(J)/GT                                                  CHIS 950
      IF(E-1.0) 135, 140, 140                                           CHIS 960
  135 IERR=1                                                            CHIS 970
  140 CS=CS+(A(IJ)-E)*(A(IJ)-E)/E                                       CHIS 980
      RETURN                                                            CHIS 990
      END                                                               CHIS1000
```

Subroutine KRANK

The subroutine computes the Kendall rank correlation coefficient, given two vectors of n observations for two variables, A and B. The observations on each variable are ranked from 1 to n. Tied observations are assigned the average of the tied ranks. Ranks are sorted in sequence of variable A.

A correction factor for ties is obtained:

$$T_a = \sum \frac{t(t-1)}{2} \quad \text{for variable A}$$

$$T_b = \sum \frac{t(t-1)}{2} \quad \text{for variable B} \qquad (1)$$

where t = number of observations tied for a given rank

The Kendall rank correlation coefficient is then computed for the following two cases:

(a) if T_a and T_b are zero,

$$\tau = \frac{S}{\frac{1}{2} n (n-1)} \qquad (2)$$

where n = number of ranks

S = total score calculated for ranks in variable B by selecting each rank in turn, adding 1 for each larger rank to its right, subtracting 1 for each smaller rank to its right

(b) if T_a and/or T_b are not zero,

$$\tau = \frac{S}{\sqrt{\frac{1}{2} n (n-1) - T_a}\ \sqrt{\frac{1}{2} n (n-1) - T_b}} \qquad (3)$$

The standard deviation is calculated:

$$s = \sqrt{\frac{2(2n+5)}{9n(n-1)}} \qquad (4)$$

The significance of τ can be measured by

$$z = \frac{\tau}{s} \qquad (5)$$

```
C                                                                       KRAN  10
C     .................................................................KRAN  20
C                                                                       KRAN  30
C        SUBROUTINE KRANK                                               KRAN  40
C                                                                       KRAN  50
C        PURPOSE                                                        KRAN  60
C           TEST CORRELATION BETWEEN TWO VARIABLES BY MEANS OF KENDALL  KRAN  70
C           RANK CORRELATION COEFFICIENT                                KRAN  80
C                                                                       KRAN  90
C        USAGE                                                          KRAN 100
C           CALL KRANK(A,B,R,N,TAU,SD,Z,NR)                             KRAN 110
C                                                                       KRAN 120
C        DESCRIPTION OF PARAMETERS                                      KRAN 130
C           A   - INPUT VECTOR OF N OBSERVATIONS FOR FIRST VARIABLE     KRAN 140
C           B   - INPUT VECTOR OF N OBSERVATIONS FOR SECOND VARIABLE    KRAN 150
C           R   - OUTPUT VECTOR OF RANKED DATA OF LENGTH 2*N. SMALLEST  KRAN 160
C                 OBSERVATION IS RANKED 1, LARGEST IS RANKED N. TIES    KRAN 170
C                 ARE ASSIGNED AVERAGE OF TIED RANKS.                   KRAN 180
C           N   - NUMBER OF OBSERVATIONS                                KRAN 190
C           TAU - KENDALL RANK CORRELATION COEFFICIENT (OUTPUT)         KRAN 200
C           SD  - STANDARD DEVIATION (OUTPUT)                           KRAN 210
C           Z   - TEST OF SIGNIFICANCE OF TAU IN TERMS OF NORMAL        KRAN 220
C                 DISTRIBUTION (OUTPUT)                                 KRAN 230
C           NR  - CODE, 0 FOR UNRANKED DATA IN A AND B, 1 FOR RANKED    KRAN 240
C                 DATA IN A AND B (INPUT)                               KRAN 250
C                                                                       KRAN 260
C        REMARKS                                                        KRAN 270
C           SD AND Z ARE SET TO ZERO IF N IS LESS THAN TEN              KRAN 280
C                                                                       KRAN 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  KRAN 300
C           RANK                                                        KRAN 310
C           TIE                                                         KRAN 320
C                                                                       KRAN 330
C                                                                       KRAN 340
C        METHOD                                                         KRAN 350
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   KRAN 360
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          KRAN 370
C           CHAPTER 9                                                   KRAN 380
C     .................................................................KRAN 390
C                                                                       KRAN 400
      SUBROUTINE KRANK(A,B,R,N,TAU,SD,Z,NR)                             KRAN 410
      DIMENSION A(1),B(1),R(1)                                          KRAN 420
C                                                                       KRAN 430
      SD=0.0                                                            KRAN 440
      Z=0.0                                                             KRAN 450
      FN=N                                                              KRAN 460
      FN1=N*(N-1)                                                       KRAN 470
C                                                                       KRAN 480
C        DETERMINE WHETHER DATA IS RANKED                               KRAN 490
C                                                                       KRAN 500
      IF(NR-1) 5, 10, 5                                                 KRAN 510
C                                                                       KRAN 520
C        RANK DATA IN A AND B VECTORS AND ASSIGN TIED OBSERVATIONS       KRAN 530
C        AVERAGE OF TIED RANKS                                          KRAN 540
C                                                                       KRAN 550
    5 CALL RANK (A,R,N)                                                 KRAN 560
      CALL RANK (B,R(N+1),N)                                            KRAN 570
      GO TO 40                                                          KRAN 580
C                                                                       KRAN 590
C        MOVE RANKED DATA TO R VECTOR                                   KRAN 600
C                                                                       KRAN 610
   10 DO 20 I=1,N                                                       KRAN 620
   20 R(I)=A(I)                                                         KRAN 630
      DO 30 I=1,N                                                       KRAN 640
      J=I+N                                                             KRAN 650
   30 R(J)=B(I)                                                         KRAN 660
C                                                                       KRAN 670
C        SORT RANK VECTOR R IN SEQUENCE OF VARIABLE A                   KRAN 680
C                                                                       KRAN 690
   40 ISORT=0                                                           KRAN 700
      DO 50 I=2,N                                                       KRAN 710
      IF(R(I)-R(I-1)) 45,50,50                                          KRAN 720
   45 ISORT=ISORT+1                                                     KRAN 730
      RSAVE=R(I)                                                        KRAN 740
      R(I)=R(I-1)                                                       KRAN 750
      R(I-1)=RSAVE                                                      KRAN 760
      I2=I+N                                                            KRAN 770
      SAVER=R(I2)                                                       KRAN 780
      R(I2)=R(I2-1)                                                     KRAN 790
      R(I2-1)=SAVER                                                     KRAN 800
   50 CONTINUE                                                          KRAN 810
      IF(ISORT) 40,55,40                                                KRAN 820
C                                                                       KRAN 830
C        COMPUTE S ON VARIABLE B. STARTING WITH THE FIRST RANK, ADD 1   KRAN 840
C        TO S FOR EACH LARGER RANK TO ITS RIGHT AND SUBTRACT 1 FOR EACH KRAN 850
C        SMALLER RANK.  REPEAT FOR ALL RANKS.                           KRAN 860
C                                                                       KRAN 870
   55 S=0.0                                                             KRAN 880
      NM=N-1                                                            KRAN 890
      DO 60 I=1,NM                                                      KRAN 900
      J=N+I                                                             KRAN 910
      DO 60 L=I,N                                                       KRAN 920
      K=N+L                                                             KRAN 930
      IF(R(K)-R(J)) 56,60,57                                            KRAN 940
   56 S=S-1.0                                                           KRAN 950
      GO TO 60                                                          KRAN 960
   57 S=S+1.0                                                           KRAN 970
   60 CONTINUE                                                          KRAN 980
C                                                                       KRAN 990
C        COMPUTE TIED SCORE INDEX FOR BOTH VARIABLES                    KRAN1000
C                                                                       KRAN1010
      KT=2                                                              KRAN1020
      CALL TIE(R,N,KT,TA)                                               KRAN1030
      CALL TIE(R(N+1),N,KT,TB)                                          KRAN1040
C                                                                       KRAN1050
C        COMPUTE TAU                                                    KRAN1060
C                                                                       KRAN1070
      IF(TA) 70,65,70                                                   KRAN1080
   65 IF(TB) 70,67,70                                                   KRAN1090
   67 TAU=S/(0.5*FN1)                                                   KRAN1100
      GO TO 80                                                          KRAN1110
   70 TAU=S/((SQRT(0.5*FN1-TA))*(SQRT(0.5*FN1-TB)))                     KRAN1120
C                                                                       KRAN1130
C     COMPUTE STANDARD DEVIATION AND Z IF N IS 10 OR LARGER             KRAN1140
C                                                                       KRAN1150
   80 IF(N-10) 90,85,85                                                 KRAN1160
   85 SD=(SQRT((2.0*(FN+FN+5.0))/(9.0*FN1)))                            KRAN1170
      Z=TAU/SD                                                          KRAN1180
   90 RETURN                                                            KRAN1190
      END                                                               KRAN1200
```

Subroutine MPAIR

This subroutine performs the Wilcoxon matched-pairs signed-ranks test, given two vectors of n observations of matched samples. The computational steps are as follows:

1. For each matched pair, determine the signed difference (d_j) between the two scores.

2. Rank these d's without respect to sign. In doing so, (a) disregard those d's equal to zero (0), and (b) with tied d's, assign the average of the tied ranks.

3. Affix to each rank the sign (+ or -) of the d in step 1 above.

4. Compute T = the sum of positive ranks or the sum of negative ranks, whichever is smaller.

5. Compute mean:

$$\mu = \frac{K(K+1)}{4} \qquad (1)$$

where K = the total number of d's which are not zero (0).

6. Compute standard deviation:

$$\sigma = \sqrt{\frac{K(K+1)\ (2K+1)}{24}} \qquad (2)$$

7. Compute Z:

$$Z = \frac{T - \mu}{\sigma} \qquad (3)$$

Z is approximately normally distributed with zero mean and unit variance.

8. Compute the probability, p, associated with the value as extreme as Z by the subroutine NDTR.

Note: p is the probability for a one-tailed test; thus for a two-tailed test, the user should double the value of p.

For reference see:

(1) S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 5.

(2) F. Wilcoxon, Some Rapid Approximate Statistical Procedures, American Cyanamid Co., Stamford, Conn., 1949.

```
C                                                                       MPAI  10
C     ...................................................................MPAI  20
C                                                                       MPAI  30
C        SUBROUTINE MPAIR                                               MPAI  40
C                                                                       MPAI  50
C        PURPOSE                                                        MPAI  60
C           PERFORM THE WILCOXON MATCHED-PAIRS SIGNED-RANKS TEST, GIVEN MPAI  70
C           TWO VECTORS OF N OBSERVATIONS OF THE MATCHED SAMPLES.       MPAI  80
C                                                                       MPAI  90
C        USAGE                                                          MPAI 100
C           CALL MPAIR (N,A,B,K,T,Z,P,D,E,L,IE)                         MPAI 110
C                                                                       MPAI 120
C        DESCRIPTION OF PARAMETERS                                      MPAI 130
C           N - NUMBER OF OBSERVATIONS IN THE VECTORS A AND B           MPAI 140
C           A - INPUT VECTOR OF LENGTH N CONTAINING DATA FROM THE FIRST MPAI 150
C               SAMPLE                                                  MPAI 160
C           B - INPUT VECTOR OF LENGTH N CONTAINING DATA FROM THE SECONDMPAI 170
C               SAMPLE                                                  MPAI 180
C           K - OUTPUT VARIABLE CONTAINING THE NUMBER OF PAIRS OF THE   MPAI 190
C               MATCHED SAMPLES WHOSE DIFFERENCES ARE NON ZERO (0)      MPAI 200
C           T - OUTPUT VARIABLE CONTAINING THE SUM OF THE RANKS OF PLUS MPAI 210
C               OR MINUS DIFFERENCES, WHICHEVER IS SMALLER              MPAI 220
C           Z - VALUE OF THE STANDARDIZED NORMAL SCORE COMPUTED FOR THE MPAI 230
C               WILCOXON MATCHED-PAIRS SIGNED-RANKS TEST                MPAI 240
C           P - COMPUTED PROBABILITY OF OBTAINING A VALUE OF Z AS       MPAI 250
C               EXTREME AS THE ONE FOUND BY THE TEST                    MPAI 260
C           D - WORKING VECTOR OF LENGTH N                              MPAI 270
C           E - WORKING VECTOR OF LENGTH N                              MPAI 280
C           L - WORKING VECTOR OF LENGTH N                              MPAI 290
C           IE- 1, IF SAMPLES A AND B ARE IDENTICAL.                    MPAI 300
C               0 OTHERWISE.  IF IE=1, THEN T=P=0, AND Z=-10**75        MPAI 310
C                                                                       MPAI 320
C        REMARKS                                                        MPAI 330
C           THE COMPUTED PROBABILTY IS FOR A ONE-TAILED TEST.           MPAI 340
C           MULTIPLYING P BY 2 WILL GIVE THE VALUE FOR A TWO-TAILED     MPAI 350
C           TEST.                                                       MPAI 360
C                                                                       MPAI 370
C        SUBROUTINES AND FUNCTIONS SUBPROGRAMS REQUIRED                 MPAI 380
C           RANK                                                        MPAI 390
C           NDTR                                                        MPAI 400
C                                                                       MPAI 410
C        METHOD                                                         MPAI 420
C           REFER TO DIXON AND MASSEY, AN INTRODUCTION TO STATISTICAL   MPAI 430
C           ANALYSIS (MC GRAW-HILL, 1957)                               MPAI 440
C                                                                       MPAI 450
C     ...................................................................MPAI 460
C                                                                       MPAI 470
      SUBROUTINE MPAIR (N,A,B,K,T,Z,P,D,E,L,IE)                         MPAI 480
C                                                                       MPAI 490
      DIMENSION A(1),B(1),D(1),E(1),L(1)                                MPAI 500
C                                                                       MPAI 510
      IE=0                                                              MPAI 520
      K=N                                                               MPAI 530
C                                                                       MPAI 540
C        FIND DIFFERENCES OF MATCHED-PAIRS                              MPAI 550
C                                                                       MPAI 560
      BIG=0.0                                                           MPAI 570
      DO 55 I=1,N                                                       MPAI 580
      DIF=A(I)-B(I)                                                     MPAI 590
      IF(DIF) 10, 20, 30                                                MPAI 600
C                                                                       MPAI 610
C        DIFFERENCE HAS A NEGATIVE SIGN (-)                             MPAI 620
C                                                                       MPAI 630
   10 L(I)=1                                                            MPAI 640
      GO TO 40                                                          MPAI 650
C                                                                       MPAI 660
C        DIFFERENCE IS ZERO (0)                                         MPAI 670
C                                                                       MPAI 680
   20 L(I)=2                                                            MPAI 690
      K=K-1                                                             MPAI 700
      GO TO 40                                                          MPAI 710
C                                                                       MPAI 720
C        DIFFERENCE HAS A POSITIVE SIGN (+)                             MPAI 730
C                                                                       MPAI 740
   30 L(I)=3                                                            MPAI 750
C                                                                       MPAI 760
   40 DIF= ABS(DIF)                                                     MPAI 770
      IF(BIG-DIF) 45, 50, 50                                            MPAI 780
   45 BIG=DIF                                                           MPAI 790
   50 D(I)=DIF                                                          MPAI 800
C                                                                       MPAI 810
   55 CONTINUE                                                          MPAI 820
      IF(K) 57,57,59                                                    MPAI 830
   57 IE=1                                                              MPAI 840
      T=0.0                                                             MPAI 850
      Z=-1.0E75                                                         MPAI 860
      P=0                                                               MPAI 870
      GO TO 100                                                         MPAI 880
C                                                                       MPAI 890
C        STORE A LARGE VALUE IN PLACE OF 0 DIFFERENCE IN ORDER TO       MPAI 900
C        ASSIGN A LARGE RANK (LARGER THAN K), SO THAT ABSOLUTE VALUES   MPAI 910
C        OF SIGNED DIFFERENCES WILL BE PROPERLY RANKED                  MPAI 920
C                                                                       MPAI 930
   59 BIG=BIG*2.0                                                       MPAI 940
      DO 65 I=1,N                                                       MPAI 950
      IF(L(I)-2) 65, 60, 65                                             MPAI 960
   60 D(I)=BIG                                                          MPAI 970
   65 CONTINUE                                                          MPAI 980
C                                                                       MPAI 990
      CALL RANK (D,E,N)                                                 MPAI1000
C                                                                       MPAI1010
C        FIND SUMS OF RANKS OF (+) DIFFERENCES AND (-) DIFFERENCES      MPAI1020
C                                                                       MPAI1030
      SUMP=0.0                                                          MPAI1040
      SUMM=0.0                                                          MPAI1050
      DO 80 I=1,N                                                       MPAI1060
      IF(L(I)-2) 70, 80, 75                                             MPAI1070
   70 SUMM=SUMM+E(I)                                                    MPAI1080
      GO TO 80                                                          MPAI1090
   75 SUMP=SUMP+E(I)                                                    MPAI1100
   80 CONTINUE                                                          MPAI1110
C                                                                       MPAI1120
C        SET T = SMALLER SUM                                            MPAI1130
C                                                                       MPAI1140
      IF(SUMP-SUMM) 85, 85, 90                                          MPAI1150
   85 T=SUMP                                                            MPAI1160
      GO TO 95                                                          MPAI1170
   90 T=SUMM                                                            MPAI1180
C                                                                       MPAI1190
C        COMPUTE MEAN, STANDARD DEVIATION, AND Z                        MPAI1200
C                                                                       MPAI1210
   95 FK=K                                                              MPAI1220
      U=FK*(FK+1.0)/4.0                                                 MPAI1230
      S= SQRT((FK*(FK+1.0)*(2.0*FK+1.0))/24.0)                          MPAI1240
      Z=(T-U)/S                                                         MPAI1250
C                                                                       MPAI1260
C        COMPUTE THE PROBABILITY OF A VALUE AS EXTREME AS Z             MPAI1270
C                                                                       MPAI1280
      CALL NDTR (Z,P,BIG)                                               MPAI1290
C                                                                       MPAI1300
  100 RETURN                                                            MPAI1310
      END                                                               MPAI1320
```

Subroutine QTEST

This subroutine determines the Cochran Q-test statistic, given a matrix A of dichotomous data with n rows (sets) and m columns (groups).

Row and column totals are calculated:

$$L_i = \sum_{j=1}^{m} A_{ij} \quad \text{(row totals)} \tag{1}$$

where $i = 1, 2, \ldots, n$

$$G_j = \sum_{i=1}^{n} A_{ij} \quad \text{(column totals)} \tag{2}$$

where $j = 1, 2, \ldots, m$

The Cochran Q statistic is computed:

$$Q = \frac{(m-1)\left[m\sum_{j=1}^{m} G_j^2 - \left(\sum_{j=1}^{m} G_j\right)^2\right]}{m\sum_{i=1}^{n} L_i - \sum_{i=1}^{n} L_i^2} \tag{3}$$

The degrees of freedom are:

$$\text{d.f.} = m - 1 \tag{4}$$

```
C                                                                       QTES  10
C     ..................................................................QTES  20
C                                                                       QTES  30
C        SUBROUTINE QTEST                                               QTES  40
C                                                                       QTES  50
C        PURPOSE                                                        QTES  60
C           TEST WHETHER THREE OR MORE MATCHED GROUPS OF DICHOTOMOUS    QTES  70
C           DATA DIFFER SIGNIFICANTLY BY THE COCHRAN Q-TEST             QTES  80
C                                                                       QTES  90
C        USAGE                                                          QTES 100
C           CALL QTEST(A,N,M,Q,NDF)                                     QTES 110
C                                                                       QTES 120
C        DESCRIPTION OF PARAMETERS                                      QTES 130
C           A   - INPUT MATRIX, N BY M, OF DICHOTOMOUS DATA (0 AND 1)   QTES 140
C           N   - NUMBER OF SETS IN EACH GROUP                          QTES 150
C           M   - NUMBER OF GROUPS                                      QTES 160
C           Q   - COCHRAN Q STATISTIC (OUTPUT)                          QTES 170
C           NDF - NUMBER OF DEGREES OF FREEDOM (OUTPUT)                 QTES 180
C                                                                       QTES 190
C        REMARKS                                                        QTES 200
C           M MUST BE THREE OR GREATER                                  QTES 210
C                                                                       QTES 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QTES 230
C           NONE                                                        QTES 240
C                                                                       QTES 250
C        METHOD                                                         QTES 260
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   QTES 270
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          QTES 280
C           CHAPTER 7                                                   QTES 290
C                                                                       QTES 300
C     ..................................................................QTES 310
C                                                                       QTES 320
      SUBROUTINE QTEST(A,N,M,Q,NDF)                                     QTES 330
      DIMENSION A(1)                                                    QTES 340
C                                                                       QTES 350
C        COMPUTE SUM OF SQUARES OF ROW TOTALS, RSQ, AND GRAND TOTAL OF  QTES 360
C        ALL ELEMENTS, GD                                               QTES 370
C                                                                       QTES 380
      RSQ=0.0                                                           QTES 390
      GD=0.0                                                            QTES 400
      DO 20 I=1,N                                                       QTES 410
      TR=0.0                                                            QTES 420
      IJ=I-N                                                            QTES 430
      DO 10 J=1,M                                                       QTES 440
      IJ=IJ+N                                                           QTES 450
   10 TR=TR+A(IJ)                                                       QTES 460
      GD=GD+TR                                                          QTES 470
   20 RSQ=RSQ+TR*TR                                                     QTES 480
C                                                                       QTES 490
C        COMPUTE SUM OF SQUARES OF COLUMN TOTALS, CSQ                   QTES 500
C                                                                       QTES 510
      CSQ=0.0                                                           QTES 520
      IJ=0                                                              QTES 530
      DO 40 J=1,M                                                       QTES 540
      TC=0.0                                                            QTES 550
      DO 30 I=1,N                                                       QTES 560
      IJ=IJ+1                                                           QTES 570
   30 TC=TC+A(IJ)                                                       QTES 580
   40 CSQ=CSQ+TC*TC                                                     QTES 590
C                                                                       QTES 600
C        COMPUTE COCHRAN Q TEST VALUE                                   QTES 610
C                                                                       QTES 620
      FM=M                                                              QTES 630
      Q=(FM-1.0)*(FM*CSQ-GD*GD)/(FM*GD-RSQ)                             QTES 640
C                                                                       QTES 650
C        FIND DEGREES OF FREEDOM                                        QTES 660
C                                                                       QTES 670
      NDF=M-1                                                           QTES 680
      RETURN                                                            QTES 690
      END                                                               QTES 700
```

Subroutine RANK

```
C                                                                       RANK  10
C     ..................................................................RANK  20
C                                                                       RANK  30
C        SUBROUTINE RANK                                                RANK  40
C                                                                       RANK  50
C        PURPOSE                                                        RANK  60
C           RANK A VECTOR OF VALUES                                     RANK  70
C                                                                       RANK  80
C        USAGE                                                          RANK  90
C           CALL RANK(A,R,N)                                            RANK 100
C                                                                       RANK 110
C        DESCRIPTION OF PARAMETERS                                      RANK 120
C           A - INPUT VECTOR OF N VALUES                                RANK 130
C           R - OUTPUT VECTOR OF LENGTH N. SMALLEST VALUE IS RANKED 1,  RANK 140
C               LARGEST IS RANKED N. TIES ARE ASSIGNED AVERAGE OF TIED  RANK 150
C               RANKS                                                   RANK 160
C           N - NUMBER OF VALUES                                        RANK 170
C                                                                       RANK 180
C        REMARKS                                                        RANK 190
C           NONE                                                        RANK 200
C                                                                       RANK 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RANK 220
C           NONE                                                        RANK 230
C                                                                       RANK 240
C        METHOD                                                         RANK 250
C           VECTOR IS SEARCHED FOR SUCCESSIVELY LARGER ELEMENTS. IF TIESRANK 260
C           OCCUR, THEY ARE LOCATED AND THEIR RANK VALUE COMPUTED.      RANK 270
C           FOR EXAMPLE, IF 2 VALUES ARE TIED FOR SIXTH RANK, THEY ARE  RANK 280
C           ASSIGNED A RANK OF 6.5 (=(6+7)/2)                           RANK 290
C                                                                       RANK 300
C     ..................................................................RANK 310
C                                                                       RANK 320
      SUBROUTINE RANK(A,R,N)                                            RANK 330
      DIMENSION A(1),R(1)                                               RANK 340
C                                                                       RANK 350
C        INITIALIZATION                                                 RANK 360
C                                                                       RANK 370
      DO 10 I=1,N                                                       RANK 380
   10 R(I)=0.0                                                          RANK 390
C                                                                       RANK 400
C        FIND RANK OF DATA                                              RANK 410
C                                                                       RANK 420
      DO 100 I=1,N                                                      RANK 430
C                                                                       RANK 440
C        TEST WHETHER DATA POINT IS ALREADY RANKED                      RANK 450
C                                                                       RANK 460
      IF(R(I)) 20, 20, 100                                              RANK 470
C                                                                       RANK 480
C        DATA POINT TO BE RANKED                                        RANK 490
C                                                                       RANK 500
   20 SMALL=0.0                                                         RANK 510
      EQUAL=0.0                                                         RANK 520
      X=A(I)                                                            RANK 530
      DO 50 J=1,N                                                       RANK 540
      IF(A(J)-X) 30, 40, 50                                             RANK 550
C        COUNT NUMBER OF DATA POINTS WHICH ARE SMALLER                  RANK 560
C                                                                       RANK 570
C                                                                       RANK 580
   30 SMALL=SMALL+1.0                                                   RANK 590
      GO TO 50                                                          RANK 600
C        COUNT NUMBER OF DATA POINTS WHICH ARE EQUAL                    RANK 610
C                                                                       RANK 620
   40 EQUAL=EQUAL+1.0                                                   RANK 630
      R(J)=-1.0                                                         RANK 640
   50 CONTINUE                                                          RANK 650
C                                                                       RANK 660
C        TEST FOR TIE                                                   RANK 670
C                                                                       RANK 680
      IF(EQUAL-1.0) 60, 60, 70                                          RANK 690
C                                                                       RANK 700
C        STORE RANK OF DATA POINT WHERE NO TIE                          RANK 710
C                                                                       RANK 720
   60 R(I)=SMALL+1.0                                                    RANK 730
      GO TO 100                                                         RANK 740
C        CALCULATE RANK OF TIED DATA POINTS                             RANK 750
C                                                                       RANK 760
   70 P=SMALL + (EQUAL + 1.0)*0.5                                       RANK 770
      DO 90 J=1,N                                                       RANK 780
      IF(R(J)+1.0) 90, 80, 90                                           RANK 790
   80 R(J)=P                                                            RANK 800
   90 CONTINUE                                                          RANK 810
  100 CONTINUE                                                          RANK 820
      RETURN                                                            RANK 830
      END                                                               RANK 840
```

Subroutine SIGNT

This subroutine performs a sign test, given two vectors of n observations of two matched samples. The computational steps are as follows:

1. Find the sign of the difference between the two numbers of each pair.

2. Find K = the number of pairs whose differences are not zero (0). Disregard those pairs whose differences are zero (0).

3. Find M = the number of (+) differences or the number of (-) differences, whichever is fewer.

4. If K is less than or equal to 25, the probability associated with a value as small as the observed value of M is given by the binomial distribution as:

$$p = \sum_{i=0}^{M} \binom{K}{i} P^i Q^{K-i} \qquad (1)$$

where $P = Q = 0.5$

$$\binom{K}{i} = \frac{K!}{i!\ (K-i)!}$$

The equation (1) is rewritten to simplify the calculation as follows:

$$p = \frac{\sum_{i=0}^{M} \binom{K}{i}}{2^K} \qquad (2)$$

If K is greater than 25, the probability is calculated by the normal approximation to the binomial distribution as follows:

Mean: $$\mu = KP = \frac{1}{2} K \qquad (3)$$

Standard deviation: $$\sigma = \sqrt{KPQ} = \frac{1}{2}\sqrt{K} \qquad (4)$$

Value of Z: $$Z = \frac{(M+0.5) - \mu}{\sigma} \qquad (5)$$

Then the probability, p, associated with the value as extreme as Z is obtained by the subroutine NDTR.

Note: p computed by this subroutine is the probability for a one-tailed test; thus for a two-tailed test, the user should double the value of p.

For reference see S. Siegel, Nonparametric Statistics for the Behavioral Sciences, McGraw-Hill, New York, 1956, chapter 5.

```
C                                                                       SIGN  10
C     ..................................................................SIGN  20
C                                                                       SIGN  30
C        SUBROUTINE SIGNT                                               SIGN  40
C                                                                       SIGN  50
C        PURPOSE                                                        SIGN  60
C           TO PERFORM A NON-PARAMETRIC SIGN TEST, GIVEN TWO SETS OF    SIGN  70
C           MATCHED OBSERVATIONS.  IT TESTS THE NULL HYPOTHESIS THAT THESIGN  80
C           DIFFERENCES BETWEEN EACH PAIR OF MATCHED OBSERVATIONS HAS A SIGN  90
C           MEDIAN EQUAL TO ZERO.                                       SIGN 100
C                                                                       SIGN 110
C        USAGE                                                          SIGN 120
C           CALL SIGNT (N,A,B,K,M,P,IE)                                 SIGN 130
C                                                                       SIGN 140
C        DESCRIPTION OF PARAMETERS                                      SIGN 150
C           N - NUMBER OF OBSERVATIONS IN SETS A AND B                  SIGN 160
C           A - INPUT VECTOR OF LENGTH N CONTAINING DATA FROM THE FIRST SIGN 170
C               SAMPLE, A                                               SIGN 180
C           B - INPUT VECTOR OF LENGTH N CONTAINING DATA FROM THE SECONDSIGN 190
C               SAMPLE, B                                               SIGN 200
C           K - OUTPUT VARIABLE CONTAINING THE NUMBER OF PAIRS OF       SIGN 210
C               OBSERVATIONS FROM THE TWO SAMPLES WHOSE DIFFERENCES ARE SIGN 220
C               NON-ZERO                                                SIGN 230
C           M - OUTPUT VARIABLE CONTAINING THE NUMBER OF PLUS OR MINUS  SIGN 240
C               DIFFERENCES, WHICHEVER IS FEWER.                        SIGN 250
C           P - COMPUTED PROBABILITY OF AS FEW AS M NUMBER OF PAIRS     SIGN 260
C               HAVING THE SAME SIGN, ASSUMING THAT THE SAMPLES CAME    SIGN 270
C               FROM THE SAME POPULATION.                               SIGN 280
C           IE- 0, IF THERE IS NO ERROR.                                SIGN 290
C               1, IF K IS ZERO.  IN THIS CASE, P IS SET TO 1.0 AND     SIGN 300
C               M TO 0.                                                 SIGN 310
C                                                                       SIGN 320
C        REMARKS                                                        SIGN 330
C           IF K IS LESS THAN OR EQUAL TO 25, THE PROBABILITY WILL BE   SIGN 340
C           COMPUTED USING THE BINOMIAL DISTRIBUTION.  IF K IS GREATER  SIGN 350
C           THAN 25, THE PROBABILITY WILL BE COMPUTED USING THE NORMAL  SIGN 360
C           APPROXIMATION TO THE BINOMIAL DISTRIBUTION.                 SIGN 370
C           P COMPUTED IS THE PROBABILITY FOR A ONE-TAILED TEST.  THUS, SIGN 380
C           FOR A TWO TAILED TEST, DOUBLE THE VALUE FOR P.              SIGN 390
C                                                                       SIGN 400
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SIGN 410
C           NDTR                                                        SIGN 420
C                                                                       SIGN 430
C        METHOD                                                         SIGN 440
C           REFER TO DIXON AND MASSEY, INTRODUCTION TO STATISTICAL      SIGN 450
C           ANALYSIS (MCGRAW-HILL, 1957).                               SIGN 460
C                                                                       SIGN 470
C     ..................................................................SIGN 480
C                                                                       SIGN 490
      SUBROUTINE SIGNT (N,A,B,K,M,P,IE)                                 SIGN 500
C                                                                       SIGN 510
      DIMENSION A(1),B(1)                                               SIGN 520
      DOUBLE PRECISION FN,FD                                            SIGN 530
C                                                                       SIGN 540
C        INITIALIZATION                                                 SIGN 550
C                                                                       SIGN 560
      IE=0                                                              SIGN 570
      K=0                                                               SIGN 580
      MPLUS=0                                                           SIGN 590
      MMINS=0                                                           SIGN 600
C                                                                       SIGN 610
C        FIND (+) OR (-) DIFFERENCE                                     SIGN 620
C                                                                       SIGN 630
      DO 40 I=1,N                                                       SIGN 640
      D=A(I)-B(I)                                                       SIGN 650
      IF(D) 20, 40, 30                                                  SIGN 660
C                                                                       SIGN 670
C        (-) DIFFERENCE                                                 SIGN 680
C                                                                       SIGN 690
   20 K=K+1                                                             SIGN 700
      MMINS=MMINS+1                                                     SIGN 710
      GO TO 40                                                          SIGN 720
C                                                                       SIGN 730
C        (+) DIFFERENCE                                                 SIGN 740
C                                                                       SIGN 750
   30 K=K+1                                                             SIGN 760
      MPLUS=MPLUS+1                                                     SIGN 770
C                                                                       SIGN 780
   40 CONTINUE                                                          SIGN 790
      IF(K) 41,41,42                                                    SIGN 800
   41 IE=1                                                              SIGN 810
      P=1.0                                                             SIGN 820
      M=0                                                               SIGN 830
      GO TO 95                                                          SIGN 840
   42 FK=K                                                              SIGN 850
C                                                                       SIGN 860
C        FIND THE NUMBER OF FEWER SIGNS                                 SIGN 870
C                                                                       SIGN 880
      IF(MPLUS-MMINS) 45, 45, 50                                        SIGN 890
   45 M=MPLUS                                                           SIGN 900
      GO TO 55                                                          SIGN 910
   50 M=MMINS                                                           SIGN 920
C                                                                       SIGN 930
C        TEST WHETHER K IS GREATER THAN 25                              SIGN 940
C                                                                       SIGN 950
   55 IF(K-25) 60, 60, 77                                               SIGN 960
C                                                                       SIGN 970
C        K IS LESS THAN OR EQUAL TO 25                                  SIGN 980
C                                                                       SIGN 990
   60 P=1.0                                                             SIGN1000
      IF(M) 75, 75, 65                                                  SIGN1010
   65 FN=1.0                                                            SIGN1020
      FD=1.0                                                            SIGN1030
      DO 70 I=1,M                                                       SIGN1040
      FI=I                                                              SIGN1050
      FN=FN*(FK-(FI-1.0))                                               SIGN1060
      FD=FD*FI                                                          SIGN1070
   70 P=P+FN/FD                                                         SIGN1080
C                                                                       SIGN1090
   75 P=P/(2.0**K)                                                      SIGN1100
      GO TO 95                                                          SIGN1110
C                                                                       SIGN1120
C        K IS GREATER THAN 25.  COMPUTE MEAN, STANDARD DEVIATION, AND Z SIGN1130
C                                                                       SIGN1140
   77 U=0.5*FK                                                          SIGN1150
      S=0.5*SQRT(FK)                                                    SIGN1160
      FM=M                                                              SIGN1170
      IF(FM-U) 80, 85, 85                                               SIGN1180
   80 CON=0.5                                                           SIGN1190
      GO TO 90                                                          SIGN1200
   85 CON=0.0                                                           SIGN1210
   90 Z=(FM+CON-U)/S                                                    SIGN1220
C                                                                       SIGN1230
C        COMPUTE P ASSOCIATED WITH THE VALUE AS EXTREME AS Z            SIGN1240
C                                                                       SIGN1250
      CALL NDTR (Z,P,D)                                                 SIGN1260
C                                                                       SIGN1270
   95 RETURN                                                            SIGN1280
      END                                                               SIGN1290
```

Subroutine SRANK

This subroutine measures the correlation between two variables by means of the Spearman rank correlation coefficient, given two vectors of n observations for the variables.

The observations on each variable are ranked from 1 to n. Tied observations are assigned the average of the tied ranks.

The sum of squares of rank differences is calculated:

$$D = \sum_{i=1}^{n} (A_i - B_i)^2 \qquad (1)$$

where A_i = first ranked vector

B_i = second ranked vector

n = number of ranks

A correction factor for ties is obtained:

$$T_a = \sum \frac{t^3 - t}{12} \quad \text{over variable A} \qquad (2)$$

$$T_b = \sum \frac{t^3 - t}{12} \quad \text{over variable B}$$

where t = number of observations tied for a given rank

The Spearman rank correlation coefficient is then computed for the following two cases:

(a) if T_a and T_b are zero,

$$r_s = 1 - \frac{6D}{n^3 - n} \qquad (3)$$

(b) if T_a and/or T_b are not zero,

$$r_s = \frac{X + Y - D}{2\sqrt{XY}} \qquad (4)$$

where $X = \frac{n^3 - n}{12} - T_a$ (5)

$$Y = \frac{n^3 - n}{12} - T_b \qquad (6)$$

The statistic used to measure the significance of r_s is:

$$t = r_s \sqrt{\frac{n - 2}{1 - r_s^2}} \qquad (7)$$

The degrees of freedom are:

d.f. = n - 2 (8)

```
C     ..................................................................SRAN  10
C                                                                       SRAN  20
C                                                                       SRAN  30
C        SUBROUTINE SRANK                                               SRAN  40
C                                                                       SRAN  50
C        PURPOSE                                                        SRAN  60
C           TEST CORRELATION BETWEEN TWO VARIABLES BY MEANS OF SPEARMAN SRAN  70
C           RANK CORRELATION COEFFICIENT                                SRAN  80
C                                                                       SRAN  90
C                                                                       SRAN 100
C        USAGE                                                          SRAN 110
C           CALL SRANK(A,B,R,N,RS,T,NDF,NR)                             SRAN 120
C                                                                       SRAN 130
C        DESCRIPTION OF PARAMETERS                                      SRAN 140
C           A   - INPUT VECTOR OF N OBSERVATIONS FOR FIRST VARIABLE     SRAN 150
C           B   - INPUT VECTOR OF N OBSERVATIONS FOR SECOND VARIABLE    SRAN 160
C           R   - OUTPUT VECTOR FOR RANKED DATA, LENGTH IS 2*N. SMALLESTSRAN 170
C                 OBSERVATION IS RANKED 1, LARGEST IS RANKED N. TIES    SRAN 180
C                 ARE ASSIGNED AVERAGE OF TIED RANKS.                   SRAN 190
C           N   - NUMBER OF OBSERVATIONS                                SRAN 200
C           RS  - SPEARMAN RANK CORRELATION COEFFICIENT (OUTPUT)        SRAN 210
C           T   - TEST OF SIGNIFICANCE OF RS (OUTPUT)                   SRAN 220
C           NDF - NUMBER OF DEGREES OF FREEDOM (OUTPUT)                 SRAN 230
C           NR  - CODE, 0 FOR UNRANKED DATA IN A AND B, 1 FOR RANKED    SRAN 240
C                 DATA IN A AND B (INPUT)                               SRAN 250
C                                                                       SRAN 260
C        REMARKS                                                        SRAN 270
C           T IS SET TO ZERO IF N IS LESS THAN TEN                      SRAN 280
C                                                                       SRAN 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SRAN 300
C           RANK                                                        SRAN 310
C           TIE                                                         SRAN 320
C                                                                       SRAN 330
C        METHOD                                                         SRAN 340
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   SRAN 350
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          SRAN 360
C           CHAPTER 9                                                   SRAN 370
C     ..................................................................SRAN 380
      SUBROUTINE SRANK(A,B,R,N,RS,T,NDF,NR)                             SRAN 390
      DIMENSION A(1),B(1),R(1)                                          SRAN 400
C                                                                       SRAN 410
      FNNN=N*N*N-N                                                      SRAN 420
C                                                                       SRAN 430
C        DETERMINE WHETHER DATA IS RANKED                               SRAN 440
C                                                                       SRAN 450
      IF(NR-1) 5, 10, 5                                                 SRAN 460
C                                                                       SRAN 470
C        RANK DATA IN A AND B VECTORS AND ASSIGN TIED OBSERVATIONS       SRAN 480
C        AVERAGE OF TIED RANKS                                          SRAN 490
C                                                                       SRAN 500
    5 CALL RANK (A,R,N)                                                 SRAN 510
      CALL RANK (B,R(N+1),N)                                            SRAN 520
      GO TO 40                                                          SRAN 530
C                                                                       SRAN 540
C        MOVE RANKED DATA TO R VECTOR                                   SRAN 550
C                                                                       SRAN 560
   10 DO 20 I=1,N                                                       SRAN 570
   20 R(I)=A(I)                                                         SRAN 580
      DO 30 I=1,N                                                       SRAN 590
      J=I+N                                                             SRAN 600
   30 R(J)=B(I)                                                         SRAN 610
C                                                                       SRAN 620
C        COMPUTE SUM OF SQUARES OF RANK DIFFERENCES                     SRAN 630
C                                                                       SRAN 640
   40 D=0.0                                                             SRAN 650
      DO 50 I=1,N                                                       SRAN 660
      J=I+N                                                             SRAN 670
   50 D=D+(R(I)-R(J))*(R(I)-R(J))                                       SRAN 680
C                                                                       SRAN 690
C        COMPUTE TIED SCORE INDEX                                       SRAN 700
C                                                                       SRAN 710
      KT=1                                                              SRAN 720
      CALL TIE (R,N,KT,TSA)                                             SRAN 730
      CALL TIE (R(N+1),N,KT,TSB)                                        SRAN 740
C                                                                       SRAN 750
C        COMPUTE SPEARMAN RANK CORRELATION COEFFICIENT                  SRAN 760
C                                                                       SRAN 770
      IF(TSA) 60,55,60                                                  SRAN 780
   55 IF(TSB) 60,57,60                                                  SRAN 790
   57 RS=1.0-6.0*D/FNNN                                                 SRAN 800
      GO TO 70                                                          SRAN 810
   60 X=FNNN/12.0-TSA                                                   SRAN 820
      Y=X+TSA-TSB                                                       SRAN 830
      RS=(X+Y-D)/(2.0*(SQRT(X*Y)))                                      SRAN 840
C                                                                       SRAN 850
C        COMPUTE T AND DEGREES OF FREEDOM IF N IS 10 OR LARGER          SRAN 860
C                                                                       SRAN 870
      T=0.0                                                             SRAN 880
   70 IF(N-10) 80,75,75                                                 SRAN 890
   75 T=RS*SQRT(FLOAT(N-2)/(1.0-RS*RS))                                 SRAN 900
   80 NDF=N-2                                                           SRAN 910
      RETURN                                                            SRAN 920
      END                                                               SRAN 930
                                                                        SRAN 940
```

Subroutine TIE

```
C
C     ..................................................................TIE   10
C                                                                       TIE   20
C        SUBROUTINE TIE                                                 TIE   30
C                                                                       TIE   40
C        PURPOSE                                                        TIE   50
C           CALCULATE CORRECTION FACTOR DUE TO TIES                     TIE   60
C                                                                       TIE   70
C        USAGE                                                          TIE   80
C           CALL TIE(R,N,KT,T)                                          TIE   90
C                                                                       TIE  100
C        DESCRIPTION OF PARAMETERS                                      TIE  110
C           R  - INPUT VECTOR OF RANKS OF LENGTH N CONTAINING VALUES    TIE  120
C                1 TO N                                                 TIE  130
C           N  - NUMBER OF RANKED VALUES                                TIE  140
C           KT - INPUT CODE FOR CALCULATION OF CORRECTION FACTOR        TIE  150
C                      1   SOLVE EQUATION 1                            TIE  160
C                      2   SOLVE EQUATION 2                            TIE  170
C           T  - CORRECTION FACTOR (OUTPUT)                             TIE  180
C                EQUATION 1   T=SUM(CT**3-CT)/12                        TIE  190
C                EQUATION 2   T=SUM(CT*(CT-1)/2)                        TIE  200
C                WHERE CT IS THE NUMBER OF OBSERVATIONS TIED FOR A      TIE  210
C                      GIVEN RANK                                       TIE  220
C                                                                       TIE  230
C        REMARKS                                                        TIE  240
C           NONE                                                        TIE  250
C                                                                       TIE  260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TIE  270
C           NONE                                                        TIE  280
C                                                                       TIE  290
C        METHOD                                                         TIE  300
C           VECTOR IS SEARCHED FOR SUCCESSIVELY LARGER RANKS. TIES ARE  TIE  310
C           COUNTED AND CORRECTION FACTOR 1 OR 2 SUMMED.                TIE  320
C                                                                       TIE  330
C     ..................................................................TIE  340
C                                                                       TIE  350
      SUBROUTINE TIE(R,N,KT,T)                                          TIE  360
      DIMENSION R(1)                                                    TIE  370
C                                                                       TIE  380
C        INITIALIZATION                                                 TIE  390
C                                                                       TIE  400
      T=0.0                                                             TIE  410
      Y=0.0                                                             TIE  420
    5 X=1.0E38                                                          TIE  430
      IND=0                                                             TIE  440
C                                                                       TIE  450
C        FIND NEXT LARGEST RANK                                         TIE  460
C                                                                       TIE  470
      DO 30 I=1,N                                                       TIE  480
      IF(R(I)-Y) 30,30,10                                               TIE  490
   10 IF(R(I)-X) 20,30,30                                               TIE  500
   20 X=R(I)                                                            TIE  510
      IND=IND+1                                                         TIE  520
   30 CONTINUE                                                          TIE  530
C                                                                       TIE  540
C        IF ALL RANKS HAVE BEEN TESTED, RETURN                          TIE  550
C                                                                       TIE  560
      IF(IND) 90,90,40                                                  TIE  570
   40 Y=X                                                               TIE  580
      CT=0.0                                                            TIE  590
C                                                                       TIE  600
C        COUNT TIES                                                     TIE  610
C                                                                       TIE  620
      DO 60 I=1,N                                                       TIE  630
      IF(R(I)-X) 60,50,60                                               TIE  640
   50 CT=CT+1.0                                                         TIE  650
   60 CONTINUE                                                          TIE  660
C                                                                       TIE  670
C        CALCULATE CORRECTION FACTOR                                    TIE  680
C                                                                       TIE  690
      IF(CT) 70,5,70                                                    TIE  700
   70 IF(KT-1) 75,80,75                                                 TIE  710
   75 T=T+CT*(CT-1.)/2.0                                                TIE  720
      GO TO 5                                                           TIE  730
   80 T=T+(CT*CT*CT-CT)/12.0                                            TIE  740
      GO TO 5                                                           TIE  750
   90 RETURN                                                            TIE  760
      END                                                               TIE  770
                                                                        TIE  780
```

Subroutine TWOAV

This subroutine determines the Friedman two-way analysis of variance statistic, given a matrix A with n rows (groups) and m columns (cases). Data in each group is ranked from 1 to m. Tied observations are assigned the average of the tied ranks.

The sum of ranks is calculated:

$$R_j = \sum_{i=1}^{n} A_{ij} \qquad (1)$$

Friedman's statistic is then computed:

$$\chi_r^2 = \frac{12}{nm(m+1)} \sum_{j=1}^{m} (R_j)^2 - 3n(m+1) \qquad (2)$$

The degrees of freedom are:

$$d.f. = m - 1 \qquad (3)$$

```
C                                                                       TWOA  10
C     ..................................................................TWOA  20
C                                                                       TWOA  30
C        SUBROUTINE TWOAV                                               TWOA  40
C                                                                       TWOA  50
C        PURPOSE                                                        TWOA  60
C           TEST WHETHER A NUMBER OF SAMPLES ARE FROM THE SAME          TWOA  70
C           POPULATION BY THE FRIEDMAN TWO-WAY ANALYSIS OF VARIANCE TESTTWOA  80
C                                                                       TWOA  90
C        USAGE                                                          TWOA 100
C           CALL TWOAV(A,R,N,M,W,XR,NDF,NR)                             TWOA 110
C                                                                       TWOA 120
C        DESCRIPTION OF PARAMETERS                                      TWOA 130
C           A   - INPUT MATRIX, N BY M, OF ORIGINAL DATA                TWOA 140
C           R   - OUTPUT MATRIX, N BY M, OF RANKED DATA                 TWOA 150
C           N   - NUMBER OF GROUPS                                      TWOA 160
C           M   - NUMBER OF CASES IN EACH GROUP                         TWOA 170
C           W   - WORK AREA OF LENGTH 2*M                               TWOA 180
C           XR  - FRIEDMAN STATISTIC (OUTPUT)                           TWOA 190
C           NDF - NUMBER OF DEGREES OF FREEDOM (OUTPUT)                 TWOA 200
C           NR  - CODE, 0 FOR UNRANKED DATA IN A, 1 FOR RANKED DATA     TWOA 210
C                 IN A (INPUT)                                          TWOA 220
C                                                                       TWOA 230
C        REMARKS                                                        TWOA 240
C           NONE                                                        TWOA 250
C                                                                       TWOA 260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TWOA 270
C           RANK                                                        TWOA 280
C                                                                       TWOA 290
C        METHOD                                                         TWOA 300
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   TWOA 310
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          TWOA 320
C           CHAPTER 7                                                   TWOA 330
C                                                                       TWOA 340
C     ..................................................................TWOA 350
      SUBROUTINE TWOAV (A,R,N,M,W,XR,NDF,NR)                            TWOA 360
      DIMENSION A(1),R(1),W(1)                                          TWOA 370
C                                                                       TWOA 380
C        DETERMINE WHETHER DATA IS RANKED                               TWOA 390
C                                                                       TWOA 400
      IF(NR-1) 10, 30, 10                                               TWOA 410
C                                                                       TWOA 420
C        RANK DATA IN EACH GROUP AND ASSIGN TIED OBSERVATIONS AVERAGE   TWOA 430
C        OF TIED RANK                                                   TWOA 440
C                                                                       TWOA 450
   10 DO 20 I=1,N                                                       TWOA 460
      IJ=I-N                                                            TWOA 470
      IK=IJ                                                             TWOA 480
      DO 15 J=1,M                                                       TWOA 490
      IJ=IJ+N                                                           TWOA 500
   15 W(J)=A(IJ)                                                        TWOA 510
      CALL RANK (W,W(M+1),M)                                            TWOA 520
      DO 20 J=1,M                                                       TWOA 530
      IK=IK+N                                                           TWOA 540
      IW=M+J                                                            TWOA 550
   20 R(IK)=W(IW)                                                       TWOA 560
      GO TO 35                                                          TWOA 570
   30 NM=N*M                                                            TWOA 580
      DO 32 I=1,NM                                                      TWOA 590
   32 R(I)=A(I)                                                         TWOA 600
C                                                                       TWOA 610
C        CALCULATE SUM OF SQUARES OF SUMS OF RANKS                      TWOA 620
C                                                                       TWOA 630
   35 RTSQ=0.0                                                          TWOA 640
      IR=0                                                              TWOA 650
      DO 50 J=1,M                                                       TWOA 660
      RT=0.0                                                            TWOA 670
      DO 40 I=1,N                                                       TWOA 680
      IR=IR+1                                                           TWOA 690
   40 RT=RT+R(IR)                                                       TWOA 700
   50 RTSQ=RTSQ+RT*RT                                                   TWOA 710
C                                                                       TWOA 720
C        CALCULATE FRIEDMAN TEST VALUE, XR                              TWOA 730
C                                                                       TWOA 740
      FNM=N*(M+1)                                                       TWOA 750
      FM=M                                                              TWOA 760
      XR=(12.0/(FM*FNM))*RTSQ-3.0*FNM                                   TWOA 770
C                                                                       TWOA 780
C        FIND DEGREES OF FREEDOM                                        TWOA 790
C                                                                       TWOA 800
      NDF=M-1                                                           TWOA 810
      RETURN                                                            TWOA 820
      END                                                               TWOA 830
                                                                        TWOA 840
```

Subroutine UTEST

This subroutine tests whether two independent groups are from the same population by means of the Mann-Whitney U-test, given an input vector A with the smaller group preceding the larger group. The scores for both groups are ranked together in ascending order. Tied observations are assigned the average of the tied ranks.

The sum of ranks in the larger group, R2, is calculated. The U statistic is then computed as follows:

$$U' = n_1 n_2 + \frac{n_2 (n_2 + 1)}{2} - R_2 \qquad (1)$$

where n_1 = number of cases in smaller group

n_2 = number of cases in larger group

$U = n_1 n_2 - U'$

if $U' < U$, set $U = U'$ (2)

A correction factor for ties is obtained:

$$T = \sum \frac{t^3 - t}{12} \qquad (3)$$

where t = number of observations tied for a given rank

The standard deviation is computed for two cases:

(a) if $T = 0$

$$s = \sqrt{\frac{n_1 n_2 (n_1 + n_2 + 1)}{12}} \qquad (4)$$

(b) if $T > 0$

$$s = \sqrt{\left(\frac{n_1 n_2}{N(N-1)}\right)\left(\frac{N^3 - N}{12} - T\right)} \qquad (5)$$

where N = total number of cases $(n_1 + n_2)$

The significance of U can be measured by

$$Z = \frac{U - \overline{X}}{s} \qquad (6)$$

where $\overline{X}$ = mean $= \frac{n_1 n_2}{2}$

Z is set to zero if n_2 is less than 20.

```
C                                                                       UTES  10
C     ..................................................................UTES  20
C                                                                       UTES  30
C        SUBROUTINE UTEST                                               UTES  40
C                                                                       UTES  50
C        PURPOSE                                                        UTES  60
C           TEST WHETHER TWO INDEPENDENT GROUPS ARE FROM THE SAME       UTES  70
C           POPULATION BY MEANS OF MANN-WHITNEY U-TEST                  UTES  80
C                                                                       UTES  90
C        USAGE                                                          UTES 100
C           CALL UTEST(A,R,N1,N2,U,Z,IER)                               UTES 110
C                                                                       UTES 120
C        DESCRIPTION OF PARAMETERS                                      UTES 130
C           A  - INPUT VECTOR OF CASES CONSISTING OF TWO INDEPENDENT    UTES 140
C                GROUPS . SMALLER GROUP PRECEDES LARGER GROUP. LENGTH   UTES 150
C                IS N1+N2.                                              UTES 160
C           R  - OUTPUT VECTOR OF RANKS. SMALLEST VALUE IS RANKED 1,    UTES 170
C                LARGEST IS RANKED N. TIES ARE ASSIGNED AVERAGE OF TIED UTES 180
C                RANKS. LENGTH IS N1+N2.                                UTES 190
C           N1 - NUMBER OF CASES IN SMALLER GROUP                       UTES 200
C           N2 - NUMBER OF CASES IN LARGER GROUP                        UTES 210
C           U  - STATISTIC USED TO TEST HOMOGENEITY OF THE TWO          UTES 220
C                GROUPS (OUTPUT)                                        UTES 230
C           Z  - MEASURE OF SIGNIFICANCE OF U IN TERMS OF NORMAL        UTES 240
C                DISTRIBUTION (OUTPUT)                                  UTES 250
C           IER- 0, IF NO ERROR.                                        UTES 251
C                1, IF ALL VALUES OF ONE GROUP ARE TIED.                UTES 252
C                                                                       UTES 260
C        REMARKS                                                        UTES 270
C           Z IS SET TO ZERO IF N2 IS LESS THAN 20                      UTES 280
C                                                                       UTES 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  UTES 300
C           RANK                                                        UTES 310
C           TIE                                                         UTES 320
C                                                                       UTES 330
C        METHOD                                                         UTES 340
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   UTES 350
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          UTES 360
C           CHAPTER 6                                                   UTES 370
C                                                                       UTES 380
C     ..................................................................UTES 390
C                                                                       UTES 400
      SUBROUTINE UTEST(A,R,N1,N2,U,Z)                                   UTES 410
      DIMENSION A(1),R(1)                                               UTES 420
C                                                                       UTES 430
C        RANK SCORES FROM BOTH GROUP TOGETHER IN ASCENDING ORDER, AND   UTES 440
C        ASSIGN TIED OBSERVATIONS AVERAGE OF TIED RANKS                 UTES 450
C                                                                       UTES 460
      N=N1+N2                                                           UTES 470
      CALL RANK(A,R,N)                                                  UTES 480
      Z=0.0                                                             UTES 490
C                                                                       UTES 500
C        SUM RANKS IN LARGER GROUP                                      UTES 510
C                                                                       UTES 520
      R2=0.0                                                            UTES 530
      NF=N1+1                                                           UTES 540
      DO 1C I=NF,N                                                      UTES 550
   1C R2=R2+R(I)                                                        UTES 560
C                                                                       UTES 570
C        CALCULATE U                                                    UTES 580
C                                                                       UTES 590
      FNX=N1*N2                                                         UTES 600
      FN=N                                                              UTES 610
      FN2=N2                                                            UTES 620
      LF=FNX+FN2*((FN2+1.0)/2.0)-R2                                     UTES 630
      U=FNX-LF                                                          UTES 640
      IF(U-LF) 2C,2C,2C                                                 UTES 650
   2C U=LF                                                              UTES 660
C                                                                       UTES 670
C        TEST FOR N2 LESS THAN 20                                       UTES 680
C                                                                       UTES 690
   3C IF(N2-2C) 8C,4C,4C                                                UTES 700
C                                                                       UTES 710
C        COMPUTE STANDARD DEVIATION                                     UTES 720
C                                                                       UTES 730
                                                                        UTES 740
   4C KT=1                                                              UTES 750
      CALL TIE(R,N,KT,TS)                                               UTES 760
      IF(TS) 5C,6C,5C                                                   UTES 761
   5C IF (TS-(FN*FN*FN-FN)/12)52,51,52                                  UTES 762
   51 IER=1                                                             UTES 763
      GO TO 8C                                                          UTES 770
   52 S=SQRT((FNX/(FN*(FN-1.0)))*(((FN*FN*FN-FN)/12.0)-TS))             UTES 780
      GO TO 7C                                                          UTES 790
   6C S=SQRT((FN)*(FN+1.0)/12.0)                                        UTES 800
C                                                                       UTES 810
C        COMPUTE Z                                                      UTES 820
C                                                                       UTES 830
   7C Z=(U-FN)*0.5)/S                                                   UTES 840
   8C RETURN                                                            UTES 850
      END
```

Subroutine WTEST

This subroutine computes the Kendall coefficient of concordance, given a matrix A of n rows (variables) and m columns (cases). The observations on all variables are ranked from 1 to m. Tied observations are assigned the average of the tied ranks.

A correction factor for ties is obtained:

$$T = \sum_{i=1}^{n} \frac{t^3 - t}{12} \qquad (1)$$

where t = number of observations tied for a given rank

Sums of ranks are calculated:

$$Y_j = \sum_{i=1}^{n} R_{ij} \qquad (2)$$

where j = 1, 2, . . . , m

From these, the mean of sums of ranks is found:

$$\bar{R} = \frac{\sum_{j=1}^{m} Y_j}{m} \qquad (3)$$

The sum of squares of deviations is derived:

$$s = \sum_{j=1}^{m} (Y_j - \bar{R})^2 \qquad (4)$$

The Kendall coefficient of concordance is then computed:

$$W = \frac{s}{\frac{1}{12} n^2 (m^3 - m) - n T} \qquad (5)$$

For m larger than 7, chi-square is:

$$\chi^2 = n (m - 1) W \qquad (6)$$

The degrees of freedom are:

$$\text{d.f.} = n - 1 \qquad (7)$$

```
C                                                                       WTES  10
C     ...............................................................   WTES  20
C                                                                       WTES  30
C        SUBROUTINE WTEST                                               WTES  40
C                                                                       WTES  50
C        PURPOSE                                                        WTES  60
C           TEST DEGREE OF ASSOCIATION AMONG A NUMBER OF VARIABLES BY   WTES  70
C           THE KENDALL COEFFICIENT OF CONCORDANCE                      WTES  80
C                                                                       WTES  90
C        USAGE                                                          WTES 100
C           CALL WTEST(A,R,N,M,WA,W,CS,NDF,NR)                          WTES 110
C                                                                       WTES 120
C        DESCRIPTION OF PARAMETERS                                      WTES 130
C           A   - INPUT MATRIX, N BY M, OF ORIGINAL DATA                WTES 140
C           R   - OUTPUT MATRIX, N BY M, OF RANKED DATA.SMALLEST VALUE  WTES 150
C                 IS RANKED 1, LARGEST IS RANKED N. TIES ARE ASSIGNED   WTES 160
C                 AVERAGE OF TIED RANKS                                 WTES 170
C           N   - NUMBER OF VARIABLES                                   WTES 180
C           M   - NUMBER OF CASES                                       WTES 190
C           WA  - WORK AREA VECTOR OF LENGTH 2*M                        WTES 200
C           W   - KENDALL COEFFICIENT OF CONCORDANCE(OUTPUT)            WTES 210
C           CS  - CHI-SQUARE (OUTPUT)                                   WTES 220
C           NDF - NUMBER OF DEGREES OF FREEDOM (OUTPUT)                 WTES 230
C           NR  - CODE, 2 FOR UNRANKED DATA IN A, 1 FOR RANKED DATA     WTES 240
C                 IN A (INPUT)                                          WTES 250
C                                                                       WTES 260
C        REMARKS                                                        WTES 270
C           CHI-SQUARE IS SET TO ZERO IF M IS 7 OR SMALLER              WTES 280
C                                                                       WTES 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  WTES 300
C           RANK                                                        WTES 310
C           TIE                                                         WTES 320
C                                                                       WTES 330
C        METHOD                                                         WTES 340
C           DESCRIBED IN S. SIEGEL, 'NONPARAMETRIC STATISTICS FOR THE   WTES 350
C           BEHAVIORAL SCIENCES', MCGRAW-HILL, NEW YORK, 1956,          WTES 360
C           CHAPTER 9                                                   WTES 370
C     ...............................................................   WTES 380
C                                                                       WTES 390
      SUBROUTINE WTEST (A,R,N,M,WA,W,CS,NDF,NR)                         WTES 400
      DIMENSION A(1),R(1),WA(1)                                         WTES 410
C                                                                       WTES 420
      FN=M                                                              WTES 430
      FN=N                                                              WTES 440
C                                                                       WTES 450
C        DETERMINE WHETHER DATA IS RANKED                               WTES 460
C        RANK DATA FOR ALL VARIABLES ASSIGNING TIED OBSERVATIONS AVERAGEWTES 470
C        OF TIED RANKS AND COMPUTE CORRECTION FOR TIED SCORES           WTES 480
C                                                                       WTES 490
      T=0.0                                                             WTES 500
      KT=1                                                              WTES 510
      DO 20 I=1,N                                                       WTES 520
      IJ=I-N                                                            WTES 530
      IK=IJ                                                             WTES 540
      IF(NR-1) 3,2,5                                                    WTES 550
    2 DO 4 J=1,M                                                        WTES 560
      IJ=IJ+N                                                           WTES 570
      K=M+J                                                             WTES 580
    4 WA(K)=A(IJ)                                                       WTES 590
      GO TO 15                                                          WTES 600
    5 DO 10 J=1,M                                                       WTES 610
      IJ=IJ+N                                                           WTES 620
   10 WA(J)=A(IJ)                                                       WTES 630
      CALL RANK(WA,WA(M+1),M)                                           WTES 640
   15 CALL TIE(WA(M+1),M,KT,TI)                                         WTES 650
      T=T+TI                                                            WTES 660
      DO 20 J=1,M                                                       WTES 670
      IK=IK+N                                                           WTES 680
      IM=M+J                                                            WTES 690
   20 R(IK)=WA(IM)                                                      WTES 700
C                                                                       WTES 710
C        CALCULATE VECTOR OF SUMS OF RANKS                              WTES 720
C                                                                       WTES 730
      IR=0                                                              WTES 740
      DO 40 J=1,M                                                       WTES 750
      WA(J)=0.0                                                         WTES 760
      DO 40 I=1,N                                                       WTES 770
      IR=IR+1                                                           WTES 780
   40 WA(J)=WA(J)+R(IR)                                                 WTES 790
C                                                                       WTES 800
C        COMPUTE MEAN OF SUMS OF RANKS                                  WTES 810
C                                                                       WTES 820
      SM=0.0                                                            WTES 830
      DO 50 J=1,M                                                       WTES 840
   50 SM=SM+WA(J)                                                       WTES 850
      SM=SM/FM                                                          WTES 860
C                                                                       WTES 870
C        COMPUTE SUM OF SQUARES OF DEVIATIONS                           WTES 880
C                                                                       WTES 890
      S=0.0                                                             WTES 900
      DO 60 J=1,M                                                       WTES 910
   60 S=S+(WA(J)-SM)*(WA(J)-SM)                                         WTES 920
C                                                                       WTES 930
C        COMPUTE W                                                      WTES 940
C                                                                       WTES 950
      W=S/(((FN*FN)*(FM*FM*FM-FM)/12.0)-FN*T)                           WTES 960
C                                                                       WTES 970
C        COMPUTE DEGREES OF FREEDOM AND CHI-SQUARE IF M IS OVER 7       WTES 980
C                                                                       WTES 990
      CS=0.0                                                            WTES1000
      NDF=0                                                             WTES1010
      IF(M-7) 70,70,65                                                  WTES1020
   65 CS=FN*(FM-1.0)*W                                                  WTES1030
      NDF=M-1                                                           WTES1040
   70 RETURN                                                            WTES1050
      END                                                               WTES1060
```

Generation of Random Variates; Distribution Functions

Generators

Subroutine RANDU

```
C                                                                       RAND  10
C     ..................................................................RAND  20
C                                                                       RAND  30
C        SUBROUTINE RANDU                                               RAND  40
C                                                                       RAND  50
C        PURPOSE                                                        RAND  60
C           COMPUTES UNIFORMLY DISTRIBUTED RANDOM REAL NUMBERS BETWEEN  RAND  70
C           0 AND 1.0 AND RANDOM INTEGERS BETWEEN ZERO AND              RAND  80
C           2**31.  EACH ENTRY USES AS INPUT AN INTEGER RANDOM NUMBER   RAND  90
C           AND PRODUCES A NEW INTEGER AND REAL RANDOM NUMBER.          RAND 100
C                                                                       RAND 110
C        USAGE                                                          RAND 120
C           CALL RANDU(IX,IY,YFL)                                       RAND 130
C                                                                       RAND 140
C        DESCRIPTION OF PARAMETERS                                      RAND 150
C           IX - FOR THE FIRST ENTRY THIS MUST CONTAIN ANY ODD INTEGER  RAND 160
C                NUMBER WITH NINE OR LESS DIGITS. AFTER THE FIRST ENTRY,RAND 170
C                IX SHOULD BE THE PREVIOUS VALUE OF IY COMPUTED BY THIS RAND 180
C                SUBROUTINE.                                            RAND 190
C           IY - A RESULTANT INTEGER RANDOM NUMBER REQUIRED FOR THE NEXTRAND 200
C                ENTRY TO THIS SUBROUTINE. THE RANGE OF THIS NUMBER IS  RAND 210
C                BETWEEN ZERO AND 2**31                                 RAND 220
C           YFL- THE RESULTANT UNIFORMLY DISTRIBUTED, FLOATING POINT,   RAND 230
C                RANDOM NUMBER IN THE RANGE 0 TO 1.0                    RAND 240
C                                                                       RAND 250
C        REMARKS                                                        RAND 260
C           THIS SUBROUTINE IS SPECIFIC TO SYSTEM/360 AND WILL PRODUCE  RAND 270
C           2**29 TERMS BEFORE REPEATING.  THE REFERENCE BELOW DISCUSSESRAND 280
C           SEEDS (65539 HERE), RUN PROBLEMS, AND PROBLEMS CONCERNING   RAND 290
C           RANDOM DIGITS USING THIS GENERATION SCHEME.  MACLAREN AND   RAND 300
C           MARSAGLIA, JACM 12, P. 83-89, DISCUSS CONGRUENTIAL          RAND 310
C           GENERATION METHODS AND TESTS.  THE USE OF TWO GENERATORS OF RAND 320
C           THE RANDU TYPE, ONE FILLING A TABLE AND ONE PICKING FROM THERAND 330
C           TABLE, IS OF BENEFIT IN SOME CASES.  65549 HAS BEEN         RAND 340
C           SUGGESTED AS A SEED WHICH HAS BETTER STATISTICAL PROPERTIES RAND 350
C           FOR HIGH ORDER BITS OF THE GENERATED DEVIATE.               RAND 360
C           SEEDS SHOULD BE CHOSEN IN ACCORDANCE WITH THE DISCUSSION    RAND 370
C           GIVEN IN THE REFERENCE BELOW.  ALSO, IT SHOULD BE NOTED THATRAND 380
C           IF FLOATING POINT RANDOM NUMBERS ARE DESIRED, AS ARE        RAND 390
C           AVAILABLE FROM RANDU, THE RANDOM CHARACTERISTICS OF THE     RAND 400
C           FLOATING POINT DEVIATES ARE MODIFIED AND IN FACT THESE      RAND 410
C           DEVIATES HAVE HIGH PROBABILITY OF HAVING A TRAILING LOW     RAND 420
C           ORDER ZERO BIT IN THEIR FRACTIONAL PART.                    RAND 430
C                                                                       RAND 440
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RAND 450
C           NONE                                                        RAND 460
C                                                                       RAND 470
C        METHOD                                                         RAND 480
C           POWER RESIDUE METHOD DISCUSSED IN IBM MANUAL C20-8011,      RAND 490
C           RANDOM NUMBER GENERATION AND TESTING                        RAND 500
C                                                                       RAND 510
C     ..................................................................RAND 520
C                                                                       RAND 530
      SUBROUTINE RANDU(IX,IY,YFL)                                       RAND 540
      IY=IX*65539                                                       RAND 550
      IF(IY)5,6,6                                                       RAND 560
    5 IY=IY+2147483647+1                                                RAND 570
    6 YFL=IY                                                            RAND 580
      YFL=YFL*.4656613E-9                                               RAND 590
      RETURN                                                            RAND 600
      END                                                               RAND 610
```

Subroutine GAUSS

This subroutine computes a normally distributed random number with a given mean and standard deviation.

An approximation to normally distributed random numbers Y can be found from a sequence of uniform random numbers† using the formula:

$$Y = \frac{\sum_{i=1}^{K} X_i - \frac{K}{2}}{\sqrt{K/12}} \qquad (1)$$

where X_i is a uniformly distributed random number, $0 < X_i < 1$

K is the number of values X_i to be used

Y approaches a true normal distribution asymptotically as K approaches infinity. For this subroutine, K was chosen as 12 to reduce execution time. Equation (1) thus becomes:

$$Y = \sum_{i=1}^{12} X_i - 6.0$$

The adjustment for the required mean and standard deviation is then:

$$Y' = Y * S + AM \qquad (2)$$

where Y' is the required normally distributed random number

S is the required standard deviation

AM is the required mean

```
C                                                                       GAUS  10
C     ..................................................................GAUS  20
C                                                                       GAUS  30
C        SUBROUTINE GAUSS                                               GAUS  40
C                                                                       GAUS  50
C        PURPOSE                                                        GAUS  60
C           COMPUTES A NORMALLY DISTRIBUTED RANDOM NUMBER WITH A GIVEN  GAUS  70
C           MEAN AND STANDARD DEVIATION                                 GAUS  80
C                                                                       GAUS  90
C        USAGE                                                          GAUS 100
C           CALL GAUSS(IX,S,AM,V)                                       GAUS 110
C                                                                       GAUS 120
C        DESCRIPTION OF PARAMETERS                                      GAUS 130
C           IX -IX MUST CONTAIN AN ODD INTEGER NUMBER WITH NINE OR      GAUS 140
C               LESS DIGITS ON THE FIRST ENTRY TO GAUSS. THEREAFTER     GAUS 150
C               IT WILL CONTAIN A UNIFORMLY DISTRIBUTED INTEGER RANDOM  GAUS 160
C               NUMBER GENERATED BY THE SUBROUTINE FOR USE ON THE NEXT  GAUS 170
C               ENTRY TO THE SUBROUTINE.                                GAUS 180
C           S  -THE DESIRED STANDARD DEVIATION OF THE NORMAL            GAUS 190
C               DISTRIBUTION.                                           GAUS 200
C           AM -THE DESIRED MEAN OF THE NORMAL DISTRIBUTION             GAUS 210
C           V  -THE VALUE OF THE COMPUTED NORMAL RANDOM VARIABLE        GAUS 220
C                                                                       GAUS 230
C        REMARKS                                                        GAUS 240
C           THIS SUBROUTINE USES RANDU WHICH IS MACHINE SPECIFIC        GAUS 250
C                                                                       GAUS 260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GAUS 270
C           RANDU                                                       GAUS 280
C                                                                       GAUS 290
C        METHOD                                                         GAUS 300
C           USES 12 UNIFORM RANDOM NUMBERS TO COMPUTE NORMAL RANDOM     GAUS 310
C           NUMBERS BY CENTRAL LIMIT THEOREM. THE RESULT IS THEN        GAUS 320
C           ADJUSTED TO MATCH THE GIVEN MEAN AND STANDARD DEVIATION.    GAUS 330
C           THE UNIFORM RANDOM NUMBERS COMPUTED WITHIN THE SUBROUTINE   GAUS 340
C           ARE FOUND BY THE POWER RESIDUE METHOD.                      GAUS 350
C                                                                       GAUS 360
C     ..................................................................GAUS 370
C                                                                       GAUS 380
      SUBROUTINE GAUSS(IX,S,AM,V)                                       GAUS 390
      A=0.0                                                             GAUS 400
      DO 50 I=1,12                                                      GAUS 410
      CALL RANDU(IX,IY,Y)                                               GAUS 420
      IX=IY                                                             GAUS 430
   50 A=A+Y                                                             GAUS 440
      V=(A-6.0)*S+AM                                                    GAUS 450
      RETURN                                                            GAUS 460
      END                                                               GAUS 470
```

† R. W. Hamming, Numerical Methods for Scientists and Engineers, McGraw-Hill, N.Y., 1962, pages 34 and 389.

Distribution Functions

Subroutine NDTR

This subroutine computes y = P(x) = Prob ($X \le x$), where X is a random variable distributed normally with mean zero and variance one.

$$P(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-u^2/2)du$$

The following approximation† is used:

$$P(x) = 1 - f(x) \sum_{i=1}^{5} a_i w^i ; \quad x \ge 0$$

where:

$$w = 1/(1 + px)$$

$$f(x) = \exp(-x^2/2) / \sqrt{2\pi}$$

$$P = 0.2316419$$

$$a_1 = 0.3193815$$

$$a_2 = -0.3565638$$

$$a_3 = 1.781478$$

$$a_4 = -1.821256$$

$$a_5 = 1.330274$$

The maximum error is $7(10^{-7})$; f(x) is also presented in output.

†C. Hastings, Approximations for Digital Computers. Princeton University Press, Princeton, N.J., 1955.
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. Dover Publications, Inc., N.Y., equation 26.2.17.

```
C                                                                       NDTR  10
C.....................................................................NDTR  20
C                                                                       NDTR  30
C       SUBROUTINE NDTR                                                 NDTR  40
C                                                                       NDTR  50
C       PURPOSE                                                         NDTR  60
C          COMPUTES Y = P(X) = PROBABILITY THAT THE RANDOM VARIABLE  U,NDTR  70
C          DISTRIBUTED NORMALLY(0,1), IS LESS THAN OR EQUAL TO X.       NDTR  80
C          F(X), THE ORDINATE OF THE NORMAL DENSITY AT X, IS ALSO       NDTR  90
C          COMPUTED.                                                    NDTR 100
C                                                                       NDTR 110
C       USAGE                                                           NDTR 120
C          CALL NDTR(X,P,D)                                             NDTR 130
C                                                                       NDTR 140
C       DESCRIPTION OF PARAMETERS                                       NDTR 150
C          X--INPUT SCALAR FOR WHICH P(X) IS COMPUTED.                  NDTR 160
C          P--OUTPUT PROBABILITY.                                       NDTR 170
C          D--OUTPUT DENSITY.                                           NDTR 180
C                                                                       NDTR 190
C       REMARKS                                                         NDTR 200
C          MAXIMUM ERROR IS 0.0000007.                                  NDTR 210
C                                                                       NDTR 220
C       SUBROUTINES AND SUBPROGRAMS REQUIRED                            NDTR 230
C          NONE                                                         NDTR 240
C                                                                       NDTR 250
C       METHOD                                                          NDTR 260
C          BASED ON APPROXIMATIONS IN C. HASTINGS, APPROXIMATIONS FOR   NDTR 270
C          DIGITAL COMPUTERS, PRINCETON UNIV. PRESS, PRINCETON, N.J.,   NDTR 280
C          1955.  SEE EQUATION 26.2.17, HANDBOOK OF MATHEMATICAL        NDTR 290
C          FUNCTIONS, ABRAMOWITZ AND STEGUN, DOVER PUBLICATIONS, INC.,  NDTR 300
C          NEW YORK.                                                    NDTR 310
C                                                                       NDTR 320
C.....................................................................NDTR 330
C                                                                       NDTR 340
      SUBROUTINE NDTR(X,P,D)                                            NDTR 350
C                                                                       NDTR 360
      AX=ABS(X)                                                         NDTR 370
      T=1.0/(1.0+.2316419*AX)                                           NDTR 380
      D=0.3989423*EXP(-X*X/2.0)                                         NDTR 390
      P = 1.0 - D*T*(((((1.330274*T - 1.821256)*T + 1.781478)*T -       NDTR 400
     1  0.3565638)*T + 0.3193815)                                       NDTR 410
      IF(X)1,2,2                                                        NDTR 420
    1 P=1.0-P                                                           NDTR 430
    2 RETURN                                                            NDTR 440
      END                                                               NDTR 450
```

Subroutine BDTR

This subroutine computes $P=I_x(m,n)=\text{Prob}(X \le x)$ where X is a random variable following the beta distribution with degrees of freedom (continuous parameters) m and n. For computation to take place, $0 \le x \le 1$, $0.5 \le m \le 10^{+5}$, and $0.5 \le n \le 10^{+5}$. D, the ordinate of the beta density at x, is also presented in the output.

For $0 \le x \le 1$, $I_x(m,n)$ may be written as:

$$I_x(m,n) = \int_0^x f(m,n,y)\,dy$$

where:

$$f(m,n,y) = \frac{1}{B(m,n)} y^{m-1}(1-y)^{n-1} \qquad (1)$$

$$B(m,n) = \frac{\Gamma(m)\,\Gamma(n)}{\Gamma(m+n)}; \quad D = f(m,n,x)$$

$I_x(m,n)$ can be reduced to a binomial partial sum which can be evaluated by means of a continued fraction expansion.

Let $N = m+n-1$ and $r = m-1$. Then:

$$I_x(m,n) = I_x(r+1,\ N-r)$$

$$I_x(r+1,\ N-r) = \sum_{s=r+1}^{N} \binom{N}{s} x^s (1-x)^{N-s} \qquad (2)$$

$$= \binom{N}{r+1} x^{r+1} (1-x)^{N-r-1} S$$

where $0 \le s \le N$

S is a continued fraction, with 80 terms being sufficient for the desired accuracy.

$$S = \frac{1}{1-}\frac{c_1}{1+}\frac{d_1}{1-}\frac{c_2}{1+}\frac{d_2}{1-}\ \cdots\ \frac{c_{80}}{1+}\frac{d_{80}}{1} \qquad (3)$$

$$c_i = \frac{(N-i-r)(r+i)}{(r+2i-1)(r+2i)} \frac{x}{1-x} \qquad (4)$$

$$d_i = \frac{i(N+i)}{(r+2i+1)(r+2i)} \frac{x}{1-x} \qquad (5)$$

The above continued fraction expansion of $I_x(m,n)$ holds for positive m and n (integers or nonintegers), $N \geq 0$ $(m+n \geq 1)$, and $r \geq 0$ $(m \geq 1)$. In order to fulfill these last two conditions, if $m < 1$, the following transformation must be made before computation of $I_x(m,n)$ can take place:

$$I_x(m,n) = \frac{\Gamma(m+n)}{\Gamma(m+1)\Gamma(n)} x^m (1-x)^n + I_x(m+1,n) \quad (6)$$

The quantities on the right-hand side of equation (6) are those which are computed.

It is known that $I_x(m,n) = I_{1-x}(n,m)$. Thus, either of the two parameter sets indicated by this equation may be used in computing the beta integral. The parameter set selection is made by applying the following empirically derived rule:

> Let p and q be the degrees of freedom corresponding to z, where $z = x$ if $x \leq .5$ or $(1-x)$ otherwise. If the quantity $[(p-1) - (p+q-1) z^{6/5} + 2]$ is positive, use the parameter set corresponding to z. Otherwise, use the parameter set corresponding to (1-z).

If $0 \leq x \leq 10^{-8}$ or $0 \leq 1-x \leq 10^{-8}$, the approximation is made that x = 0 or 1 respectively. P and D are then set according to the following table:

$0 \leq x \leq 10^{-8}$		$0 \leq 1-x \leq 10^{-8}$	
P = 0		P = 1	
If:	then:	If:	then:
A < 1	$D = 10^{75}$	B < 1	$D = 10^{75}$
A = 1	D = 1/B(m,n)	B = 1	D = 1/B(m,n)
A > 1	D = 0	B > 1	D = 0

If either or both m and n are within 10^{-8} of 1, the beta integral is solved explicitly for m = 1, n = 1, or m = n = 1:

If:	then:
A = 1, B = 1	P = x
A = 1, B ≠ 1	$P = 1 - (1-x)^n$
A ≠ 1, B = 1	$P = x^m$

If m or n is greater than 1000, the chi-square approximation is used:

$z_1 = 2m(1-x)/x$ is distributed as χ^2 with 2n degrees of freedom and $P = 1 - P_{\chi 2}(z_1)$ for m > 1000.

$z_2 = 2nx/(1-x)$ is distributed as χ^2 with 2 m degrees of freedom and $P = P_{\chi 2}(z_2)$ for n > 1000.

If both m and n are greater than 1000, the approximation corresponding to z_1 is used.

The values of P very near zero or one may be somewhat imprecise. To eliminate possible misinterpretation of results, if $0 \leq P \leq 10^{-8}$ or $0 \leq 1-P \leq 10^{-8}$, P is set to 0 or 1 respectively.

For reference see:

(1) R. E. Bargmann and S. P. Ghosh, Statistical Description Programs For a Computer Language. IBM Research Report RC-1094, 1963.

(2) M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. U. S. Department of Commerce, National Bureau of Standards Applied Mathematics Series, 1966.


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C                                                                       BDTR  10
C     ..................................................................BDTF  20
C                                                                       BDTR  30
C        SUBROUTINE BDTR                                                BDTF  40
C                                                                       BDTF  50
C        PURPOSE                                                        BDTR  60
C           COMPUTES P(X) = PROBABILITY THAT THE RANDOM VARIABLE U,      BDTR  70
C           DISTRIBUTED ACCORDING TO THE BETA DISTRIBUTION WITH         BDTF  80
C           PARAMETERS A AND B, IS LESS THAN OR EQUAL TO X.  F(A,B,X),  BDTR  90
C           THE ORDINATE OF THE BETA DENSITY AT X, IS ALSO COMPUTED.    BDTR 100
C                                                                       BDTR 110
C        USAGE                                                          BDTR 120
C           CALL BDTR(X,A,B,P,D,IER)                                    BDTR 130
C                                                                       BDTF 140
C        DESCRIPTION OF PARAMETERS                                      BDTR 150
C           X   - INPUT SCALAR FOR WHICH P(X) IS COMPUTED.              BDTR 160
C           A   - BETA DISTRIBUTION PARAMETER (CONTINUOUS).             BDTR 170
C           B   - BETA DISTRIBUTION PARAMETER (CONTINUOUS).             BDTR 180
C           P   - OUTPUT PROBABILITY.                                   BDTR 190
C           D   - OUTPUT DENSITY.                                       BDTR 200
C           IER - RESULTANT ERROR CODE WHERE                            BDTR 210
C               IER= 0 --- NO ERROR                                     BDTR 220
C               IER=-1,+1  CDTF HAS BEEN CALLED AND AN ERROR HAS        BDTF 230
C                          OCCURRED.  SEE CDTR.                         BDTF 240
C               IER=-2 --- AN INPUT PARAMETER IS INVALID.  X IS LESS    BDTR 250
C                          THAN 0.0 OR GREATER THAN 1.0, OR EITHER A OR BDTR 260
C                          B IS LESS THAN 0.5 OR GREATER THAN 10**(+5).  BDTR 270
C                          P AND D ARE SET TO -1.E75.                   BDTR 280
C               IER=+2 --- INVALID OUTPUT.  P IS LESS THAN ZERO OR      BDTR 290
C                          GREATER THAN ONE.  P IS SET TO 1.E75.         BDTR 300
C                                                                       BDTR 310
C        REMARKS                                                        BDTR 320
C           SEE MATHEMATICAL DESCRIPTION.                               BDTR 330
C                                                                       BDTR 340
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  BDTR 350
C           DLGAM                                                       BDTR 360
C           NDTR                                                        BDTR 370
C           CDTF                                                        BDTR 380
C                                                                       BDTR 390
C        METHOD                                                         BDTR 400
C           REFER TO R.E. BARGMANN AND S.P. GHOSH, STATISTICAL          BDTR 410
C           DISTRIBUTION PROGRAMS FOR A COMPUTER LANGUAGE,              BDTR 420
C           IBM RESEARCH REPORT RC-1094, 1963.                          BDTR 430
C                                                                       BDTR 440
C     ..................................................................BDTR 450
C                                                                       BDTF 460
      SUBROUTINE BDTF(X,A,B,P,D,IER)                                    BDTR 470
      DOUBLE PRECISION XX,DLXX,DL1X,AA,BB,G1,G2,G3,G4,DD,PP,XO,FF,FN,   BDTR 480
     1XI,SS,CC,RR,DLBETA                                                BDTF 490
C                                                                       BDTR 500
C        TEST FOR VALID INPUT DATA                                      BDTR 510
C                                                                       BDTF 520
      IF(A-(.5-1.E-5)) 640,10,10                                        BDTR 530
   10 IF(B-(.5-1.E-5)) 640,20,20                                        BDTR 540
   20 IF(A-1.E+5) 30,30,640                                             BDTF 550
   30 IF(B-1.E+5) 40,40,640                                             BDTR 560
   40 IF(X) 640,50,50                                                   BDTR 570
   50 IF(1.-X) 640,60,60                                                BDTF 580
C                                                                       BDTR 590
```

```
C        COMPUTE LOG(BETA(A,B))                                          BDTR 600
C                                                                        BDTR 610
   60 AA=DBLE(A)                                                         BDTR 620
      BB=DBLE(B)                                                         BDTR 630
      CALL DLGAM(AA,G1,IOK)                                              BDTR 640
      CALL DLGAM(BB,G2,IOK)                                              BDTR 650
      CALL DLGAM(AA+BB,G3,IOK)                                           BDTR 660
      DLBETA=G1+G2-G3                                                    BDTR 670
C                                                                        BDTR 680
C        TEST FOR X NEAR 0.0 OR 1.0                                      BDTR 690
C                                                                        BDTR 700
      IF(X-1.E-8) 80,80,70                                               BDTR 710
   70 IF((1.-X)-1.E-8) 130,130,140                                       BDTR 720
   80 P=0.0                                                              BDTR 730
      IF(A-1.) 90,100,120                                                BDTR 740
   90 D=1.E+75                                                           BDTR 750
      GO TO 660                                                          BDTR 760
  100 DD=-DLBETA                                                         BDTR 770
      IF(DD+1.68D02)  120,120,110                                        BDTR 780
  110 DD=DEXP(DD)                                                        BDTR 790
      D=SNGL(DD)                                                         BDTR 800
      GO TO 660                                                          BDTR 810
  120 D=0.0                                                              BDTR 820
      GO TO 660                                                          BDTR 830
  130 P=1.0                                                              BDTR 840
      IF(B-1.) 90,100,120                                                BDTR 850
C                                                                        BDTR 860
C        SET PROGRAM PARAMETERS                                          BDTR 870
C                                                                        BDTR 880
  140 XX=DBLE(X)                                                         BDTR 890
      DLXX=DLOG(XX)                                                      BDTR 900
      DL1X=DLOG(1.D0-XX)                                                 BDTR 910
      XO=XX/(1.D0-XX)                                                    BDTR 920
      ID=0                                                               BDTR 930
C                                                                        BDTR 940
C        COMPUTE ORDINATE                                                BDTR 950
C                                                                        BDTR 960
      DD=(AA-1.D0)*DLXX+(BB-1.D0)*DL1X-DLBETA                            BDTR 970
      IF(DD-1.68D02) 150,150,160                                         BDTR 980
  150 IF(DD+1.68D02) 170,170,180                                         BDTR 990
  160 D=1.E75                                                            BDTR1000
      GO TO 190                                                          BDTR1010
  170 D=0.0                                                              BDTR1020
      GO TO 190                                                          BDTR1030
  180 DD=DEXP(DD)                                                        BDTR1040
      D=SNGL(DD)                                                         BDTR1050
C                                                                        BDTR1060
C        A OR B OR BOTH WITHIN 1.E-8 OF 1.0                              BDTR1070
C                                                                        BDTR1080
  190 IF(ABS(A-1.)-1.E-8)  200,200,210                                   BDTR1090
  200 IF(ABS(B-1.)-1.E-8)  220,220,230                                   BDTR1100
  210 IF(ABS(B-1.)-1.E-8)  260,260,290                                   BDTR1110
  220 P=X                                                                BDTR1120
      GO TO 660                                                          BDTR1130
  230 PP=BB*DL1X                                                         BDTR1140
      IF(PP+1.68D02) 240,240,250                                         BDTR1150
  240 P=1.0                                                              BDTR1160
      GO TO 660                                                          BDTR1170
  250 PP=DEXP(PP)                                                        BDTR1180
      PP=1.D0-PP                                                         BDTR1190
      P=SNGL(PP)                                                         BDTR1200
      GO TO 600                                                          BDTR1210
  260 PP=AA*DLXX                                                         BDTR1220
      IF(PP+1.68D02) 270,270,280                                         BDTR1230
  270 P=0.0                                                              BDTR1240
      GO TO 660                                                          BDTR1250
  280 PP=DEXP(PP)                                                        BDTR1260
      P=SNGL(PP)                                                         BDTR1270
      GO TO 600                                                          BDTR1280
C                                                                        BDTR1290
C        TEST FOR A OR B GREATER THAN 1000.0                             BDTR1300
C                                                                        BDTR1310
  290 IF(A-1000.) 300,300,310                                            BDTR1320
  300 IF(B-1000.) 330,330,320                                            BDTR1330
  310 XX=2.D0*AA/XO                                                      BDTR1340
      XS=SNGL(XX)                                                        BDTR1350
      AA=2.D0*BB                                                         BDTR1360
      DF=SNGL(AA)                                                        BDTR1370
      CALL CDTR(XS,DF,P,DUMMY,IER)                                       BDTR1380
      P=1.0-P                                                            BDTR1390
      GO TO 670                                                          BDTR1400
  320 XX=2.D0*BB*XO                                                      BDTR1410
      XS=SNGL(XX)                                                        BDTR1420
      AA=2.D0*AA                                                         BDTR1430
      DF=SNGL(AA)                                                        BDTR1440
      CALL CDTR(XS,DF,P,DUMMY,IER)                                       BDTR1450
      GO TO 670                                                          BDTR1460
C                                                                        BDTR1470
C        SELECT PARAMETERS FOR CONTINUED FRACTION COMPUTATION            BDTR1480
C                                                                        BDTR1490
  330 IF(X-.5) 340,340,380                                               BDTR1500
  340 IF(AA-1.D0) 350,350,360                                            BDTR1510
  350 RR=AA+1.D0                                                         BDTR1520
      GO TO 370                                                          BDTR1530
  360 RR=AA                                                              BDTR1540
  370 DD=DLXX/5.D0                                                       BDTR1550
      DD=DEXP(DD)                                                        BDTR1560
      DD=(RR-1.D0)-(RR+BB-1.D0)*XX*DD +2.D0                              BDTR1570
      IF(DD) 420,420,430                                                 BDTR1580
  380 IF(BB-1.D0) 390,390,400                                            BDTR1590
  390 RR=BB+1.D0                                                         BDTR1600
      GO TO 410                                                          BDTR1610
  400 RR=BB                                                              BDTR1620
  410 DD=DL1X/5.D0                                                       BDTR1630
      DD=DEXP(DD)                                                        BDTR1640
      DD=(RR-1.D0)-(AA+RR-1.D0)*(1.D0-XX)*DD +2.D0                       BDTR1650
      IF(DD) 430,430,420                                                 BDTR1660
  420 ID=1                                                               BDTR1670
      FF=DL1X                                                            BDTR1680
      DL1X=DLXX                                                          BDTR1690
      DLXX=FF                                                            BDTR1700
      XO=1.D0/XO                                                         BDTR1710
      FF=AA                                                              BDTR1720
      AA=BB                                                              BDTR1730
      BB=FF                                                              BDTR1740
      G2=G1                                                              BDTR1750
C                                                                        BDTR1760
C        TEST FOR A LESS THAN 1.0                                        BDTR1770
C                                                                        BDTR1780
  430 FF=0.D0                                                            BDTR1790
      IF(AA-1.D0) 440,440,470                                            BDTR1800
  440 CALL DLGAM(AA+1.D0,G4,IOK)                                         BDTR1810
      DD=AA*DLXX+BB*DL1X+G3-G2-G4                                        BDTR1820
      IF(DD+1.68D02) 460,460,450                                         BDTR1830
  450 FF=FF+DEXP(DD)                                                     BDTR1840
  460 AA=AA+1.D0                                                         BDTR1850
C                                                                        BDTR1860
C        COMPUTE P USING CONTINUED FRACTION EXPANSION                    BDTR1870
C                                                                        BDTR1880
  470 FN=AA+BB-1.D0                                                      BDTR1890
      RR=AA-1.D0                                                         BDTR1900
      II=80                                                              BDTR1910
      XI=DFLOAT(II)                                                      BDTR1920
      SS=((BB-XI)*(RR+XI))/((RR+2.D0*XI-1.D0)*(RR+2.D0*XI))              BDTR1930
      SS=SS*XO                                                           BDTR1940
      DO 480 I=1,79                                                      BDTR1950
      II=80-I                                                            BDTR1960
      XI=DFLOAT(II)                                                      BDTR1970
      DD=(XI*(FN+XI))/((RR+2.D0*XI+1.D0)*(RR+2.D0*XI))                   BDTR1980
      DD=DD*XO                                                           BDTR1990
      CC=((BB-XI)*(RR+XI))/((RR+2.D0*XI-1.D0)*(RR+2.D0*XI))              BDTR2000
      CC=CC*XO                                                           BDTR2010
      SS=CC/(1.D0+DD/(1.D0-SS))                                          BDTR2020
  480 CONTINUE                                                           BDTR2030
      SS=1.D0/(1.D0-SS)                                                  BDTR2040
      IF(SS) 650,650,490                                                 BDTR2050
  490 CALL DLGAM(AA+BB,G1,IOK)                                           BDTR2060
      CALL DLGAM(AA+1.D0,G4,IOK)                                         BDTR2070
      CC=G1-G2-G4+AA*DLXX+(BB-1.D0)*DL1X                                 BDTR2080
      PP=CC+DLOG(SS)                                                     BDTR2090
      IF(PP+1.68D02) 500,500,510                                         BDTR2100
  500 PP=FF                                                              BDTR2110
      GO TO 520                                                          BDTR2120
  510 PP=DEXP(PP)+FF                                                     BDTR2130
  520 IF(ID) 540,540,530                                                 BDTR2140
  530 PP=1.D0-PP                                                         BDTR2150
  540 P=SNGL(PP)                                                         BDTR2160
C                                                                        BDTR2170
C        SET ERROR INDICATOR                                             BDTR2180
C                                                                        BDTR2190
      IF(P) 550,570,570                                                  BDTR2200
  550 IF(ABS(P)-1.E-7) 560,560,650                                       BDTR2210
  560 P=0.0                                                              BDTR2220
      GO TO 660                                                          BDTR2230
  570 IF(1.-P) 580,600,600                                               BDTR2240
  580 IF(ABS(1.-P)-1.E-7) 590,590,650                                    BDTR2250
  590 P=1.0                                                              BDTR2260
      GO TO 660                                                          BDTR2270
  600 IF(P-1.E-8) 610,610,620                                            BDTR2280
  610 P=0.0                                                              BDTR2290
      GO TO 660                                                          BDTR2300
  620 IF((1.0-P)-1.E-8) 630,630,660                                      BDTR2310
  630 P=1.0                                                              BDTR2320
      GO TO 660                                                          BDTR2330
  640 IER=-2                                                             BDTR2340
      D=-1.E75                                                           BDTR2350
      P=-1.E75                                                           BDTR2360
      GO TO 670                                                          BDTR2370
  650 IEP=+2                                                             BDTR2380
      P= 1.E75                                                           BDTR2390
      GO TO 670                                                          BDTR2400
  660 IER=0                                                              BDTR2410
  670 RETURN                                                             BDTR2420
      END                                                                BDTR2430
```

Subroutine CDTR

This subroutine computes P = P (x) = Prob. $(X \leq x)$, where X is a random variable following the χ^2 distribution with continuous parameter m. The value of x must be greater than or equal to zero and $0.5 \leq m \leq 2\ (10^5)$ for computation to take place. D, the ordinate of the χ^2 density at x, is also presented in the output.

For $x \geq 0$, P(x) may be written as:

$$P(x) = \int_0^x f(m,y)\, dy \qquad (1)$$

where $f(m,y) = y^{(m-2)/2}\ e^{-y/2} / (2^{m/2}\, \Gamma(\frac{m}{2}))$

and D = f(m,x)

To evaluate the integral, $\theta = \frac{m}{2} - [\frac{m}{2}]$ is first defined where $[\frac{m}{2}]$ denotes the largest integer less than or equal to $\frac{m}{2}$. θ is thus the fractional part of $\frac{m}{2}$.

Substituting this expression into the integral and performing the proper reductions, the following results are obtained.

If:	then:
$0 < m < 2$	P (x) = T1 + T2
$2 \leq m < 4$	P (x) = T1
$m \geq 4$	P (x) = T1 - 2T3

where:

$$T1 = \int_0^x \frac{y^{\theta}\ e^{-y/2}\, dy}{2^{1+\theta}\, \Gamma(1+\theta)}$$

$$T2 = f(2+2\theta, x)$$

$$T3 = \sum_{i=2}^{[\frac{m}{2}]} f(2i+2\theta, x)$$

T2 and T3 may be evaluated directly using logs and antilogs.

If $\theta = 0$ ($\frac{m}{2}$ is an integer), T1 is easily evaluated as:

$$T1 = 1 - e^{-x/2}$$

If $\theta > 0$, T1 can be expanded in the following infinite series:

$$T1 = \frac{z^{\theta}}{\Gamma(1+\theta)}\left(\frac{z}{1+\theta} - \frac{z^2}{2+\theta} + \frac{z^3}{2!\,(3+\theta)} - \frac{z^4}{3!\,(4+\theta)} \cdots\right) \qquad (2)$$

where $Z = \frac{x}{2}$

This series is used in the range $10^{-8} < x \leq 10$, and not more than 30 terms are necessary to ensure convergence within error bounds of 10^{-9}.

For $x > 10$, 1-T1 is evaluated by the Euler-McLaurin formula up to third-derivative terms (see reference (2), equation 23.1.30). One finds:

$$1 - T1 = \int_0^N h(u)\, du \qquad (3)$$

where $h(u) = \frac{1}{\Gamma(1+\theta)} (\frac{2u}{Nx})^{-(1+\theta)} u^{-1}\ e^{-Nx/2u}$

and $\int_0^N h(u)du = \sum_{u=o}^{N-1} h(u) + \frac{1}{2} h(N) - \frac{1}{12} h'(N)$

$$+ \frac{1}{720} h'''(N)$$ (Note: $h' = h'''$ = 0 at 0)

In order to achieve accuracy consistent with that obtained by the method of equation (2), N = 26 is used in equation (3).

If $0 \leq x \leq 10^{-8}$, the approximation x = 0 is made. P is set to 0; and D is set to 10^{75}, 0.5, or 0, corresponding to m less than 2, equal to 2, or greater than 2 respectively.

If m > 1000, Wilson and Hilferty's approximation is used. $(\chi^2/m)^{1/3}$ is approximately normally distributed with mean 1 - 2/9m and variance 2/9m (see reference (2), equation 26.4.14). If $m \leq 1000$ and $x > 2000$, or $m > 1000$ and $x > 10^6$, P is set to 1.

Since T1 may have an error of about 10^{-9}, values of P(x) very near zero or one may be somewhat imprecise. To eliminate possible misinterpretation of results, if $0 \leq P(x) \leq 10^{-8}$ or $0 \leq 1-P(x) \leq 10^{-8}$, P(x) is set to 0 or 1 respectively.

The χ^2 distribution is a member of the gamma family of probability distributions. The general form for distributions of this class is:

$$P_G(x) = \int_0^x G(n, A, \psi; u)\, du$$

where $G(n, a, \psi; u) = (u-a)^{n-1}\, e^{-(u-a)/\psi} / (\psi^n \Gamma(n))$

This subroutine may, therefore, also be used to compute the probability integral from zero to x and the corresponding ordinate at x for any member of this gamma family by setting:

$x = 2(u-a) / \psi$ and $m = 2n$

Then P(x) will be the desired probability and $2f(m,x)/\psi$ will be the desired ordinate.

For reference see:

(1) R. E. Bargmann and S. P. Ghosh, Statistical Distribution Programs For a Computer Language. IBM Research Report RC-1094, 1963

(2) M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. U. S. Department of Commerce, National Bureau of Standards Applied Mathematics Series, 1966.


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C                                                                       CDTR  10
C ......................................................................CDTR  20
C                                                                       CDTR  30
C     SUBROUTINE CDTR                                                   CDTR  40
C                                                                       CDTR  50
C     PURPOSE                                                           CDTR  60
C        COMPUTES P(X) = PROBABILITY THAT THE RANDOM VARIABLE U,        CDTR  70
C        DISTRIBUTED ACCORDING TO THE CHI-SQUARE DISTRIBUTION WITH G    CDTR  80
C        DEGREES OF FREEDOM, IS LESS THAN OR EQUAL TO X.  F(G,X), THE   CDTR  90
C        ORDINATE OF THE CHI-SQUARE DENSITY AT X, IS ALSO COMPUTED.     CDTR 100
C                                                                       CDTR 110
C     USAGE                                                             CDTR 120
C        CALL CDTR(X,G,P,D,IER)                                         CDTR 130
C                                                                       CDTR 140
C     DESCRIPTION OF PARAMETERS                                         CDTR 150
C        X   - INPUT SCALAR FOR WHICH P(X) IS COMPUTED.                 CDTR 160
C        G   - NUMBER OF DEGREES OF FREEDOM OF THE CHI-SQUARE           CDTR 170
C              DISTRIBUTION.  G IS A CONTINUOUS PARAMETER.              CDTR 180
C        P   - OUTPUT PROBABILITY.                                      CDTR 190
C        D   - OUTPUT DENSITY.                                          CDTR 200
C        IER - RESULTANT ERROR CODE WHERE                               CDTR 210
C              IER= 0 --- NO ERROR                                      CDTR 220
C              IER=-1 --- AN INPUT PARAMETER IS INVALID.  X IS LESS     CDTR 230
C                         THAN 0.0, OR G IS LESS THAN 0.5 OR GREATER    CDTR 240
C                         THAN 2*10**(+5).  P AND D ARE SET TO -1.E75.   CDTR 250
C              IER=+1 --- INVALID OUTPUT.  P IS LESS THAN ZERO OR       CDTR 260
C                         GREATER THAN ONE, OR SERIES FOR T1 (SEE       CDTR 270
C                         MATHEMATICAL DESCRIPTION) HAS FAILED TO       CDTR 280
C                         CONVERGE.  P IS SET TO 1.E75.                 CDTR 290
C                                                                       CDTR 300
C     REMARKS                                                           CDTR 310
C        SEE MATHEMATICAL DESCRIPTION.                                  CDTR 320
C                                                                       CDTR 330
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     CDTR 340
C        DLGAM                                                          CDTR 350
C        NDTR                                                           CDTR 360
C                                                                       CDTR 370
C     METHOD                                                            CDTR 380
C        REFER TO R.E. BARGMANN AND S.P. GHOSH, STATISTICAL             CDTR 390
C        DISTRIBUTION PROGRAMS FOR A COMPUTER LANGUAGE,                 CDTR 400
C        IBM RESEARCH REPORT RC-1094, 1963.                             CDTR 410
C                                                                       CDTR 420
C ......................................................................CDTR 430
C                                                                       CDTR 440
      SUBROUTINE CDTR(X,G,P,D,IER)                                      CDTR 450
      DOUBLE PRECISION XX,DLXX,X2,DLX2,GG,G2,DLT3,THETA,THP1,           CDTR 460
     1GLG2,DD,T11,SER,CC,XI,FAC,TLOG,TERM,GTH,A2,A,B,C,DT2,DT3,THPI     CDTR 470
C                                                                       CDTR 480
C        TEST FOR VALID INPUT DATA                                      CDTR 490
C                                                                       CDTR 500
      IF(G-(.5-1.E-5)) 590,10,10                                        CDTR 510
   10 IF(G-2.E+5) 20,20,590                                             CDTR 520
   20 IF(X) 590,30,30                                                   CDTR 530
C                                                                       CDTR 540
C        TEST FOR X NEAR 0.0                                            CDTR 550
C                                                                       CDTR 560
   30 IF(X-1.E-8) 40,40,80                                              CDTR 570
   40 P=0.0                                                             CDTR 580
      IF(G-2.) 50,60,70                                                 CDTR 590
   50 D=1.E75                                                           CDTR 600
      GO TO 610                                                         CDTR 610
   60 D=0.5                                                             CDTR 620
      GO TO 610                                                         CDTR 630
   70 D=0.0                                                             CDTR 640
      GO TO 610                                                         CDTR 650
C                                                                       CDTR 660
C        TEST FOR X GREATER THAN 1.E+6                                  CDTR 670
C                                                                       CDTR 680
   80 IF(X-1.E+6) 100,100,90                                            CDTR 690
   90 D=0.0                                                             CDTR 700
      P=1.0                                                             CDTR 710
      GO TO 610                                                         CDTR 720
C                                                                       CDTR 730
C        SET PROGRAM PARAMETERS                                         CDTR 740
C                                                                       CDTR 750
  100 XX=DBLE(X)                                                        CDTR 760
      DLXX=DLOG(XX)                                                     CDTR 770
      X2=XX/2.D0                                                        CDTR 780
      DLX2=DLOG(X2)                                                     CDTR 790
      GG=DBLE(G)                                                        CDTR 800
      G2=GG/2.D0                                                        CDTR 810
C                                                                       CDTR 820
C        COMPUTE ORDINATE                                               CDTR 830
C                                                                       CDTR 840
      CALL DLGAM(G2,GLG2,IOK)                                           CDTR 850
      DD=(G2-1.D0)*DLXX-X2-G2*.6931471805599453 -GLG2                   CDTR 860
      IF(DD-1.68D02) 110,110,120                                        CDTR 870
  110 IF(DD+1.68D02) 130,130,140                                        CDTR 880
  120 D=1.E75                                                           CDTR 890
      GO TO 150                                                         CDTR 900
  130 D=0.0                                                             CDTR 910
      GO TO 150                                                         CDTR 920
  140 DD=DEXP(DD)                                                       CDTR 930
      D=SNGL(DD)                                                        CDTR 940
C                                                                       CDTR 950
C        TEST FOR G GREATER THAN 1000.0                                 CDTR 960
C        TEST FOR X GREATER THAN 2000.0                                 CDTR 970
C                                                                       CDTR 980
  150 IF(G-1000.) 160,160,180                                           CDTR 990
  160 IF(X-2000.) 190,190,170                                           CDTR1000
  170 P=1.0                                                             CDTR1010
      GO TO 610                                                         CDTR1020
  180 A=DLOG(XX/GG)/3.D0                                                CDTR1030
      A=DEXP(A)                                                         CDTR1040
      B=2.D0/(9.D0*GG)                                                  CDTR1050
      C=(A-1.D0+B)/DSQRT(B)                                             CDTR1060
      SC=SNGL(C)                                                        CDTR1070
      CALL NDTR(SC,P,DUMMY)                                             CDTR1080
      GO TO 490                                                         CDTR1090
C                                                                       CDTR1100
C        COMPUTE THETA                                                  CDTR1110
C                                                                       CDTR1120
  190 K= IDINT(G2)                                                      CDTR1130
      THETA=G2-DFLOAT(K)                                                CDTR1140
      IF(THETA-1.D-8) 200,200,210                                       CDTR1150
  200 THETA=0.D0                                                        CDTR1160
  210 THP1=THETA+1.D0                                                   CDTR1170
C                                                                       CDTR1180
C        SELECT METHOD OF COMPUTING T1                                  CDTR1190
C                                                                       CDTR1200
      IF(THETA) 230,230,220                                             CDTR1210
  220 IF(XX-16.D0) 260,260,320                                          CDTR1220
C                                                                       CDTR1230
C        COMPUTE T1 FOR THETA EQUALS 0.0                                CDTR1240
C                                                                       CDTR1250
  230 IF(X2-1.68D02) 250,240,240                                        CDTR1260
  240 T1=1.0                                                            CDTR1270
      GO TO 400                                                         CDTR1280
  250 T11=1.D0-DEXP(-X2)                                                CDTR1290
      T1=SNGL(T11)                                                      CDTR1300
      GO TO 400                                                         CDTR1310
C                                                                       CDTR1320
C        COMPUTE T1 FOR THETA GREATER THAN 0.0 AND                      CDTR1330
C        X LESS THAN OR EQUAL TO 10.0                                   CDTR1340
C                                                                       CDTR1350
  260 SER=X2*(1.D0/THP1 -X2/(THP1+1.D0))                               CDTR1360
      J=+1                                                              CDTR1370
      CC=DFLOAT(J)                                                      CDTR1380
      DO 270 IT1=3,30                                                   CDTR1390
      XI=DFLOAT(IT1)                                                    CDTR1400
      CALL DLGAM(XI,FAC,IOK)                                            CDTR1410
      TLOG= XI*DLX2-FAC-DLOG(XI+THETA)                                  CDTR1420
      TERM=DEXP(TLOG)                                                   CDTR1430
      TERM=DSIGN(TERM,CC)                                               CDTR1440
      SER=SER+TERM                                                      CDTR1450
      CC=-CC                                                            CDTR1460
      IF(DABS(TERM)-1.D-9) 280,270,270                                  CDTR1470
  270 CONTINUE                                                          CDTR1480
      GO TO 600                                                         CDTR1490
  280 IF(SER) 600,600,290                                               CDTR1500
  290 CALL DLGAM(THP1,GTH,IOK)                                          CDTR1510
      TLOG=THETA*DLX2+DLOG(SER)-GTH                                     CDTR1520
      IF(TLOG+1.68D02) 300,300,310                                      CDTR1530
  300 T1=0.0                                                            CDTR1540
      GO TO 400                                                         CDTR1550
  310 T11=DEXP(TLOG)                                                    CDTR1560
      T1=SNGL(T11)                                                      CDTR1570
      GO TO 400                                                         CDTR1580
C                                                                       CDTR1590
C        COMPUTE T1 FOR THETA GREATER THAN 0.0 AND                      CDTR1600
C        X GREATER THAN 10.0 AND LESS THAN 2000.0                       CDTR1610
C                                                                       CDTR1620
  320 A2=0.D0                                                           CDTR1630
      DO 340 I=1,25                                                     CDTR1640
      XI=DFLOAT(I)                                                      CDTR1650
      CALL DLGAM(THP1,GTH,IOK)                                          CDTR1660
      T11=-(13.D0*XX)/XI +THP1*DLOG(13.D0*XX/XI) -GTH-DLOG(XI)          CDTR1670
      IF(T11+1.68D02) 340,340,330                                       CDTR1680
  330 T11=DEXP(T11)                                                     CDTR1690
      A2=A2+T11                                                         CDTR1700
  340 CONTINUE                                                          CDTR1710
      A=1.01282051*THETA/156.D0-XX/312.D0                               CDTR1720
      B=DABS(A)                                                         CDTR1730
      C= -X2+THP1*DLX2+DLOG(B)-GTH-3.951243718581427                    CDTR1740
      IF(C+1.68D02) 370,370,350                                         CDTR1750
  350 IF (A) 360,370,380                                                CDTR1760
  360 C=-DEXP(C)                                                        CDTR1770
      GO TO 390                                                         CDTR1780
  370 C=0.D0                                                            CDTR1790
      GO TO 390                                                         CDTR1800
  380 C=DEXP(C)                                                         CDTR1810
  390 C=A2+C                                                            CDTR1820
      T11=1.D0-C                                                        CDTR1830
      T1=SNGL(T11)                                                      CDTR1840
C                                                                       CDTR1850
C        SELECT PROPER EXPRESSION FOR P                                 CDTR1860
C                                                                       CDTR1870
  400 IF(G-2.) 420,410,410                                              CDTR1880
  410 IF(G-4.) 450,460,460                                              CDTR1890
C                                                                       CDTR1900
C        COMPUTE P FOR G GREATER THAN ZERO AND LESS THAN 2.0            CDTR1910
C                                                                       CDTR1920
  420 CALL DLGAM(THP1,GTH,IOK)                                          CDTR1930
      DT2=THETA*DLXX-X2-THP1*.6931471805599453 -GTH                     CDTR1940
```

```
      IF(DT2+1.68D02) 430,430,440
  430 P=T1
      GO TO 490
  440 DT2=DEXP(DT2)
      T2=SNGL(DT2)
      P=T1+T2+T2
      GO TO 490
C
C        COMPUTE P FOR G GREATER THAN OR EQUAL TO 2.0
C        AND LESS THAN 4.0
C
  450 P=T1
      GO TO 490
C
C        COMPUTE P FOR G GREATER THAN OR EQUAL TO 4.0
C        AND LESS THAN OR EQUAL TO 1000.0
C
  460 DT3=0.D0
      DO 480 I3=2,K
      THPI=DFLOAT(I3)+THETA
      CALL DLGAM(THPI,GTH,IOK)
      DLT3=THPI*DLX2-DLXX-X2-GTH
      IF(DLT3+1.68D02) 480,480,470
  470 DT3=DT3+DEXP(DLT3)
  480 CONTINUE
      T3=SNGL(DT3)
      P=T1-T3-T3
C
C        SET ERROR INDICATOR
C
  490 IF(P) 500,520,520
  500 IF(ABS(P)-1.E-7) 510,510,600
  510 P=0.0
      GO TO 610
  520 IF(1.-P) 530,550,550
  530 IF(ABS(1.-P)-1.E-7) 540,540,600
  540 P=1.0
      GO TO 610
  550 IF(P-1.E-8) 560,560,570
  560 P=0.0
      GO TO 610
  570 IF((1.0-P)-1.E-8) 580,580,610
  580 P=1.0
      GO TO 610
  590 IER=-1
      D=-1.E75
      P=-1.E75
      GO TO 620
  600 IER=+1
      P= 1.E75
      GO TO 620
  610 IER=0
  620 RETURN
      END
```

```
CDTR1950
CDTR1960
CDTR1970
CDTR1980
CDTR1990
CDTR2000
CDTR2010
CDTR2020
CDTR2030
CDTR2040
CDTR2050
CDTR2060
CDTR2070
CDTR2080
CDTR2090
CDTR2100
CDTR2110
CDTR2120
CDTR2130
CDTR2140
CDTR2150
CDTR2160
CDTR2170
CDTR2180
CDTR2190
CDTR2200
CDTR2210
CDTR2220
CDTR2230
CDTF2240
CDTR2250
CDTR2260
CDTR2270
CDTR2280
CDTR2290
CDTF2300
CDTR2310
CDTR2320
CDTF2330
CDTR2340
CDTR2350
CDTF2360
CDTR2370
CDTR2380
CDTF2390
CDTR2400
CDTR2410
CDTF2420
CDTR2430
CDTR2440
CDTF2450
CDTR2460
CDTR2470
CDTF2480
```

Subroutine NDTRI

This subroutine computes $x = p^{-1}(y)$ such that $y = P(x) = \text{Prob}\ (X \leq x)$ where X is a random variable distributed normally with mean zero and variance one.
That is, given P(x), the following is solved for x:

$$P(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-u^2/2)du$$

The following approximation† is used:

$$x = w - \sum_{i=0}^{2} a_i w^i \Big/ \sum_{i=0}^{3} b_i w^i \qquad (1)$$

where:

$$w = \sqrt{\ln(1/p^2)} \quad (0 < p \leq .5) \qquad (2)$$

$$a_0 = 2.515517$$

$$a_1 = 0.802853$$

$$a_2 = 0.010328$$

$$b_1 = 1.432788$$

$$b_2 = 0.189269$$

$$b_3 = 0.001308$$

If P(x) is greater than 0.5, 1 - P(x) is used as p in (2) above, and the result of (1), x, is negated.
The maximum error is 0.00045; f(x) is also calculated.

---

†C. Hastings, Approximations for Digital Computers. Princeton University Press, Princeton, N.J., 1955
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions. Dover Publications, Inc., N.Y., equation 26.2.23.

```
C                                                                       NTRI  10
C***********************************************************************NTRI  20
C                                                                       NTRI  30
C       SUBROUTINE NCTRI                                                NTRI  40
C                                                                       NTRI  50
C       PURPOSE                                                         NTRI  60
C         COMPUTES X = P**(-1)(Y), THE ARGUMENT X SUCH THAT Y= P(X) =   NTRI  70
C         THE PROBABILITY THAT THE RANDOM VARIABLE U, DISTRIBUTED       NTRI  80
C         NORMALLY(0,1), IS LESS THAN OR EQUAL TO X.  P(X), THE         NTRI  90
C         ORDINATE OF THE NORMAL DENSITY, AT X, IS ALSO COMPUTED.       NTRI 100
C                                                                       NTRI 110
C       USAGE                                                           NTRI 120
C         CALL NCTRI(P,X,C,IER)                                         NTRI 130
C                                                                       NTRI 140
C       DESCRIPTION OF PARAMETERS                                       NTRI 150
C         P   - INPUT PROBABILITY.                                      NTRI 160
C         X   - OUTPUT ARGUMENT SUCH THAT P = Y = THE PROBABILITY THAT  NTRI 170
C                 U, THE RANDOM VARIABLE, IS LESS THAN OR EQUAL TO X.   NTRI 180
C         C   - OUTPUT DENSITY, F(X).                                   NTRI 190
C         IER - OUTPUT ERROR CODE                                       NTRI 200
C               = -1 IF P IS NOT IN THE INTERVAL (0,1), INCLUSIVE.      NTRI 210
C                 X=C=.999999E+74 IN THIS CASE                          NTRI 211
C               = 0 IF THERE IS NO ERROR.  SEE REMARKS, BELOW.          NTRI 220
C                                                                       NTRI 230
C       REMARKS                                                         NTRI 240
C         MAXIMUM ERROR IS 0.00045.                                     NTRI 250
C         IF P = 0, X IS SET TO -(10)**74.  C IS SET TO 0.              NTRI 260
C         IF P = 1, X IS SET TO  (10)**74.  C IS SET TO 0.              NTRI 270
C                                                                       NTRI 280
C       SUBROUTINES AND SUBPROGRAMS REQUIRED                            NTRI 290
C         NONE                                                          NTRI 300
C                                                                       NTRI 310
C       METHOD                                                          NTRI 320
C         BASED ON APPROXIMATIONS IN C. HASTINGS, APPROXIMATIONS FOR    NTRI 330
C         DIGITAL COMPUTERS, PRINCETON UNIV. PRESS, PRINCETON, N.J.,    NTRI 340
C         1955.  SEE EQUATION 26.2.23, HANDBOOK OF MATHEMATICAL         NTRI 350
C         FUNCTIONS, ABRAMOWITZ AND STEGUN, DOVER PUBLICATIONS, INC.,   NTRI 360
C         NEW YORK.                                                     NTRI 370
C                                                                       NTRI 380
C***********************************************************************NTRI 390
C                                                                       NTRI 400
      SUBROUTINE NCTRI(P,X,C,IE)                                        NTRI 410
C                                                                       NTRI 420
      IE=0                                                              NTRI 430
      X=.999999E+74                                                     NTRI 431
      C=X                                                               NTRI 432
      IF(P)1,4,2                                                        NTRI 440
    1 IE=-1                                                             NTRI 450
      GO TO 12                                                          NTRI 460
    2 IF (P-1.0)7,5,1                                                   NTRI 470
    4 X=-.999999E+74                                                    NTRI 480
    5 C=0.0                                                             NTRI 490
      GO TO 12                                                          NTRI 500
C                                                                       NTRI 510
C                                                                       NTRI 520
    7 C=P                                                               NTRI 530
      IF(C-0.5)9,9,8                                                    NTRI 540
    8 C=1.0-C                                                           NTRI 550
    9 T2=ALOG(1.0/(C*C))                                                NTRI 560
      T=SQRT(T2)                                                        NTRI 570
      X=T-(2.515517+0.802853*T+0.010328*T2)/(1.0+1.432788*T+0.189269*T2 NTRI 580
     1  +0.001308*T*T2)                                                NTRI 590
      IF(P-0.5)10,10,11                                                 NTRI 600
   10 X=-X                                                              NTRI 610
   11 C=0.398942280*EXP(-X*X/2.0)                                       NTRI 620
   12 RETURN                                                            NTRI 630
      END                                                               NTRI 640
```

Subroutine MOMEN

This subroutine computes four moments for grouped data $F_1, F_2, \ldots, F_n$ on equal class intervals. The number of class intervals is computed as follows:

$$n = (UBO_3 - UBO_1)/UBO_2 \qquad (1)$$

where UBO_1 = given lower bound

UBO_2 = given class interval

UBO_3 = given upper bound

and the total frequency as follows:

$$T = \sum_{i=1}^{n} F_i \qquad (2)$$

where F_i = frequency count in i^{th} interval.

Then, the following are computed.

First moment (mean):

$$ANS_1 = \frac{\sum_{i=1}^{n} F_i \left[UBO_1 + (i-0.5)\ UBO_2\right]}{T} \qquad (3)$$

j^{th} moment:

$$ANS_j = \frac{\sum_{i=1}^{n} F_i \left[UBO_1 + (i-0.5)\ UBO_2 - ANS_1\right]^j}{T} \qquad (4)$$

$$j = 2,\ 3,\ 4$$

These moments are biased and not corrected for grouping.

```
C                                                                       MOME  10
C     ..................................................................MOME  20
C                                                                       MOME  30
C        SUBROUTINE MOMEN                                               MOME  40
C                                                                       MOME  50
C        PURPOSE                                                        MOME  60
C           TO FIND THE THE FIRST FOUR MOMENTS FOR GROUPED DATA ON      MOME  70
C           EQUAL CLASS INTERVALS.                                      MOME  80
C                                                                       MOME  90
C        USAGE                                                          MOME 100
C           CALL MOMEN (F,LBC,NCP,ANS)                                  MOME 110
C                                                                       MOME 120
C        DESCRIPTION OF PARAMETERS                                      MOME 130
C           F   - GROUPED DATA (FREQUENCIES).  GIVEN AS A VECTOR OF     MOME 140
C                 LENGTH (LBC(3)-LBC(1))/UBC(2)                         MOME 150
C           LBC - 3 CELL VECTOR. LBC(1) IS LOWER BOUND AND LBC(3) UPPER MOME 160
C                 BOUND ON DATA.  UBC(2) IS CLASS INTERVAL.  NOTE THAT  MOME 170
C                 UBC(3) MUST BE GREATER THAN UBC(1).                   MOME 180
C           NCP - OPTION PARAMETER.  IF NCP = 1, ANS(1) = MEAN.  IF     MOME 190
C                 NCP = 2, ANS(2) = SECOND MOMENT.  IF NCP = 3, ANS(3) =MOME 200
C                 THIRD MOMENT.  IF NCP = 4, ANS(4) = FOURTH MOMENT.    MOME 210
C                 IF NCP = 5, ALL FOUR MOMENTS ARE FILLED IN.           MOME 220
C           ANS - OUTPUT VECTOR OF LENGTH 4 INTO WHICH MOMENTS ARE PUT. MOME 230
C                                                                       MOME 240
C        REMARKS                                                        MOME 250
C           NOTE THAT THE FIRST MOMENT IS NOT CENTRAL BUT THE VALUE OF  MOME 260
C           THE MEAN ITSELF.  THE MEAN IS ALWAYS CALCULATED.  MOMENTS   MOME 270
C           ARE BIASED AND NOT CORRECTED FOR GROUPING.                  MOME 280
C                                                                       MOME 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MOME 300
C           NONE                                                        MOME 310
C                                                                       MOME 320
C        METHOD                                                         MOME 330
C           REFER TO M. G. KENDALL, 'THE ADVANCED THEORY OF STATISTICS',MOME 340
C           V.1, HAFNER PUBLISHING COMPANY, 1958, CHAPTER 3.            MOME 350
C                                                                       MOME 360
C     ..................................................................MOME 370
C                                                                       MOME 380
      SUBROUTINE MOMEN (F,LBC,NCP,ANS)                                  MOME 390
      DIMENSION F(1),LBC(1),ANS(1)                                      MOME 400
C                                                                       MOME 410
      DO 100 I=1,4                                                      MOME 420
  100 ANS(I)=0.0                                                        MOME 430
C                                                                       MOME 440
C     CALCULATE THE NUMBER OF CLASS INTERVALS                           MOME 450
C                                                                       MOME 460
      N=(UBC(3)-LBC(1))/UBC(2)+0.5                                      MOME 470
C                                                                       MOME 480
C     CALCULATE TOTAL FREQUENCY                                         MOME 490
C                                                                       MOME 500
      T=0.0                                                             MOME 510
      DO 110 I=1,N                                                      MOME 520
  110 T=T+F(I)                                                          MOME 530
C                                                                       MOME 540
      IF(NCP-5) 130, 120, 115                                           MOME 550
  115 NCP=5                                                             MOME 560
  120 JUMP=1                                                            MOME 570
      GO TO 150                                                         MOME 580
  130 JUMP=2                                                            MOME 590
C                                                                       MOME 600
C        FIRST MOMENT                                                   MOME 610
C                                                                       MOME 620
  150 DO 160 I=1,N                                                      MOME 630
      FI=I                                                              MOME 640
  160 ANS(1)=ANS(1)+F(I)*(LBC(1)+(FI-0.5)*UBC(2))                       MOME 650
      ANS(1)=ANS(1)/T                                                   MOME 660
C                                                                       MOME 670
      GO TO (255,200,255,300,200), NCP                                  MOME 680
C                                                                       MOME 690
C        SECOND MOMENT                                                  MOME 700
C                                                                       MOME 710
  200 DO 210 I=1,N                                                      MOME 720
      FI=I                                                              MOME 730
  210 ANS(2)=ANS(2)+F(I)*(LBC(1)+(FI-0.5)*UBC(2)-ANS(1))**2             MOME 740
      ANS(2)=ANS(2)/T                                                   MOME 750
      GO TO (255,355), JUMP                                             MOME 760
C                                                                       MOME 770
C        THIRD MOMENT                                                   MOME 780
C                                                                       MOME 790
  255 DO 260 I=1,N                                                      MOME 800
      FI=I                                                              MOME 810
  260 ANS(3)=ANS(3)+F(I)*(LBC(1)+(FI-0.5)*UBC(2)-ANS(1))**3             MOME 820
      ANS(3)=ANS(3)/T                                                   MOME 830
      GO TO (300,355), JUMP                                             MOME 840
C                                                                       MOME 850
C        FOURTH MOMENT                                                  MOME 860
C                                                                       MOME 870
  300 DO 310 I=1,N                                                      MOME 880
      FI=I                                                              MOME 890
  310 ANS(4)=ANS(4)+F(I)*(LBC(1)+(FI-0.5)*UBC(2)-ANS(1))**4             MOME 900
      ANS(4)=ANS(4)/T                                                   MOME 910
  355 RETURN                                                            MOME 920
      END                                                               MOME 930
```

Subroutine TTEST

This subroutine computes certain t-statistics on the means of populations under various hypotheses.

The sample means of $A_1, A_2, \ldots, A_{NA}$, and $B_1, B_2, \ldots, B_{NB}$ are normally found by the following formulas:

$$\bar{A} = \frac{\sum_{i=1}^{NA} A_i}{NA}; \qquad \bar{B} = \frac{\sum_{i=1}^{NB} B_i}{NB} \tag{1}$$

and the corresponding sample variances by:

$$SA^2 = \frac{\sum_{i=1}^{NA} (A_i - \bar{A})^2}{NA - 1}; \qquad SB^2 = \frac{\sum_{i=1}^{NB} (B_i - \bar{B})^2}{NB - 1} \tag{2}$$

The quantities μ and σ^2 stand respectively for population mean and variance in the following hypotheses.

Hypothesis: $\mu_B = A$; A = a given value (Option 1)

Let $\bar{B}$ = estimate of μ_B and set NA = 1. (A is stored in location A_1).

The subroutine computes:

$$ANS = \frac{\bar{B} - A}{SB} \cdot \sqrt{NB} \quad \text{(t-statistics)} \tag{3}$$

$$NDF = NB - 1 \quad \text{(degrees of freedom)} \tag{4}$$

Hypothesis: $\mu_A = \mu_B \left(\sigma_A^2 = \sigma_B^2\right)$ (Option 2)

The subroutine computes:

$$ANS = \frac{\bar{B} - \bar{A}}{S} \cdot \frac{1}{\sqrt{\frac{1}{NA} + \frac{1}{NB}}} \quad \text{(t-statistics)} \tag{5}$$

$$NDF = NA + NB - 2 \quad \text{(degrees of freedom)} \tag{6}$$

where $S = \sqrt{\frac{(NA-1)\,SA^2 + (NB-1)\,SB^2}{NA + NB - 2}}$ (7)

Hypothesis: $\mu_A = \mu_B \left(\sigma_A^2 \neq \sigma_B^2\right)$ (Option 3)

The subroutine computes:

$$ANS = \frac{\bar{B} - \bar{A}}{\sqrt{\frac{SA^2}{NA} + \frac{SB^2}{NB}}} \quad \text{(t-statistics)} \tag{8}$$

$$NDF = \frac{\left(\frac{SA^2}{NA} + \frac{SB^2}{NB}\right)^2}{\left(\frac{SA^2}{NA}\right)^2 \Big/ (NA+1) + \left(\frac{SB^2}{NB}\right)^2 \Big/ (NB+1)} - 2 \tag{9}$$

(degrees of freedom)

Note: The program returns a rounded NDF, not a truncated NDF.

Hypothesis: $\mu_A = \mu_B \left(\text{no assumption on } \sigma^2\right)$ (Option 4)

The subroutine computes:

$$ANS = \frac{\bar{D}}{SD} \cdot \sqrt{NB} \quad \text{(t-statistics)} \tag{10}$$

$$NDF = NB - 1 \quad \text{(degrees of freedom)} \tag{11}$$

where $\bar{D} = \bar{B} - \bar{A}$ (12)

$$SD = \sqrt{\frac{\sum_{i=1}^{NB} (B_i - A_i - \bar{D})^2}{NB - 1}} \tag{13}$$

NA = NB

```
C
C     ..................................................................   TTES  10
C                                                                          TTES  20
C     SUBROUTINE TTEST                                                     TTES  30
C                                                                          TTES  40
C     PURPOSE                                                              TTES  50
C        TO FIND CERTAIN T-STATISTICS ON THE MEANS OF POPULATIONS.         TTES  60
C                                                                          TTES  70
C     USAGE                                                                TTES  80
C        CALL TTEST (A,NA,B,NB,NOP,NDF,ANS)                                TTES  90
C                                                                          TTES 100
C     DESCRIPTION OF PARAMETERS                                            TTES 110
C        A   - INPUT VECTOR OF LENGTH NA CONTAINING DATA.                  TTES 120
C        NA  - NUMBER OF OBSERVATIONS IN A.                                TTES 130
C        B   - INPUT VECTOR OF LENGTH NB CONTAINING DATA.                  TTES 140
C        NB  - NUMBER OF OBSERVATIONS IN B.                                TTES 150
C        NOP - OPTIONS FOR VARIOUS HYPOTHESES..                            TTES 160
C              NOP=1--- THAT POPULATION MEAN OF B = GIVEN VALUE A.         TTES 170
C                       (SET NA=1)                                         TTES 180
C              NOP=2--- THAT POPULATION MEAN OF B = POPULATION MEAN        TTES 190
C                       OF A, GIVEN THAT THE VARIANCE OF B = THE           TTES 200
C                       VARIANCE OF A.                                     TTES 210
C              NOP=3--- THAT POPULATION MEAN OF B = POPULATION MEAN        TTES 220
C                       OF A, GIVEN THAT THE VARIANCE OF B IS NOT          TTES 230
C                       EQUAL TO THE VARIANCE OF A.                        TTES 240
C              NOP=4--- THAT POPULATION MEAN OF B = POPULATION MEAN        TTES 250
C                       OF A, GIVEN NO INFORMATION ABOUT VARIANCES OF      TTES 260
C                       A AND B.  (SET NA=NB)                              TTES 270
C        NDF - OUTPUT VARIABLE CONTAINING DEGREES OF FREEDOM ASSOCI-       TTES 280
C              ATED WITH T-STATISTIC CALCULATED.                           TTES 290
C        ANS - T-STATISTIC FOR GIVEN HYPOTHESIS.                           TTES 300
C                                                                          TTES 310
C     REMARKS                                                              TTES 320
C        NA AND NB MUST BE GREATER THAN 1, EXCEPT THAT NA=1 IN             TTES 330
C        OPTION 1.  NA AND NB MUST BE THE SAME IN OPTION 4.                TTES 340
C        IF NOP IS OTHER THAN 1, 2, 3 OR 4, DEGREES OF FREEDOM AND         TTES 350
C        T-STATISTIC WILL NOT BE CALCULATED.  NDF AND ANS WILL BE          TTES 360
C        SET TO ZERO.                                                      TTES 370
C                                                                          TTES 380
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                        TTES 390
C        NONE                                                              TTES 400
C                                                                          TTES 410
C     METHOD                                                               TTES 420
C        REFER TO OSTLE, BERNARD, 'STATISTICS IN RESEARCH', IOWA           TTES 430
C        STATE COLLEGE PRESS, 1954, CHAPTER 5.                             TTES 440
C                                                                          TTES 450
C     ..................................................................   TTES 460
C                                                                          TTES 470
      SUBROUTINE TTEST (A,NA,B,NB,NOP,NDF,ANS)                             TTES 480
      DIMENSION A(1),B(1)                                                  TTES 490
C                                                                          TTES 500
C     INITIALIZATION                                                       TTES 510
C                                                                          TTES 520
      NDF=0                                                                TTES 530
      ANS=0.0                                                              TTES 540
C                                                                          TTES 550
C     CALCULATE THE MEAN OF A                                              TTES 560
C                                                                          TTES 570
      AMEAN=0.0                                                            TTES 580
      DO 110 I=1,NA                                                        TTES 590
                                                                           TTES 600
```

```
  110 AMEAN=AMEAN+A(I)                                                  TTES 610
      FNA=NA                                                            TTES 620
      AMEAN=AMEAN/FNA                                                   TTES 630
C                                                                       TTES 640
C     CALCULATE THE MEAN OF B                                           TTES 650
C                                                                       TTES 660
  115 BMEAN=0.0                                                         TTES 670
      DO 120 I=1,NB                                                     TTES 680
  120 BMEAN=BMEAN+B(I)                                                  TTES 690
      FNB=NB                                                            TTES 700
      BMEAN=BMEAN/FNB                                                   TTES 710
C                                                                       TTES 720
      IF(NOP-4) 122, 180, 200                                           TTES 730
  122 IF(NOP-1) 200, 135, 125                                           TTES 740
C                                                                       TTES 750
C     CALCULATE THE VARIANCE OF A                                       TTES 760
C                                                                       TTES 770
  125 SA2=0.0                                                           TTES 780
      DO 130 I=1,NA                                                     TTES 790
  130 SA2=SA2+(A(I)-AMEAN)**2                                           TTES 800
      SA2=SA2/(FNA-1.0)                                                 TTES 810
C                                                                       TTES 820
C     CALCULATE THE VARIANCE OF B                                       TTES 830
C                                                                       TTES 840
  135 SB2=0.0                                                           TTES 850
      DO 140 I=1,NB                                                     TTES 860
  140 SB2=SB2+(B(I)-BMEAN)**2                                           TTES 870
      SB2=SB2/(FNB-1.0)                                                 TTES 880
C                                                                       TTES 890
      GO TO (150,160,170), NOP                                          TTES 900
C                                                                       TTES 910
C        OPTION 1                                                       TTES 920
C                                                                       TTES 930
  150 ANS=((BMEAN-AMEAN)/SQRT(SB2))*SQRT(FNB)                           TTES 940
      NDF=NB-1                                                          TTES 950
      GO TO 200                                                         TTES 960
C                                                                       TTES 970
C        OPTION 2                                                       TTES 980
C                                                                       TTES 990
  160 NDF=NA+NB-2                                                       TTES1000
      FNDF=NDF                                                          TTES1010
      S=SQRT(((FNA-1.0)*SA2+(FNB-1.0)*SB2)/FNDF)                        TTES1020
      ANS=((BMEAN-AMEAN)/S)*(1.0/SQRT(1.0/FNA+1.0/FNB))                 TTES1030
      GO TO 200                                                         TTES1040
C                                                                       TTES1050
C        OPTION 3                                                       TTES1060
C                                                                       TTES1070
  170 ANS=(BMEAN-AMEAN)/SQRT(SA2/FNA+SB2/FNB)                           TTES1080
      A1=(SA2/FNA+SB2/FNB)**2                                           TTES1090
      A2=(SA2/FNA)**2/(FNA+1.0)+(SB2/FNB)**2/(FNB+1.0)                  TTES1100
      NDF=A1/A2-2.0+0.5                                                 TTES1110
      GO TO 200                                                         TTES1120
C                                                                       TTES1130
C        OPTION 4                                                       TTES1140
C                                                                       TTES1150
  180 SD=0.0                                                            TTES1160
      D=BMEAN-AMEAN                                                     TTES1170
      DO 190 I=1,NB                                                     TTES1180
  190 SD=SD+(B(I)-A(I)-D)**2                                            TTES1190
      SD=SQRT(SD/(FNB-1.0))                                             TTES1200
      ANS=(D/SD)*SQRT(FNB)                                              TTES1210
      NDF=NB-1                                                          TTES1220
C                                                                       TTES1230
  200 RETURN                                                            TTES1240
      END                                                               TTES1250
```

Subroutine BISER

This subroutine computes a biserial coefficient of correlation between two continuous variables when one has been artificially dichotomized. The computational steps are as follows:

1. Compute the mean of the continuously measured variable, A:

$$\bar{A} = \frac{\sum_{i=1}^{N} A_i}{N} \qquad (1)$$

where N = number of observations in the sample.

2. Compute the standard deviation of the continuously measured variable, A:

$$s = \sqrt{\frac{\sum_{i=1}^{N} A^2_i - \frac{\left(\sum_{i=1}^{N} A_i\right)^2}{N}}{N-1}} \qquad (2)$$

3. Obtain the following information for the dichotomous variable, B:

p = proportion of the cases in the higher group

q = proportion of the cases in the lower group

y = ordinate of the normal distribution curve at the point of division between p and q proportions

4. Obtain $\bar{A}_p$ = mean of A values whose corresponding B values are in the higher group.

5. Then, compute the biserial coefficient of correlation, r_b, by the use of the following formula:

$$r_b = \frac{\bar{A}_p - \bar{A}}{s} \cdot \frac{p}{y} \qquad (3)$$

6. The standard error of r_b is estimated by the formula:

$$s_{r_b} = \frac{\sqrt{\frac{pq}{y} - r_b^2}}{\sqrt{N}} \qquad (4)$$

For reference see:

(1) J. P. Guilford, Fundamental Statistics in Psychology and Education. McGraw-Hill, New York, 1956, chapter 13.

(2) J. W. Dunlop, "Note on Computation of Biserial Correlations in Item Evaluation", Psychometrika, 1936, I, pp. 51-60.

```
C                                                                       BISE  10
C     ...................................................................BISE  20
C                                                                       BISE  30
C        SUBROUTINE BISER                                               BISE  40
C                                                                       BISE  50
C        PURPOSE                                                        BISE  60
C           TO COMPUTE THE BISERIAL CORRELATION COEFFICIENT BETWEEN TWO  BISE  70
C           CONTINUOUS VARIABLES WHEN ONE OF THEM HAS BEEN ARTIFICIALLY BISE  80
C           DICHOTOMIZED.                                               BISE  90
C                                                                       BISE 100
C        USAGE                                                          BISE 110
C           CALL BISER (N,A,B,HI,ANS,IER)                               BISE 120
C                                                                       BISE 130
C        DESCRIPTION OF PARAMETERS                                      BISE 140
C           N   - NUMBER OF OBSERVATIONS                                BISE 150
C           A   - INPUT VECTOR OF LENGTH N CONTAINING THE CONTINUOUS    BISE 160
C                 VARIABLE                                              BISE 170
C           B   - INPUT VECTOR OF LENGTH N CONTAINING THE DICHOTOMIZED  BISE 180
C                 VARIABLE                                              BISE 190
C           HI  - INPUT - NUMERICAL CODE TO INDICATE THE HIGHER CATEGORYBISE 200
C                 OF THE DICHOTOMIZED VARIABLE.  ANY VALUE IN VECTOR B  BISE 210
C                 EQUAL TO OR GREATER THAN HI WILL BE CLASSIFIED INTO   BISE 220
C                 THE HIGHER CATEGORY.                                  BISE 230
C           ANS - OUTPUT VECTOR OF LENGTH 8 CONTAINING THE FOLLOWING    BISE 240
C                 ANS(1) - MEAN OF VARIABLE A                           BISE 250
C                 ANS(2) - STANDARD DEVIATION OF VARIABLE A             BISE 260
C                 ANS(3) - PROPORTION OF THE CASES IN THE HIGHER        BISE 270
C                          CATEGORY OF VARIABLE B                       BISE 280
C                 ANS(4) - PROPORTION OF THE CASES IN THE LOWER         BISE 290
C                          CATEGORY OF VARIABLE B                       BISE 300
C                 ANS(5) - MEAN OF VARIABLE A FOR THOSE CASES FALLING   BISE 310
C                          INTO THE HIGHER CATEGORY OF VARIABLE B       BISE 320
C                 ANS(6) - MEAN OF VARIABLE A FOR THOSE CASES FALLING   BISE 330
C                          INTO THE LOWER CATEGORY OF VARIABLE B        BISE 340
C                 ANS(7) - BISERIAL CORRELATION COEFFICIENT             BISE 350
C                 ANS(8) - STANDARD ERROR OF BISERIAL CORRELATION       BISE 360
C                          COEFFICIENT                                  BISE 370
C           IER -  1, IF NO CASES ARE IN THE LOWER CATEGORY OF VARIABLE BISE 380
C                  B.                                                   BISE 390
C                 -1, IF ALL CASES ARE IN THE LOWER CATEGORY OF         BISE 400
C                  VARIABLE B.                                          BISE 410
C                  0, OTHERWISE.                                       BISE 420
C                  IF IER IS NON-ZERO, ANS(I)=1.E**75,I=5,...,8.       BISE 430
C                                                                       BISE 440
C        REMARKS                                                        BISE 450
C           THE VALUES OF THE DICHOTOMIZED VARIABLE, B, MUST BE IN      BISE 460
C           NUMERIC FORM.  THEY CANNOT BE SPECIFIED BY MEANS OF         BISE 470
C           ALPHABETIC OR SPECIAL CHARACTERS.                           BISE 480
C                                                                       BISE 490
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  BISE 500
C           NDTRI                                                       BISE 510
C                                                                       BISE 520
C        METHOD                                                         BISE 530
C           REFER TO P. HORST, 'PSYCHOLOGICAL MEASUREMENT AND           BISE 540
C           PREDICTION', P.95-96 (WADSWORTH, 1966).                     BISE 550
C                                                                       BISE 560
C     ...................................................................BISE 570
C                                                                       BISE 580
      SUBROUTINE BISER (N,A,B,HI,ANS,IER)                               BISE 590
C                                                                       BISE 600
      DIMENSION A(1),B(1),ANS(1)                                        BISE 610
C                                                                       BISE 620
C        COMPUTE MEAN AND STANDARD DEVIATION OF VARIABLE A              BISE 630
C                                                                       BISE 640
      IER=0                                                             BISE 650
      SUM=0.0                                                           BISE 660
      SUM2=0.0                                                          BISE 670
      DO 10 I=1,N                                                       BISE 680
      SUM=SUM+A(I)                                                      BISE 690
   10 SUM2=SUM2+A(I)*A(I)                                               BISE 700
      FN=N                                                              BISE 710
      ANS(1)=SUM/FN                                                     BISE 720
      ANS(2)=(SUM2-ANS(1)*SUM)/(FN-1.0)                                 BISE 730
      ANS(2)= SQRT(ANS(2))                                              BISE 740
C                                                                       BISE 750
C        FIND PROPORTIONS OF CASES IN THE HIGHER AND LOWER CATEGORIES   BISE 760
C                                                                       BISE 770
      P=0.0                                                             BISE 780
      SUM=0.0                                                           BISE 790
      SUM2=0.0                                                          BISE 800
      DO 30 I=1,N                                                       BISE 810
      IF(B(I)-HI) 20, 25, 25                                            BISE 820
   20 SUM2=SUM2+A(I)                                                    BISE 830
      GO TO 30                                                          BISE 840
   25 P=P+1.0                                                           BISE 850
      SUM=SUM+A(I)                                                      BISE 860
   30 CONTINUE                                                          BISE 870
      ANS(4)=1.0                                                        BISE 880
      ANS(3)=0.0                                                        BISE 890
      Q=FN-P                                                            BISE 900
      IF (P) 35,35,40                                                   BISE 910
   35 IER=-1                                                            BISE 920
      GO TO 50                                                          BISE 930
   40 ANS(5)=SUM/P                                                      BISE 940
      IF (Q) 45,45,60                                                   BISE 950
   45 IER=1                                                             BISE 960
      ANS(4)=0.0                                                        BISE 970
      ANS(3)=1.0                                                        BISE 980
   50 DO 55 I=5,8                                                       BISE 990
   55 ANS(I)=1.E75                                                      BISE1000
      GO TO 65                                                          BISE1010
   60 ANS(6)=SUM2/Q                                                     BISE1020
      P=P/FN                                                            BISE1030
      Q=1.0-P                                                           BISE1040
C                                                                       BISE1050
C        FIND ORDINATE OF THE NORMAL DISTRIBUTION CURVE AT THE POINT OF BISE1060
C        DIVISION BETWEEN SEGMENTS CONTAINING P AND Q PROPORTIONS       BISE1070
C                                                                       BISE1080
      CALL NDTRI (Q,X,Y,ER)                                             BISE1090
C                                                                       BISE1100
C        COMPUTE THE BISERIAL COEFFICIENT OF CORRELATION                BISE1110
C                                                                       BISE1120
      R=((ANS(5)-ANS(1))/ANS(2))*(P/Y)                                  BISE1130
C                                                                       BISE1140
C        COMPUTE THE STANDARD ERROR OF R                                BISE1150
C                                                                       BISE1160
      ANS(8)=( SQRT(P*Q)/Y-R*R)/SQRT(FN)                                BISE1170
C                                                                       BISE1180
C        STORE RESULTS                                                  BISE1190
C                                                                       BISE1200
      ANS(3)=P                                                          BISE1210
      ANS(4)=Q                                                          BISE1220
      ANS(7)=R                                                          BISE1230
C                                                                       BISE1240
   65 RETURN                                                            BISE1250
      END                                                               BISE1260
```

Subroutine PHI

This subroutine computes a phi coefficient between two variables which are dichotomous. The computational steps are as follows:

1. Two dichotomous variables are summarized in a 2 x 2 table as shown below:

		Variable 1: High	Variable 1: Low
Variable 2	High	A	B
	Low	C	D

A, B, C, and D stand for frequencies.

2. Compute the phi coefficient by the formula:

$$\phi = \frac{AD - BC}{\sqrt{(A+B)\,(C+D)\,(A+C)\,(B+D)}} \qquad (1)$$

3. Compute χ^2 as a function of phi coefficient as follows:

$$\chi^2 = N\,\phi^2 \qquad (2)$$

where N = number of observations.

χ^2, with one degree of freedom, may be tested at a required level of significance. If it is significant, the obtained phi coefficient is also significant.

4. Compute the maximal phi coefficient that can be attainable in a given problem by the formula:

$$\phi_{max} = \sqrt{\left(\frac{p_j}{q_j}\right)\left(\frac{q_i}{p_i}\right)} \qquad (3)$$

where p_i is the largest marginal proportion in a 2 x 2 contingency table, and p_j is the corresponding marginal proportion in the other variable.

For reference see:

(1) J. P. Guilford, Fundamental Statistics in Psychology and Education. McGraw-Hill, New York, 1956, chapter 13.

(2) G. U. Yule, "On the Methods of Measuring the Association Between Two Attributes", Journal of Royal Statistical Association, 1912, 75, pp. 576-642.

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C                                                                       PHI   10
C     ...................................................................PHI   20
C                                                                       PHI   30
C        SUBROUTINE PHI                                                 PHI   40
C                                                                       PHI   50
C        PURPOSE                                                        PHI   60
C           TO COMPUTE THE PHI COEFFICIENT BETWEEN TWO VARIABLES  WHICH PHI   70
C           ARE DICHOTOMOUS.                                           PHI   80
C                                                                       PHI   90
C        USAGE                                                          PHI  100
C           CALL PHI (N,U,V,HU,HV,P,CH,XP,IE)                           PHI  110
C                                                                       PHI  120
C        DESCRIPTION OF PARAMETERS                                      PHI  130
C           N  - NUMBER OF OBSERVATIONS                                 PHI  140
C           U  - INPUT VECTOR OF LENGTH N CONTAINING THE FIRST DICHOTO- PHI  150
C                MOUS VARIABLE                                          PHI  160
C           V  - INPUT VECTOR OF LENGTH N CONTAINING THE SECOND DICHOTO-PHI  170
C                MOUS VARIABLE                                          PHI  180
C           HU - INPUT NUMERICAL CODE WHICH INDICATES THE HIGHER        PHI  190
C                CATEGORY OF THE FIRST VARIABLE.  ANY OBSERVATION IN    PHI  200
C                VECTOR U WHICH HAS A VALUE EQUAL TO OR GREATER THAN HU PHI  210
C                WILL BE CLASSIFIED IN THE HIGHER CATEGORY.             PHI  220
C           HV - INPUT NUMERICAL CODE FOR VECTOR V, SIMILAR TO HU       PHI  230
C           P  - PHI COEFFICIENT COMPUTED                               PHI  240
C           CH - CHI-SQUARE COMPUTED AS A FUNCTION OF PHI COEFFICIENT   PHI  250
C                (DEGREES OF FREEDOM FOR CHI-SQUARE = 1)                PHI  260
C           XP - COMPUTED VALUE OF THE MAXIMAL PHI COEFFICIENT THAT     PHI  270
C                CAN BE ATTAINED IN THE PROBLEM                         PHI  280
C           IE - IF IE IS NON-ZERO, SOME CELL IN THE 2 BY 2 TABLE IS    PHI  290
C                NULL.  IF SO, P, CH, AND XP ARE SET TO 10**75.         PHI  300
C                                                                       PHI  310
C        REMARKS                                                        PHI  320
C           VARIABLES U AND V MUST BE SPECIFIED NUMERIC.                PHI  330
C           THE PHI COEFFICIENT IS A SPECIAL CASE OF THE                PHI  340
C           PEARSON PRODUCT-MOMENT CORRELATION WHEN BOTH VARIABLES ARE  PHI  350
C           BINARY.                                                     PHI  360
C                                                                       PHI  370
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PHI  380
C           NONE                                                        PHI  390
C                                                                       PHI  400
C        METHOD                                                         PHI  410
C           REFER TO P. HORST, 'PSYCHOLOGICAL MEASUREMENT AND           PHI  420
C           PREDICTION', P. 94 (WADSWORTH, 1966).                       PHI  430
C                                                                       PHI  440
C     ...................................................................PHI  450
C                                                                       PHI  460
      SUBROUTINE PHI (N,U,V,HU,HV,P,CH,XP,IE)                           PHI  470
C                                                                       PHI  480
      DIMENSION U(1),V(1)                                               PHI  490
C                                                                       PHI  500
C        CONSTRUCT A 2X2 CONTINGENCY TABLE                              PHI  510
C                                                                       PHI  520
      IE=0                                                              PHI  530
      A=0.0                                                             PHI  540
      B=0.0                                                             PHI  550
      C=0.0                                                             PHI  560
      D=0.0                                                             PHI  570
C                                                                       PHI  580
      DO 40 I=1,N                                                       PHI  590
      IF(U(I)-HU) 10,25,25                                              PHI  600
   10 IF(V(I)-HV) 15,20,20                                              PHI  610
   15 D=D+1.0                                                           PHI  620
      GO TO 40                                                          PHI  630
   20 B=B+1.0                                                           PHI  640
      GO TO 40                                                          PHI  650
   25 IF(V(I)-HV) 30,35,35                                              PHI  660
   30 C=C+1.0                                                           PHI  670
      GO TO 40                                                          PHI  680
   35 A=A+1.0                                                           PHI  690
   40 CONTINUE                                                          PHI  700
      IF(A) 100,100,41                                                  PHI  710
   41 IF(B) 100,100,42                                                  PHI  720
   42 IF(C) 100,100,43                                                  PHI  730
   43 IF(D) 100,100,44                                                  PHI  740
C                                                                       PHI  750
C        COMPUTE THE PHI COEFFICIENT                                    PHI  760
C                                                                       PHI  770
   44 P=(A*D-B*C)/ SQRT((A+B)*(C+D)*(A+C)*(B+D))                        PHI  780
C                                                                       PHI  790
C        COMPUTE CHI-SQURE                                              PHI  800
C                                                                       PHI  810
      T=N                                                               PHI  820
      CH=T*P*P                                                          PHI  830
C                                                                       PHI  840
C        COMPUTE THE MAXIMAL PHI COEFFICIENT                            PHI  850
C                                                                       PHI  860
      P1=(A+C)/T                                                        PHI  870
      P2=(B+D)/T                                                        PHI  880
      P3=(A+B)/T                                                        PHI  890
      P4=(C+D)/T                                                        PHI  900
      IF(P1-P2) 75, 45, 45                                              PHI  910
   45 IF(P3-P4) 65, 50, 50                                              PHI  920
   50 IF(P1-P3) 60, 55, 55                                              PHI  930
   55 XP=SQRT((P3/P4)*(P2/P1))                                          PHI  940
      GO TO 95                                                          PHI  950
   60 XP=SQRT((P1/P2)*(P4/P3))                                          PHI  960
      GO TO 95                                                          PHI  970
   65 IF(P1-P4) 70, 55, 55                                              PHI  980
   70 XP=SQRT((P2/P1)*(P3/P4))                                          PHI  990
      GO TO 95                                                          PHI 1000
   75 IF(P3-P4) 90, 80, 80                                              PHI 1010
   80 IF(P2-P3) 60, 85, 85                                              PHI 1020
   85 XP=SQRT((P4/P3)*(P1/P2))                                          PHI 1030
      GO TO 95                                                          PHI 1040
   90 IF(P2-P4) 70, 85, 85                                              PHI 1050
C                                                                       PHI 1060
   95 RETURN                                                            PHI 1070
  100 IE=1                                                              PHI 1080
      P=1.E75                                                           PHI 1090
      CH=1.E75                                                          PHI 1100
      XP=1.E75                                                          PHI 1110
      GO TO 95                                                          PHI 1120
      END                                                               PHI 1130
```

Subroutine POINT

This subroutine computes a point-biserial correlation coefficient between two variables, one binary (dichotomized) and one continuous. The computational steps are as follows:

1. Compute the mean of the continuously measured variable, A:

$$\bar{A} = \frac{\sum_{i=1}^{N} A_i}{N} \tag{1}$$

where N = number of observations in the sample.

2. Compute the standard deviation of the continuously measured variable, A:

$$s = \sqrt{\frac{\sum_{i=1}^{N} A^2_i - \frac{\left(\sum_{i=1}^{N} A_i\right)^2}{N}}{N-1}} \tag{2}$$

3. Obtain the following information for the dichotomous variable, B:

N_p = number of cases in the higher group

N_q = number of cases in the lower group

4. Obtain $\bar{A}_p$ = mean of A values whose corresponding B values are in the higher group.

5. Then, compute the point-biserial correlation, r_{pb}:

$$r_{pb} = \frac{\bar{A}_p - \bar{A}}{s} \sqrt{\frac{N_p}{N_q}} \tag{3}$$

6. Compute the t ratio used to test the hypothesis of zero correlation:

$$t = r_{pb} \sqrt{\frac{N-2}{1-r^2_{pb}}} \tag{4}$$

7. The degrees of freedom for the t ratio are obtained by:

$$\text{d.f.} = N-2 \tag{5}$$

For reference see:

(1) J. P. Guilford, Fundamental Statistics in Psychology and Education. McGraw-Hill, New York, 1956, chapter 13.

(2) N. C. Perry and W. B. Michael, "The Reliability of a Point-Biserial Coefficient of Correlation". Psychometrika, 1954, 16, pp. 313-325.

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C     ...............................................................POIN  10
C                                                                    POIN  20
C                                                                    POIN  30
C        SUBROUTINE POINT                                            POIN  40
C                                                                    POIN  50
C        PURPOSE                                                     POIN  60
C           TO COMPUTE THE POINT-BISERIAL CORRELATION COEFFICIENT    POIN  70
C           BETWEEN TWO VARIABLES, WHEN ONE OF THE VARIABLES IS A BINARYPOIN  80
C           VARIABLE AND ONE IS CONTINUOUS.  THIS IS A SPECIAL CASE OF POIN  90
C           THE PEARSON PRODUCT-MOMENT CORRELATION COEFFICIENT.      POIN 100
C                                                                    POIN 110
C        USAGE                                                       POIN 120
C           CALL POINT (N,A,B,HI,ANS,IER)                            POIN 130
C                                                                    POIN 140
C        DESCRIPTION OF PARAMETERS                                   POIN 150
C           N   - NUMBER OF OBSERVATIONS                             POIN 160
C           A   - INPUT VECTOR OF LENGTH N CONTAINING THE CONTINUOUS POIN 170
C                 VARIABLE                                           POIN 180
C           B   - INPUT VECTOR OF LENGTH N CONTAINING THE DICHOTOMOUS POIN 190
C                 (BINARY) VARIABLE                                  POIN 200
C           HI  - INPUT NUMERICAL CODE TO INDICATE THE HIGHER CATEGORY. POIN 210
C                 ANY VALUE OF THE BINARY VARIABLE NOT LESS THAN HI WILLPOIN 220
C                 BE CLASSIFIED IN THE HIGHER OF THE TWO CATEGORIES.  POIN 230
C           ANS - OUTPUT VECTOR OF LENGTH 9 CONTAINING THE FOLLOWING POIN 240
C                 RESULTS                                            POIN 250
C                    ANS(1)- MEAN OF VARIABLE A                      POIN 260
C                    ANS(2)- STANDARD DEVIATION OF VARIABLE A        POIN 270
C                    ANS(3)- NUMBER OF OBSERVATIONS IN THE HIGHER    POIN 280
C                            CATEGORY OF VARIABLE B                  POIN 290
C                    ANS(4)- NUMBER OF OBSERVATIONS IN THE LOWER     POIN 300
C                            CATEGORY OF VARIABLE B                  POIN 310
C                    ANS(5)- MEAN OF VARIABLE A FOR ONLY THOSE       POIN 320
C                            OBSERVATIONS IN THE HIGHER CATEGORY OF  POIN 330
C                            VARIABLE B                              POIN 340
C                    ANS(6)- MEAN OF VARIABLE A FOR ONLY THOSE       POIN 350
C                            OBSERVATIONS IN THE LOWER CATEGORY OF   POIN 360
C                            VARIABLE B                              POIN 370
C                    ANS(7)- POINT-BISERIAL CORRELATION COEFFICIENT  POIN 380
C                    ANS(8)- T-TEST FOR THE SIGNIFICANCE OF THE      POIN 390
C                            DIFFERENCE BETWEEN THE MEANS OF VARIABLE A POIN 400
C                            FOR THE HIGHER AND LOWER CATEGORIES     POIN 410
C                            RESPECTIVELY.                           POIN 420
C                    ANS(9)- DEGREES OF FREEDOM FOR THE T-TEST       POIN 430
C           IER- 1, IF ALL ELEMENTS OF B ARE NOT LESS THAN HI.       POIN 440
C                -1, IF ALL ELEMENTS OF B ARE LESS THAN HI.          POIN 450
C                0, OTHERWISE.  IF IER IS NON-ZERO, ANS(I), I=5,...,9, POIN 460
C                IS SET TO 10**75.                                   POIN 470
C                                                                    POIN 480
C        REMARKS                                                     POIN 490
C           THE SYMBOLS USED TO IDENTIFY THE VALUES OF THE TWO CATEGORIESPOIN 500
C           OF VARIABLE B MUST BE NUMERIC.  ALPHABETIC OR SPECIAL    POIN 510
C           CHARACTERS CANNOT BE USED.                               POIN 520
C           THE T-TEST(ANS(8)) IS A TEST OF WHETHER THE POINT-BISERIAL POIN 530
C           COEFFICIENT DIFFERS SIGNIFICANTLY FROM ZERO.             POIN 540
C                                                                    POIN 550
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED               POIN 560
C           NONE                                                     POIN 570
C                                                                    POIN 580
C        METHOD                                                      POIN 590
C           REFER TO P. HORST, 'PSYCHOLOGICAL MEASUREMENT AND        POIN 600
C           PREDICTION', P. 91 (WADSWORTH, 1966).                    POIN 610
C                                                                    POIN 620
C     ...............................................................POIN 630
C                                                                    POIN 640
      SUBROUTINE POINT (N,A,B,HI,ANS,IER)                            POIN 650
C                                                                    POIN 660
      DIMENSION A(1),B(1),ANS(1)                                     POIN 670
C                                                                    POIN 680
C        COMPUTE MEAN AND STANDARD DEVIATION OF VARIABLE A           POIN 690
C                                                                    POIN 700
      IER=0                                                          POIN 710
      SUM=0.0                                                        POIN 720
      SUM2=0.0                                                       POIN 730
      DO 10 I=1,N                                                    POIN 740
      SUM=SUM+A(I)                                                   POIN 750
   10 SUM2=SUM2+A(I)*A(I)                                            POIN 760
      FN=N                                                           POIN 770
      ANS(1)=SUM/FN                                                  POIN 780
      ANS(2)=(SUM2-ANS(1)*SUM)/(FN-1.0)                              POIN 790
      ANS(2)= SQRT(ANS(2))                                           POIN 800
C                                                                    POIN 810
C        FIND NUMBERS OF CASES IN THE HIGHER AND LOWER CATEGORIES    POIN 820
C                                                                    POIN 830
      P=0.0                                                          POIN 840
      SUM=0.0                                                        POIN 850
      SUM2=0.0                                                       POIN 860
      DO 30 I=1,N                                                    POIN 870
      IF(B(I)-HI) 20, 25, 25                                         POIN 880
   20 SUM2=SUM2+A(I)                                                 POIN 890
      GO TO 30                                                       POIN 900
   25 P=P+1.0                                                        POIN 910
      SUM=SUM+A(I)                                                   POIN 920
   30 CONTINUE                                                       POIN 930
C                                                                    POIN 940
      Q=FN-P                                                         POIN 950
      ANS(3)=P                                                       POIN 960
      ANS(4)=Q                                                       POIN 970
      IF (P) 35,35,40                                                POIN 980
   35 IER=-1                                                         POIN 990
      GO TO 50                                                       POIN1000
   40 ANS(5)=SUM/P                                                   POIN1010
      IF (Q) 45,45,60                                                POIN1020
   45 IER=1                                                          POIN1030
   50 DO 55 I=5,9                                                    POIN1040
   55 ANS(I)=1.E75                                                   POIN1050
      GO TO 65                                                       POIN1060
   60 ANS(6)=SUM2/Q                                                  POIN1070
C                                                                    POIN1080
C        COMPUTE THE POINT-BISERIAL CORRELATION                      POIN1090
C                                                                    POIN1100
      R=((ANS(5)-ANS(1))/ANS(2))* SQRT(P/Q)                          POIN1110
      ANS(7)=R                                                       POIN1120
C                                                                    POIN1130
C        COMPUTE T RATIO USED TO TEST THE HYPOTHESIS OF ZERO CORRELATIONPOIN1140
C                                                                    POIN1150
      T=R* SQRT((FN-2.0)/(1.0-R*R))                                  POIN1160
      ANS(8)=T                                                       POIN1170
C                                                                    POIN1180
C        COMPUTE DEGREES OF FREEDOM                                  POIN1190
C                                                                    POIN1200
      ANS(9)=FN-2                                                    POIN1210
C                                                                    POIN1220
   65 RETURN                                                         POIN1230
      END                                                            POIN1240
```

Subroutine TETRA

This subroutine computes a tetrachoric correlation coefficient between two variables where both of the variables have been reduced artifically to two categories. The computational steps are as follows:

1. Two dichotomous variables are summarized in a 2 x 2 table such as the one shown below.

		Variable 1: High	Variable 1: Low
Variable 2	High	A	B
	Low	C	D

A, B, C, and D stand for frequencies. If any frequency is zero (0), the tetrachoric correlation will not be computed.

2. Obtain the proportions of marginal totals:

$$p_1 = (A+C)/N \quad (1)$$

$$q_1 = (B+D)/N \quad (2)$$

$$p_2 = (A+B)/N \quad (3)$$

$$q_2 = (C+D)/N \quad (4)$$

where N = number of observations.

3. Obtain:

y_1 = ordinate of the normal distribution curve at the point of division between p_1 and q_1 proportions

y_2 = same as y_1 using p_2 and q_2 proportions

z_1 = standard normal variable corresponding to y_1

z_2 = standard normal variable corresponding to y_2

4. Then, compute the tetrachoric correlation coefficient by the use of the following formula:

$$\frac{AD - BC}{y_1 y_2 N^2} = r_t + \frac{1}{2} z_1 z_2 r_t^2 + \frac{1}{6}\left(z_1^2 - 1\right)\left(z_2^2 - 1\right) r_t^3 + \frac{1}{24} z_1 \left(z_1^2 - 3\right) z_2 \left(z_2^2 - 3\right) r_t^4 + \frac{1}{120}\left(z_1^4 - 6z_1^2 + 3\right)\left(z_2^4 - 6z_2^2 + 3\right) r_t^5 + \frac{1}{720} z_1 \left(z_1^4 - 10z_1^2 + 15\right) z_2 \left(z_2^4 - 10z_2^2 + 15\right) r_t^6 + \frac{1}{5040}\left(z_1^6 - 15z_1^4 + 45z_1^2 - 15\right)\left(z_2^6 - 15z_2^4 + 45z_2^2 - 15\right) r_t^7 \quad (5)$$

Note: r_t is found by the subroutine POLRT -- Newton-Raphson method of approximation to the root of the above equation.

5. For the purpose of testing $r_t = 0.0$, the standard error is estimated by the formula:

$$s_{r_t} = \frac{\sqrt{p_1 p_2 q_1 q_2}}{y_1 y_2 \sqrt{N}} \qquad (6)$$

6. In selecting the real root in $[-1, 1]$, if $r_t = a + bi$, and

$$|b| \leq .5(10^{-6})\,|a|$$

r_t is considered to be a real root.

For reference see:

(1) J. P. Guilford, Fundamental Statistics in Psychology and Education. McGraw-Hill, New York, 1956, chapter 13.

(2) W. P. Elderton, Frequency Curves and Correlation, 4th Edition. Cambridge University Press, 1953, chapter 9.

```
C                                                                       TETR  10
C     ..................................................................TETR  20
C                                                                       TETR  30
C        SUBROUTINE TETRA                                               TETR  40
C                                                                       TETR  50
C        PURPOSE                                                        TETR  60
C           COMPUTE A TETRACHORIC CORRELATION COEFFICIENT BETWEEN TWO    TETR  70
C           VARIABLES WHERE DATA IN BOTH VARIABLES HAVE BEEN REDUCED     TETR  80
C           ARTIFICIALLY TO TWO CATEGORIES.                             TETR  90
C                                                                       TETR 100
C        USAGE                                                          TETR 110
C           CALL TETRA (N,U,V,HU,HV,R,RS,IE)                            TETR 120
C                                                                       TETR 130
C        DESCRIPTION OF PARAMETERS                                      TETR 140
C           N  - NUMBER OF OBSERVATIONS                                 TETR 150
C           U  - INPUT VECTOR OF LENGTH N CONTAINING THE FIRST VARIABLE TETR 160
C                REDUCED TO TWO CATEGORIES                              TETR 170
C           V  - INPUT VECTOR OF LENGTH N CONTAINING THE SECOND VARIABLETETR 180
C                REDUCED TO TWO CATEGORIES                              TETR 190
C           HU - INPUT NUMERICAL CODE INDICATING THE HIGHER CATEGORY OF TETR 200
C                THE FIRST VARIABLE.  IF ANY VALUE OF VARIABLE U IS     TETR 210
C                EQUAL TO OR GREATER THAN HU, IT WILL BE CLASSIFIED AS  TETR 220
C                THE HIGHER CATEGORY, OTHERWISE AS THE LOWER CATEGORY.  TETR 230
C           HV - SAME AS HU EXCEPT THAT HV IS FOR THE SECOND VARIABLE.  TETR 240
C           R  - TETRACHORIC CORRELATION COMPUTED                       TETR 250
C           RS - STANDARD ERROR OF TETRACHORIC CORRELATION COMPUTED     TETR 260
C           IE - ERROR CODE                                             TETR 270
C                0 - NO ERROR                                           TETR 280
C                1 - UNABLE TO COMPUTE A TETRACHORIC CORRELATION DUE TO TETR 290
C                    THE FACT THAT AT LEAST ONE CELL SHOWS ZERO FRE-    TETR 300
C                    QUENCY IN THE 2X2 CONTINGENCY TABLE CONSTRUCTED    TETR 310
C                    FROM INPUT DATA.  IN THIS CASE, R AND RS ARE SET   TETR 320
C                    TO 10**75.  (SEE GUILFORD, 1956)                   TETR 330
C                2 - THE ROOT SOLVER GIVES MULTIPLE ROOTS, OR NO ROOTS, TETR 340
C                    R, IN THE INTERVAL (-1,1) INCLUSIVE.  R AND RS ARE TETR 350
C                    SET TO 10**75.                                     TETR 360
C                3 - UNABLE TO COMPUTE A SATISFACTORY VALUE OF TETRA-   TETR 370
C                    CHORIC CORRELATION USING NEWTON-RAPHSON METHOD OF  TETR 380
C                    APPROXIMATION TO THE ROOT OF THE EQUATION.  R AND  TETR 390
C                    RS ARE SET TO 10**75.  SEE SUBROUTINE POLRT ERROR  TETR 400
C                    INDICATORS.                                        TETR 410
C                4 - HIGH ORDER COEFFICIENT OF THE POLYNOMIAL IS ZERO.  TETR 420
C                    SEE SUBROUTINE POLRT ERROR INDICATORS.             TETR 430
C                                                                       TETR 440
C        REMARKS                                                        TETR 450
C           VALUES OF VARIABLES U AND V MUST BE NUMERICAL, AND          TETR 460
C           ALPHABETIC AND SPECIAL CHARACTERS MUST NOT BE USED.         TETR 470
C           FOR A DEPENDABLE RESULT FOR TETRACHORIC CORRELATION,        TETR 480
C           IT IS RECOMMENDED THAT N BE AT LEAST 200 OR GREATER.        TETR 490
C                                                                       TETR 500
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TETR 510
C           NDTRI                                                       TETR 520
C           POLRT--THIS POLYNOMIAL ROOT ROUTINE WAS SELECTED BECAUSE OF TETR 530
C                  ITS SMALL STORAGE REQUIREMENT.  OTHER SSP ROUTINES   TETR 540
C                  WHICH COULD REPLACE POLRT ARE PROD AND PRBM.  THEIR  TETR 550
C                  USE WOULD REQUIRE MODIFICATION OF TETRA.             TETR 560
C                                                                       TETR 570
C                                                                       TETR 580
C        METHOD                                                         TETR 590
C           REFER TO J. P. GUILFORD, 'FUNDAMENTAL STATISTICS IN PSYCHO- TETR 600
C           LOGY AND EDUCATION', MCGRAW-HILL, NEW YORK, 1956, CHAPTER 13TETR 610
C           AND W. P. ELDERTON, 'FREQUENCY CURVES AND CORRELATION' 4-TH TETR 620
C           ED., CAMBRIDGE UNIVERSITY PRESS, 1953, CHAPTER 9.           TETR 630
C                                                                       TETR 640
C     ..................................................................TETR 650
C                                                                       TETR 660
      SUBROUTINE TETRA (N,U,V,HU,HV,R,RS,IE)                            TETR 670
C                                                                       TETR 680
      DIMENSION XCOF(8),COF(8),ROOTR(7),ROOTI(7)                        TETR 690
      DIMENSION U(1),V(1)                                               TETR 700
      DOUBLE PRECISION X31,X32,X312,X322                                TETR 710
C                                                                       TETR 720
C        CONSTRUCT A 2X2 CONTINGENCY TABLE                              TETR 730
C                                                                       TETR 740
      A=0.0                                                             TETR 750
      B=0.0                                                             TETR 760
      C=0.0                                                             TETR 770
      D=0.0                                                             TETR 780
      DO 40 I=1,N                                                       TETR 790
      IF(U(I)-HU) 10, 25, 25                                            TETR 800
   10 IF(V(I)-HV) 15, 20, 20                                            TETR 810
   15 D=D+1.0                                                           TETR 820
      GO TO 40                                                          TETR 830
   20 B=B+1.0                                                           TETR 840
      GO TO 40                                                          TETR 850
   25 IF(V(I)-HV) 30, 35, 35                                            TETR 860
   30 C=C+1.0                                                           TETR 870
      GO TO 40                                                          TETR 880
   35 A=A+1.0                                                           TETR 890
   40 CONTINUE                                                          TETR 900
C                                                                       TETR 910
C        TEST WHETHER ANY CELL IN THE CONTINGENCY TABLE IS ZERO.        TETR 920
C        IF SO, RETURN TO THE CALLING ROUTINE WITH R=0.0 AND IE=1.      TETR 930
C                                                                       TETR 940
      IE=0                                                              TETR 950
      IF(A) 60, 60, 45                                                  TETR 960
   45 IF(B) 60, 60, 50                                                  TETR 970
   50 IF(C) 60, 60, 55                                                  TETR 980
   55 IF(D) 60, 60, 70                                                  TETR 990
   60 IE=1                                                              TETR1000
      GO TO 86                                                          TETR1010
C                                                                       TETR1020
C        COMPUTE P1, Q1, P2, AND Q2                                     TETR1030
C                                                                       TETR1040
   70 FN=N                                                              TETR1050
      P1=(A+C)/FN                                                       TETR1060
      Q1=(B+D)/FN                                                       TETR1070
      P2=(A+B)/FN                                                       TETR1080
      Q2=(C+D)/FN                                                       TETR1090
C                                                                       TETR1100
C        FIND THE STANDARD NORMAL DEVIATES AT Q1 AND Q2, AND THE        TETR1110
C        ORDINATES AT THOSE POINTS                                      TETR1120
C                                                                       TETR1130
      CALL NDTRI (Q1,X1,Y1,ER)                                          TETR1140
      CALL NDTRI (Q2,X2,Y2,ER)                                          TETR1150
C                                                                       TETR1160
C        COMPUTE THE TETRACHORIC CORRELATION COEFFICIENT                TETR1170
C                                                                       TETR1180
      IF(X1) 76, 72, 76                                                 TETR1190
   72 IF(X2) 76, 74, 76                                                 TETR1200
   74 R=0.0                                                             TETR1210
      GO TO 90                                                          TETR1220
   76 XCOF(1)=-((A*D-B*C)/(Y1*Y2*FN*FN))                                TETR1230
      XCOF(2)=1.0                                                       TETR1240
      XCOF(3)=X1*X2/2.0                                                 TETR1250
      XCOF(4)=(X1*X1-1.0)*(X2*X2-1.0)/6.0                               TETR1260
      X31=DBLE(X1)                                                      TETR1270
      X32=DBLE(X2)                                                      TETR1280
      X312=X31**2                                                       TETR1290
      X322=X32**2                                                       TETR1300
      XCOF(5)=SNGL(X31*(X312-3.000)*X32*(X322-3.000)/24.000)            TETR1310
      XCOF(6)=SNGL((X312*(X312-6.000)+3.000)*(X322*(X322-6.000)+3.000)  TETR1320
     1        /120.000)                                                 TETR1330
      XCOF(7)=SNGL(X31*(X312*(X312-10.000)+15.000)*X32*(X322*(X322-10.0 TETR1340
     1        00)+15.000)/720.000)                                      TETR1350
      XCOF(8)=SNGL((((X312-15.000)*X312+45.000)*X312-15.000)*(((X322-   TETR1360
     1        15.000)*X322+45.000)*X322-15.000)/5040.000)               TETR1370
C                                                                       TETR1380
      CALL POLRT (XCOF,COF,7,ROOTR,ROOTI,IER)                           TETR1390
C                                                                       TETR1400
      J=0                                                               TETR1410
      IF(IER) 78, 78, 84                                                TETR1420
   78 DO 82 I=1,7                                                       TETR1430
      IF(ABS(ROOTI(I))-.5*ABS(ROOTR(I))*1.0E-6)79,79,82                 TETR1440
   79 R=ROOTR(I)                                                        TETR1450
      IF(ABS(R)-1.0)81,81,80                                            TETR1460
   80 R=1.E75                                                           TETR1470
      GO TO 82                                                          TETR1480
   81 J=J+1                                                             TETR1490
   82 CONTINUE                                                          TETR1500
      IF(J-1)83,88,83                                                   TETR1510
   83 IE=2                                                              TETR1520
      GO TO 86                                                          TETR1530
C                                                                       TETR1540
C        UNABLE TO COMPUTE R                                            TETR1550
C                                                                       TETR1560
   84 IE=IER                                                            TETR1570
   86 R=1.0E75                                                          TETR1580
      RS=R                                                              TETR1590
      GO TO 100                                                         TETR1600
   88 IF(R-1.0E75)90,83,83                                              TETR1610
C                                                                       TETR1620
C        STANDARD ERROR OF R=0.0                                        TETR1630
C                                                                       TETR1640
   90 RS= SQRT(P1*P2*Q1*Q2)/(Y1*Y2* SQRT(FN))                           TETR1650
C                                                                       TETR1660
  100 RETURN                                                            TETR1670
      END
```

Subroutine SRATE

This subroutine computes the survival rates of subjects alive n periods after diagnosis or treatment. The survival rate for each period is computed successively for each of K periods where K is specified and $K \leq n$. An example of the input to this subroutine is presented in Table 2.

Table 2. Example of Input to Subroutine SRATE

Periods after diagnosis	Alive at beginning of period	Died during period	Lost during period	Withdrawn alive during period
(i)	(L_i)	(D_i)	(U_i)	(W_i)
1	130	40	4	10
2	76	6	2	8
3	60	2	1	5
4	52	1	0	4
5	47	0	0	47

The input information includes:

- Periods after diagnosis. This column shows the time period elapsed from the date of diagnosis or treatment. A period may be any time interval.
- Alive at beginning of period. The first entry in this column indicates the initial number of subjects; in Table 2, $L_1 = 130$. Each entry thereafter is obtained by subtracting from the preceding number of subjects the total of those who are no longer in the program; in Table 2, $L_2 = L_1 - (D_1 + U_1 + W_1) = 130 - (40 + 4 + 10) = 76$.
- Died during period. This column indicates the number of subjects that died during the period.
- Lost during period. This column indicates the number of subjects whose survival status became unknown during the period.
- Withdrawn alive during period. This column indicates the number of living subjects withdrawn from the study during the period.

For the value of $i = 1, 2, \ldots, K$, the subroutine computes the following information:

1. Effective number exposed to risk of dying during period:

$$E_i = L_i - (U_i + W_i)/2 \qquad (1)$$

2. Proportion dying during period:

$$Q_i = \frac{D_i}{E_i} \qquad (2)$$

3. Proportion surviving during period:

$$P_i = 1 - Q_i \qquad (3)$$

4. i^{th} period survival rate:

$$R_i = \prod_{j=1}^{i} P_i \qquad (4)$$

5. Standard error of survival rate:

$$s_i = R_i \sqrt{\sum_{j=1}^{i} \frac{Q_j}{E_j - D_j}} \qquad (5)$$

For reference see: S. J. Cutler and F. Ederer, "Maximum Utilization of the Life Table Method in Analyzing Survival", Journal of Chronic Diseases, December, 1958. pp 699-712.

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C                                                                       SRAT  10
C     ..................................................................SRAT  20
C                                                                       SRAT  30
C       SUBROUTINE SRATE                                                SRAT  40
C                                                                       SRAT  50
C       PURPOSE                                                         SRAT  60
C          TO COMPUTE THE PROPORTION OF SUBJECTS SURVIVING, THE         SRAT  70
C          SURVIVAL RATES AND THE STANDARD ERRORS FOR SUCCESSIVELY      SRAT  80
C          REDUCED TIME PERIODS.  THE SURVIVAL RATE IS COMPUTED FOR     SRAT  90
C          EACH OF K PERIODS, WHERE K IS A CONSTANT TO BE SPECIFIED ANDSRAT 100
C          IS LESS THAN OR EQUAL TO N (WHERE N = TOTAL NUMBER OF        SRAT 110
C          PERIODS).                                                    SRAT 120
C                                                                       SRAT 130
C       USAGE                                                           SRAT 140
C          CALL SRATE (N,K,X,IE)                                        SRAT 150
C                                                                       SRAT 160
C       DESCRIPTION OF PARAMETERS                                       SRAT 170
C          N - THE TOTAL NUMBER OF PERIODS AFTER TREATMENT OR DIAGNOSISSRAT 180
C          K - THE SPECIFIED PERIOD UP TO WHICH SURVIVAL RATES ARE TO   SRAT 190
C              BE CALCULATED                                            SRAT 200
C          X - AN INPUT AND OUTPUT MATRIX (N X 9) CONTAINING THE        SRAT 210
C              FOLLOWING INFORMATION                                    SRAT 220
C              FOR INPUT--STORED IN THE N ROWS OF EACH COLUMN           SRAT 230
C                 COL 1 - NUMBER OF SUBJECTS ALIVE AT THE BEGINNING OF  SRAT 240
C                         PERIOD                                        SRAT 250
C                 COL 2 - NUMBER OF SUBJECTS WHICH DIED DURING THE      SRAT 260
C                         PERIOD                                        SRAT 270
C                 COL 3 - NUMBER OF SUBJECTS LOST TO FOLLOW-UP DURING   SRAT 280
C                         THE PERIOD                                    SRAT 290
C                 COL 4 - NUMBER OF SUBJECTS WITHDRAWN ALIVE DURING THESRAT 300
C                         PERIOD                                        SRAT 310
C                FOR OUTPUT--STORED IN THE FIRST K ROWS OF EACH         SRAT 320
C                COLUMN                                                 SRAT 330
C                 COL 5 - EFFECTIVE NUMBER EXPOSED TO THE RISK OF DYINGSRAT 340
C                 COL 6 - PROPORTION WHO DIED DURING THE PERIOD         SRAT 350
C                 COL 7 - PROPORTION WHO SURVIVED DURING THE PERIOD     SRAT 360
C                 COL 8 - SURVIAL RATE                                  SRAT 370
C                 COL 9 - STANDARD ERROR OF THE SURVIVAL RATE           SRAT 380
C          IE- 1, IF K IS NOT IN THE CLOSED INTERVAL (0,N).             SRAT 390
C              2, IF THE NUMBER OF SUBJECTS ALIVE AT THE BEGINNING      SRAT 400
C              OF PERIOD I IS LESS THAN THE SUM OF THOSE WHICH DIED,    SRAT 410
C              WERE LOST, OR WERE WITHDRAWN DURING PERIOD I (I=1,...N)  SRAT 420
C              3, IF THE NUMBER OF SUBJECTS WHICH DIED, WERE LOST, OR   SRAT 430
C              WERE WITHDRAWN IN PERIOD I IS NOT EQUAL TO THE NUMBER    SRAT 440
C              ALIVE AT THE BEGINNING OF PERIOD I LESS THE NUMBER       SRAT 450
C              ALIVE AT THE BEGINNING OF PERIOD I + 1 (I=1,...N-1)      SRAT 460
C                                                                       SRAT 470
C       REMARKS                                                         SRAT 480
C          IF THE SUBJECTS IN A GIVEN GROUP ARE ALL DIAGNOSED OR        SRAT 490
C          TREATED AT THE SAME TIME, THE CONSTANT K MAY BE SET EQUAL TOSRAT 500
C          N .  IF THE SUBJECTS IN A GIVEN GOUP ENTER THE STUDY AT      SRAT 510
C          VARYING TIMES, K CAN BE NO GREATER THAN N-1.                 SRAT 520
C                                                                       SRAT 530
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   SRAT 540
C          NONE                                                         SRAT 550
C                                                                       SRAT 560
C       METHOD                                                          SRAT 570
C          REFER TO S. J. CUTLER AND F. EDERER 'MAXIMUM UTILIZATION OF  SRAT 580
C          THE LIFE TABLE METHOD IN ANALYZING SURVIVAL', JOURNAL OF     SRAT 590
C          CHRONIC DISEASES, DECEMBER, 1958.  PP 699-712.               SRAT 600
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C                                                                       SRAT 610
C     ..................................................................SRAT 620
C                                                                       SRAT 630
      SUBROUTINE SRATE (N,K,X,IE)                                       SRAT 640
C                                                                       SRAT 650
      DIMENSION X(1)                                                    SRAT 660
C                                                                       SRAT 670
C        INITIALIZATION AND ERROR CHECKING                              SRAT 680
C                                                                       SRAT 690
      IE=0                                                              SRAT 700
      NP4=4*N+1                                                         SRAT 710
      NP9=NP4+NP4+N-2                                                   SRAT 720
      DO 1 I=NP4,NP9                                                    SRAT 730
    1 X(I)=0.0                                                          SRAT 740
      IF (K) 2,2,3                                                      SRAT 750
    2 IE=1                                                              SRAT 760
      GO TO 45                                                          SRAT 770
    3 IF(K-N) 4,4,2                                                     SRAT 780
    4 DO 9 I=1,N                                                        SRAT 790
      NP4=I+N                                                           SRAT 800
      NP9=NP4+N                                                         SRAT 810
      NP1=NP9+N                                                         SRAT 820
      IF(INT(X(I)-X(NP4)-X(NP9)-X(NP1)+.01)) 5,6,6                      SRAT 830
    5 IE=2                                                              SRAT 840
      GO TO 45                                                          SRAT 850
    6 IF(I-N) 7,9,9                                                     SRAT 860
    7 IF (INT(X(I+1)-X(I)+X(NP4)+X(NP9)+X(NP1)+.01)) 8,9,8              SRAT 870
    8 IE=3                                                              SRAT 880
      GO TO 45                                                          SRAT 890
    9 CONTINUE                                                          SRAT 900
   15 L1=0                                                              SRAT 910
      L2=L1+N                                                           SRAT 920
      L3=L2+N                                                           SRAT 930
      L4=L3+N                                                           SRAT 940
      L5=L4+N                                                           SRAT 950
      L6=L5+N                                                           SRAT 960
      L7=L6+N                                                           SRAT 970
      L8=L7+N                                                           SRAT 980
      L9=L8+N                                                           SRAT 990
      LD=L2                                                            SRAT1000
      LE=L5                                                            SRAT1010
      LQ=L6                                                            SRAT1020
      SUM=0.0                                                          SRAT1030
C                                                                      SRAT1040
      DO 40 I=1,K                                                      SRAT1050
C                                                                      SRAT1060
C        COMPUTE EFFECTIVE NUMBER EXPOSED TO RISK OF DYING             SRAT1070
C                                                                      SRAT1080
      L1=L1+1                                                          SRAT1090
      L3=L3+1                                                          SRAT1100
      L4=L4+1                                                          SRAT1110
      L5=L5+1                                                          SRAT1120
      X(L5)=X(L1)-(X(L3)+X(L4))/2.0                                    SRAT1130
C                                                                      SRAT1140
C        COMPUTE PROPORTION OF DYING                                   SRAT1150
C                                                                      SRAT1160
      L2=L2+1                                                          SRAT1170
      L6=L6+1                                                          SRAT1180
      X(L6)=X(L2)/X(L5)                                                SRAT1190
C                                                                      SRAT1200
C        COMPUTE PROPORTION OF SURVIVING                               SRAT1210
C                                                                      SRAT1220
      L7=L7+1                                                          SRAT1230
      X(L7)=1.0-X(L6)                                                  SRAT1240
C                                                                      SRAT1250
C        COMPUTE SURVIVAL RATE                                         SRAT1260
C                                                                      SRAT1270
      L8=L8+1                                                          SRAT1280
      IF (I-1) 20, 20, 25                                              SRAT1290
   20 X(LE)=X(L7)                                                      SRAT1300
      GO TO 30                                                         SRAT1310
   25 X(L8)=X(L8-1)*X(L7)                                              SRAT1320
C                                                                      SRAT1330
C        COMPUTE STANDARD ERROR OF SURVIVAL RATE                       SRAT1340
C                                                                      SRAT1350
   30 L9=L9+1                                                          SRAT1360
      SUM=SUM+X(L6)/(X(L5)-X(L2))                                      SRAT1370
   40 X(L9)=X(L8)*SQRT(SUM)                                            SRAT1380
C                                                                      SRAT1390
   45 RETURN                                                           SRAT1400
      END                                                              SRAT1410
```

Matrices: Storage

Subroutine MCPY

```
C                                                                       MCPY  10
C     ...................................................................MCPY  20
C                                                                       MCPY  30
C        SUBROUTINE MCPY                                                MCPY  40
C                                                                       MCPY  50
C        PURPOSE                                                        MCPY  60
C           COPY ENTIRE MATRIX                                          MCPY  70
C                                                                       MCPY  80
C        USAGE                                                          MCPY  90
C           CALL MCPY (A,R,N,M,MS)                                      MCPY 100
C                                                                       MCPY 110
C        DESCRIPTION OF PARAMETERS                                      MCPY 120
C           A - NAME OF INPUT MATRIX                                    MCPY 130
C           R - NAME OF OUTPUT MATRIX                                   MCPY 140
C           N - NUMBER OF ROWS IN A OR R                                MCPY 150
C           M - NUMBER OF COLUMNS IN A OR R                             MCPY 160
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R) MCPY 170
C                 0 - GENERAL                                           MCPY 180
C                 1 - SYMMETRIC                                         MCPY 190
C                 2 - DIAGONAL                                          MCPY 200
C                                                                       MCPY 210
C        REMARKS                                                        MCPY 220
C           NONE                                                        MCPY 230
C                                                                       MCPY 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MCPY 250
C           LOC                                                         MCPY 260
C                                                                       MCPY 270
C        METHOD                                                         MCPY 280
C           EACH ELEMENT OF MATRIX A IS MOVED TO THE CORRESPONDING      MCPY 290
C           ELEMENT OF MATRIX R                                         MCPY 300
C                                                                       MCPY 310
C     ...................................................................MCPY 320
C                                                                       MCPY 330
      SUBROUTINE MCPY(A,R,N,M,MS)                                       MCPY 340
      DIMENSION A(1),R(1)                                               MCPY 350
C                                                                       MCPY 360
C        COMPUTE VECTOR LENGTH, IT                                      MCPY 370
C                                                                       MCPY 380
      CALL LOC(N,M,IT,N,M,MS)                                           MCPY 390
C                                                                       MCPY 400
C        COPY MATRIX                                                    MCPY 410
C                                                                       MCPY 420
      DO 1 I=1,IT                                                       MCPY 430
    1 R(I)=A(I)                                                         MCPY 440
      RETURN                                                            MCPY 450
      END                                                               MCPY 460
```

Subroutine RCPY

```
C                                                                       RCPY  10
C     ...................................................................RCPY  20
C                                                                       RCPY  30
C        SUBROUTINE RCPY                                                RCPY  40
C                                                                       RCPY  50
C        PURPOSE                                                        RCPY  60
C           COPY SPECIFIED ROW OF A MATRIX INTO A VECTOR                RCPY  70
C                                                                       RCPY  80
C        USAGE                                                          RCPY  90
C           CALL RCPY (A,L,R,N,M,MS)                                    RCPY 100
C                                                                       RCPY 110
C        DESCRIPTION OF PARAMETERS                                      RCPY 120
C           A - NAME OF INPUT MATRIX                                    RCPY 130
C           L - ROW OF A TO BE MOVED TO R                               RCPY 140
C           R - NAME OF OUTPUT VECTOR OF LENGTH M                       RCPY 150
C           N - NUMBER OF ROWS IN A                                     RCPY 160
C           M - NUMBER OF COLUMNS IN A                                  RCPY 170
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         RCPY 180
C                 0 - GENERAL                                           RCPY 190
C                 1 - SYMMETRIC                                         RCPY 200
C                 2 - DIAGONAL                                          RCPY 210
C                                                                       RCPY 220
C        REMARKS                                                        RCPY 230
C           NONE                                                        RCPY 240
C                                                                       RCPY 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RCPY 260
C           LOC                                                         RCPY 270
C                                                                       RCPY 280
C        METHOD                                                         RCPY 290
C           ELEMENTS OF ROW L ARE MOVED TO CORRESPONDING POSITIONS      RCPY 300
C           OF VECTOR R                                                 RCPY 310
C                                                                       RCPY 320
C     ...................................................................RCPY 330
C                                                                       RCPY 340
      SUBROUTINE RCPY(A,L,R,N,M,MS)                                     RCPY 350
      DIMENSION A(1),R(1)                                               RCPY 360
C                                                                       RCPY 370
      DO 3 J=1,M                                                        RCPY 380
C                                                                       RCPY 390
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     RCPY 400
C                                                                       RCPY 410
      CALL LOC(L,J,LJ,N,M,MS)                                           RCPY 420
C                                                                       RCPY 430
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RCPY 440
C                                                                       RCPY 450
      IF(LJ) 1,2,1                                                      RCPY 460
C                                                                       RCPY 470
C        MOVE ELEMENT TO R                                              RCPY 480
C                                                                       RCPY 490
    1 R(J)=A(LJ)                                                        RCPY 500
      GO TO 3                                                           RCPY 510
    2 R(J)=0.0                                                          RCPY 520
    3 CONTINUE                                                          RCPY 530
      RETURN                                                            RCPY 540
      END                                                               RCPY 550
```

Subroutine CCPY

```
C                                                                       CCPY  10
C     ...................................................................CCPY  20
C                                                                       CCPY  30
C       SUBROUTINE CCPY                                                 CCPY  40
C                                                                       CCPY  50
C       PURPOSE                                                         CCPY  60
C          COPY SPECIFIED COLUMN OF A MATRIX INTO A VECTOR              CCPY  70
C                                                                       CCPY  80
C       USAGE                                                           CCPY  90
C          CALL CCPY(A,L,R,N,M,MS)                                      CCPY 100
C                                                                       CCPY 110
C       DESCRIPTION OF PARAMETERS                                       CCPY 120
C          A - NAME OF INPUT MATRIX                                     CCPY 130
C          L - COLUMN OF A TO BE MOVED TO R                             CCPY 140
C          R - NAME OF OUTPUT VECTOR OF LENGTH N                        CCPY 150
C          N - NUMBER OR ROWS IN A                                      CCPY 160
C          M - NUMBER OF COLUMNS IN A                                   CCPY 170
C          MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A          CCPY 180
C                0 - GENERAL                                            CCPY 190
C                1 - SYMMETRIC                                          CCPY 200
C                2 - DIAGONAL                                           CCPY 210
C                                                                       CCPY 220
C       REMARKS                                                         CCPY 230
C          NONE                                                         CCPY 240
C                                                                       CCPY 250
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   CCPY 260
C          LOC                                                          CCPY 270
C                                                                       CCPY 280
C       METHOD                                                          CCPY 290
C          ELEMENTS OF COLUMN L ARE MOVED TO CORRESPONDING POSITIONS    CCPY 300
C          OF VECTOR R                                                  CCPY 310
C                                                                       CCPY 320
C     ...................................................................CCPY 330
      SUBROUTINE CCPY(A,L,R,N,M,MS)                                     CCPY 340
      DIMENSION A(1),R(1)                                               CCPY 350
C                                                                       CCPY 360
      DO 3 I=1,N                                                        CCPY 370
C                                                                       CCPY 380
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     CCPY 390
C                                                                       CCPY 400
      CALL LOC(I,L,IL,N,M,MS)                                           CCPY 410
C                                                                       CCPY 420
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       CCPY 430
C                                                                       CCPY 440
      IF(IL) 1,2,1                                                      CCPY 450
C                                                                       CCPY 460
C        MOVE ELEMENT TO R                                              CCPY 470
C                                                                       CCPY 480
    1 R(I)=A(IL)                                                        CCPY 490
      GO TO 3                                                           CCPY 500
    2 R(I)=0.0                                                          CCPY 510
    3 CONTINUE                                                          CCPY 520
      RETURN                                                            CCPY 530
      END                                                               CCPY 540
                                                                        CCPY 550
```

Subroutine DCPY

```
C                                                                       DCPY  10
C     ...................................................................DCPY  20
C                                                                       DCPY  30
C       SUBROUTINE DCPY                                                 DCPY  40
C                                                                       DCPY  50
C       PURPOSE                                                         DCPY  60
C          COPY DIAGONAL ELEMENTS OF A MATRIX INTO A VECTOR             DCPY  70
C                                                                       DCPY  80
C       USAGE                                                           DCPY  90
C          CALL DCPY (A,R,N,MS)                                         DCPY 100
C                                                                       DCPY 110
C       DESCRIPTION OF PARAMETERS                                       DCPY 120
C          A - NAME OF INPUT MATRIX                                     DCPY 130
C          R - NAME OF OUTPUT VECTOR OF LENGTH N                        DCPY 140
C          N - NUMBER OF ROWS AND COLUMNS IN MATRIX A                   DCPY 150
C          MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A          DCPY 160
C                0 - GENERAL                                            DCPY 170
C                1 - SYMMETRIC                                          DCPY 180
C                2 - DIAGONAL                                           DCPY 190
C                                                                       DCPY 200
C       REMARKS                                                         DCPY 210
C          INPUT MATRIX MUST BE A SQUARE MATRIX                         DCPY 220
C                                                                       DCPY 230
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DCPY 240
C          LOC                                                          DCPY 250
C                                                                       DCPY 260
C       METHOD                                                          DCPY 270
C          ELEMENTS ON DIAGONAL OF MATRIX ARE MOVED TO CORRESPONDING    DCPY 280
C          POSITIONS OF VECTOR R                                        DCPY 290
C                                                                       DCPY 300
C     ...................................................................DCPY 310
      SUBROUTINE DCPY(A,R,N,MS)                                         DCPY 320
      DIMENSION A(1),R(1)                                               DCPY 330
C                                                                       DCPY 340
      DO 3 J=1,N                                                        DCPY 350
C                                                                       DCPY 360
C        LOCATE DIAGONAL ELEMENT FOR ANY MATRIX STORAGE MODE            DCPY 370
C                                                                       DCPY 380
      CALL LOC(J,J,IJ,N,N,MS)                                           DCPY 390
C                                                                       DCPY 400
C        MOVE DIAGONAL ELEMENT TO VECTOR R                              DCPY 410
C                                                                       DCPY 420
    3 R(J)=A(IJ)                                                        DCPY 430
      RETURN                                                            DCPY 440
      END                                                               DCPY 450
                                                                        DCPY 460
```

Subroutine XCPY

```
C                                                                       XCPY  10
C     ...................................................................XCPY  20
C                                                                       XCPY  30
C        SUBROUTINE XCPY                                                XCPY  40
C                                                                       XCPY  50
C        PURPOSE                                                        XCPY  60
C           COPY A PORTION OF A MATRIX                                  XCPY  70
C                                                                       XCPY  80
C        USAGE                                                          XCPY  90
C           CALL XCPY(A,R,L,K,NR,MR,NA,MA,MS)                           XCPY 100
C                                                                       XCPY 110
C        DESCRIPTION OF PARAMETERS                                      XCPY 120
C           A  - NAME OF INPUT MATRIX                                   XCPY 130
C           R  - NAME OF OUTPUT MATRIX                                  XCPY 140
C           L  - ROW OF A WHERE FIRST ELEMENT OF R CAN BE FOUND         XCPY 150
C           K  - COLUMN OF A WHERE FIRST ELEMENT OF R CAN BE FOUND      XCPY 160
C           NR - NUMBER OF ROWS TO BE COPIED INTO R                     XCPY 170
C           MR - NUMBER OF COLUMNS TO BE COPIED INTO R                  XCPY 180
C           NA - NUMBER OF ROWS IN A                                    XCPY 190
C           MA - NUMBER OF COLUMNS IN A                                 XCPY 200
C           MS - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A          XCPY 210
C                0 - GENERAL                                            XCPY 220
C                1 - SYMMETRIC                                          XCPY 230
C                2 - DIAGONAL                                           XCPY 240
C                                                                       XCPY 250
C        REMARKS                                                        XCPY 260
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         XCPY 270
C           MATRIX R IS ALWAYS A GENERAL MATRIX                         XCPY 280
C                                                                       XCPY 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  XCPY 300
C           LOC                                                         XCPY 310
C                                                                       XCPY 320
C        METHOD                                                         XCPY 330
C           MATRIX R IS FORMED BY COPYING A PORTION OF MATRIX A. THIS   XCPY 340
C           IS DONE BY EXTRACTING NR ROWS AND MR COLUMNS OF MATRIX A,   XCPY 350
C           STARTING WITH ELEMENT AT ROW L, COLUMN K                    XCPY 360
C                                                                       XCPY 370
C     ...................................................................XCPY 380
C                                                                       XCPY 390
      SUBROUTINE XCPY(A,R,L,K,NR,MR,NA,MA,MS)                           XCPY 400
      DIMENSION A(1),R(1)                                               XCPY 410
C                                                                       XCPY 420
C        INITIALIZE                                                     XCPY 430
C                                                                       XCPY 440
      IR=0                                                              XCPY 450
      L2=L+NR-1                                                         XCPY 460
      K2=K+MR-1                                                         XCPY 470
C                                                                       XCPY 480
      DO 5 J=K,K2                                                       XCPY 490
      DO 5 I=L,L2                                                       XCPY 500
      IR=IR+1                                                           XCPY 510
      R(IR)=0.0                                                         XCPY 520
C                                                                       XCPY 530
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     XCPY 540
C                                                                       XCPY 550
      CALL LOC(I,J,IA,NA,MA,MS)                                         XCPY 560
C                                                                       XCPY 570
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       XCPY 580
C                                                                       XCPY 590
      IF(IA) 4,5,4                                                      XCPY 600
    4 R(IR)=A(IA)                                                       XCPY 610
    5 CONTINUE                                                          XCPY 620
      RETURN                                                            XCPY 630
      END                                                               XCPY 640
```

Subroutine MSTR

```
C                                                                       MSTR  10
C     ...................................................................MSTR  20
C                                                                       MSTR  30
C        SUBROUTINE MSTR                                                MSTR  40
C                                                                       MSTR  50
C        PURPOSE                                                        MSTR  60
C           CHANGE STORAGE MODE OF A MATRIX                             MSTR  70
C                                                                       MSTR  80
C        USAGE                                                          MSTR  90
C           CALL MSTR(A,R,N,MSA,MSR)                                    MSTR 100
C                                                                       MSTR 110
C        DESCRIPTION OF PARAMETERS                                      MSTR 120
C           A - NAME OF INPUT MATRIX                                    MSTR 130
C           R - NAME OF OUTPUT MATRIX                                   MSTR 140
C           N - NUMBER OF ROWS AND COLUMNS IN A AND R                   MSTR 150
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         MSTR 160
C                 0 - GENERAL                                           MSTR 170
C                 1 - SYMMETRIC                                         MSTR 180
C                 2 - DIAGONAL                                          MSTR 190
C           MSR - SAME AS MSA EXCEPT FOR MATRIX R                       MSTR 200
C                                                                       MSTR 210
C        REMARKS                                                        MSTR 220
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         MSTR 230
C           MATRIX A MUST BE A SQUARE MATRIX                            MSTR 240
C                                                                       MSTR 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MSTR 260
C           LOC                                                         MSTR 270
C                                                                       MSTR 280
C        METHOD                                                         MSTR 290
C           MATRIX A IS RESTRUCTURED TO FORM MATRIX R.                  MSTR 300
C            MSA MSR                                                    MSTR 310
C              0   0  MATRIX A IS MOVED TO MATRIX R                     MSTR 320
C              0   1  THE UPPER TRIANGLE ELEMENTS OF A GENERAL MATRIX   MSTR 330
C                     ARE USED TO FORM A SYMMETRIC MATRIX               MSTR 340
C              0   2  THE DIAGONAL ELEMENTS OF A GENERAL MATRIX ARE USED MSTR 350
C                     TO FORM A DIAGONAL MATRIX                         MSTR 360
C              1   0  A SYMMETRIC MATRIX IS EXPANDED TO FORM A GENERAL  MSTR 370
C                     MATRIX                                            MSTR 380
C              1   1  MATRIX A IS MOVED TO MATRIX R                     MSTR 390
C              1   2  THE DIAGONAL ELEMENTS OF A SYMMETRIC MATRIX ARE   MSTR 400
C                     USED TO FORM A DIAGONAL MATRIX                    MSTR 410
C              2   0  A DIAGONAL MATRIX IS EXPANDED BY INSERTING MISSING MSTR 420
C                     ZERO ELEMENTS TO FORM A GENERAL MATRIX            MSTR 430
C              2   1  A DIAGONAL MATRIX IS EXPANDED BY INSERTING MISSING MSTR 440
C                     ZERO ELEMENTS TO FORM A SYMMETRIC MATRIX          MSTR 450
C              2   2  MATRIX A IS MOVED TO MATRIX R                     MSTR 460
C                                                                       MSTR 470
C     ...................................................................MSTR 480
C                                                                       MSTR 490
      SUBROUTINE MSTR(A,R,N,MSA,MSR)                                    MSTR 500
      DIMENSION A(1),R(1)                                               MSTR 510
C                                                                       MSTR 520
      DO 20 I=1,N                                                       MSTR 530
      DO 20 J=1,N                                                       MSTR 540
C                                                                       MSTR 550
C        IF R IS GENERAL, FORM ELEMENT                                  MSTR 560
C                                                                       MSTR 570
      IF(MSR) 5,10,5                                                    MSTR 580
C                                                                       MSTR 590
C        IF IN LOWER TRIANGLE OF SYMMETRIC OR DIAGONAL R, BYPASS        MSTR 600
C                                                                       MSTR 610
    5 IF(I-J) 10,10,20                                                  MSTR 620
   10 CALL LOC(I,J,IR,N,N,MSR)                                          MSTR 630
C                                                                       MSTR 640
C        IF IN UPPER AND OFF DIAGONAL  OF DIAGONAL R, BYPASS            MSTR 650
C                                                                       MSTR 660
      IF(IR) 20,20,15                                                   MSTR 670
C                                                                       MSTR 680
C        OTHERWISE, FORM R(I,J)                                         MSTR 690
C                                                                       MSTR 700
   15 R(IR)=0.0                                                         MSTR 710
      CALL LOC(I,J,IA,N,N,MSA)                                          MSTR 720
C                                                                       MSTR 730
C        IF THERE IS NO A(I,J), LEAVE R(I,J) AT C.0                     MSTR 740
C                                                                       MSTR 750
      IF(IA) 20,20,18                                                   MSTR 760
   18 R(IR)=A(IA)                                                       MSTR 770
   20 CONTINUE                                                          MSTR 780
      RETURN                                                            MSTR 790
      END                                                               MSTR 800
```

Subroutine LOC

```
C
C     ...................................................................
C
C        SUBROUTINE LOC
C
C        PURPOSE
C           COMPUTE A VECTOR SUBSCRIPT FOR AN ELEMENT IN A MATRIX OF
C           SPECIFIED STORAGE MODE
C
C        USAGE
C           CALL LOC (I,J,IR,N,M,MS)
C
C        DESCRIPTION OF PARAMETERS
C           I   - ROW NUMBER OF ELEMENT
C           J   - COLUMN NUMBER OF ELEMENT
C           IR  - RESULTANT VECTOR SUBSCRIPT
C           N   - NUMBER OF ROWS IN MATRIX
C           M   - NUMBER OF COLUMNS IN MATRIX
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX
C                 0 - GENERAL
C                 1 - SYMMETRIC
C                 2 - DIAGONAL
C
C        REMARKS
C           NONE
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           MS=0   SUBSCRIPT IS COMPUTED FOR A MATRIX WITH N*M ELEMENTS
C                  IN STORAGE (GENERAL MATRIX)
C           MS=1   SUBSCRIPT IS COMPUTED FOR A MATRIX WITH N*(N+1)/2 IN
C                  STORAGE (UPPER TRIANGLE OF SYMMETRIC MATRIX). IF
C                  ELEMENT IS IN LOWER TRIANGULAR PORTION, SUBSCRIPT IS
C                  CORRESPONDING ELEMENT IN UPPER TRIANGLE.
C           MS=2   SUBSCRIPT IS COMPUTED FOR A MATRIX WITH N ELEMENTS
C                  IN STORAGE (DIAGONAL ELEMENTS OF DIAGONAL MATRIX).
C                  IF ELEMENT IS NOT ON DIAGONAL (AND THEREFORE NOT IN
C                  STORAGE), IR IS SET TO ZERO.
C
C     ...................................................................
C
      SUBROUTINE LOC(I,J,IR,N,M,MS)
C
      IX=I
      JX=J
      IF(MS-1) 10,20,30
   10 IR=N*(JX-1)+IX
      GO TO 36
   20 IF(IX-JX) 22,24,24
   22 IR=IX+(JX*JX-JX)/2
      GO TO 36
   24 IR=JX+(IX*IX-IX)/2
      GO TO 36
   30 IR=0
      IF(IX-JX) 36,32,36
   32 IR=IX
   36 IR=IR
      RETURN
      END
```

Subroutine CONVT

```
C
C     ...................................................................
C
C        SUBROUTINE CONVT
C
C        PURPOSE
C           CONVERT NUMBERS FROM SINGLE PRECISION TO DOUBLE PRECISION
C           OR FROM DOUBLE PRECISION TO SINGLE PRECISION.
C
C        USAGE
C           CALL CONVT (N,M,MODE,S,D,MS)
C
C        DESCRIPTION OF PARAMETERS
C           N    - NUMBER OF ROWS IN MATRICES S AND D.
C           M    - NUMBER OF COLUMNS IN MATRICES S AND D.
C           MODE - CODE INDICATING TYPE OF CONVERSION
C                    1 - FROM SINGLE PRECISION TO DOUBLE PRECISION
C                    2 - FROM DOUBLE PRECISION TO SINGLE PRECISION
C           S    - IF MODE=1, THIS MATRIX CONTAINS SINGLE PRECISION
C                  NUMBERS AS INPUT.  IF MODE=2, IT CONTAINS SINGLE
C                  PRECISION NUMBERS AS OUTPUT.  THE SIZE OF MATRIX S
C                  IS N BY M.
C           D    - IF MODE=1, THIS MATRIX CONTAINS DOUBLE PRECISION
C                  NUMBERS AS OUTPUT.  IF MODE=2, IT CONTAINS DOUBLE
C                  PRECISION NUMBERS AS INPUT.  THE SIZE OF MATRIX D IS
C                  N BY M.
C           MS   - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX
C                    0 - GENERAL
C                    1 - SYMMETRIC
C                    2 - DIAGONAL
C
C        REMARKS
C           MATRIX D CANNOT BE IN THE SAME LOCATION AS MATRIX S.
C           MATRIX D MUST BE DEFINED BY A DOUBLE PRECISION STATEMENT IN
C           THE CALLING PROGRAM.
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           ACCORDING TO THE TYPE OF CONVERSION INDICATED IN MODE, THIS
C           SUBROUTINE COPIES NUMBERS FROM MATRIX S TO MATRIX D OR FROM
C           MATRIX D TO MATRIX S.
C
C     ...................................................................
C
      SUBROUTINE CONVT (N,M,MODE,S,D,MS)
      DIMENSION S(1),D(1)
      DOUBLE PRECISION D
C
C        FIND STORAGE MODE OF MATRIX AND NUMBER OF DATA POINTS
C
      IF(MS-1) 2, 4, 6
    2 NM=N*M
      GO TO 8
    4 NM=((N+1)*N)/2
      GO TO 8
    6 NM=N
C
C        TEST TYPE OF CONVERSION
C
    8 IF(MODE-1) 10, 10, 20
C
C        SINGLE PRECISION TO DOUBLE PRECISION
C
   10 DO 15 L=1,NM
   15 D(L)=S(L)
      GO TO 30
C
C        DOUBLE PRECISION TO SINGLE PRECISION
C
   20 DO 25 L=1,NM
   25 S(L)=D(L)
C
   30 RETURN
      END
```

Subroutine GMADD

```
C                                                                       ARRA  10
C     ...................................................................ARRA  20
C                                                                       ARRA  30
C        SUBROUTINE ARRAY                                               ARRA  40
C                                                                       ARRA  50
C        PURPOSE                                                        ARRA  60
C           CONVERT DATA ARRAY FROM SINGLE TO DOUBLE DIMENSION OR VICE  ARRA  70
C           VERSA.  THIS SUBROUTINE IS USED TO LINK THE USER PROGRAM    ARRA  80
C           WHICH HAS DOUBLE DIMENSION ARRAYS AND THE SSP SUBROUTINES   ARRA  90
C           WHICH OPERATE ON ARRAYS OF DATA IN A VECTOR FASHION.        ARRA 100
C                                                                       ARRA 110
C        USAGE                                                          ARRA 120
C           CALL ARRAY (MODE,I,J,N,M,S,D)                               ARRA 130
C                                                                       ARRA 140
C        DESCRIPTION OF PARAMETERS                                      ARRA 150
C           MODE - CODE INDICATING TYPE OF CONVERSION                   ARRA 160
C                  1 - FROM SINGLE TO DOUBLE DIMENSION                  ARRA 170
C                  2 - FROM DOUBLE TO SINGLE DIMENSION                  ARRA 180
C           I    - NUMBER OF ROWS IN ACTUAL DATA MATRIX                 ARRA 190
C           J    - NUMBER OF COLUMNS IN ACTUAL DATA MATRIX              ARRA 200
C           N    - NUMBER OF ROWS SPECIFIED FOR THE MATRIX D IN         ARRA 210
C                  DIMENSION STATEMENT                                  ARRA 220
C           M    - NUMBER OF COLUMNS SPECIFIED FOR THE MATRIX D IN      ARRA 230
C                  DIMENSION STATEMENT                                  ARRA 240
C           S    - IF MODE=1, THIS VECTOR IS INPUT WHICH CONTAINS THE   ARRA 250
C                  ELEMENTS OF A DATA MATRIX OF SIZE I BY J. COLUMN I+1 ARRA 260
C                  OF DATA MATRIX FOLLOWS COLUMN I, ETC. IF MODE=2,     ARRA 270
C                  THIS VECTOR IS OUTPUT REPRESENTING A DATA MATRIX OF  ARRA 280
C                  SIZE I BY J CONTAINING ITS COLUMNS CONSECUTIVELY.    ARRA 290
C                  THE LENGTH OF S IS IJ, WHERE IJ=I*J.                 ARRA 300
C           D    - IF MODE=1, THIS MATRIX OF SIZE N BY M IS OUTPUT,      ARRA 310
C                  CONTAINING A DATA MATRIX OF SIZE I BY J IN THE FIRST ARRA 320
C                  I ROWS AND J COLUMNS. IF MODE=2, THIS N BY M MATRIX  ARRA 330
C                  IS INPUT CONTAINING A DATA MATRIX OF SIZE I BY J IN  ARRA 340
C                  THE FIRST I ROWS AND J COLUMNS.                      ARRA 350
C                                                                       ARRA 360
C        REMARKS                                                        ARRA 370
C           VECTOR S CAN BE IN THE SAME LOCATION AS MATRIX D.  VECTOR S ARRA 380
C           IS REFERRED AS A MATRIX IN OTHER SSP ROUTINES, SINCE IT     ARRA 390
C           CONTAINS A DATA MATRIX.                                     ARRA 400
C           THIS SUBROUTINE CONVERTS ONLY GENERAL DATA MATRICES (STORAGEARRA 410
C           MODE OF 0).                                                 ARRA 420
C                                                                       ARRA 430
C        SUBROUTINES AND FUNCTION SUBROUTINES REQUIRED                  ARRA 440
C           NONE                                                        ARRA 450
C                                                                       ARRA 460
C        METHOD                                                         ARRA 470
C           REFER TO THE DISCUSSION ON VARIABLE DATA SIZE IN THE SECTIONARRA 480
C           DESCRIBING OVERALL RULES FOR USAGE IN THIS MANUAL.          ARRA 490
C                                                                       ARRA 500
C     ...................................................................ARRA 510
C                                                                       ARRA 520
      SUBROUTINE ARRAY (MODE,I,J,N,M,S,D)                               ARRA 530
      DIMENSION S(1),D(1)                                               ARRA 540
C                                                                       ARRA 550
      NI=N-I                                                            ARRA 560
C                                                                       ARRA 570
C        TEST TYPE OF CONVERSION                                        ARRA 580
C                                                                       ARRA 590
      IF(MODE-1) 100, 100, 120                                          ARRA 600
C                                                                       ARRA 610
C        CONVERT FROM SINGLE TO DOUBLE DIMENSION                        ARRA 620
C                                                                       ARRA 630
  100 IJ=I*J+1                                                          ARRA 640
      NM=N*J+1                                                          ARRA 650
      DO 110 K=1,J                                                      ARRA 660
      NM=NM-NI                                                          ARRA 670
      DO 110 L=1,I                                                      ARRA 680
      IJ=IJ-1                                                           ARRA 690
      NM=NM-1                                                           ARRA 700
  110 D(NM)=S(IJ)                                                       ARRA 710
      GO TO 140                                                         ARRA 720
C                                                                       ARRA 730
C        CONVERT FROM DOUBLE TO SINGLE DIMENSION                        ARRA 740
C                                                                       ARRA 750
  120 IJ=0                                                              ARRA 760
      NM=0                                                              ARRA 770
      DO 130 K=1,J                                                      ARRA 780
      DO 125 L=1,I                                                      ARRA 790
      IJ=IJ+1                                                           ARRA 800
      NM=NM+1                                                           ARRA 810
  125 S(IJ)=D(NM)                                                       ARRA 820
  130 NM=NM+NI                                                          ARRA 830
C                                                                       ARRA 840
  140 RETURN                                                            ARRA 850
      END                                                               ARRA 860
```

```
C                                                                       GMAD  10
C     ...................................................................GMAD  20
C                                                                       GMAD  30
C        SUBROUTINE GMADD                                               GMAD  40
C                                                                       GMAD  50
C        PURPOSE                                                        GMAD  60
C           ADD TWO GENERAL MATRICES TO FORM RESULTANT GENERAL MATRIX   GMAD  70
C                                                                       GMAD  80
C        USAGE                                                          GMAD  90
C           CALL GMADD(A,B,R,N,M)                                       GMAD 100
C                                                                       GMAD 110
C        DESCRIPTION OF PARAMETERS                                      GMAD 120
C           A - NAME OF FIRST INPUT MATRIX                              GMAD 130
C           B - NAME OF SECOND INPUT MATRIX                             GMAD 140
C           R - NAME OF OUTPUT MATRIX                                   GMAD 150
C           N - NUMBER OF ROWS IN A,B,R                                 GMAD 160
C           M - NUMBER OF COLUMNS IN A,B,R                              GMAD 170
C                                                                       GMAD 180
C        REMARKS                                                        GMAD 190
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GMAD 200
C                                                                       GMAD 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMAD 220
C           NONE                                                        GMAD 230
C                                                                       GMAD 240
C        METHOD                                                         GMAD 250
C           ADDITION IS PERFORMED ELEMENT BY ELEMENT                    GMAD 260
C                                                                       GMAD 270
C     ...................................................................GMAD 280
C                                                                       GMAD 290
      SUBROUTINE GMADD(A,B,R,N,M)                                       GMAD 300
      DIMENSION A(1),B(1),R(1)                                          GMAD 310
C                                                                       GMAD 320
C        CALCULATE NUMBER OF ELEMENTS                                   GMAD 330
C                                                                       GMAD 340
      NM=N*M                                                            GMAD 350
C                                                                       GMAD 360
C        ADD MATRICES                                                   GMAD 370
C                                                                       GMAD 380
      DO 10 I=1,NM                                                      GMAD 390
   10 R(I)=A(I)+B(I)                                                    GMAD 400
      RETURN                                                            GMAD 410
      END                                                               GMAD 420
```

Subroutine GMSUB

```
C                                                                       GMSU  10
C     ...................................................................GMSU  20
C                                                                       GMSU  30
C        SUBROUTINE GMSUB                                               GMSU  40
C                                                                       GMSU  50
C        PURPOSE                                                        GMSU  60
C           SUBTRACT ONE GENERAL MATRIX FROM ANOTHER TO FORM RESULTANT   GMSU  70
C           MATRIX                                                      GMSU  80
C                                                                       GMSU  90
C        USAGE                                                          GMSU 100
C           CALL GMSUB(A,B,R,N,M)                                       GMSU 110
C                                                                       GMSU 120
C        DESCRIPTION OF PARAMETERS                                      GMSU 130
C           A - NAME OF FIRST INPUT MATRIX                              GMSU 140
C           B - NAME OF SECOND INPUT MATRIX                             GMSU 150
C           R - NAME OF OUTPUT MATRIX                                   GMSU 160
C           N - NUMBER OF ROWS IN A,B,R                                 GMSU 170
C           M - NUMBER OF COLUMNS IN A,B,R                              GMSU 180
C                                                                       GMSU 190
C        REMARKS                                                        GMSU 200
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GMSU 210
C                                                                       GMSU 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMSU 230
C           NONE                                                        GMSU 240
C                                                                       GMSU 250
C        METHOD                                                         GMSU 260
C           MATRIX B ELEMENTS ARE SUBTRACTED FROM CORRESPONDING MATRIX AGMSU 270
C           ELEMENTS                                                    GMSU 280
C                                                                       GMSU 290
C     ...................................................................GMSU 300
C                                                                       GMSU 310
      SUBROUTINE GMSUB(A,B,R,N,M)                                       GMSU 320
      DIMENSION A(1),B(1),R(1)                                          GMSU 330
C                                                                       GMSU 340
C        CALCULATE NUMBER OF ELEMENTS                                   GMSU 350
C                                                                       GMSU 360
      NM=N*M                                                            GMSU 370
C                                                                       GMSU 380
C        SUBTRACT MATRICES                                              GMSU 390
C                                                                       GMSU 400
      DO 10 I=1,NM                                                      GMSU 410
   10 R(I)=A(I)-B(I)                                                    GMSU 420
      RETURN                                                            GMSU 430
      END                                                               GMSU 440
```

Subroutine GMPRD

```
C                                                                       GMPR  10
C     ...................................................................GMPR  20
C                                                                       GMPR  30
C        SUBROUTINE GMPRD                                               GMPR  40
C                                                                       GMPR  50
C        PURPOSE                                                        GMPR  60
C           MULTIPLY TWO GENERAL MATRICES TO FORM A RESULTANT GENERAL    GMPR  70
C           MATRIX                                                      GMPR  80
C                                                                       GMPR  90
C        USAGE                                                          GMPR 100
C           CALL GMPRD(A,B,R,N,M,L)                                     GMPR 110
C                                                                       GMPR 120
C        DESCRIPTION OF PARAMETERS                                      GMPR 130
C           A - NAME OF FIRST INPUT MATRIX                              GMPR 140
C           B - NAME OF SECOND INPUT MATRIX                             GMPR 150
C           R - NAME OF OUTPUT MATRIX                                   GMPR 160
C           N - NUMBER OF ROWS IN A                                     GMPR 170
C           M - NUMBER OF COLUMNS IN A AND ROWS IN B                    GMPR 180
C           L - NUMBER OF COLUMNS IN B                                  GMPR 190
C                                                                       GMPR 200
C        REMARKS                                                        GMPR 210
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GMPR 220
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         GMPR 230
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX B         GMPR 240
C           NUMBER OF COLUMNS OF MATRIX A MUST BE EQUAL TO NUMBER OF ROWGMPR 250
C           OF MATRIX B                                                 GMPR 260
C                                                                       GMPR 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMPR 280
C           NONE                                                        GMPR 290
C                                                                       GMPR 300
C        METHOD                                                         GMPR 310
C           THE M BY L MATRIX B IS PREMULTIPLIED BY THE N BY M MATRIX A GMPR 320
C           AND THE RESULT IS STORED IN THE N BY L MATRIX R.            GMPR 330
C                                                                       GMPR 340
C     ...................................................................GMPR 350
C                                                                       GMPR 360
      SUBROUTINE GMPRD(A,B,R,N,M,L)                                     GMPR 370
      DIMENSION A(1),B(1),R(1)                                          GMPR 380
C                                                                       GMPR 390
      IR=0                                                              GMPR 400
      IK=-M                                                             GMPR 410
      DO 10 K=1,L                                                       GMPR 420
      IK=IK+M                                                           GMPR 430
      DO 10 J=1,N                                                       GMPR 440
      IR=IR+1                                                           GMPR 450
      JI=J-N                                                            GMPR 460
      IB=IK                                                             GMPR 470
      R(IR)=0                                                           GMPR 480
      DO 10 I=1,M                                                       GMPR 490
      JI=JI+N                                                           GMPR 500
      IB=IB+1                                                           GMPR 510
   10 R(IR)=R(IR)+A(JI)*B(IB)                                           GMPR 520
      RETURN                                                            GMPR 530
      END                                                               GMPR 540
```

Subroutine GMTRA

```
C                                                                       GMTR  10
C     ...................................................................GMTR  20
C                                                                       GMTR  30
C        SUBROUTINE GMTRA                                               GMTR  40
C                                                                       GMTR  50
C        PURPOSE                                                        GMTR  60
C           TRANSPOSE A GENERAL MATRIX                                  GMTR  70
C                                                                       GMTR  80
C        USAGE                                                          GMTR  90
C           CALL GMTRA(A,R,N,M)                                         GMTR 100
C                                                                       GMTR 110
C        DESCRIPTION OF PARAMETERS                                      GMTR 120
C           A - NAME OF MATRIX TO BE TRANSPOSED                         GMTR 130
C           R - NAME OF RESULTANT MATRIX                                GMTR 140
C           N - NUMBER OF ROWS OF A AND COLUMNS OF R                    GMTR 150
C           M - NUMBER OF COLUMNS OF A AND ROWS OF R                    GMTR 160
C                                                                       GMTR 170
C        REMARKS                                                        GMTR 180
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         GMTR 190
C           MATRICES A AND R MUST BE STORED AS GENERAL MATRICES         GMTR 200
C                                                                       GMTR 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMTR 220
C           NONE                                                        GMTR 230
C                                                                       GMTR 240
C        METHOD                                                         GMTR 250
C           TRANSPOSE N BY M MATRIX A TO FORM M BY N MATRIX R           GMTR 260
C                                                                       GMTR 270
C     ...................................................................GMTR 280
C                                                                       GMTR 290
      SUBROUTINE GMTRA(A,R,N,M)                                         GMTR 300
      DIMENSION A(1),R(1)                                               GMTR 310
C                                                                       GMTR 320
      IR=0                                                              GMTR 330
      DO 10 I=1,N                                                       GMTR 340
      IJ=I-N                                                            GMTR 350
      DO 10 J=1,M                                                       GMTR 360
      IJ=IJ+N                                                           GMTR 370
      IR=IR+1                                                           GMTR 380
   10 R(IR)=A(IJ)                                                       GMTR 390
      RETURN                                                            GMTR 400
      END                                                               GMTR 410
```

Subroutine GTPRD

```
C                                                                       GTPR  10
C     ...................................................................GTPR  20
C                                                                       GTPR  30
C        SUBROUTINE GTPRD                                               GTPR  40
C                                                                       GTPR  50
C        PURPOSE                                                        GTPR  60
C           PREMULTIPLY A GENERAL MATRIX BY THE TRANSPOSE OF ANOTHER    GTPR  70
C           GENERAL MATRIX                                              GTPR  80
C                                                                       GTPR  90
C        USAGE                                                          GTPR 100
C           CALL GTPRD(A,B,R,N,M,L)                                     GTPR 110
C                                                                       GTPR 120
C        DESCRIPTION OF PARAMETERS                                      GTPR 130
C           A - NAME OF FIRST INPUT MATRIX                              GTPR 140
C           B - NAME OF SECOND INPUT MATRIX                             GTPR 150
C           R - NAME OF OUTPUT MATRIX                                   GTPR 160
C           N - NUMBER OF ROWS IN A AND B                               GTPR 170
C           M - NUMBER OF COLUMNS IN A AND ROWS IN R                    GTPR 180
C           L - NUMBER OF COLUMNS IN B AND R                            GTPR 190
C                                                                       GTPR 200
C        REMARKS                                                        GTPR 210
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         GTPR 220
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX B         GTPR 230
C           ALL MATRICES MUST BE STORED AS GENERAL MATRICES             GTPR 240
C                                                                       GTPR 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GTPR 260
C           NONE                                                        GTPR 270
C                                                                       GTPR 280
C        METHOD                                                         GTPR 290
C           MATRIX TRANSPOSE OF A IS NOT ACTUALLY CALCULATED. INSTEAD,  GTPR 300
C           ELEMENTS OF MATRIX A ARE TAKEN COLUMNWISE RATHER THAN       GTPR 310
C           ROWWISE FOR POSTMULTIPLICATION BY MATRIX B.                 GTPR 320
C                                                                       GTPR 330
C     ...................................................................GTPR 340
C                                                                       GTPR 350
      SUBROUTINE GTPRD(A,B,R,N,M,L)                                     GTPR 360
      DIMENSION A(1),B(1),R(1)                                          GTPR 370
C                                                                       GTPR 380
      IR=0                                                              GTPR 390
      IK=-N                                                             GTPR 400
      DO 10 K=1,L                                                       GTPR 410
      IJ=0                                                              GTPR 420
      IK=IK+N                                                           GTPR 430
      DO 10 J=1,M                                                       GTPR 440
      IB=IK                                                             GTPR 450
      IR=IR+1                                                           GTPR 460
      R(IR)=0                                                           GTPR 470
      DO 10 I=1,N                                                       GTPR 480
      IJ=IJ+1                                                           GTPR 490
      IB=IB+1                                                           GTPR 500
   10 R(IR)=R(IR)+A(IJ)*B(IB)                                           GTPR 510
      RETURN                                                            GTPR 520
      END                                                               GTPR 530
```

Subroutine MADD

```
C                                                                       MADD  10
C  ***********************************************************************MADD  20
C                                                                       MADD  30
C        SUBROUTINE MADD                                                MADD  40
C                                                                       MADD  50
C        PURPOSE                                                        MADD  60
C           ADD TWO MATRICES ELEMENT BY ELEMENT TO FORM RESULTANT       MADD  70
C           MATRIX                                                      MADD  80
C                                                                       MADD  90
C        USAGE                                                          MADD 100
C           CALL MADD(A,B,R,N,M,MSA,MSB)                                MADD 110
C                                                                       MADD 120
C        DESCRIPTION OF PARAMETERS                                      MADD 130
C           A - NAME OF INPUT MATRIX                                    MADD 140
C           B - NAME OF INPUT MATRIX                                    MADD 150
C           R - NAME OF OUTPUT MATRIX                                   MADD 160
C           N - NUMBER OF ROWS IN A,B,R                                 MADD 170
C           M - NUMBER OF COLUMNS IN A,B,R                              MADD 180
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         MADD 190
C                 0 - GENERAL                                           MADD 200
C                 1 - SYMMETRIC                                         MADD 210
C                 2 - DIAGONAL                                          MADD 220
C           MSB - SAME AS MSA EXCEPT FOR MATRIX B                       MADD 230
C                                                                       MADD 240
C        REMARKS                                                        MADD 250
C           NONE                                                        MADD 260
C                                                                       MADD 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MADD 280
C           LOC                                                         MADD 290
C                                                                       MADD 300
C        METHOD                                                         MADD 310
C           STORAGE MODE OF OUTPUT MATRIX IS FIRST DETERMINED. ADDITION MADD 320
C           OF CORRESPONDING ELEMENTS IS THEN PERFORMED.                MADD 330
C           THE FOLLOWING TABLE SHOWS THE STORAGE MODE OF THE OUTPUT    MADD 340
C           MATRIX FOR ALL COMBINATIONS OF INPUT MATRICES               MADD 350
C                       A              B              R                MADD 360
C                 GENERAL        GENERAL        GENERAL                MADD 370
C                 GENERAL        SYMMETRIC      GENERAL                MADD 380
C                 GENERAL        DIAGONAL       GENERAL                MADD 390
C                 SYMMETRIC      GENERAL        GENERAL                MADD 400
C                 SYMMETRIC      SYMMETRIC      SYMMETRIC              MADD 410
C                 SYMMETRIC      DIAGONAL       SYMMETRIC              MADD 420
C                 DIAGONAL       GENERAL        GENERAL                MADD 430
C                 DIAGONAL       SYMMETRIC      SYMMETRIC              MADD 440
C                 DIAGONAL       DIAGONAL       DIAGONAL               MADD 450
C                                                                       MADD 460
C  ***********************************************************************MADD 470
C                                                                       MADD 480
      SUBROUTINE MADD(A,B,R,N,M,MSA,MSB)                                MADD 490
      DIMENSION A(1),B(1),R(1)                                          MADD 500
C                                                                       MADD 510
C        DETERMINE STORAGE MODE OF OUTPUT MATRIX                        MADD 520
C                                                                       MADD 530
      IF(MSA-MSB) 7,5,7                                                 MADD 540
    5 CALL LOC(N,M,NM,N,M,MSA)                                          MADD 550
      GO TO 10C                                                         MADD 560
    7 MTEST=MSA*MSB                                                     MADD 570
      MSA=0                                                             MADD 580
      IF(MTEST) 20,20,10                                                MADD 590
   10 MSA=1                                                             MADD 600
   20 IF(MTEST-2) 35,35,30                                              MADD 610
   30 MSA=2                                                             MADD 620
C                                                                       MADD 630
C        LOCATE ELEMENTS AND PERFORM ADDITION                           MADD 640
C                                                                       MADD 650
   35 DO 90 J=1,M                                                       MADD 660
      DO 90 I=1,N                                                       MADD 670
      CALL LOC(I,J,IJR,N,M,MSA)                                         MADD 680
      IF(IJR) 40,90,40                                                  MADD 690
   40 CALL LOC(I,J,IJA,N,M,MSA)                                         MADD 700
      AEL=0.0                                                           MADD 710
      IF(IJA) 50,60,50                                                  MADD 720
   50 AEL=A(IJA)                                                        MADD 730
   60 CALL LOC(I,J,IJB,N,M,MSB)                                         MADD 740
      BEL=0.0                                                           MADD 750
      IF(IJB) 70,80,70                                                  MADD 760
   70 BEL=B(IJB)                                                        MADD 770
   80 R(IJR)=AEL+BEL                                                    MADD 780
   90 CONTINUE                                                          MADD 790
      RETURN                                                            MADD 800
C                                                                       MADD 810
C        ADD MATRICES FOR OTHER CASES                                   MADD 820
C                                                                       MADD 830
  100 DO 110 I=1,NM                                                     MADD 840
  110 R(I)=A(I)+B(I)                                                    MADD 850
      RETURN                                                            MADD 860
      END                                                               MADD 870
```

Subroutine MSUB

```
C                                                                       MSUB  10
C  ***********************************************************************MSUB  20
C                                                                       MSUB  30
C        SUBROUTINE MSUB                                                MSUB  40
C                                                                       MSUB  50
C        PURPOSE                                                        MSUB  60
C           SUBTRACT TWO MATRICES ELEMENT BY ELEMENT TO FORM RESULTANT  MSUB  70
C           MATRIX                                                      MSUB  80
C                                                                       MSUB  90
C        USAGE                                                          MSUB 100
C           CALL MSUB(A,B,R,N,M,MSA,MSB)                                MSUB 110
C                                                                       MSUB 120
C        DESCRIPTION OF PARAMETERS                                      MSUB 130
C           A - NAME OF INPUT MATRIX                                    MSUB 140
C           B - NAME OF INPUT MATRIX                                    MSUB 150
C           R - NAME OF OUTPUT MATRIX                                   MSUB 160
C           N - NUMBER OF ROWS IN A,B,R                                 MSUB 170
C           M - NUMBER OF COLUMNS IN A,B,R                              MSUB 180
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         MSUB 190
C                 0 - GENERAL                                           MSUB 200
C                 1 - SYMMETRIC                                         MSUB 210
C                 2 - DIAGONAL                                          MSUB 220
C           MSB - SAME AS MSA EXCEPT FOR MATRIX B                       MSUB 230
C                                                                       MSUB 240
C        REMARKS                                                        MSUB 250
C           NONE                                                        MSUB 260
C                                                                       MSUB 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MSUB 280
C           LOC                                                         MSUB 290
C                                                                       MSUB 300
C        METHOD                                                         MSUB 310
C           STRUCTURE OF OUTPUT MATRIX IS FIRST DETERMINED. SUBTRACTION MSUB 320
C           OF MATRIX B ELEMENTS FROM CORRESPONDING MATRIX A ELEMENTS   MSUB 330
C           IS THEN PERFORMED.                                          MSUB 340
C           THE FOLLOWING TABLE SHOWS THE STORAGE MODE OF THE OUTPUT    MSUB 350
C           MATRIX FOR ALL COMBINATIONS OF INPUT MATRICES               MSUB 360
C                       A              B              R                MSUB 370
C                 GENERAL        GENERAL        GENERAL                MSUB 380
C                 GENERAL        SYMMETRIC      GENERAL                MSUB 390
C                 GENERAL        DIAGONAL       GENERAL                MSUB 400
C                 SYMMETRIC      GENERAL        GENERAL                MSUB 410
C                 SYMMETRIC      SYMMETRIC      SYMMETRIC              MSUB 420
C                 SYMMETRIC      DIAGONAL       SYMMETRIC              MSUB 430
C                 DIAGONAL       GENERAL        GENERAL                MSUB 440
C                 DIAGONAL       SYMMETRIC      SYMMETRIC              MSUB 450
C                 DIAGONAL       DIAGONAL       DIAGONAL               MSUB 460
C                                                                       MSUB 470
C  ***********************************************************************MSUB 480
C                                                                       MSUB 490
      SUBROUTINE MSUB(A,B,R,N,M,MSA,MSB)                                MSUB 500
      DIMENSION A(1),B(1),R(1)                                          MSUB 510
C                                                                       MSUB 520
C        DETERMINE STORAGE MODE OF OUTPUT MATRIX                        MSUB 530
C                                                                       MSUB 540
      IF(MSA-MSB) 7,5,7                                                 MSUB 550
    5 CALL LOC(N,M,NM,N,M,MSA)                                          MSUB 560
      GO TO 100                                                         MSUB 570
    7 MTEST=MSA*MSB                                                     MSUB 580
      MSA=0                                                             MSUB 590
      IF(MTEST) 20,20,10                                                MSUB 600
   10 MSA=1                                                             MSUB 610
   20 IF(MTEST-2) 35,35,30                                              MSUB 620
   30 MSA=2                                                             MSUB 630
C                                                                       MSUB 640
C        LOCATE ELEMENTS AND PERFORM SUBTRACTION                        MSUB 650
C                                                                       MSUB 660
   35 DO 90 J=1,M                                                       MSUB 670
      DO 90 I=1,N                                                       MSUB 680
      CALL LOC(I,J,IJR,N,M,MSA)                                         MSUB 690
      IF(IJR) 40,90,40                                                  MSUB 700
   40 CALL LOC(I,J,IJA,N,M,MSA)                                         MSUB 710
      AEL=0.0                                                           MSUB 720
      IF(IJA) 50,60,50                                                  MSUB 730
   50 AEL=A(IJA)                                                        MSUB 740
   60 CALL LOC(I,J,IJB,N,M,MSB)                                         MSUB 750
      BEL=0.0                                                           MSUB 760
      IF(IJB) 70,80,70                                                  MSUB 770
   70 BEL=B(IJB)                                                        MSUB 780
   80 R(IJR)=AEL-BEL                                                    MSUB 790
   90 CONTINUE                                                          MSUB 800
      RETURN                                                            MSUB 810
C                                                                       MSUB 820
C        SUBTRACT MATRICES FOR OTHER CASES                              MSUB 830
C                                                                       MSUB 840
  100 DO 110 I=1,NM                                                     MSUB 850
  110 R(I)=A(I)-B(I)                                                    MSUB 860
      RETURN                                                            MSUB 870
      END                                                               MSUB 880
```

Subroutine MPRD

```
C                                                                       MPRD  10
C     ******************************************************************MPRD  20
C                                                                       MPRD  30
C        SUBROUTINE MPRD                                                MPRD  40
C                                                                       MPRD  50
C        PURPOSE                                                        MPRD  60
C           MULTIPLY TWO MATRICES TO FORM A RESULTANT MATRIX            MPRD  70
C                                                                       MPRD  80
C        USAGE                                                          MPRD  90
C           CALL MPRD(A,B,R,N,M,MSA,MSB,L)                              MPRD 100
C                                                                       MPRD 110
C        DESCRIPTION OF PARAMETERS                                      MPRD 120
C           A - NAME OF FIRST INPUT MATRIX                              MPRD 130
C           B - NAME OF SECOND INPUT MATRIX                             MPRD 140
C           R - NAME OF OUTPUT MATRIX                                   MPRD 150
C           N - NUMBER OF ROWS IN A AND R                               MPRD 160
C           M - NUMBER OF COLUMNS IN A AND ROWS IN B                    MPRD 170
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         MPRD 180
C                 0 - GENERAL                                           MPRD 190
C                 1 - SYMMETRIC                                         MPRD 200
C                 2 - DIAGONAL                                          MPRD 210
C           MSB - SAME AS MSA EXCEPT FOR MATRIX B                       MPRD 220
C           L - NUMBER OF COLUMNS IN B AND R                            MPRD 230
C                                                                       MPRD 240
C        REMARKS                                                        MPRD 250
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRICES A OR B  MPRD 260
C           NUMBER OF COLUMNS OF MATRIX A MUST BE EQUAL TO NUMBER OF ROWMPRD 270
C           OF MATRIX B                                                 MPRD 280
C                                                                       MPRD 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MPRD 300
C           LOC                                                         MPRD 310
C                                                                       MPRD 320
C        METHOD                                                         MPRD 330
C           THE M BY L MATRIX B IS PREMULTIPLIED BY THE N BY M MATRIX A MPRD 340
C           AND THE RESULT IS STORED IN THE N BY L MATRIX R. THIS IS A  MPRD 350
C           ROW INTO COLUMN PRODUCT.                                    MPRD 360
C           THE FOLLOWING TABLE SHOWS THE STORAGE MODE OF THE OUTPUT    MPRD 370
C           MATRIX FOR ALL COMBINATIONS OF INPUT MATRICES               MPRD 380
C                        A              B              R                MPRD 390
C                  GENERAL        GENERAL        GENERAL               MPRD 400
C                  GENERAL        SYMMETRIC      GENERAL               MPRD 410
C                  GENERAL        DIAGONAL       GENERAL               MPRD 420
C                  SYMMETRIC      GENERAL        GENERAL               MPRD 430
C                  SYMMETRIC      SYMMETRIC      GENERAL               MPRD 440
C                  SYMMETRIC      DIAGONAL       GENERAL               MPRD 450
C                  DIAGONAL       GENERAL        GENERAL               MPRD 460
C                  DIAGONAL       SYMMETRIC      GENERAL               MPRD 470
C                  DIAGONAL       DIAGONAL       DIAGONAL              MPRD 480
C                                                                       MPRD 490
C     ******************************************************************MPRD 500
C                                                                       MPRD 510
      SUBROUTINE MPRD(A,B,R,N,M,MSA,MSB,L)                              MPRD 520
      DIMENSION A(1),B(1),R(1)                                          MPRD 530
C                                                                       MPRD 540
C        SPECIAL CASE FOR DIAGONAL BY DIAGONAL                          MPRD 550
C                                                                       MPRD 560
      MS=MSA*10+MSB                                                     MPRD 570
      IF(MS-22) 30,10,30                                                MPRD 580
   10 DO 20 I=1,N                                                       MPRD 590
   20 R(I)=A(I)*B(I)                                                    MPRD 600
      RETURN                                                            MPRD 610
C                                                                       MPRD 620
C        ALL OTHER CASES                                                MPRD 630
C                                                                       MPRD 640
   30 IR=1                                                              MPRD 650
      DO 90 K=1,L                                                       MPRD 660
      DO 90 J=1,N                                                       MPRD 670
      R(IR)=0                                                           MPRD 680
      DO 80 I=1,M                                                       MPRD 690
      IF(MS) 40,60,40                                                   MPRD 700
   40 CALL LOC(J,I,IA,N,M,MSA)                                          MPRD 710
      CALL LOC(I,K,IB,M,L,MSB)                                          MPRD 720
      IF(IA) 50,80,50                                                   MPRD 730
   50 IF(IB) 70,80,70                                                   MPRD 740
   60 IA=N*(I-1)+J                                                      MPRD 750
      IB=M*(K-1)+I                                                      MPRD 760
   70 R(IR)=R(IR)+A(IA)*B(IB)                                           MPRD 770
   80 CONTINUE                                                          MPRD 780
   90 IR=IR+1                                                           MPRD 790
      RETURN                                                            MPRD 800
      END                                                               MPRD 810
```

Subroutine MTRA

```
C                                                                       MTRA  10
C     ******************************************************************MTRA  20
C                                                                       MTRA  30
C        SUBROUTINE MTRA                                                MTRA  40
C                                                                       MTRA  50
C        PURPOSE                                                        MTRA  60
C           TRANSPOSE A MATRIX                                          MTRA  70
C                                                                       MTRA  80
C        USAGE                                                          MTRA  90
C           CALL MTRA(A,R,N,M,MS)                                       MTRA 100
C                                                                       MTRA 110
C        DESCRIPTION OF PARAMETERS                                      MTRA 120
C           A - NAME OF MATRIX TO BE TRANSPOSED                         MTRA 130
C           R - NAME OF OUTPUT MATRIX                                   MTRA 140
C           N - NUMBER OF ROWS OF A AND COLUMNS OF R                    MTRA 150
C           M - NUMBER OF COLUMNS OF A AND ROWS OF R                    MTRA 160
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R) MTRA 170
C                 0 - GENERAL                                           MTRA 180
C                 1 - SYMMETRIC                                         MTRA 190
C                 2 - DIAGONAL                                          MTRA 200
C                                                                       MTRA 210
C        REMARKS                                                        MTRA 220
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         MTRA 230
C                                                                       MTRA 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MTRA 250
C           MCPY                                                        MTRA 260
C                                                                       MTRA 270
C        METHOD                                                         MTRA 280
C           TRANSPOSE N BY M MATRIX A TO FORM M BY N MATRIX R BY MOVING MTRA 290
C           EACH ROW OF A INTO THE CORRESPONDING COLUMN OF R. IF MATRIX MTRA 300
C           A IS SYMMETRIC OR DIAGONAL, MATRIX R IS THE SAME AS A.      MTRA 310
C                                                                       MTRA 320
C     ******************************************************************MTRA 330
C                                                                       MTRA 340
      SUBROUTINE MTRA(A,R,N,M,MS)                                       MTRA 350
      DIMENSION A(1),R(1)                                               MTRA 360
C                                                                       MTRA 370
C        IF MS IS 1 OR 2, COPY A                                        MTRA 380
C                                                                       MTRA 390
      IF(MS) 10,20,10                                                   MTRA 400
   10 CALL MCPY(A,R,N,N,MS)                                             MTRA 410
      RETURN                                                            MTRA 420
C                                                                       MTRA 430
C        TRANSPOSE GENERAL MATRIX                                       MTRA 440
C                                                                       MTRA 450
   20 IR=0                                                              MTRA 460
      DO 30 I=1,N                                                       MTRA 470
      IJ=I-N                                                            MTRA 480
      DO 30 J=1,M                                                       MTRA 490
      IJ=IJ+N                                                           MTRA 500
      IR=IR+1                                                           MTRA 510
   30 R(IR)=A(IJ)                                                       MTRA 520
      RETURN                                                            MTRA 530
      END                                                               MTRA 540
```

Subroutine TPRD

```
C                                                                       TPRD  10
C     ...................................................................TPRD  20
C                                                                       TPRD  30
C        SUBROUTINE TPRD                                                TPRD  40
C                                                                       TPRD  50
C        PURPOSE                                                        TPRD  60
C           TRANSPOSE A MATRIX AND POSTMULTIPLY BY ANOTHER TO FORM      TPRD  70
C           A RESULTANT MATRIX                                          TPRD  80
C                                                                       TPRD  90
C        USAGE                                                          TPRD 100
C           CALL TPRD(A,B,R,N,M,MSA,MSB,L)                              TPRD 110
C                                                                       TPRD 120
C        DESCRIPTION OF PARAMETERS                                      TPRD 130
C           A - NAME OF FIRST INPUT MATRIX                              TPRD 140
C           B - NAME OF SECOND INPUT MATRIX                             TPRD 150
C           R - NAME OF OUTPUT MATRIX                                   TPRD 160
C           N - NUMBER OF ROWS IN A AND B                               TPRD 170
C           M - NUMBER OF COLUMNS IN A AND ROWS IN R                    TPRD 180
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         TPRD 190
C                 0 - GENERAL                                           TPRD 200
C                 1 - SYMMETRIC                                         TPRD 210
C                 2 - DIAGONAL                                          TPRD 220
C           MSB - SAME AS MSA EXCEPT FOR MATRIX B                       TPRD 230
C           L - NUMBER OF COLUMNS IN B AND R                            TPRD 240
C                                                                       TPRD 250
C        REMARKS                                                        TPRD 260
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRICES A OR B  TPRD 270
C                                                                       TPRD 280
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TPRD 290
C           LOC                                                         TPRD 300
C                                                                       TPRD 310
C        METHOD                                                         TPRD 320
C           MATRIX TRANSPOSE OF A IS NOT ACTUALLY CALCULATED. INSTEAD,  TPRD 330
C           ELEMENTS IN MATRIX A ARE TAKEN COLUMNWISE RATHER THAN       TPRD 340
C           ROWWISE FOR MULTIPLICATION BY MATRIX B.                     TPRD 350
C           THE FOLLOWING TABLE SHOWS THE STORAGE MODE OF THE OUTPUT    TPRD 360
C           MATRIX FOR ALL COMBINATIONS OF INPUT MATRICES               TPRD 370
C                       A                B                R             TPRD 380
C                   GENERAL          GENERAL          GENERAL           TPRD 390
C                   GENERAL          SYMMETRIC        GENERAL           TPRD 400
C                   GENERAL          DIAGONAL         GENERAL           TPRD 410
C                   SYMMETRIC        GENERAL          GENERAL           TPRD 420
C                   SYMMETRIC        SYMMETRIC        GENERAL           TPRD 430
C                   SYMMETRIC        DIAGONAL         GENERAL           TPRD 440
C                   DIAGONAL         GENERAL          GENERAL           TPRD 450
C                   DIAGONAL         SYMMETRIC        GENERAL           TPRD 460
C                   DIAGONAL         DIAGONAL         DIAGONAL          TPRD 470
C                                                                       TPRD 480
C     ...................................................................TPRD 490
C                                                                       TPRD 500
      SUBROUTINE TPRD(A,B,R,N,M,MSA,MSB,L)                              TPRD 510
      DIMENSION A(1),B(1),R(1)                                          TPRD 520
C                                                                       TPRD 530
C        SPECIAL CASE FOR DIAGONAL BY DIAGONAL                          TPRD 540
C                                                                       TPRD 550
      MS=MSA*10+MSB                                                     TPRD 560
      IF(MS-22) 30,10,30                                                TPRD 570
   10 DO 20 I=1,N                                                       TPRD 580
   20 R(I)=A(I)*B(I)                                                    TPRD 590
      RETURN                                                            TPRD 600
C                                                                       TPRD 610
C        MULTIPLY TRANSPOSE OF A BY B                                   TPRD 620
C                                                                       TPRD 630
   30 IR=1                                                              TPRD 640
      DO 90 K=1,L                                                       TPRD 650
      DO 90 J=1,M                                                       TPRD 660
      R(IR)=0.0                                                         TPRD 670
      DO 80 I=1,N                                                       TPRD 680
      IF(MS) 40,60,40                                                   TPRD 690
   40 CALL LOC(I,J,IA,N,M,MSA)                                          TPRD 700
      CALL LOC(I,K,IB,N,L,MSB)                                          TPRD 710
      IF(IA) 50,80,50                                                   TPRD 720
   50 IF(IB) 70,80,70                                                   TPRD 730
   60 IA=N*(J-1)+I                                                      TPRD 740
      IB=N*(K-1)+I                                                      TPRD 750
   70 R(IR)=R(IR)+A(IA)*B(IB)                                           TPRD 760
   80 CONTINUE                                                          TPRD 770
   90 IR=IR+1                                                           TPRD 780
      RETURN                                                            TPRD 790
      END                                                               TPRD 800
```

Subroutine MATA

```
C                                                                       MATA  10
C     ...................................................................MATA  20
C                                                                       MATA  30
C        SUBROUTINE MATA                                                MATA  40
C                                                                       MATA  50
C        PURPOSE                                                        MATA  60
C           PREMULTIPLY A MATRIX BY ITS TRANSPOSE TO FORM A             MATA  70
C           SYMMETRIC MATRIX                                            MATA  80
C                                                                       MATA  90
C        USAGE                                                          MATA 100
C           CALL MATA(A,R,N,M,MS)                                       MATA 110
C                                                                       MATA 120
C        DESCRIPTION OF PARAMETERS                                      MATA 130
C           A  - NAME OF INPUT MATRIX                                   MATA 140
C           R  - NAME OF OUTPUT MATRIX                                  MATA 150
C           N  - NUMBER OF ROWS IN A                                    MATA 160
C           M  - NUMBER OF COLUMNS IN A. ALSO NUMBER OF ROWS AND        MATA 170
C                NUMBER OF COLUMNS OF R.                                MATA 180
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         MATA 190
C                 0 - GENERAL                                           MATA 200
C                 1 - SYMMETRIC                                         MATA 210
C                 2 - DIAGONAL                                          MATA 220
C                                                                       MATA 230
C        REMARKS                                                        MATA 240
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         MATA 250
C           MATRIX R IS ALWAYS A SYMMETRIC MATRIX WITH A STORAGE MODE=1 MATA 260
C                                                                       MATA 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MATA 280
C           LOC                                                         MATA 290
C                                                                       MATA 300
C        METHOD                                                         MATA 310
C           CALCULATION OF (A TRANSPOSE A) RESULTS IN A SYMMETRIC MATRIXMATA 320
C           REGARDLESS OF THE STORAGE MODE OF THE INPUT MATRIX. THE     MATA 330
C           ELEMENTS OF MATRIX A ARE NOT CHANGED.                       MATA 340
C                                                                       MATA 350
C     ...................................................................MATA 360
C                                                                       MATA 370
      SUBROUTINE MATA(A,R,N,M,MS)                                       MATA 380
      DIMENSION A(1),R(1)                                               MATA 390
C                                                                       MATA 400
      DO 60 K=1,M                                                       MATA 410
      KX=(K*K-K)/2                                                      MATA 420
      DO 60 J=1,M                                                       MATA 430
      IF(J-K) 10,10,60                                                  MATA 440
   10 IR=J+KX                                                           MATA 450
      R(IR)=0                                                           MATA 460
      DO 60 I=1,N                                                       MATA 470
      IF(MS) 20,40,20                                                   MATA 480
   20 CALL LOC(I,J,IA,N,M,MS)                                           MATA 490
      CALL LOC(I,K,IB,N,M,MS)                                           MATA 500
      IF(IA) 30,60,30                                                   MATA 510
   30 IF(IB) 50,60,50                                                   MATA 520
   40 IA=N*(J-1)+I                                                      MATA 530
      IB=N*(K-1)+I                                                      MATA 540
   50 R(IR)=R(IR)+A(IA)*A(IB)                                           MATA 550
   60 CONTINUE                                                          MATA 560
      RETURN                                                            MATA 570
      END                                                               MATA 580
```

Subroutine SADD

```
C                                                                       SADD  10
C  ***********************************************************************SADD  20
C                                                                       SADD  30
C       SUBROUTINE SADD                                                 SADD  40
C                                                                       SADD  50
C       PURPOSE                                                         SADD  60
C          ADD A SCALAR TO EACH ELEMENT OF A MATRIX TO FORM A RESULTANT SADD  70
C          MATRIX                                                       SADD  80
C                                                                       SADD  90
C       USAGE                                                           SADD 100
C          CALL SADD(A,C,R,N,M,MS)                                      SADD 110
C                                                                       SADD 120
C       DESCRIPTION OF PARAMETERS                                       SADD 130
C          A - NAME OF INPUT MATRIX                                     SADD 140
C          C - SCALAR                                                   SADD 150
C          R - NAME OF OUTPUT MATRIX                                    SADD 160
C          N - NUMBER OF ROWS IN MATRIX A AND R                         SADD 170
C          M - NUMBER OF COLUMNS IN MATRIX A AND R                      SADD 180
C          MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R)  SADD 190
C                0 - GENERAL                                            SADD 200
C                1 - SYMMETRIC                                          SADD 210
C                2 - DIAGONAL                                           SADD 220
C                                                                       SADD 230
C       REMARKS                                                         SADD 240
C          NONE                                                         SADD 250
C                                                                       SADD 260
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   SADD 270
C          LOC                                                          SADD 280
C                                                                       SADD 290
C       METHOD                                                          SADD 300
C          SCALAR IS ADDED TO EACH ELEMENT OF MATRIX                    SADD 310
C                                                                       SADD 320
C  ***********************************************************************SADD 330
C                                                                       SADD 340
      SUBROUTINE SADD(A,C,R,N,M,MS)                                     SADD 350
      DIMENSION A(1),R(1)                                               SADD 360
C                                                                       SADD 370
C        COMPUTE VECTOR LENGTH, IT                                      SADD 380
C                                                                       SADD 390
      CALL LOC(N,M,IT,N,M,MS)                                           SADD 400
C                                                                       SADD 410
C        ADD SCALAR                                                     SADD 420
C                                                                       SADD 430
      DO 1 I=1,IT                                                       SADD 440
    1 R(I)=A(I)+C                                                       SADD 450
      RETURN                                                            SADD 460
      END                                                               SADD 470
```

Subroutine SSUB

```
C                                                                       SSUB  10
C  ***********************************************************************SSUB  20
C                                                                       SSUB  30
C       SUBROUTINE SSUB                                                 SSUB  40
C                                                                       SSUB  50
C       PURPOSE                                                         SSUB  60
C          SUBTRACT A SCALAR FROM EACH ELEMENT OF A MATRIX TO FORM A    SSUB  70
C          RESULTANT MATRIX                                             SSUB  80
C                                                                       SSUB  90
C       USAGE                                                           SSUB 100
C          CALL SSUB(A,C,R,N,M,MS)                                      SSUB 110
C                                                                       SSUB 120
C       DESCRIPTION OF PARAMETERS                                       SSUB 130
C          A - NAME OF INPUT MATRIX                                     SSUB 140
C          C - SCALAR                                                   SSUB 150
C          R - NAME OF OUTPUT MATRIX                                    SSUB 160
C          N - NUMBER OF ROWS IN MATRIX A AND R                         SSUB 170
C          M - NUMBER OF COLUMNS IN MATRIX A AND R                      SSUB 180
C          MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R)  SSUB 190
C                0 - GENERAL                                            SSUB 200
C                1 - SYMMETRIC                                          SSUB 210
C                2 - DIAGONAL                                           SSUB 220
C                                                                       SSUB 230
C       REMARKS                                                         SSUB 240
C          NONE                                                         SSUB 250
C                                                                       SSUB 260
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   SSUB 270
C          LOC                                                          SSUB 280
C                                                                       SSUB 290
C       METHOD                                                          SSUB 300
C          SCALAR IS SUBTRACTED FROM EACH EACH ELEMENT OF MATRIX        SSUB 310
C                                                                       SSUB 320
C  ***********************************************************************SSUB 330
C                                                                       SSUB 340
      SUBROUTINE SSUB(A,C,R,N,M,MS)                                     SSUB 350
      DIMENSION A(1),R(1)                                               SSUB 360
C                                                                       SSUB 370
C        COMPUTE VECTOR LENGTH, IT                                      SSUB 380
C                                                                       SSUB 390
      CALL LOC(N,M,IT,N,M,MS)                                           SSUB 400
C                                                                       SSUB 410
C        SUBTRACT SCALAR                                                SSUB 420
C                                                                       SSUB 430
      DO 1 I=1,IT                                                       SSUB 440
    1 R(I)=A(I)-C                                                       SSUB 450
      RETURN                                                            SSUB 460
      END                                                               SSUB 470
```

Subroutine SMPY

```
C                                                                       SMPY  10
C     ...................................................................SMPY  20
C                                                                       SMPY  30
C        SUBROUTINE SMPY                                                SMPY  40
C                                                                       SMPY  50
C        PURPOSE                                                        SMPY  60
C           MULTIPLY EACH ELEMENT OF A MATRIX BY A SCALAR TO FORM A     SMPY  70
C           RESULTANT MATRIX                                            SMPY  80
C                                                                       SMPY  90
C        USAGE                                                          SMPY 100
C           CALL SMPY(A,C,R,N,M,MS)                                     SMPY 110
C                                                                       SMPY 120
C        DESCRIPTION OF PARAMETERS                                      SMPY 130
C           A - NAME OF INPUT MATRIX                                    SMPY 140
C           C - SCALAR                                                  SMPY 150
C           R - NAME OF OUTPUT MATRIX                                   SMPY 160
C           N - NUMBER OF ROWS IN MATRIX A AND R                        SMPY 170
C           M - NUMBER OF COLUMNS IN MATRIX A AND R                     SMPY 180
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R) SMPY 190
C                 0 - GENERAL                                           SMPY 200
C                 1 - SYMMETRIC                                         SMPY 210
C                 2 - DIAGONAL                                          SMPY 220
C                                                                       SMPY 230
C        REMARKS                                                        SMPY 240
C           NONE                                                        SMPY 250
C                                                                       SMPY 260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SMPY 270
C           LOC                                                         SMPY 280
C                                                                       SMPY 290
C        METHOD                                                         SMPY 300
C           SCALAR IS MULTIPLIED BY EACH ELEMENT OF MATRIX              SMPY 310
C                                                                       SMPY 320
C     ...................................................................SMPY 330
C                                                                       SMPY 340
      SUBROUTINE SMPY(A,C,R,N,M,MS)                                     SMPY 350
      DIMENSION A(1),R(1)                                               SMPY 360
C                                                                       SMPY 370
C        COMPUTE VECTOR LENGTH, IT                                      SMPY 380
C                                                                       SMPY 390
      CALL LOC(N,M,IT,N,M,MS)                                           SMPY 400
C                                                                       SMPY 410
C        MULTIPLY BY SCALAR                                             SMPY 420
C                                                                       SMPY 430
      DO 1 I=1,IT                                                       SMPY 440
    1 R(I)=A(I)*C                                                       SMPY 450
      RETURN                                                            SMPY 460
      END                                                               SMPY 470
```

Subroutine SDIV

```
C                                                                       SDIV  10
C     ...................................................................SDIV  20
C                                                                       SDIV  30
C        SUBROUTINE SDIV                                                SDIV  40
C                                                                       SDIV  50
C        PURPOSE                                                        SDIV  60
C           DIVIDE EACH ELEMENT OF A MATRIX BY A SCALAR TO FORM A       SDIV  70
C           RESULTANT MATRIX                                            SDIV  80
C                                                                       SDIV  90
C        USAGE                                                          SDIV 100
C           CALL SDIV(A,C,R,N,M,MS)                                     SDIV 110
C                                                                       SDIV 120
C        DESCRIPTION OF PARAMETERS                                      SDIV 130
C           A - NAME OF INPUT MATRIX                                    SDIV 140
C           C - SCALAR                                                  SDIV 150
C           R - NAME OF OUTPUT MATRIX                                   SDIV 160
C           N - NUMBER OF ROWS IN MATRIX A AND R                        SDIV 170
C           M - NUMBER OF COLUMNS IN MATRIX A AND R                     SDIV 180
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R) SDIV 190
C                 0 - GENERAL                                           SDIV 200
C                 1 - SYMMETRIC                                         SDIV 210
C                 2 - DIAGONAL                                          SDIV 220
C                                                                       SDIV 230
C        REMARKS                                                        SDIV 240
C           IF SCALAR IS ZERO, DIVISION IS PERFORMED ONLY ONCE TO CAUSE SDIV 250
C           FLOATING POINT OVERFLOW CONDITION                           SDIV 260
C                                                                       SDIV 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SDIV 280
C           LOC                                                         SDIV 290
C                                                                       SDIV 300
C        METHOD                                                         SDIV 310
C           EACH ELEMENT OF MATRIX IS DIVIDED BY SCALAR                 SDIV 320
C                                                                       SDIV 330
C     ...................................................................SDIV 340
C                                                                       SDIV 350
      SUBROUTINE SDIV(A,C,R,N,M,MS)                                     SDIV 360
      DIMENSION A(1),R(1)                                               SDIV 370
C                                                                       SDIV 380
C        COMPUTE VECTOR LENGTH, IT                                      SDIV 390
C                                                                       SDIV 400
      CALL LOC(N,M,IT,N,M,MS)                                           SDIV 410
C                                                                       SDIV 420
C        DIVIDE BY SCALAR (IF SCALAR IS ZERO, DIVIDE ONLY ONCE)         SDIV 430
C                                                                       SDIV 440
      IF(C) 2,1,2                                                       SDIV 450
    1 IT=1                                                              SDIV 460
    2 DO 3 I=1,IT                                                       SDIV 470
    3 R(I)=A(I)/C                                                       SDIV 480
      RETURN                                                            SDIV 490
      END                                                               SDIV 500
```

Subroutine SCLA

```
C                                                                       SCLA  10
C     ***************************************************************SCLA  20
C                                                                       SCLA  30
C        SUBROUTINE SCLA                                                SCLA  40
C                                                                       SCLA  50
C        PURPOSE                                                        SCLA  60
C           SET EACH ELEMENT OF A MATRIX EQUAL TO A GIVEN SCALAR        SCLA  70
C                                                                       SCLA  80
C        USAGE                                                          SCLA  90
C           CALL SCLA (A,C,N,M,MS)                                      SCLA 100
C                                                                       SCLA 110
C        DESCRIPTION OF PARAMETERS                                      SCLA 120
C           A - NAME OF INPUT MATRIX                                    SCLA 130
C           C - SCALAR                                                  SCLA 140
C           N - NUMBER OF ROWS IN MATRIX A                              SCLA 150
C           M - NUMBER OF COLUMNS IN MATRIX A                           SCLA 160
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         SCLA 170
C                 0 - GENERAL                                           SCLA 180
C                 1 - SYMMETRIC                                         SCLA 190
C                 2 - DIAGONAL                                          SCLA 200
C                                                                       SCLA 210
C        REMARKS                                                        SCLA 220
C           NONE                                                        SCLA 230
C                                                                       SCLA 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SCLA 250
C           LOC                                                         SCLA 260
C                                                                       SCLA 270
C        METHOD                                                         SCLA 280
C           EACH ELEMENT OF MATRIX A IS REPLACED BY SCALAR C            SCLA 290
C                                                                       SCLA 300
C     ***************************************************************SCLA 310
C                                                                       SCLA 320
      SUBROUTINE SCLA(A,C,N,M,MS)                                       SCLA 330
      DIMENSION A(1)                                                    SCLA 340
C                                                                       SCLA 350
C        COMPUTE VECTOR LENGTH, IT                                      SCLA 360
C                                                                       SCLA 370
      CALL LOC(N,M,IT,N,M,MS)                                           SCLA 380
C                                                                       SCLA 390
C        REPLACE BY SCALAR                                              SCLA 400
C                                                                       SCLA 410
      DO 1 I=1,IT                                                       SCLA 420
    1 A(I)=C                                                            SCLA 430
      RETURN                                                            SCLA 440
      END                                                               SCLA 450
```

Subroutine DCLA

```
C                                                                       DCLA  10
C     ***************************************************************DCLA  20
C                                                                       DCLA  30
C        SUBROUTINE DCLA                                                DCLA  40
C                                                                       DCLA  50
C        PURPOSE                                                        DCLA  60
C           SET EACH DIAGONAL ELEMENT OF A MATRIX EQUAL TO A SCALAR     DCLA  70
C                                                                       DCLA  80
C        USAGE                                                          DCLA  90
C           CALL DCLA (A,C,N,MS)                                        DCLA 100
C                                                                       DCLA 110
C        DESCRIPTION OF PARAMETERS                                      DCLA 120
C           A - NAME OF INPUT MATRIX                                    DCLA 130
C           C - SCALAR                                                  DCLA 140
C           N - NUMBER OF ROWS AND COLUMNS IN MATRIX A                  DCLA 150
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         DCLA 160
C                 0 - GENERAL                                           DCLA 170
C                 1 - SYMMETRIC                                         DCLA 180
C                 2 - DIAGONAL                                          DCLA 190
C                                                                       DCLA 200
C        REMARKS                                                        DCLA 210
C           INPUT MATRIX MUST BE A SQUARE MATRIX                        DCLA 220
C                                                                       DCLA 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DCLA 240
C           LOC                                                         DCLA 250
C                                                                       DCLA 260
C        METHOD                                                         DCLA 270
C           EACH ELEMENT ON DIAGONAL OF MATRIX IS REPLACED BY SCALAR C  DCLA 280
C                                                                       DCLA 290
C     ***************************************************************DCLA 300
C                                                                       DCLA 310
      SUBROUTINE DCLA(A,C,N,MS)                                         DCLA 320
      DIMENSION A(1)                                                    DCLA 330
C                                                                       DCLA 340
      DO 3 I=1,N                                                        DCLA 350
C                                                                       DCLA 360
C        LOCATE DIAGONAL ELEMENT FOR ANY MATRIX STORAGE MODE            DCLA 370
C                                                                       DCLA 380
      CALL LOC(I,I,ID,N,N,MS)                                           DCLA 390
C                                                                       DCLA 400
C        REPLACE DIAGONAL ELEMENTS                                      DCLA 410
C                                                                       DCLA 420
    3 A(ID)=C                                                           DCLA 430
      RETURN                                                            DCLA 440
      END                                                               DCLA 450
```

Subroutine RADD

```
C                                                                       RADD  10
C     ...................................................................RADD  20
C                                                                       RADD  30
C        SUBROUTINE RADD                                                RADD  40
C                                                                       RADD  50
C        PURPOSE                                                        RADD  60
C           ADD ROW OF ONE MATRIX TO ROW OF ANOTHER MATRIX              RADD  70
C                                                                       RADD  80
C        USAGE                                                          RADD  90
C           CALL RADD(A,IRA,R,IRR,N,M,MS,L)                             RADD 100
C                                                                       RADD 110
C        DESCRIPTION OF PARAMETERS                                      RADD 120
C           A   - NAME OF INPUT MATRIX                                  RADD 130
C           IRA - ROW IN MATRIX A TO BE ADDED TO ROW IRR OF MATRIX R    RADD 140
C           R   - NAME OF OUTPUT MATRIX                                 RADD 150
C           IRR - ROW IN MATRIX R WHERE SUMMATION IS DEVELOPED          RADD 160
C           N   - NUMBER OF ROWS IN A                                   RADD 170
C           M   - NUMBER OF COLUMNS IN A AND R                          RADD 180
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         RADD 190
C                 0 - GENERAL                                           RADD 200
C                 1 - SYMMETRIC                                         RADD 210
C                 2 - DIAGONAL                                          RADD 220
C           L   - NUMBER OF ROWS IN R                                   RADD 230
C                                                                       RADD 240
C        REMARKS                                                        RADD 250
C           MATRIX R MUST BE A GENERAL MATRIX                           RADD 260
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A UNLESS  RADD 270
C           A IS GENERAL                                                RADD 280
C                                                                       RADD 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RADD 300
C           LOC                                                         RADD 310
C                                                                       RADD 320
C        METHOD                                                         RADD 330
C           EACH ELEMENT OF ROW IRA OF MATRIX A IS ADDED TO             RADD 340
C           CORRESPONDING ELEMENT OF ROW IRR OF MATRIX R                RADD 350
C                                                                       RADD 360
C     ...................................................................RADD 370
C                                                                       RADD 380
      SUBROUTINE RADD(A,IRA,R,IRR,N,M,MS,L)                             RADD 390
      DIMENSION A(1),R(1)                                               RADD 400
C                                                                       RADD 410
      IR=IRR-L                                                          RADD 420
      DO 2 J=1,M                                                        RADD 430
      IR=IR+L                                                           RADD 440
C                                                                       RADD 450
C        LOCATE INPUT ELEMENT FOR ANY MATRIX STORAGE MODE               RADD 460
C                                                                       RADD 470
      CALL LOC(IRA,J,IA,N,M,MS)                                         RADD 480
C                                                                       RADD 490
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RADD 500
C                                                                       RADD 510
      IF(IA) 1,2,1                                                      RADD 520
C                                                                       RADD 530
C        ADD ELEMENTS                                                   RADD 540
C                                                                       RADD 550
    1 R(IR)=R(IR)+A(IA)                                                 RADD 560
    2 CONTINUE                                                          RADD 570
      RETURN                                                            RADD 580
      END                                                               RADD 590
```

Subroutine CADD

```
C                                                                       CADD  10
C     ...................................................................CADD  20
C                                                                       CADD  30
C        SUBROUTINE CADD                                                CADD  40
C                                                                       CADD  50
C        PURPOSE                                                        CADD  60
C           ADD COLUMN OF ONE MATRIX TO COLUMN OF ANOTHER MATRIX        CADD  70
C                                                                       CADD  80
C        USAGE                                                          CADD  90
C           CALL CADD(A,ICA,R,ICR,N,M,MS,L)                             CADD 100
C                                                                       CADD 110
C        DESCRIPTION OF PARAMETERS                                      CADD 120
C           A   - NAME OF INPUT MATRIX                                  CADD 130
C           ICA - COLUMN IN MATRIX A TO BE ADDED TO COLUMN ICR OF R     CADD 140
C           R   - NAME OF OUTPUT MATRIX                                 CADD 150
C           ICR - COLUMN IN MATRIX R WHERE SUMMATION IS DEVELOPED       CADD 160
C           N   - NUMBER OF ROWS IN A AND R                             CADD 170
C           M   - NUMBER OF COLUMNS IN A                                CADD 180
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         CADD 190
C                 0 - GENERAL                                           CADD 200
C                 1 - SYMMETRIC                                         CADD 210
C                 2 - DIAGONAL                                          CADD 220
C           L   - NUMBER OF COLUMNS IN R                                CADD 230
C                                                                       CADD 240
C        REMARKS                                                        CADD 250
C           MATRIX R MUST BE A GENERAL MATRIX                           CADD 260
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A UNLESS  CADD 270
C           A IS GENERAL                                                CADD 280
C                                                                       CADD 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CADD 300
C           LOC                                                         CADD 310
C                                                                       CADD 320
C        METHOD                                                         CADD 330
C           EACH ELEMENT OF COLUMN ICA OF MATRIX A IS ADDED TO          CADD 340
C           CORRESPONDING ELEMENT OF COLUMN ICR OF MATRIX R             CADD 350
C                                                                       CADD 360
C     ...................................................................CADD 370
C                                                                       CADD 380
      SUBROUTINE CADD(A,ICA,R,ICR,N,M,MS,L)                             CADD 390
      DIMENSION A(1),R(1)                                               CADD 400
C                                                                       CADD 410
      IR=N*(ICR-1)                                                      CADD 420
      DO 2 I=1,M                                                        CADD 430
      IR=IR+1                                                           CADD 440
C                                                                       CADD 450
C        LOCATE INPUT ELEMENT FOR ANY MATRIX STORAGE MODE               CADD 460
C                                                                       CADD 470
      CALL LOC(I,ICA,IA,N,M,MS)                                         CADD 480
C                                                                       CADD 490
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       CADD 500
C                                                                       CADD 510
      IF(IA) 1,2,1                                                      CADD 520
C                                                                       CADD 530
C        ADD ELEMENTS                                                   CADD 540
C                                                                       CADD 550
    1 R(IR)=R(IR)+A(IA)                                                 CADD 560
    2 CONTINUE                                                          CADD 570
      RETURN                                                            CADD 580
      END                                                               CADD 590
```

Subroutine SRMA

```
C                                                                       SRMA  10
C     ***************************************************************SRMA  20
C                                                                       SRMA  30
C        SUBROUTINE SRMA                                                SRMA  40
C                                                                       SRMA  50
C        PURPOSE                                                        SRMA  60
C           MULTIPLY ROW OF MATRIX BY A SCALAR AND ADD TO ANOTHER ROW   SRMA  70
C           OF THE SAME MATRIX                                          SRMA  80
C                                                                       SRMA  90
C        USAGE                                                          SRMA 100
C           CALL SRMA(A,C,N,M,LA,LB)                                    SRMA 110
C                                                                       SRMA 120
C        DESCRIPTION OF PARAMETERS                                      SRMA 130
C           A  - NAME OF MATRIX                                         SRMA 140
C           C  - SCALAR                                                 SRMA 150
C           N  - NUMBER OF ROWS IN A                                    SRMA 160
C           M  - NUMBER OF COLUMNS IN A                                 SRMA 170
C           LA - ROW IN A TO BE MULTIPLIED BY SCALAR                    SRMA 180
C           LB - ROW IN A TO WHICH PRODUCT IS ADDED                     SRMA 190
C                IF 0 IS SPECIFIED, PRODUCT REPLACES ELEMENTS IN ROW LA SRMA 200
C                                                                       SRMA 210
C        REMARKS                                                        SRMA 220
C           MATRIX A MUST BE A GENERAL MATRIX                           SRMA 230
C                                                                       SRMA 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SRMA 250
C           NONE                                                        SRMA 260
C                                                                       SRMA 270
C        METHOD                                                         SRMA 280
C           EACH ELEMENT OF ROW LA IS MULTIPLIED BY SCALAR C AND THE    SRMA 290
C           PRODUCT IS ADDED TO THE CORRESPONDING ELEMENT OF ROW LB.    SRMA 300
C           ROW LA REMAINS UNAFFECTED BY THE OPERATION.                 SRMA 310
C           IF PARAMETER LB CONTAINS ZERO, MULTIPLICATION BY THE SCALAR SRMA 320
C           IS PERFORMED AND THE PRODUCT REPLACES ELEMENTS IN ROW LA.    SRMA 330
C                                                                       SRMA 340
C     ***************************************************************SRMA 350
C                                                                       SRMA 360
      SUBROUTINE SRMA(A,C,N,M,LA,LB)                                    SRMA 370
      DIMENSION A(1)                                                    SRMA 380
C                                                                       SRMA 390
      LAJ=LA-N                                                          SRMA 400
      LBJ=LB-N                                                          SRMA 410
      DO 3 J=1,M                                                        SRMA 420
C                                                                       SRMA 430
C        LOCATE ELEMENT IN BOTH ROWS                                    SRMA 440
C                                                                       SRMA 450
      LAJ=LAJ+N                                                         SRMA 460
      LBJ=LBJ+N                                                         SRMA 470
C                                                                       SRMA 480
C        CHECK LB FOR ZERO                                              SRMA 490
C                                                                       SRMA 500
      IF(LB) 1,2,1                                                      SRMA 510
C                                                                       SRMA 520
C        IF NOT, MULTIPLY BY CONSTANT AND ADD TO OTHER ROW              SRMA 530
C                                                                       SRMA 540
    1 A(LBJ)=A(LAJ)*C+A(LBJ)                                            SRMA 550
      GO TO 3                                                           SRMA 560
C                                                                       SRMA 570
C        OTHERWISE, MULTIPLY ROW BY CONSTANT                            SRMA 580
C                                                                       SRMA 590
    2 A(LAJ)=A(LAJ)*C                                                   SRMA 600
    3 CONTINUE                                                          SRMA 610
      RETURN                                                            SRMA 620
      END                                                               SRMA 630
```

Subroutine SCMA

```
C                                                                       SCMA  10
C     ***************************************************************SCMA  20
C                                                                       SCMA  30
C        SUBROUTINE SCMA                                                SCMA  40
C                                                                       SCMA  50
C        PURPOSE                                                        SCMA  60
C           MULTIPLY COLUMN OF MATRIX BY A SCALAR AND ADD TO ANOTHER    SCMA  70
C           COLUMN OF THE SAME MATRIX                                   SCMA  80
C                                                                       SCMA  90
C        USAGE                                                          SCMA 100
C           CALL SCMA(A,C,N,LA,LB)                                      SCMA 110
C                                                                       SCMA 120
C        DESCRIPTION OF PARAMETERS                                      SCMA 130
C           A  - NAME OF MATRIX                                         SCMA 140
C           C  - SCALAR                                                 SCMA 150
C           N  - NUMBER OF ROWS IN A                                    SCMA 160
C           LA - COLUMN IN A TO BE MULTIPLIED BY SCALAR                 SCMA 170
C           LB - COLUMN IN A TO WHICH PRODUCT IS ADDED                  SCMA 180
C                IF 0 IS SPECIFIED, PRODUCT REPLACES ELEMENTS IN LA     SCMA 190
C                                                                       SCMA 200
C        REMARKS                                                        SCMA 210
C           MATRIX A MUST BE A GENERAL MATRIX                           SCMA 220
C                                                                       SCMA 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SCMA 240
C           NONE                                                        SCMA 250
C                                                                       SCMA 260
C        METHOD                                                         SCMA 270
C           EACH ELEMENT OF COLUMN LA IS MULTIPLIED BY SCALAR C AND THE SCMA 280
C           PRODUCT IS ADDED TO THE CORRESPONDING ELEMENT OF COLUMN LB. SCMA 290
C           COLUMN LA REMAINS UNAFFECTED BY THE OPERATION.              SCMA 300
C           IF PARAMETER LB CONTAINS ZERO, MULTIPLICATION BY THE SCALAR SCMA 310
C           IS PERFORMED AND THE PRODUCT REPLACES ELEMENTS IN LA.       SCMA 320
C                                                                       SCMA 330
C     ***************************************************************SCMA 340
C                                                                       SCMA 350
      SUBROUTINE SCMA(A,C,N,LA,LB)                                      SCMA 360
      DIMENSION A(1)                                                    SCMA 370
C                                                                       SCMA 380
C        LOCATE STARTING POINT OF BOTH COLUMNS                          SCMA 390
C                                                                       SCMA 400
      ILA=N*(LA-1)                                                      SCMA 410
      ILB=N*(LB-1)                                                      SCMA 420
C                                                                       SCMA 430
      DO 3 I=1,N                                                        SCMA 440
      ILA=ILA+1                                                         SCMA 450
      ILB=ILB+1                                                         SCMA 460
C                                                                       SCMA 470
C        CHECK LB FOR ZERO                                              SCMA 480
C                                                                       SCMA 490
      IF(LB) 1,2,1                                                      SCMA 500
C                                                                       SCMA 510
C        IF NOT MULTIPLY BY CONSTANT AND ADD TO SECOND COLUMN           SCMA 520
C                                                                       SCMA 530
    1 A(ILB)=A(ILA)*C+A(ILB)                                            SCMA 540
      GO TO 3                                                           SCMA 550
C                                                                       SCMA 560
C        OTHERWISE, MULTIPLY COLUMN BY CONSTANT                         SCMA 570
C                                                                       SCMA 580
    2 A(ILA)=A(ILA)*C                                                   SCMA 590
    3 CONTINUE                                                          SCMA 600
      RETURN                                                            SCMA 610
      END                                                               SCMA 620
```

Subroutine RINT

```
C                                                                       RINT  10
C   ***************************************************************** RINT  20
C                                                                       RINT  30
C       SUBROUTINE RINT                                                 RINT  40
C                                                                       RINT  50
C       PURPOSE                                                         RINT  60
C          INTERCHANGE TWO ROWS OF A MATRIX                             RINT  70
C                                                                       RINT  80
C       USAGE                                                           RINT  90
C          CALL RINT(A,N,M,LA,LB)                                       RINT 100
C                                                                       RINT 110
C       DESCRIPTION OF PARAMETERS                                       RINT 120
C          A  - NAME OF MATRIX                                          RINT 130
C          N  - NUMBER OF ROWS IN A                                     RINT 140
C          M  - NUMBER OF COLUMNS IN A                                  RINT 150
C          LA - ROW TO BE INTERCHANGED WITH ROW LB                      RINT 160
C          LB - ROW TO BE INTERCHANGED WITH ROW LA                      RINT 170
C                                                                       RINT 180
C       REMARKS                                                         RINT 190
C          MATRIX A MUST BE A GENERAL MATRIX                            RINT 200
C                                                                       RINT 210
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   RINT 220
C          NONE                                                         RINT 230
C                                                                       RINT 240
C       METHOD                                                          RINT 250
C          EACH ELEMENT OF ROW LA IS INTERCHANGED WITH CORRESPONDING     RINT 260
C          ELEMENT OF ROW LB                                            RINT 270
C                                                                       RINT 280
C   ***************************************************************** RINT 290
C                                                                       RINT 300
      SUBROUTINE RINT(A,N,M,LA,LB)                                      RINT 310
      DIMENSION A(1)                                                    RINT 320
C                                                                       RINT 330
      LAJ=LA-N                                                          RINT 340
      LBJ=LB-N                                                          RINT 350
      DO 3 J=1,M                                                        RINT 360
C                                                                       RINT 370
C        LOCATE ELEMENTS IN BOTH ROWS                                   RINT 380
C                                                                       RINT 390
      LAJ=LAJ+N                                                         RINT 400
      LBJ=LBJ+N                                                         RINT 410
C                                                                       RINT 420
C        INTERCHANGE ELEMENTS                                           RINT 430
C                                                                       RINT 440
      SAVE=A(LAJ)                                                       RINT 450
      A(LAJ)=A(LBJ)                                                     RINT 460
    3 A(LBJ)=SAVE                                                       RINT 470
      RETURN                                                            RINT 480
      END                                                               RINT 490
```

Subroutine CINT

```
C                                                                       CINT  10
C   ***************************************************************** CINT  20
C                                                                       CINT  30
C       SUBROUTINE CINT                                                 CINT  40
C                                                                       CINT  50
C       PURPOSE                                                         CINT  60
C          INTERCHANGE TWO COLUMNS OF A MATRIX                          CINT  70
C                                                                       CINT  80
C       USAGE                                                           CINT  90
C          CALL CINT(A,N,LA,LB)                                         CINT 100
C                                                                       CINT 110
C       DESCRIPTION OF PARAMETERS                                       CINT 120
C          A  - NAME OF MATRIX                                          CINT 130
C          N  - NUMBER OF ROWS IN A                                     CINT 140
C          LA - COLUMN TO BE INTERCHANGED WITH COLUMN LB                CINT 150
C          LB - COLUMN TO BE INTERCHANGED WITH COLUMN LA                CINT 160
C                                                                       CINT 170
C       REMARKS                                                         CINT 180
C          MATRIX A MUST BE A GENERAL MATRIX                            CINT 190
C                                                                       CINT 200
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   CINT 210
C          NONE                                                         CINT 220
C                                                                       CINT 230
C       METHOD                                                          CINT 240
C          EACH ELEMENT OF COLUMN LA IS INTERCHANGED WITH CORRESPONDINGCINT 250
C          ELEMENT OF COLUMN LB                                         CINT 260
C                                                                       CINT 270
C   ***************************************************************** CINT 280
C                                                                       CINT 290
      SUBROUTINE CINT(A,N,LA,LB)                                        CINT 300
      DIMENSION A(1)                                                    CINT 310
C                                                                       CINT 320
C        LOCATE STARTING POINT OF BOTH COLUMNS                          CINT 330
C                                                                       CINT 340
      ILA=N*(LA-1)                                                      CINT 350
      ILB=N*(LB-1)                                                      CINT 360
C                                                                       CINT 370
      DO 3 I=1,N                                                        CINT 380
      ILA=ILA+1                                                         CINT 390
      ILB=ILB+1                                                         CINT 400
C                                                                       CINT 410
C        INTERCHANGE ELEMENTS                                           CINT 420
C                                                                       CINT 430
      SAVE=A(ILA)                                                       CINT 440
      A(ILA)=A(ILB)                                                     CINT 450
    3 A(ILB)=SAVE                                                       CINT 460
      RETURN                                                            CINT 470
      END                                                               CINT 480
```

Subroutine RSUM

```
C                                                                       RSUM  10
C     ***************************************************************RSUM  20
C                                                                       RSUM  30
C        SUBROUTINE RSUM                                                RSUM  40
C                                                                       RSUM  50
C        PURPOSE                                                        RSUM  60
C           SUM ELEMENTS OF EACH ROW TO FORM COLUMN VECTOR              RSUM  70
C                                                                       RSUM  80
C        USAGE                                                          RSUM  90
C           CALL RSUM (A,R,N,M,MS)                                      RSUM 100
C                                                                       RSUM 110
C        DESCRIPTION OF PARAMETERS                                      RSUM 120
C           A - NAME OF INPUT MATRIX                                    RSUM 130
C           R - NAME OF VECTOR OF LENGTH N                              RSUM 140
C           N - NUMBER OF ROWS IN A                                     RSUM 150
C           M - NUMBER OF COLUMNS IN A                                  RSUM 160
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         RSUM 170
C                 0 - GENERAL                                           RSUM 180
C                 1 - SYMMETRIC                                         RSUM 190
C                 2 - DIAGONAL                                          RSUM 200
C                                                                       RSUM 210
C        REMARKS                                                        RSUM 220
C           VECTOR R CANNOT BE IN THE SAME LOCATION AS MATRIX A         RSUM 230
C           UNLESS A IS GENERAL                                         RSUM 240
C                                                                       RSUM 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RSUM 260
C           LOC                                                         RSUM 270
C                                                                       RSUM 280
C        METHOD                                                         RSUM 290
C           ELEMENTS ARE SUMMED ACROSS EACH ROW INTO A CORRESPONDING    RSUM 300
C           ELEMENT OF OUTPUT COLUMN VECTOR R                           RSUM 310
C                                                                       RSUM 320
C     ***************************************************************RSUM 330
C                                                                       RSUM 340
      SUBROUTINE RSUM(A,R,N,M,MS)                                       RSUM 350
      DIMENSION A(1),R(1)                                               RSUM 360
C                                                                       RSUM 370
      DO 3 I=1,N                                                        RSUM 380
C                                                                       RSUM 390
C        CLEAR OUTPUT LOCATION                                          RSUM 400
C                                                                       RSUM 410
      R(I)=0.0                                                          RSUM 420
C                                                                       RSUM 430
      DO 3 J=1,M                                                        RSUM 440
C                                                                       RSUM 450
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     RSUM 460
C                                                                       RSUM 470
      CALL LOC(I,J,IJ,N,M,MS)                                           RSUM 480
C                                                                       RSUM 490
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RSUM 500
C                                                                       RSUM 510
      IF(IJ) 2,3,2                                                      RSUM 520
C                                                                       RSUM 530
C        ACCUMULATE IN OUTPUT VECTOR                                    RSUM 540
C                                                                       RSUM 550
    2 R(I)=R(I)+A(IJ)                                                   RSUM 560
    3 CONTINUE                                                          RSUM 570
      RETURN                                                            RSUM 580
      END                                                               RSUM 590
```

Subroutine CSUM

```
C                                                                       CSUM  10
C     ***************************************************************CSUM  20
C                                                                       CSUM  30
C        SUBROUTINE CSUM                                                CSUM  40
C                                                                       CSUM  50
C        PURPOSE                                                        CSUM  60
C           SUM ELEMENTS OF EACH COLUMN TO FORM ROW VECTOR              CSUM  70
C                                                                       CSUM  80
C        USAGE                                                          CSUM  90
C           CALL CSUM(A,R,N,M,MS)                                       CSUM 100
C                                                                       CSUM 110
C        DESCRIPTION OF PARAMETERS                                      CSUM 120
C           A - NAME OF INPUT MATRIX                                    CSUM 130
C           R - NAME OF VECTOR OF LENGTH M                              CSUM 140
C           N - NUMBER OF ROWS IN A                                     CSUM 150
C           M - NUMBER OF COLUMNS IN A                                  CSUM 160
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         CSUM 170
C                 0 - GENERAL                                           CSUM 180
C                 1 - SYMMETRIC                                         CSUM 190
C                 2 - DIAGONAL                                          CSUM 200
C                                                                       CSUM 210
C        REMARKS                                                        CSUM 220
C           VECTOR R CANNOT BE IN THE SAME LOCATION AS MATRIX A         CSUM 230
C           UNLESS A IS GENERAL                                         CSUM 240
C                                                                       CSUM 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CSUM 260
C           LOC                                                         CSUM 270
C                                                                       CSUM 280
C        METHOD                                                         CSUM 290
C           ELEMENTS ARE SUMMED DOWN EACH COLUMN INTO A CORRESPONDING   CSUM 300
C           ELEMENT OF OUTPUT ROW VECTOR R                              CSUM 310
C                                                                       CSUM 320
C     ***************************************************************CSUM 330
C                                                                       CSUM 340
      SUBROUTINE CSUM(A,R,N,M,MS)                                       CSUM 350
      DIMENSION A(1),R(1)                                               CSUM 360
C                                                                       CSUM 370
      DO 3 J=1,M                                                        CSUM 380
C                                                                       CSUM 390
C        CLEAR OUTPUT LOCATION                                          CSUM 400
C                                                                       CSUM 410
      R(J)=0.0                                                          CSUM 420
C                                                                       CSUM 430
      DO 3 I=1,N                                                        CSUM 440
C                                                                       CSUM 450
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     CSUM 460
C                                                                       CSUM 470
      CALL LOC(I,J,IJ,N,M,MS)                                           CSUM 480
C                                                                       CSUM 490
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       CSUM 500
C                                                                       CSUM 510
      IF(IJ) 2,3,2                                                      CSUM 520
C                                                                       CSUM 530
C        ACCUMULATE IN OUTPUT VECTOR                                    CSUM 540
C                                                                       CSUM 550
    2 R(J)=R(J)+A(IJ)                                                   CSUM 560
    3 CONTINUE                                                          CSUM 570
      RETURN                                                            CSUM 580
      END                                                               CSUM 590
```

Subroutine RTAB

The function of this subroutine is graphically displayed by Figure 7 (see description under "Method" in the program listing).

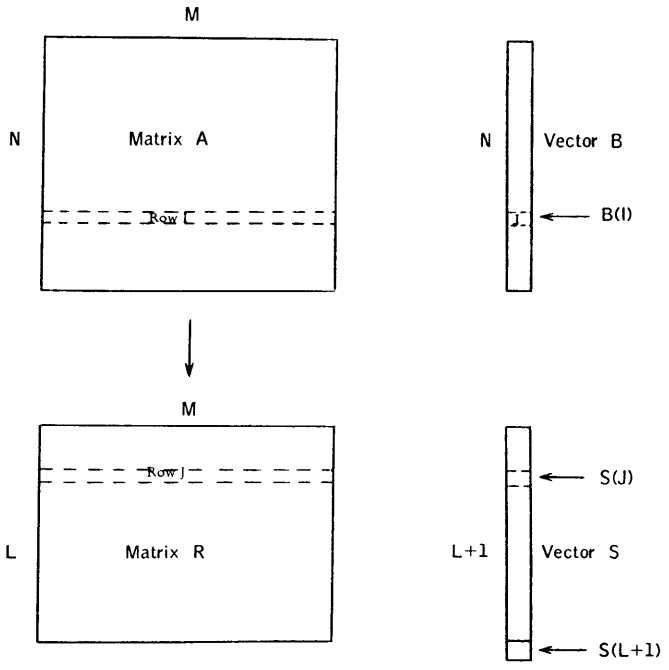

Figure 7. Row tabulation

```
C
C     ..................................................................RTAB  10
C                                                                       RTAB  20
C       SUBROUTINE RTAB                                                 RTAB  30
C                                                                       RTAB  40
C       PURPOSE                                                         RTAB  50
C          TABULATE ROWS OF A MATRIX TO FORM A SUMMARY MATRIX           RTAB  60
C                                                                       RTAB  70
C       USAGE                                                           RTAB  80
C          CALL RTAB(A,B,M,S,N,M,PS,L)                                  RTAB  90
C                                                                       RTAB 100
C       DESCRIPTION OF PARAMETERS                                       RTAB 110
C          A - NAME OF INPUT MATRIX                                     RTAB 120
C          B - NAME OF INPUT VECTOR OF LENGTH N CONTAINING KEY          RTAB 130
C          R - NAME OF OUTPUT MATRIX CONTAINING SUMMARY OF ROW DATA.    RTAB 140
C              IT IS INITIALLY SET TO ZERO BY THIS SUBROUTINE.          RTAB 150
C          S - NAME OF OUTPUT VECTOR OF LENGTH L+1 CONTAINING COUNTS    RTAB 160
C          N - NUMBER OF ROWS IN A                                      RTAB 170
C          M - NUMBER OF COLUMNS IN A AND R                             RTAB 180
C          L - NUMBER OF ROWS IN R                                      RTAB 190
C          PS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A          RTAB 200
C                0 - GENERAL                                            RTAB 210
C                1 - SYMMETRIC                                          RTAB 220
C                2 - DIAGONAL                                           RTAB 230
C                                                                       RTAB 240
C       REMARKS                                                         RTAB 250
C          MATRIX R IS ALWAYS A GENERAL MATRIX                          RTAB 260
C                                                                       RTAB 270
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   RTAB 280
C          LCC                                                          RTAB 290
C          RACE                                                         RTAB 300
C                                                                       RTAB 310
C       METHOD                                                          RTAB 320
C          ROWS OF DATA IN MATRIX A ARE TABULATED BASED ON THE KEY      RTAB 330
C          CONTAINED IN VECTOR B. THE FLOATING POINT NUMBER IN B(I) IS  RTAB 340
C          TRUNCATED TO FORM J. THE ITH ROW OF A IS ADDED TO THE JTH    RTAB 350
C          ROW OF R ELEMENT BY ELEMENT AND ONE IS ADDED TO S(J). IF J   RTAB 360
C          IS NOT BETWEEN ONE AND L, ONE IS ADDED TO S(L+1). THIS       RTAB 370
C          PROCEDURE IS REPEATED FOR EVERY ELEMENT IN VECTOR B.         RTAB 380
C          UPON COMPLETION, THE OUTPUT MATRIX R CONTAINS A SUMMARY OF   RTAB 390
C          ROW DATA AS SPECIFIED BY VECTOR B. EACH ELEMENT IN VECTOR S  RTAB 400
C          CONTAINS A COUNT OF THE NUMBER OF ROWS OF A USED TO FORM THE RTAB 410
C          CORRESPONDING ROW OF R. ELEMENT S(L+1) CONTAINS A COUNT OF   RTAB 420
C          THE NUMBER OF ROWS OF A NOT INCLUDED IN R AS A RESULT OF J   RTAB 430
C          BEING LESS THAN ONE OR GREATER THAN L.                       RTAB 440
C                                                                       RTAB 450
C     ..................................................................RTAB 460
C                                                                       RTAB 470
      SUBROUTINE RTAB(A,B,R,S,N,M,PS,L)                                 RTAB 480
      DIMENSION A(1),B(1),R(1),S(1)                                     RTAB 490
C                                                                       RTAB 500
C        CLEAR OUTPUT AREAS                                             RTAB 510
C                                                                       RTAB 520
      CALL LCC(R,L,IT,M,L,C)                                            RTAB 530
      DO 1C IR=1,IT                                                     RTAB 540
    1C R(IR)=C.C                                                        RTAB 550
      DO 2C IS=1,L                                                      RTAB 560
    2C S(IS)=C.C                                                        RTAB 570
      S(L+1)=C.C                                                        RTAB 580
C                                                                       RTAB 590
      DO 6C I=1,N                                                       RTAB 600
C                                                                       RTAB 610
C        TEST FOR THE KEY OUTSIDE THE RANGE                             RTAB 620
C                                                                       RTAB 630
      JR=B(I)                                                           RTAB 640
      IF (JR-1) 5C,4C,3C                                                RTAB 650
    3C IF (JR-L) 4C,4C,5C                                               RTAB 660
C                                                                       RTAB 670
C                                                                       RTAB 680
C        ADD ROW OF A TO ROW OF R AND 1 TO COUNT                        RTAB 690
C                                                                       RTAB 700
    4C CALL RACE (A,I,R,JR,N,M,PS,L)                                    RTAB 710
      S(JR)=S(JR)+1.C                                                   RTAB 720
      GO TO 6C                                                          RTAB 730
C                                                                       RTAB 740
    5C S(L+1)=S(L+1)+1.C                                                RTAB 750
    6C CONTINUE                                                         RTAB 760
      RETURN                                                            RTAB 770
      END                                                               RTAB 780
                                                                        RTAB 790
```

Subroutine CTAB

The function of this subroutine is graphically displayed by Figure 8 (see description under "Method" in the program listing).

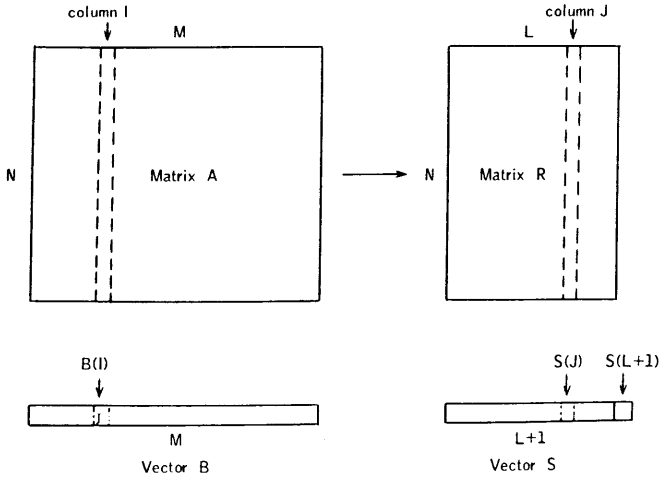

Figure 8. Column tabulation

```
C                                                                       CTAB  10
C     ..................................................................CTAB  20
C                                                                       CTAB  30
C        SUBROUTINE CTAB                                                CTAB  40
C                                                                       CTAB  50
C        PURPOSE                                                        CTAB  60
C           TABULATE COLUMNS OF A MATRIX TO FORM A SUMMARY MATRIX       CTAB  70
C                                                                       CTAB  80
C        USAGE                                                          CTAB  90
C           CALL CTAB(A,B,R,S,N,M,MS,L)                                 CTAB 100
C                                                                       CTAB 110
C        DESCRIPTION OF PARAMETERS                                      CTAB 120
C           A - NAME OF INPUT MATRIX                                    CTAB 130
C           B - NAME OF INPUT VECTOR OF LENGTH M CONTAINING KEY         CTAB 140
C           R - NAME OF OUTPUT MATRIX CONTAINING SUMMARY OF COLUMN DATA.CTAB 150
C               IT IS INITIALLY SET TO ZERO BY THIS SUBROUTINE.         CTAB 160
C           S - NAME OF OUTPUT VECTOR OF LENGTH L+1 CONTAINING COUNTS   CTAB 170
C           N - NUMBER OF ROWS IN A AND R                               CTAB 180
C           M - NUMBER OF COLUMNS IN A                                  CTAB 190
C           L - NUMBER OF COLUMNS IN R                                  CTAB 200
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         CTAB 210
C                 0 - GENERAL                                           CTAB 220
C                 1 - SYMMETRIC                                         CTAB 230
C                 2 - DIAGONAL                                          CTAB 240
C                                                                       CTAB 250
C        REMARKS                                                        CTAB 260
C           MATRIX R IS ALWAYS A GENERAL MATRIX                         CTAB 270
C                                                                       CTAB 280
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CTAB 290
C           LOC                                                         CTAB 300
C           CACC                                                        CTAB 310
C                                                                       CTAB 320
C        METHOD                                                         CTAB 330
C           COLUMNS OF DATA IN MATRIX A ARE TABULATED BASED ON THE KEY  CTAB 340
C           CONTAINED IN VECTOR B. THE FLOATING POINT NUMBER IN B(I) IS CTAB 350
C           TRUNCATED TO FORM J. THE ITH COLUMN OF A IS ADDED TO THE JTHCTAB 360
C           COLUMN OF MATRIX R AND ONE IS ADDED TO S(J). IF THE VALUE OFCTAB 370
C           J IS NOT BETWEEN 1 AND L, ONE IS ADDED TO S(L+1)            CTAB 380
C           UPON COMPLETION, THE OUTPUT MATRIX R CONTAINS A SUMMARY OF  CTAB 390
C           COLUMN DATA AS SPECIFIED BY VECTOR B. EACH ELEMENT IN VECTORCTAB 400
C           S CONTAINS A COUNT OF THE NUMBER OF COLUMNS OF A USED TO    CTAB 410
C           FORM R. ELEMENT S(L+1) CONTAINS THE NUMBER OF COLUMNS OF A  CTAB 420
C           NOT INCLUDED IN R AS A RESULT OF J BEING LESS THAN ONE OR   CTAB 430
C           GREATER THAN L.                                             CTAB 440
C                                                                       CTAB 450
C     ..................................................................CTAB 460
C                                                                       CTAB 470
      SUBROUTINE CTAB(A,B,R,S,N,M,MS,L)                                 CTAB 480
      DIMENSION A(1),B(1),R(1),S(1)                                     CTAB 490
C                                                                       CTAB 500
C        CLEAR OUTPUT AREAS                                             CTAB 510
C                                                                       CTAB 520
      CALL LOC(N,L,IT,N,L,C)                                            CTAB 530
      DO 1C I=1,IT                                                      CTAB 540
   1C R(I)=C.C                                                          CTAB 550
      DO 2C I=1,L                                                       CTAB 560
   2C S(I)=C.C                                                          CTAB 570
      S(L+1)=C.C                                                        CTAB 580
C                                                                       CTAB 590
      DO 6C I=1,M                                                       CTAB 600
C                                                                       CTAB 610
C        TEST FOR THE KEY OUTSIDE THE RANGE                             CTAB 620
C                                                                       CTAB 630
      JR=B(I)                                                           CTAB 640
      IF (JR-1) 5C,4C,3C                                                CTAB 650
   3C IF (JR-L) 4C,4C,5C                                                CTAB 660
C                                                                       CTAB 670
C                                                                       CTAB 680
C        ADD COLUMN OF A TO COLUMN OF R AND 1 TO COUNT                  CTAB 690
C                                                                       CTAB 700
   4C CALL CACC (A,I,R,JR,N,M,MS,L)                                     CTAB 710
      S(JR)=S(JR)+1.C                                                   CTAB 720
      GO TO 6C                                                          CTAB 730
C                                                                       CTAB 740
   5C S(L+1)=S(L+1)+1.C                                                 CTAB 750
   6C CONTINUE                                                          CTAB 760
      RETURN                                                            CTAB 770
      END                                                               CTAB 780
```

Subroutine RSRT

```
C                                                                       RSRT  10
C     ..................................................................RSRT  20
C                                                                       RSRT  30
C        SUBROUTINE RSRT                                                RSRT  40
C                                                                       RSRT  50
C        PURPOSE                                                        RSRT  60
C           SORT ROWS OF A MATRIX                                       RSRT  70
C                                                                       RSRT  80
C        USAGE                                                          RSRT  90
C           CALL RSRT(A,B,R,N,M,MS)                                     RSRT 100
C                                                                       RSRT 110
C        DESCRIPTION OF PARAMETERS                                      RSRT 120
C           A - NAME OF INPUT MATRIX TO BE SORTED                       RSRT 130
C           B - NAME OF INPUT VECTOR WHICH CONTAINS SORTING KEY         RSRT 140
C           R - NAME OF SORTED OUTPUT MATRIX                            RSRT 150
C           N - NUMBER OF ROWS IN A AND R AND LENGTH OF B               RSRT 160
C           M - NUMBER OF COLUMNS IN A AND R                            RSRT 170
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         RSRT 180
C                 0 - GENERAL                                           RSRT 190
C                 1 - SYMMETRIC                                         RSRT 200
C                 2 - DIAGONAL                                          RSRT 210
C                                                                       RSRT 220
C        REMARKS                                                        RSRT 230
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         RSRT 240
C           MATRIX R IS ALWAYS A GENERAL MATRIX                         RSRT 250
C           N MUST BE GREATER THAN ONE.                                 RSRT 260
C                                                                       RSRT 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RSRT 280
C           LOC                                                         RSRT 290
C                                                                       RSRT 300
C        METHOD                                                         RSRT 310
C           ROWS OF INPUT MATRIX A ARE SORTED TO FORM OUTPUT MATRIX R.  RSRT 320
C           THE SORTED ROW SEQUENCE IS DETERMINED BY THE VALUES OF      RSRT 330
C           ELEMENTS IN COLUMN VECTOR B. THE LOWEST VALUED ELEMENT IN   RSRT 340
C           B WILL CAUSE THE CORRESPONDING ROW OF A TO BE PLACED IN THE RSRT 350
C           FIRST ROW OF R. THE HIGHEST VALUED ELEMENT OF B WILL CAUSE  RSRT 360
C           THE CORRESPONDING ROW OF A TO BE PLACED IN THE LAST ROW OF  RSRT 370
C           R. IF DUPLICATE VALUES EXIST IN B, THE CORRESPONDING ROWS   RSRT 380
C           OF A ARE MOVED TO R IN THE SAME ORDER AS IN A.              RSRT 390
C                                                                       RSRT 400
C     ..................................................................RSRT 410
C                                                                       RSRT 420
      SUBROUTINE RSRT(A,B,R,N,M,MS)                                     RSRT 430
      DIMENSION A(1),B(1),R(1)                                          RSRT 440
C                                                                       RSRT 450
C        MOVE SORTING KEY VECTOR TO FIRST COLUMN OF OUTPUT MATRIX       RSRT 460
C        AND BUILD ORIGINAL SEQUENCE LIST IN SECOND COLUMN              RSRT 470
C                                                                       RSRT 480
      DO 10 I=1,N                                                       RSRT 490
      R(I)=B(I)                                                         RSRT 500
      I2=I+N                                                            RSRT 510
   10 R(I2)=I                                                           RSRT 520
C                                                                       RSRT 530
C        SORT ELEMENTS IN SORTING KEY VECTOR (ORIGINAL SEQUENCE LIST    RSRT 540
C        IS RESEQUENCED ACCORDINGLY)                                    RSRT 550
C                                                                       RSRT 560
      L=N+1                                                             RSRT 570
   20 ISORT=0                                                           RSRT 580
      L=L-1                                                             RSRT 590
      DO 40 I=2,L                                                       RSRT 600
      IF(R(I)-R(I-1)) 30,40,40                                          RSRT 610
   30 ISORT=1                                                           RSRT 620
      RSAVE=R(I)                                                        RSRT 630
      R(I)=R(I-1)                                                       RSRT 640
      R(I-1)=RSAVE                                                      RSRT 650
      I2=I+N                                                            RSRT 660
      SAVER=R(I2)                                                       RSRT 670
      R(I2)=R(I2-1)                                                     RSRT 680
      R(I2-1)=SAVER                                                     RSRT 690
   40 CONTINUE                                                          RSRT 700
      IF(ISORT) 20,50,20                                                RSRT 710
C                                                                       RSRT 720
C        MOVE ROWS FROM MATRIX A TO MATRIX R (NUMBER IN SECOND COLUMN   RSRT 730
C        OF R REPRESENTS ROW NUMBER OF MATRIX A TO BE MOVED)            RSRT 740
C                                                                       RSRT 750
   50 DO 80 I=1,N                                                       RSRT 760
C                                                                       RSRT 770
C        GET ROW NUMBER IN MATRIX A                                     RSRT 780
C                                                                       RSRT 790
      I2=I+N                                                            RSRT 800
      IN=R(I2)                                                          RSRT 810
C                                                                       RSRT 820
      IR=I-N                                                            RSRT 830
      DO 80 J=1,M                                                       RSRT 840
C                                                                       RSRT 850
C        LOCATE ELEMENT IN OUTPUT MATRIX                                RSRT 860
C                                                                       RSRT 870
      IR=IR+N                                                           RSRT 880
C                                                                       RSRT 890
C        LOCATE ELEMENT IN INPUT MATRIX                                 RSRT 900
C                                                                       RSRT 910
      CALL LOC(IN,J,IA,N,M,MS)                                          RSRT 920
C                                                                       RSRT 930
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RSRT 940
C                                                                       RSRT 950
      IF(IA) 60,70,60                                                   RSRT 960
C                                                                       RSRT 970
C        MOVE ELEMENT TO OUTPUT MATRIX                                  RSRT 980
C                                                                       RSRT 990
   60 R(IR)=A(IA)                                                       RSRT1000
      GO TO 80                                                          RSRT1010
   70 R(IR)=0                                                           RSRT1020
   80 CONTINUE                                                          RSRT1030
      RETURN                                                            RSRT1040
      END                                                               RSRT1050
```

Subroutine CSRT

```
C                                                                       CSRT  10
C     ...................................................................CSRT  20
C                                                                       CSRT  30
C        SUBROUTINE CSRT                                                CSRT  40
C                                                                       CSRT  50
C        PURPOSE                                                        CSRT  60
C           SORT COLUMNS OF A MATRIX                                    CSRT  70
C                                                                       CSRT  80
C        USAGE                                                          CSRT  90
C           CALL CSRT(A,B,R,N,M,MS)                                     CSRT 100
C                                                                       CSRT 110
C        DESCRIPTION OF PARAMETERS                                      CSRT 120
C           A - NAME OF INPUT MATRIX TO BE SORTED                       CSRT 130
C           B - NAME OF INPUT VECTOR WHICH CONTAINS SORTING KEY         CSRT 140
C           R - NAME OF SORTED OUTPUT MATRIX                            CSRT 150
C           N - NUMBER OF ROWS IN A AND R                               CSRT 160
C           M - NUMBER OF COLUMNS IN A AND R AND LENGTH OF B            CSRT 170
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         CSRT 180
C                 0 - GENERAL                                           CSRT 190
C                 1 - SYMMETRIC                                         CSRT 200
C                 2 - DIAGONAL                                          CSRT 210
C                                                                       CSRT 220
C        REMARKS                                                        CSRT 230
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRIX A         CSRT 240
C           MATRIX R IS ALWAYS A GENERAL MATRIX                         CSRT 250
C           M MUST BE GREATER THAN ONE.                                 CSRT 260
C                                                                       CSRT 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CSRT 280
C           LOC                                                         CSRT 290
C           CCPY                                                        CSRT 300
C                                                                       CSRT 310
C        METHOD                                                         CSRT 320
C           COLUMNS OF INPUT MATRIX A ARE SORTED TO FORM OUTPUT MATRIX  CSRT 330
C           R. THE SORTED COLUMN SEQUENCE IS DETERMINED BY THE VALUES OFCSRT 340
C           ELEMENTS IN ROW VECTOR B. THE LOWEST VALUED ELEMENT IN      CSRT 350
C           B WILL CAUSE THE CORRESPONDING COLUMN OF A TO BE PLACED IN  CSRT 360
C           THE FIRST COLUMN OF R. THE HIGHEST VALUED ELEMENT OF B WILL CSRT 370
C           CAUSE THE CORRESPONDING ROW OF A TO BE PLACED IN THE LAST   CSRT 380
C           COLUMN OF R. IF DUPLICATE VALUES EXIST IN B, THE            CSRT 390
C           CORRESPONDING COLUMNS OF A ARE MOVED TO R IN THE SAME ORDER CSRT 400
C           AS IN A.                                                    CSRT 410
C                                                                       CSRT 420
C     ...................................................................CSRT 430
C                                                                       CSRT 440
      SUBROUTINE CSRT(A,B,R,N,M,MS)                                     CSRT 450
      DIMENSION A(1),B(1),R(1)                                          CSRT 460
C                                                                       CSRT 470
C        MOVE SORTING KEY VECTOR TO FIRST ROW OF OUTPUT MATRIX          CSRT 480
C        AND BUILD ORIGINAL SEQUENCE LIST IN SECOND ROW                 CSRT 490
C                                                                       CSRT 500
      IK=1                                                              CSRT 510
      DO 10 J=1,M                                                       CSRT 520
      R(IK)=B(J)                                                        CSRT 530
      R(IK+1)=J                                                         CSRT 540
   10 IK=IK+N                                                           CSRT 550
C                                                                       CSRT 560
C        SORT ELEMENTS IN SORTING KEY VECTOR (ORIGINAL SEQUENCE LIST    CSRT 570
C        IS RESEQUENCED ACCORDINGLY)                                    CSRT 580
C                                                                       CSRT 590
      L=M+1                                                             CSRT 600
   20 ISORT=0                                                           CSRT 610
      L=L-1                                                             CSRT 620
      IP=1                                                              CSRT 630
      IQ=N+1                                                            CSRT 640
      DO 50 J=2,L                                                       CSRT 650
      IF(R(IQ)-R(IP)) 30,40,40                                          CSRT 660
   30 ISORT=1                                                           CSRT 670
      RSAVE=R(IQ)                                                       CSRT 680
      R(IQ)=R(IP)                                                       CSRT 690
      R(IP)=RSAVE                                                       CSRT 700
      SAVER=R(IQ+1)                                                     CSRT 710
      R(IQ+1)=R(IP+1)                                                   CSRT 720
      R(IP+1)=SAVER                                                     CSRT 730
   40 IP=IP+N                                                           CSRT 740
      IQ=IQ+N                                                           CSRT 750
   50 CONTINUE                                                          CSRT 760
      IF(ISORT) 20,60,20                                                CSRT 770
C                                                                       CSRT 780
C        MOVE COLUMNS FROM MATRIX A TO MATRIX R (NUMBER IN SECOND ROW   CSRT 790
C        OF R REPRESENTS COLUMN NUMBER OF MATRIX A TO BE MOVED)         CSRT 800
C                                                                       CSRT 810
   60 IQ=-N                                                             CSRT 820
      DO 70 J=1,M                                                       CSRT 830
      IQ=IQ+N                                                           CSRT 840
C                                                                       CSRT 850
C        GET COLUMN NUMBER IN MATRIX A                                  CSRT 860
C                                                                       CSRT 870
      I2=IQ+2                                                           CSRT 880
      IN=R(I2)                                                          CSRT 890
C                                                                       CSRT 900
C        MOVE COLUMN                                                    CSRT 910
C                                                                       CSRT 920
      IR=IQ+1                                                           CSRT 930
      CALL CCPY(A,IN,R(IR),N,M,MS)                                      CSRT 940
   70 CONTINUE                                                          CSRT 950
      RETURN                                                            CSRT 960
      END                                                               CSRT 970
```

Subroutine RCUT

```
C                                                                       RCUT  10
C     ...................................................................RCUT  20
C                                                                       RCUT  30
C        SUBROUTINE RCUT                                                RCUT  40
C                                                                       RCUT  50
C        PURPOSE                                                        RCUT  60
C           PARTITION A MATRIX BETWEEN SPECIFIED ROWS TO FORM TWO       RCUT  70
C           RESULTANT MATRICES                                          RCUT  80
C                                                                       RCUT  90
C        USAGE                                                          RCUT 100
C           CALL RCUT (A,L,R,S,N,M,MS)                                  RCUT 110
C                                                                       RCUT 120
C        DESCRIPTION OF PARAMETERS                                      RCUT 130
C           A - NAME OF INPUT MATRIX                                    RCUT 140
C           L - ROW OF A ABOVE WHICH PARTITIONING TAKES PLACE           RCUT 150
C           R - NAME OF MATRIX TO BE FORMED FROM UPPER PORTION OF A     RCUT 160
C           S - NAME OF MATRIX TO BE FORMED FROM LOWER PORTION OF A     RCUT 170
C           N - NUMBER OF ROWS IN A                                     RCUT 180
C           M - NUMBER OF COLUMNS IN A                                  RCUT 190
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         RCUT 200
C                 0 - GENERAL                                           RCUT 210
C                 1 - SYMMETRIC                                         RCUT 220
C                 2 - DIAGONAL                                          RCUT 230
C                                                                       RCUT 240
C        REMARKS                                                        RCUT 250
C           MATRIX R CANNOT BE IN SAME LOCATION AS MATRIX A             RCUT 260
C           MATRIX S CANNOT BE IN SAME LOCATION AS MATRIX A             RCUT 270
C           MATRIX R CANNOT BE IN SAME LOCATION AS MATRIX S             RCUT 280
C           MATRIX R AND MATRIX S ARE ALWAYS GENERAL MATRICES           RCUT 290
C                                                                       RCUT 300
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RCUT 310
C           LOC                                                         RCUT 320
C                                                                       RCUT 330
C        METHOD                                                         RCUT 340
C           ELEMENTS OF MATRIX A ABOVE ROW L ARE MOVED TO FORM MATRIX R RCUT 350
C           OF L-1 ROWS AND M COLUMNS. ELEMENTS OF MATRIX A IN ROW L    RCUT 360
C           AND BELOW ARE MOVED TO FORM MATRIX S OF N-L+1 ROWS AND M    RCUT 370
C           COLUMNS                                                     RCUT 380
C                                                                       RCUT 390
C     ...................................................................RCUT 400
C                                                                       RCUT 410
      SUBROUTINE RCUT(A,L,R,S,N,M,MS)                                   RCUT 420
      DIMENSION A(1),R(1),S(1)                                          RCUT 430
C                                                                       RCUT 440
      IR=0                                                              RCUT 450
      IS=0                                                              RCUT 460
      DO 70 J=1,M                                                       RCUT 470
      DO 70 I=1,N                                                       RCUT 480
C                                                                       RCUT 490
C        FIND LOCATION IN OUTPUT MATRIX AND SET TO ZERO                 RCUT 500
C                                                                       RCUT 510
      IF(I-L) 20,10,10                                                  RCUT 520
   10 IS=IS+1                                                           RCUT 530
      S(IS)=0.0                                                         RCUT 540
      GO TO 30                                                          RCUT 550
   20 IR=IR+1                                                           RCUT 560
      R(IR)=0.0                                                         RCUT 570
C                                                                       RCUT 580
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     RCUT 590
C                                                                       RCUT 600
   30 CALL LOC(I,J,IJ,N,M,MS)                                           RCUT 610
C                                                                       RCUT 620
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RCUT 630
C                                                                       RCUT 640
      IF(IJ) 40,70,40                                                   RCUT 650
C                                                                       RCUT 660
C        DETERMINE WHETHER ABOVE OR BELOW L                             RCUT 670
C                                                                       RCUT 680
   40 IF(I-L) 50,50,50                                                  RCUT 690
   50 S(IS)=A(IJ)                                                       RCUT 700
      GO TO 70                                                          RCUT 710
   60 R(IR)=A(IJ)                                                       RCUT 720
   70 CONTINUE                                                          RCUT 730
      RETURN                                                            RCUT 740
      END                                                               RCUT 750
```

Subroutine CCUT

```
C                                                                       CCUT  10
C   ....................................................................CCUT  20
C                                                                       CCUT  30
C       SUBROUTINE CCUT                                                 CCUT  40
C                                                                       CCUT  50
C       PURPOSE                                                         CCUT  60
C          PARTITION A MATRIX BETWEEN SPECIFIED COLUMNS TO FORM TWO     CCUT  70
C          RESULTANT MATRICES                                           CCUT  80
C                                                                       CCUT  90
C       USAGE                                                           CCUT 100
C          CALL CCUT (A,L,R,S,N,M,MS)                                   CCUT 110
C                                                                       CCUT 120
C       DESCRIPTION OF PARAMETERS                                       CCUT 130
C          A - NAME OF INPUT MATRIX                                     CCUT 140
C          L - COLUMN OF A TO THE LEFT OF WHICH PARTITIONING TAKES      CCUT 150
C              PLACE                                                    CCUT 160
C          R - NAME OF MATRIX TO BE FORMED FROM LEFT PORTION OF A       CCUT 170
C          S - NAME OF MATRIX TO BE FORMED FROM RIGHT PORTION OF A      CCUT 180
C          N - NUMBER OF ROWS IN A                                      CCUT 190
C          M - NUMBER OF COLUMNS IN A                                   CCUT 200
C          MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A          CCUT 210
C                0 - GENERAL                                            CCUT 220
C                1 - SYMMETRIC                                          CCUT 230
C                2 - DIAGONAL                                           CCUT 240
C                                                                       CCUT 250
C       REMARKS                                                         CCUT 260
C          MATRIX R CANNOT BE IN SAME LOCATION AS MATRIX A              CCUT 270
C          MATRIX S CANNOT BE IN SAME LOCATION AS MATRIX A              CCUT 280
C          MATRIX R CANNOT BE IN SAME LOCATION AS MATRIX S              CCUT 290
C          MATRIX R AND MATRIX S ARE ALWAYS GENERAL MATRICES            CCUT 300
C                                                                       CCUT 310
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   CCUT 320
C          LOC                                                          CCUT 330
C                                                                       CCUT 340
C       METHOD                                                          CCUT 350
C          ELEMENTS OF MATRIX A TO THE LEFT OF COLUMN L ARE MOVED TO    CCUT 360
C          FORM MATRIX R OF N ROWS AND L-1 COLUMNS. ELEMENTS OF         CCUT 370
C          MATRIX A IN COLUMN L AND TO THE RIGHT OF L ARE MOVED TO FORMCCUT 380
C          MATRIX S OF N ROWS AND M-L+1 COLUMNS.                        CCUT 390
C                                                                       CCUT 400
C   ....................................................................CCUT 410
C                                                                       CCUT 420
      SUBROUTINE CCUT(A,L,R,S,N,M,MS)                                   CCUT 430
      DIMENSION A(1),R(1),S(1)                                          CCUT 440
C                                                                       CCUT 450
      IR=0                                                              CCUT 460
      IS=0                                                              CCUT 470
      DO 70 J=1,M                                                       CCUT 480
      DO 70 I=1,N                                                       CCUT 490
C                                                                       CCUT 500
C        FIND LOCATION IN OUTPUT MATRIX AND SET TO ZERO                 CCUT 510
C                                                                       CCUT 520
      IF(J-L) 20,10,10                                                  CCUT 530
   10 IS=IS+1                                                           CCUT 540
      S(IS)=0.0                                                         CCUT 550
      GO TO 30                                                          CCUT 560
   20 IR=IR+1                                                           CCUT 570
      R(IR)=0.0                                                         CCUT 580
C                                                                       CCUT 590
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     CCUT 600
C                                                                       CCUT 610
   30 CALL LOC(I,J,II,N,M,MS)                                           CCUT 620
C                                                                       CCUT 630
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       CCUT 640
C                                                                       CCUT 650
      IF(II) 40,70,40                                                   CCUT 660
C                                                                       CCUT 670
C        DETERMINE WHETHER RIGHT OR LEFT OF L                           CCUT 680
C                                                                       CCUT 690
   40 IF(J-L) 60,50,50                                                  CCUT 700
   50 S(IS)=A(II)                                                       CCUT 710
      GO TO 70                                                          CCUT 720
   60 R(IR)=A(II)                                                       CCUT 730
   70 CONTINUE                                                          CCUT 740
      RETURN                                                            CCUT 750
      END                                                               CCUT 760
```

Subroutine RTIE

```
C                                                                       RTIE  10
C   ....................................................................RTIE  20
C                                                                       RTIE  30
C       SUBROUTINE RTIE                                                 RTIE  40
C                                                                       RTIE  50
C       PURPOSE                                                         RTIE  60
C          ADJOIN TWO MATRICES WITH SAME COLUMN DIMENSION TO FORM ONE   RTIE  70
C          RESULTANT MATRIX (SEE METHOD)                                RTIE  80
C                                                                       RTIE  90
C       USAGE                                                           RTIE 100
C          CALL RTIE(A,B,R,N,M,MSA,MSB,L)                               RTIE 110
C                                                                       RTIE 120
C       DESCRIPTION OF PARAMETERS                                       RTIE 130
C          A - NAME OF FIRST INPUT MATRIX                               RTIE 140
C          B - NAME OF SECOND INPUT MATRIX                              RTIE 150
C          R - NAME OF OUTPUT MATRIX                                    RTIE 160
C          N - NUMBER OF ROWS IN A                                      RTIE 170
C          M - NUMBER OF COLUMNS IN A,B,R                               RTIE 180
C          MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A          RTIE 190
C                0 - GENERAL                                            RTIE 200
C                1 - SYMMETRIC                                          RTIE 210
C                2 - DIAGONAL                                           RTIE 220
C          MSB - SAME AS MSA EXCEPT FOR MATRIX B                        RTIE 230
C          L - NUMBER OF ROWS IN B                                      RTIE 240
C                                                                       RTIE 250
C       REMARKS                                                         RTIE 260
C          MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRICES A OR B   RTIE 270
C          MATRIX R IS ALWAYS A GENERAL MATRIX                          RTIE 280
C          MATRIX A MUST HAVE THE SAME NUMBER OF COLUMNS AS MATRIX B    RTIE 290
C                                                                       RTIE 300
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   RTIE 310
C          LOC                                                          RTIE 320
C                                                                       RTIE 330
C       METHOD                                                          RTIE 340
C          MATRIX B IS ATTACHED TO THE BOTTOM OF MATRIX A .             RTIE 350
C          THE RESULTANT MATRIX R CONTAINS N+L ROWS AND M COLUMNS.      RTIE 360
C                                                                       RTIE 370
C   ....................................................................RTIE 380
C                                                                       RTIE 390
      SUBROUTINE RTIE(A,B,R,N,M,MSA,MSB,L)                              RTIE 400
      DIMENSION A(1),B(1),R(1)                                          RTIE 410
C                                                                       RTIE 420
      NN=N                                                              RTIE 430
      IR=0                                                              RTIE 440
      NX=NN                                                             RTIE 450
      MSX=MSA                                                           RTIE 460
      DO 9 J=1,M                                                        RTIE 470
      DO 8 II=1,2                                                       RTIE 480
      DO 7 I=1,NN                                                       RTIE 490
      IR=IR+1                                                           RTIE 500
      R(IR)=0.0                                                         RTIE 510
C                                                                       RTIE 520
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     RTIE 530
C                                                                       RTIE 540
      CALL LOC(I,J,II,NN,M,MSX)                                         RTIE 550
C                                                                       RTIE 560
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       RTIE 570
C                                                                       RTIE 580
      IF(II) 2,7,2                                                      RTIE 590
C                                                                       RTIE 600
C        MOVE ELEMENT TO MATRIX R                                       RTIE 610
C                                                                       RTIE 620
    2 GO TO(3,4),II                                                     RTIE 630
    3 R(IR)=A(II)                                                       RTIE 640
      GO TO 7                                                           RTIE 650
    4 R(IR)=B(II)                                                       RTIE 660
    7 CONTINUE                                                          RTIE 670
C                                                                       RTIE 680
C        REPEAT ABOVE FOR MATRIX B                                      RTIE 690
C                                                                       RTIE 700
      MSX=MSB                                                           RTIE 710
    8 NN=L                                                              RTIE 720
C                                                                       RTIE 730
C        RESET FOR NEXT COLUMN                                          RTIE 740
C                                                                       RTIE 750
      MSX=MSA                                                           RTIE 760
    9 NN=NX                                                             RTIE 770
      RETURN                                                            RTIE 780
      END                                                               RTIE 790
```

Subroutine CTIE

```
C                                                                       CTIE  10
C     ...................................................................CTIE  20
C                                                                       CTIE  30
C        SUBROUTINE CTIE                                                CTIE  40
C                                                                       CTIE  50
C        PURPOSE                                                        CTIE  60
C           ADJOIN TWO MATRICES WITH SAME ROW DIMENSION TO FORM ONE     CTIE  70
C           RESULTANT MATRIX (SLE METHOD)                               CTIE  80
C                                                                       CTIE  90
C        USAGE                                                          CTIE 100
C           CALL CTIE(A,B,R,N,M,MSA,MSB,L)                              CTIE 110
C                                                                       CTIE 120
C        DESCRIPTION OF PARAMETERS                                      CTIE 130
C           A - NAME OF FIRST INPUT MATRIX                              CTIE 140
C           B - NAME OF SECOND INPUT MATRIX                             CTIE 150
C           R - NAME OF OUTPUT MATRIX                                   CTIE 160
C           N - NUMBER OF ROWS IN A,B,R                                 CTIE 170
C           M - NUMBER OF COLUMNS IN A                                  CTIE 180
C           MSA - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A         CTIE 190
C                 0 - GENERAL                                           CTIE 200
C                 1 - SYMMETRIC                                         CTIE 210
C                 2 - DIAGONAL                                          CTIE 220
C           MSB - SAME AS MSA EXCEPT FOR MATRIX B                       CTIE 230
C           L - NUMBER OF COLUMNS IN B                                  CTIE 240
C                                                                       CTIE 250
C        REMARKS                                                        CTIE 260
C           MATRIX R CANNOT BE IN THE SAME LOCATION AS MATRICES A OR B  CTIE 270
C           MATRIX R IS ALWAYS A GENERAL MATRIX                         CTIE 280
C           MATRIX A MUST HAVE THE SAME NUMBER OF ROWS AS MATRIX B      CTIE 290
C                                                                       CTIE 300
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CTIE 310
C           LOC                                                         CTIE 320
C                                                                       CTIE 330
C        METHOD                                                         CTIE 340
C           MATRIX B IS ATTACHED TO THE RIGHT OF MATRIX A .             CTIE 350
C           THE RESULTANT MATRIX R CONTAINS N ROWS AND M+L COLUMNS      CTIE 360
C                                                                       CTIE 370
C     ...................................................................CTIE 380
C                                                                       CTIE 390
      SUBROUTINE CTIE(A,B,R,N,M,MSA,MSB,L)                              CTIE 400
      DIMENSION A(1),B(1),R(1)                                          CTIE 410
C                                                                       CTIE 420
      MM=M                                                              CTIE 430
      IR=0                                                              CTIE 440
      MSX=MSA                                                           CTIE 450
      DO 6 JJ=1,2                                                       CTIE 460
      DO 5 J=1,MM                                                       CTIE 470
      DO 5 I=1,N                                                        CTIE 480
      IR=IR+1                                                           CTIE 490
      R(IR)=0.0                                                         CTIE 500
C                                                                       CTIE 510
C        LOCATE ELEMENT FOR ANY MATRIX STORAGE MODE                     CTIE 520
C                                                                       CTIE 530
      CALL LOC(I,J,IJ,N,MM,MSX)                                         CTIE 540
C                                                                       CTIE 550
C        TEST FOR ZERO ELEMENT IN DIAGONAL MATRIX                       CTIE 560
C                                                                       CTIE 570
      IF(IJ) 2,5,2                                                      CTIE 580
C                                                                       CTIE 590
C        MOVE ELEMENT TO MATRIX R                                       CTIE 600
C                                                                       CTIE 610
    2 GO TO(3,4),JJ                                                     CTIE 620
    3 R(IR)=A(IJ)                                                       CTIE 630
      GO TO 5                                                           CTIE 640
    4 R(IR)=B(IJ)                                                       CTIE 650
    5 CONTINUE                                                          CTIE 660
C                                                                       CTIE 670
C        REPEAT ABOVE FOR MATRIX B                                      CTIE 680
C                                                                       CTIE 690
      MSX=MSB                                                           CTIE 700
      MM=L                                                              CTIE 710
    6 CONTINUE                                                          CTIE 720
      RETURN                                                            CTIE 730
      END                                                               CTIE 740
```

Subroutines MPRC and DMPRC

These subroutines permute the rows or columns of a given m by n matrix A according to a transposition vector ITRA = $(t_1, \ldots, t_s)$ or its inverse. (See the general discussion under "Permutations" for definitions and notation.)

1. Mathematical background

Permuting the rows or columns of A according to the transposition vector ITRA means applying the permutation $(1, t_1), \ldots, (s, t_s)$ to the rows or columns of A, while permuting according to $ITRA^{-1}$ means applying the permutation $(s, t_s), \ldots, (1, t_1)$.

2. Programming considerations

If the columns of A are to be permuted, the input parameter IROCO must be nonzero, and s = n; if the rows are to be permuted, IROCO must be zero, and s = m. Similarly, if the input parameter INV is nonzero, the rows or columns of A are permuted according to ITRA; while if INV is zero, the rows or columns of A are permuted according to $ITRA^{-1}$.

If m and n are not both positive, or if ITRA is not a transposition vector on $S = \{1, \ldots, s\}$, the subroutines are prematurely terminated and the error parameter IER is set to -1 or 1, respectively. If there is no error, IER is set to zero.

The matrix A is assumed to be stored columnwise, and the permutation of the rows or columns of A is performed in s steps. At the i^{th} step, if the permutation is according to $ITRA^{-1}$, rows or columns i and s_i are interchanged; if the permutation is according to ITRA, rows or columns $s - i + 1$ and t_{s-i+1} are interchanged.

```
C                                                                       MPRC  10
C     ...................................................................MPRC  20
C                                                                       MPRC  30
C        SUBROUTINE MPRC                                                MPRC  40
C                                                                       MPRC  50
C        PURPOSE                                                        MPRC  60
C           TO PERMUTE THE ROWS OR COLUMNS OF A GIVEN MATRIX ACCORDING  MPRC  70
C           TO A GIVEN TRANSPOSITION VECTOR OR ITS INVERSE.  (SEE THE   MPRC  80
C           DISCUSSION ON PERMUTATIONS FOR DEFINITIONS AND NOTATION.)   MPRC  90
C                                                                       MPRC 100
C        USAGE                                                          MPRC 110
C           CALL MPRC(A,M,N,ITRA,INV,IROCO,IER)                         MPRC 120
C                                                                       MPRC 130
C        DESCRIPTION OF PARAMETERS                                      MPRC 140
C           A      - GIVEN M BY N MATRIX AND RESULTING PERMUTED MATRIX  MPRC 150
C           M      - NUMBER OF ROWS OF A                                MPRC 160
C           N      - NUMBER OF COLUMNS OF A                             MPRC 170
C           ITRA   - GIVEN TRANSPOSITION VECTOR (DIMENSION M IF ROWS ARE MPRC 180
C                    PERMUTED, N IF COLUMNS ARE PERMUTED)               MPRC 190
C           INV    - INPUT PARAMETER                                    MPRC 200
C                    INV NON-ZERO  -  PERMUTE ACCORDING TO ITRA         MPRC 210
C                    INV    =  0   -  PERMUTE ACCORDING TO ITRA INVERSE MPRC 220
C           IROCO - INPUT PARAMETER                                     MPRC 230
C                    IROCO NON-ZERO  -  PERMUTE THE COLUMNS OF A        MPRC 240
C                    IROCO    =  0   -  PERMUTE THE ROWS OF A           MPRC 250
C           IER    - RESULTING ERROR PARAMETER                          MPRC 260
C                    IER = -1  -  M AND N ARE NOT BOTH POSITIVE         MPRC 270
C                    IER =  0  -  NO ERROR                              MPRC 280
C                    IER =  1  -  ITRA IS NOT A TRANSPOSITION VECTOR ON MPRC 290
C                                 1,...,M IF ROWS ARE PERMUTED, 1,...,N MPRC 300
C                                 IF COLUMNS ARE PERMUTED               MPRC 310
C                                                                       MPRC 320
C        REMARKS                                                        MPRC 330
C           (1)  IF IER=-1 THERE IS NO COMPUTATION.                     MPRC 340
C           (2)  IF IER= 1, THEN COMPUTATION HAS BEEN UNSUCCESSFUL DUE  MPRC 350
C                TO ERROR, BUT THE MATRIX A WILL REFLECT THE ROW OR     MPRC 360
C                COLUMN INTERCHANGES PERFORMED BEFORE THE ERROR WAS     MPRC 370
C                DETECTED.                                              MPRC 380
C           (3)  THE MATRIX A IS ASSUMED TO BE STORED COLUMNWISE.       MPRC 390
```

```
C                                                                       MPRC 400
C       SUBROUTINES AND SUBPROGRAMS REQUIRED                            MPRC 410
C          NONE                                                         MPRC 420
C                                                                       MPRC 430
C       METHOD                                                          MPRC 440
C          THE ROWS OR COLUMNS ARE PERMUTED ELEMENTWISE, INTERCHANGING  MPRC 450
C          ROW OR COLUMN 1 AND ITRA(1),...,ROW OR COLUMN K AND ITRA(K)  MPRC 460
C          IN THAT ORDER IF INV=0, AND OTHERWISE INTERCHANGING ROW OR   MPRC 470
C          COLUMN K AND ITRA(K),...,ROW OR COLUMN 1 AND ITRA(1), WHERE  MPRC 480
C          K IS M OR N DEPENDING ON WHETHER WE PERMUTE ROWS OR COLUMNS. MPRC 490
C                                                                       MPRC 500
C  ..................................................................   MPRC 510
C                                                                       MPRC 520
      SUBROUTINE MPRC(A,M,N,ITRA,INV,IROCO,IER)                         MPRC 530
C                                                                       MPRC 540
C                                                                       MPRC 550
      DIMENSION A(1),ITRA(1)                                            MPRC 560
C                                                                       MPRC 570
C        TEST OF DIMENSIONS                                             MPRC 580
      IF(M)14,14,1                                                      MPRC 590
    1 IF(N)14,14,2                                                      MPRC 600
C                                                                       MPRC 610
C        DETERMINE WHICH ARE TO BE PERMUTED-THE ROWS OR THE COLUMNS     MPRC 620
    2 IF(IROCO)3,4,3                                                    MPRC 630
C                                                                       MPRC 640
C        INITIALIZE FOR COLUMN INTERCHANGES                             MPRC 650
    3 MM=M                                                              MPRC 660
      MMM=-1                                                            MPRC 670
      L=M                                                               MPRC 680
      LL=N                                                              MPRC 690
      GO TO 5                                                           MPRC 700
C                                                                       MPRC 710
C        INITIALIZE FOR ROW INTERCHANGES                                MPRC 720
    4 MM=1                                                              MPRC 730
      MMM=M                                                             MPRC 740
      L=N                                                               MPRC 750
      LL=M                                                              MPRC 760
C                                                                       MPRC 770
C        INITIALIZE LOOP OVER ALL ROWS OR COLUMNS                       MPRC 780
    5 IA=1                                                              MPRC 790
      ID=1                                                              MPRC 800
C                                                                       MPRC 810
C        TEST FOR INVERSE OPERATION                                     MPRC 820
      IF(INV)6,7,6                                                      MPRC 830
    6 IA=LL                                                             MPRC 840
      ID=-1                                                             MPRC 850
    7 DO 12 I=1,LL                                                      MPRC 860
      K=ITRA(IA)                                                        MPRC 870
      IF(K-IA)9,12,9                                                    MPRC 880
    8 IF(K)13,13,10                                                     MPRC 890
    9 IF(LL-K)13,10,10                                                  MPRC 900
C                                                                       MPRC 910
C        INITIALIZE ROW OR COLUMN INTERCHANGE                           MPRC 920
   10 IL=IA*MM                                                          MPRC 930
      K=K*MM                                                            MPRC 940
C                                                                       MPRC 950
C        PERFORM ROW OR COLUMN INTERCHANGE                              MPRC 960
      DO 11 J=1,L                                                       MPRC 970
      SAVE=A(IL)                                                        MPRC 980
      A(IL)=A(K)                                                        MPRC 990
      A(K)=SAVE                                                         MPRC1000
      K=K+MMM                                                           MPRC1010
   11 IL=IL+MMM                                                         MPRC1020
C                                                                       MPRC1030
C        ADDRESS NEXT INTERCHANGE STEP                                  MPRC1040
   12 IA=IA+ID                                                          MPRC1050
C                                                                       MPRC1060
C        NORMAL EXIT                                                    MPRC1070
      IER=0                                                             MPRC1080
      RETURN                                                            MPRC1090
C                                                                       MPRC1100
C        ERROR RETURN IN CASE ITRA IS NOT A TRANSPOSITION VECTOR        MPRC1110
   13 IER=1                                                             MPRC1120
      RETURN                                                            MPRC1130
C                                                                       MPRC1140
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSIONS                     MPRC1150
   14 IER=-1                                                            MPRC1160
      RETURN                                                            MPRC1170
      END                                                               MPRC1180
```

```
C                                                                       DMPR 420
C       SUBROUTINES AND SUBPROGRAMS REQUIRED                            DMPR 430
C          NONE                                                         DMPR 440
C                                                                       DMPR 450
C       METHOD                                                          DMPR 460
C          THE ROWS OR COLUMNS ARE PERMUTED ELEMENTWISE, INTERCHANGING  DMPR 470
C          ROW OR COLUMN 1 AND ITRA(1),...,ROW OR COLUMN K AND ITRA(K)  DMPR 480
C          IN THAT ORDER IF INV=0, AND OTHERWISE INTERCHANGING ROW OR   DMPR 490
C          COLUMN K AND ITRA(K),...,ROW OR COLUMN 1 AND ITRA(1), WHERE  DMPR 500
C          K IS M OR N DEPENDING ON WHETHER WE PERMUTE ROWS OR COLUMNS. DMPR 510
C                                                                       DMPR 520
C  ..................................................................   DMPR 530
C                                                                       DMPR 540
      SUBROUTINE DMPRC(A,M,N,ITRA,INV,IROCO,IER)                        DMPR 550
C                                                                       DMPR 560
C                                                                       DMPR 570
      DIMENSION A(1),ITRA(1)                                            DMPR 580
      DOUBLE PRECISION A,SAVE                                           DMPR 590
C                                                                       DMPR 600
C        TEST OF DIMENSIONS                                             DMPR 610
      IF(M)14,14,1                                                      DMPR 620
    1 IF(N)14,14,2                                                      DMPR 630
C                                                                       DMPR 640
C        DETERMINE WHICH ARE TO BE PERMUTED-THE ROWS OR THE COLUMNS     DMPR 650
    2 IF(IROCO)3,4,3                                                    DMPR 660
C                                                                       DMPR 670
C        INITIALIZE FOR COLUMN INTERCHANGES                             DMPR 680
    3 MM=M                                                              DMPR 690
      MMM=-1                                                            DMPR 700
      L=M                                                               DMPR 710
      LL=N                                                              DMPR 720
      GO TO 5                                                           DMPR 730
C                                                                       DMPR 740
C        INITIALIZE FOR ROW INTERCHANGES                                DMPR 750
    4 MM=1                                                              DMPR 760
      MMM=M                                                             DMPR 770
      L=N                                                               DMPR 780
      LL=M                                                              DMPR 790
C                                                                       DMPR 800
C        INITIALIZE LOOP OVER ALL ROWS OR COLUMNS                       DMPR 810
    5 IA=1                                                              DMPR 820
      ID=1                                                              DMPR 830
C                                                                       DMPR 840
C        TEST FOR INVERSE OPERATION                                     DMPR 850
      IF(INV)6,7,6                                                      DMPR 860
    6 IA=LL                                                             DMPR 870
      ID=-1                                                             DMPR 880
    7 DO 12 I=1,LL                                                      DMPR 890
      K=ITRA(IA)                                                        DMPR 900
      IF(K-IA)8,12,9                                                    DMPR 910
    8 IF(K)13,13,10                                                     DMPR 920
    9 IF(LL-K)13,10,10                                                  DMPR 930
C                                                                       DMPR 940
C        INITIALIZE ROW OR COLUMN INTERCHANGE                           DMPR 950
   10 IL=IA*MM                                                          DMPR 960
      K=K*MM                                                            DMPR 970
C                                                                       DMPR 980
C        PERFORM ROW OR COLUMN INTERCHANGE                              DMPR 990
      DO 11 J=1,L                                                       DMPR1000
      SAVE=A(IL)                                                        DMPF1010
      A(IL)=A(K)                                                        DMPR1020
      A(K)=SAVE                                                         DMPR1030
      K=K+MMM                                                           DMPR1040
   11 IL=IL+MMM                                                         DMPR1050
C                                                                       DMPR1060
C        ADDRESS NEXT INTERCHANGE STEP                                  DMPR1070
   12 IA=IA+ID                                                          DMPR1080
C                                                                       DMPR1090
C        NORMAL EXIT                                                    DMPR1100
      IER=0                                                             DMPR1110
      RETURN                                                            DMPR1120
C                                                                       DMPR1130
C        ERROR RETURN IN CASE ITRA IS NOT A TRANSPOSITION VECTOR        DMPR1140
   13 IER=1                                                             DMPR1150
      RETURN                                                            DMPR1160
C                                                                       DMPR1170
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSIONS                     DMPR1180
   14 IER=-1                                                            DMPR1190
      RETURN                                                            DMPR1200
      END                                                               DMPR1210
```

```
C                                                                       DMPR  10
C  ..................................................................   DMPR  20
C                                                                       DMPR  30
C       SUBROUTINE DMPRC                                                DMPR  40
C                                                                       DMPR  50
C       PURPOSE                                                         DMPR  60
C          TO PERMUTE THE ROWS OR COLUMNS OF A GIVEN MATRIX ACCORDING   DMPR  70
C          TO A GIVEN TRANSPOSITION VECTOR OR ITS INVERSE.  (SEE THE    DMPR  80
C          DISCUSSION ON PERMUTATIONS FOR DEFINITIONS AND NOTATION.)    DMPR  90
C                                                                       DMPR 100
C       USAGE                                                           DMPR 110
C          CALL DMPRC(A,M,N,ITRA,INV,IROCO,IER)                         DMPR 120
C                                                                       DMPR 130
C       DESCRIPTION OF PARAMETERS                                       DMPR 140
C          A      - GIVEN DOUBLE PRECISION M BY N MATRIX AND RESULTING  DMPR 150
C                   PERMUTED MATRIX                                     DMPR 160
C          M      - NUMBER OF ROWS OF A                                 DMPR 170
C          N      - NUMBER OF COLUMNS OF A                              DMPR 180
C          ITRA   - GIVEN TRANSPOSITION VECTOR (DIMENSION M IF ROWS ARE DMPR 190
C                   PERMUTED, N IF COLUMNS ARE PERMUTED)                DMPR 200
C          INV    - INPUT PARAMETER                                     DMPR 210
C                   INV NON-ZERO  -  PERMUTE ACCORDING TO ITRA          DMPR 220
C                   INV    =   0  -  PERMUTE ACCORDING TO ITRA INVERSE  DMPR 230
C          IROCO  - INPUT PARAMETER                                     DMPR 240
C                   IROCO NON-ZERO  -  PERMUTE THE COLUMNS OF A         DMPR 250
C                   IROCO    =   0  -  PERMUTE THE ROWS OF A            DMPR 260
C          IER    - RESULTING ERROR PARAMETER                          DMPR 270
C                   IER = -1  -  M AND N ARE NOT BOTH POSITIVE          DMPR 280
C                   IER =  0  -  NO ERROR                               DMPR 290
C                   IER =  1  -  ITRA IS NOT A TRANSPOSITION VECTOR ON  DMPR 300
C                                1,...,M IF ROWS ARE PERMUTED, 1,...,N  DMPR 310
C                                IF COLUMNS ARE PERMUTED                DMPR 320
C                                                                       DMPR 330
C       REMARKS                                                         DMPR 340
C          (1)  IF IER=-1 THERE IS NO COMPUTATION.                      DMPR 350
C          (2)  IF IER= 1, THEN COMPUTATION HAS BEEN UNSUCCESSFUL DUE   DMPR 360
C               TO ERROR, BUT THE MATRIX A WILL REFLECT THE ROW OR      DMPR 370
C               COLUMN INTERCHANGES PERFORMED BEFORE THE ERROR WAS      DMPR 380
C               DETECTED.                                               DMPR 390
C          (3)  THE MATRIX A IS ASSUMED TO BE STORED COLUMNWISE.        DMPR 400
C                                                                       DMPR 410
```

Subroutine MFUN

```
C                                                                       MFUN  10
C     ...................................................................MFUN  20
C                                                                       MFUN  30
C        SUBROUTINE MFUN                                                MFUN  40
C                                                                       MFUN  50
C        PURPOSE                                                        MFUN  60
C           APPLY A FUNCTION TO EACH ELEMENT OF A MATRIX TO FORM A      MFUN  70
C           RESULTANT MATRIX                                            MFUN  80
C                                                                       MFUN  90
C        USAGE                                                          MFUN 100
C           CALL MFUN (A,F,R,N,M,MS)                                    MFUN 110
C           AN EXTERNAL STATEMENT MUST PRECEDE CALL STATEMENT IN ORDER  MFUN 120
C           TO IDENTIFY PARAMETER F AS THE NAME OF A FUNCTION           MFUN 130
C                                                                       MFUN 140
C        DESCRIPTION OF PARAMETERS                                      MFUN 150
C           A - NAME OF INPUT MATRIX                                    MFUN 160
C           F - NAME OF FORTRAN-FURNISHED OR USER FUNCTION SUBPROGRAM    MFUN 170
C           R - NAME OF OUTPUT MATRIX                                   MFUN 180
C           N - NUMBER OF ROWS IN MATRIX A AND R                        MFUN 190
C           M - NUMBER OF COLUMNS IN MATRIX A AND R                     MFUN 200
C           MS  - ONE DIGIT NUMBER FOR STORAGE MODE OF MATRIX A (AND R) MFUN 210
C                 0 - GENERAL                                           MFUN 220
C                 1 - SYMMETRIC                                         MFUN 230
C                 2 - DIAGONAL                                          MFUN 240
C                                                                       MFUN 250
C        REMARKS                                                        MFUN 260
C           PRECISION IS DEPENDENT UPON PRECISION OF FUNCTION USED      MFUN 270
C                                                                       MFUN 280
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MFUN 290
C           LOC                                                         MFUN 300
C                                                                       MFUN 310
C        METHOD                                                         MFUN 320
C           FUNCTION F IS APPLIED TO EACH ELEMENT OF MATRIX A           MFUN 330
C           TO FORM MATRIX R                                            MFUN 340
C                                                                       MFUN 350
C     ...................................................................MFUN 360
C                                                                       MFUN 370
      SUBROUTINE MFUN(A,F,R,N,M,MS)                                     MFUN 380
      DIMENSION A(1),R(1)                                               MFUN 390
C                                                                       MFUN 400
C        COMPUTE VECTOR LENGTH, IT                                      MFUN 410
C                                                                       MFUN 420
      CALL LOC(N,M,IT,N,M,MS)                                           MFUN 430
C                                                                       MFUN 440
C        BUILD MATRIX R FOR ANY STORAGE MODE                            MFUN 450
C                                                                       MFUN 460
      DO 5 I=1,IT                                                       MFUN 470
    5 R(I)=F(A(I))                                                      MFUN 480
      RETURN                                                            MFUN 490
      END                                                               MFUN 500
```

Subroutine RECP

```
C                                                                       RECP  10
C     ...................................................................RECP  20
C                                                                       RECP  30
C        FUNCTION RECP                                                  RECP  40
C                                                                       RECP  50
C        PURPOSE                                                        RECP  60
C           CALCULATE RECIPROCAL OF AN ELEMENT. THIS IS A FORTRAN       RECP  70
C           FUNCTION SUBPROGRAM WHICH MAY BE USED AS AN ARGUMENT BY     RECP  80
C           SUBROUTINE MFUN.                                            RECP  90
C                                                                       RECP 100
C        USAGE                                                          RECP 110
C           RECP(E)                                                     RECP 120
C                                                                       RECP 130
C        DESCRIPTION OF PARAMETERS                                      RECP 140
C           E - MATRIX ELEMENT                                          RECP 150
C                                                                       RECP 160
C        REMARKS                                                        RECP 170
C           RECIPROCAL OF ZERO IS TAKEN TO BE 1.0E75                    RECP 180
C                                                                       RECP 190
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RECP 200
C           NONE                                                        RECP 210
C                                                                       RECP 220
C        METHOD                                                         RECP 230
C           RECIPROCAL OF ELEMENT E IS PLACED IN RECP                   RECP 240
C                                                                       RECP 250
C     ...................................................................RECP 260
C                                                                       RECP 270
      FUNCTION RECP(E)                                                  RECP 280
C                                                                       RECP 290
      BIG=1.0E75                                                        RECP 300
C                                                                       RECP 310
C        TEST ELEMENT FOR ZERO                                          RECP 320
C                                                                       RECP 330
      IF(E) 1,2,1                                                       RECP 340
C                                                                       RECP 350
C        IF NON-ZERO, CALCULATE RECIPROCAL                              RECP 360
C                                                                       RECP 370
    1 RECP=1.0/E                                                        RECP 380
      RETURN                                                            RECP 390
C                                                                       RECP 400
C        IF ZERO, SET EQUAL TO INFINITY                                 RECP 410
C                                                                       RECP 420
    2 RECP=SIGN(BIG,E)                                                  RECP 430
      RETURN                                                            RECP 440
      END                                                               RECP 450
```

Matrices: Inversion, Systems of Linear Equations and Related Topics

Subroutine MINV

```
C                                                                       MINV  10
C     ..................................................................MINV  20
C                                                                       MINV  30
C        SUBROUTINE MINV                                                MINV  40
C                                                                       MINV  50
C        PURPOSE                                                        MINV  60
C           INVERT A MATRIX                                             MINV  70
C                                                                       MINV  80
C        USAGE                                                          MINV  90
C           CALL MINV(A,N,D,L,M)                                        MINV 100
C                                                                       MINV 110
C        DESCRIPTION OF PARAMETERS                                      MINV 120
C           A - INPUT MATRIX, DESTROYED IN COMPUTATION AND REPLACED BY  MINV 130
C               RESULTANT INVERSE.                                      MINV 140
C           N - ORDER OF MATRIX A                                       MINV 150
C           D - RESULTANT DETERMINANT                                   MINV 160
C           L - WORK VECTOR OF LENGTH N                                 MINV 170
C           M - WORK VECTOR OF LENGTH N                                 MINV 180
C                                                                       MINV 190
C        REMARKS                                                        MINV 200
C           MATRIX A MUST BE A GENERAL MATRIX                           MINV 210
C                                                                       MINV 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MINV 230
C           NONE                                                        MINV 240
C                                                                       MINV 250
C        METHOD                                                         MINV 260
C           THE STANDARD GAUSS-JORDAN METHOD IS USED. THE DETERMINANT   MINV 270
C           IS ALSO CALCULATED. A DETERMINANT OF ZERO INDICATES THAT    MINV 280
C           THE MATRIX IS SINGULAR.                                     MINV 290
C                                                                       MINV 300
C     ..................................................................MINV 310
C                                                                       MINV 320
      SUBROUTINE MINV(A,N,D,L,M)                                        MINV 330
      DIMENSION A(1),L(1),M(1)                                          MINV 340
C                                                                       MINV 350
C     .................................................................MINV 360
C                                                                       MINV 370
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  MINV 380
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      MINV 390
C        STATEMENT WHICH FOLLOWS.                                       MINV 400
C                                                                       MINV 410
C     DOUBLE PRECISION A,D,BIGA,HOLD                                    MINV 420
C                                                                       MINV 430
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    MINV 440
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      MINV 450
C        ROUTINE.                                                       MINV 460
C                                                                       MINV 470
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      MINV 480
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  ABS IN STATEMENT  MINV 490
C        10 MUST BE CHANGED TO DABS.                                    MINV 500
C                                                                       MINV 510
C     .................................................................MINV 520
C                                                                       MINV 530
C        SEARCH FOR LARGEST ELEMENT                                     MINV 540
C                                                                       MINV 550
      D=1.0                                                             MINV 560
      NK=-N                                                             MINV 570
      DO 80 K=1,N                                                       MINV 580
      NK=NK+N                                                           MINV 590
      L(K)=K                                                            MINV 600
      M(K)=K                                                            MINV 610
      KK=NK+K                                                           MINV 620
      BIGA=A(KK)                                                        MINV 630
      DO 20 J=K,N                                                       MINV 640
      IZ=N*(J-1)                                                        MINV 650
      DO 20 I=K,N                                                       MINV 660
      IJ=IZ+I                                                           MINV 670
   10 IF( ABS(BIGA)- ABS(A(IJ))) 15,20,20                               MINV 680
   15 BIGA=A(IJ)                                                        MINV 690
      L(K)=I                                                            MINV 700
      M(K)=J                                                            MINV 710
   20 CONTINUE                                                          MINV 720
C                                                                       MINV 730
C        INTERCHANGE ROWS                                               MINV 740
C                                                                       MINV 750
      J=L(K)                                                            MINV 760
      IF(J-K) 35,35,25                                                  MINV 770
   25 KI=K-N                                                            MINV 780
      DO 30 I=1,N                                                       MINV 790
      KI=KI+N                                                           MINV 800
      HOLD=-A(KI)                                                       MINV 810
      JI=KI-K+J                                                         MINV 820
      A(KI)=A(JI)                                                       MINV 830
   30 A(JI) =HOLD                                                       MINV 840
C                                                                       MINV 850
C        INTERCHANGE COLUMNS                                            MINV 860
C                                                                       MINV 870
   35 I=M(K)                                                            MINV 880
      IF(I-K) 45,45,38                                                  MINV 890
   38 JP=N*(I-1)                                                        MINV 900
      DO 40 J=1,N                                                       MINV 910
      JK=NK+J                                                           MINV 920
      JI=JP+J                                                           MINV 930
      HOLD=-A(JK)                                                       MINV 940
      A(JK)=A(JI)                                                       MINV 950
   40 A(JI) =HOLD                                                       MINV 960
C                                                                       MINV 970
C        DIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS        MINV 980
C        CONTAINED IN BIGA)                                             MINV 990
C                                                                       MINV1000
   45 IF(BIGA) 48,46,48                                                 MINV1010
   46 D=0.0                                                             MINV1020
      RETURN                                                            MINV1030
   48 DO 55 I=1,N                                                       MINV1040
      IF(I-K) 50,55,50                                                  MINV1050
   50 IK=NK+I                                                           MINV1060
      A(IK)=A(IK)/(-BIGA)                                               MINV1070
   55 CONTINUE                                                          MINV1080
C                                                                       MINV1090
C        REDUCE MATRIX                                                  MINV1100
C                                                                       MINV1110
      DO 65 I=1,N                                                       MINV1120
      IK=NK+I                                                           MINV1130
      HOLD=A(IK)                                                        MINV1140
      IJ=I-N                                                            MINV1150
      DO 65 J=1,N                                                       MINV1160
      IJ=IJ+N                                                           MINV1170
      IF(I-K) 60,65,60                                                  MINV1180
   60 IF(J-K) 62,65,62                                                  MINV1190
   62 KJ=IJ-I+K                                                         MINV1200
      A(IJ)=HOLD*A(KJ)+A(IJ)                                            MINV1210
   65 CONTINUE                                                          MINV1220
C                                                                       MINV1230
C        DIVIDE ROW BY PIVOT                                            MINV1240
C                                                                       MINV1250
      KJ=K-N                                                            MINV1260
      DO 75 J=1,N                                                       MINV1270
      KJ=KJ+N                                                           MINV1280
      IF(J-K) 70,75,70                                                  MINV1290
   70 A(KJ)=A(KJ)/BIGA                                                  MINV1300
   75 CONTINUE                                                          MINV1310
C                                                                       MINV1320
C        PRODUCT OF PIVOTS                                              MINV1330
C                                                                       MINV1340
      D=D*BIGA                                                          MINV1350
C                                                                       MINV1360
C        REPLACE PIVOT BY RECIPROCAL                                    MINV1370
C                                                                       MINV1380
      A(KK)=1.0/BIGA                                                    MINV1390
   80 CONTINUE                                                          MINV1400
C                                                                       MINV1410
C        FINAL ROW AND COLUMN INTERCHANGE                               MINV1420
C                                                                       MINV1430
      K=N                                                               MINV1440
  100 K=(K-1)                                                           MINV1450
      IF(K) 150,150,105                                                 MINV1460
  105 I=L(K)                                                            MINV1470
      IF(I-K) 120,120,108                                               MINV1480
  108 JQ=N*(K-1)                                                        MINV1490
      JR=N*(I-1)                                                        MINV1500
      DO 110 J=1,N                                                      MINV1510
      JK=JQ+J                                                           MINV1520
      HOLD=A(JK)                                                        MINV1530
      JI=JR+J                                                           MINV1540
      A(JK)=-A(JI)                                                      MINV1550
  110 A(JI) =HOLD                                                       MINV1560
  120 J=M(K)                                                            MINV1570
      IF(J-K) 100,100,125                                               MINV1580
  125 KI=K-N                                                            MINV1590
      DO 130 I=1,N                                                      MINV1600
      KI=KI+N                                                           MINV1610
      HOLD=A(KI)                                                        MINV1620
      JI=KI-K+J                                                         MINV1630
      A(KI)=-A(JI)                                                      MINV1640
  130 A(JI) =HOLD                                                       MINV1650
      GO TO 100                                                         MINV1660
  150 RETURN                                                            MINV1670
      END                                                               MINV1680
```

Subroutines SINV and DSINV

These subroutines invert a given symmetric positive definite matrix, using factorization by subroutines MFSD and DMFSD.

1. Mathematical background

Given an n by n symmetric positive definite matrix A, an upper triangular matrix $R=(r_{ij})$ exists such that

$$A = R^T R$$

Then $A^{-1} = R^{-1}(R^{-1})^T$. The elements $\bar{r}_{ik}$ of R^{-1} are computed using the following recursive formulas:

$$\bar{r}_{ik} = -(1/r_{ii}) \left(\sum_{m=i+1}^{k} r_{im} \bar{r}_{mk} \right) \qquad i < k$$

$$\bar{r}_{ik} = 1/r_{ii} \qquad i = k$$

$$\bar{r}_{ik} = 0 \qquad i > k$$

2. Programming considerations

The given symmetric positive definite matrix A is stored columnwise in compressed form, that is, only the upper triangular part in $\frac{n(n+1)}{2}$ successive storage locations.

Subroutine MFSD (DMFSD), which is called internally, returns the elements r_{ik} ($i \leq k$) of the upper triangular matrix R in the storage locations of A. The inverse (upper) triangular matrix R^{-1} and at last the resultant upper triangular part of the inverse matrix A^{-1} are calculated and stored columnwise in the same storage locations.

If any calculated radicand r_{kk}^2 ($k = 1, 2, 3, \ldots, N$) is not positive, further calculation is bypassed, and the error parameter IER is set to -1. This means that matrix A is not positive definite, possibly due to roundoff errors. IER is also set to -1 if the input parameter N is less than one.

Let all radicands be positive, and let r_{kk}^2 be the first radicand which is no longer greater than the internal tolerance $TOL = |EPS \cdot a_{kk}|$. The subroutine gives the warning IER = k-1; however, calculation is continued. The warning indicates that there may be loss of significance at factorization step k due to loss of significant digits in the calculation of r_{kk}^2.

```
C                                                                       SINV  10
C     ...................................................................SINV  20
C                                                                       SINV  30
C        SUBROUTINE SINV                                                SINV  40
C                                                                       SINV  50
C        PURPOSE                                                        SINV  60
C           INVERT A GIVEN SYMMETRIC POSITIVE DEFINITE MATRIX           SINV  70
C                                                                       SINV  80
C        USAGE                                                          SINV  90
C           CALL SINV(A,N,EPS,IER)                                      SINV 100
C                                                                       SINV 110
C        DESCRIPTION OF PARAMETERS                                      SINV 120
C           A      - UPPER TRIANGULAR PART OF THE GIVEN SYMMETRIC       SINV 130
C                    POSITIVE DEFINITE N BY N COEFFICIENT MATRIX.       SINV 140
C                    ON RETURN A CONTAINS THE RESULTANT UPPER           SINV 150
C                    TRIANGULAR MATRIX.                                 SINV 160
C           N      - THE NUMBER OF ROWS (COLUMNS) IN GIVEN MATRIX.      SINV 170
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS RELATIVE        SINV 180
C                    TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.        SINV 190
C           IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS         SINV 200
C                    IER=0  - NO ERROR                                  SINV 210
C                    IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARAME-  SINV 220
C                             TER N OR BECAUSE SOME RADICAND IS NON-    SINV 230
C                             POSITIVE (MATRIX A IS NOT POSITIVE        SINV 240
C                             DEFINITE, POSSIBLY DUE TO LOSS OF SIGNI-  SINV 250
C                             FICANCE)                                  SINV 260
C                    IER=K  - WARNING WHICH INDICATES LOSS OF SIGNIFI-  SINV 270
C                             CANCE. THE RADICAND FORMED AT FACTORIZA-  SINV 280
C                             TION STEP K+1 WAS STILL POSITIVE BUT NO   SINV 290
C                             LONGER GREATER THAN ABS(EPS*A(K+1,K+1)).  SINV 300
C                                                                       SINV 310
C        REMARKS                                                        SINV 320
C           THE UPPER TRIANGULAR PART OF GIVEN MATRIX IS ASSUMED TO BE  SINV 330
C           STORED COLUMNWISE IN N*(N+1)/2 SUCCESSIVE STORAGE LOCATIONS.SINV 340
C           IN THE SAME STORAGE LOCATIONS THE RESULTING UPPER TRIANGU-   SINV 350
C           LAR MATRIX IS STORED COLUMNWISE TOO.                        SINV 360
C           THE PROCEDURE GIVES RESULTS IF N IS GREATER THAN 0 AND ALL  SINV 370
C           CALCULATED RADICANDS ARE POSITIVE.                          SINV 380
C                                                                       SINV 390
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SINV 400
C           MFSD                                                        SINV 410
C                                                                       SINV 420
C        METHOD                                                         SINV 430
C           SOLUTION IS DONE USING THE FACTORIZATION BY SUBROUTINE MFSD.SINV 440
C                                                                       SINV 450
C     ...................................................................SINV 460
C                                                                       SINV 470
      SUBROUTINE SINV(A,N,EPS,IER)                                      SINV 480
C                                                                       SINV 490
C                                                                       SINV 500
      DIMENSION A(1)                                                    SINV 510
      DOUBLE PRECISION DIN,WORK                                         SINV 520
C                                                                       SINV 530
C        FACTORIZE GIVEN MATRIX BY MEANS OF SUBROUTINE MFSD             SINV 540
C        A = TRANSPOSE(T) * T                                           SINV 550
      CALL MFSD(A,N,EPS,IER)                                            SINV 560
      IF(IER) 9,1,1                                                     SINV 570
C                                                                       SINV 580
C        INVERT UPPER TRIANGULAR MATRIX T                               SINV 590
C        PREPARE INVERSION-LOOP                                         SINV 600
    1 IPIV=N*(N+1)/2                                                    SINV 610
      IND=IPIV                                                          SINV 620
C                                                                       SINV 630
C        INITIALIZE INVERSION-LOOP                                      SINV 640
      DO 6 I=1,N                                                        SINV 650
      DIN=1.D0/DBLE(A(IPIV))                                            SINV 660
      A(IPIV)=DIN                                                       SINV 670
      MIN=N                                                             SINV 680
      KEND=I-1                                                          SINV 690
      LANF=N-KEND                                                       SINV 700
      IF(KEND) 5,5,2                                                    SINV 710
    2 J=IND                                                             SINV 720
C                                                                       SINV 730
C        INITIALIZE ROW-LOOP                                            SINV 740
      DO 4 K=1,KEND                                                     SINV 750
      WORK=0.D0                                                         SINV 760
      MIN=MIN-1                                                         SINV 770
      LHOR=IPIV                                                         SINV 780
      LVER=J                                                            SINV 790
C                                                                       SINV 800
C        START INNER LOOP                                               SINV 810
      DO 3 L=LANF,MIN                                                   SINV 820
      LVER=LVER+1                                                       SINV 830
      LHOR=LHOR+L                                                       SINV 840
    3 WORK=WORK+DBLE(A(LVER)*A(LHOR))                                   SINV 850
C        END OF INNER LOOP                                              SINV 860
C                                                                       SINV 870
      A(J)=-WORK*DIN                                                    SINV 880
    4 J=J-MIN                                                           SINV 890
C        END OF ROW-LOOP                                                SINV 900
C                                                                       SINV 910
    5 IPIV=IPIV-MIN                                                     SINV 920
    6 IND=IND-1                                                         SINV 930
C        END OF INVERSION-LOOP                                          SINV 940
C                                                                       SINV 950
C        CALCULATE INVERSE(A) BY MEANS OF INVERSE(T)                    SINV 960
C        INVERSE(A) = INVERSE(T) * TRANSPOSE(INVERSE(T))                SINV 970
C        INITIALIZE MULTIPLICATION-LOOP                                 SINV 980
      DO 8 I=1,N                                                        SINV 990
      IPIV=IPIV+I                                                       SINV1000
      J=IPIV                                                            SINV1010
C                                                                       SINV1020
C        INITIALIZE ROW-LOOP                                            SINV1030
      DO 8 K=I,N                                                        SINV1040
      WORK=0.D0                                                         SINV1050
      LHOR=J                                                            SINV1060
C                                                                       SINV1070
C        START INNER LOOP                                               SINV1080
      DO 7 L=K,N                                                        SINV1090
      LVER=LHOR+K-I                                                     SINV1100
      WORK=WORK+DBLE(A(LHOR)*A(LVER))                                   SINV1110
    7 LHOR=LHOR+L                                                       SINV1120
C        END OF INNER LOOP                                              SINV1130
C                                                                       SINV1140
      A(J)=WORK                                                         SINV1150
    8 J=J+K                                                             SINV1160
C        END OF ROW- AND MULTIPLICATION-LOOP                            SINV1170
C                                                                       SINV1180
    9 RETURN                                                            SINV1190
      END                                                               SINV1200
```

```
C                                                                       DSIN  10
C     ..................................................................DSIN  20
C                                                                       DSIN  30
C         SUBROUTINE DSINV                                              DSIN  40
C                                                                       DSIN  50
C         PURPOSE                                                       DSIN  60
C            INVERT A GIVEN SYMMETRIC POSITIVE DEFINITE MATRIX          DSIN  70
C                                                                       DSIN  80
C         USAGE                                                         DSIN  90
C            CALL DSINV(A,N,EPS,IER)                                    DSIN 100
C                                                                       DSIN 110
C         DESCRIPTION OF PARAMETERS                                     DSIN 120
C            A      - DOUBLE PRECISION UPPER TRIANGULAR PART OF GIVEN   DSIN 130
C                     SYMMETRIC POSITIVE DEFINITE N BY N COEFFICIENT    DSIN 140
C                     MATRIX.                                           DSIN 150
C                     ON RETURN A CONTAINS THE RESULTANT UPPER          DSIN 160
C                     TRIANGULAR MATRIX IN DOUBLE PRECISION.            DSIN 170
C            N      - THE NUMBER OF ROWS (COLUMNS) IN GIVEN MATRIX.    DSIN 180
C            EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED    DSIN 190
C                     AS RELATIVE TOLERANCE FOR TEST ON LOSS OF         DSIN 200
C                     SIGNIFICANCE.                                     DSIN 210
C            IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS       DSIN 220
C                     IER=0  - NO ERROR                                 DSIN 230
C                     IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARAME- DSIN 240
C                              TER N OR BECAUSE SOME RADICAND IS NON-   DSIN 250
C                              POSITIVE (MATRIX A IS NOT POSITIVE       DSIN 260
C                              DEFINITE, POSSIBLY DUE TO LOSS OF SIGNI- DSIN 270
C                              FICANCE)                                 DSIN 280
C                     IER=K  - WARNING WHICH INDICATES LOSS OF SIGNIFI- DSIN 290
C                              CANCE. THE RADICAND FORMED AT FACTORIZA- DSIN 300
C                              TION STEP K+1 WAS STILL POSITIVE BUT NO  DSIN 310
C                              LONGER GREATER THAN ABS(EPS*A(K+1,K+1)). DSIN 320
C                                                                       DSIN 330
C         REMARKS                                                       DSIN 340
C            THE UPPER TRIANGULAR PART OF GIVEN MATRIX IS ASSUMED TO BE DSIN 350
C            STORED COLUMNWISE IN N*(N+1)/2 SUCCESSIVE STORAGE LOCATIONS.DSIN 360
C            IN THE SAME STORAGE LOCATIONS THE RESULTING UPPER TRIANGU- DSIN 370
C            LAR MATRIX IS STORED COLUMNWISE TOO.                       DSIN 380
C            THE PROCEDURE GIVES RESULTS IF N IS GREATER THAN 0 AND ALL DSIN 390
C            CALCULATED RADICANDS ARE POSITIVE.                         DSIN 400
C                                                                       DSIN 410
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 DSIN 420
C            DMFSD                                                      DSIN 430
C                                                                       DSIN 440
C         METHOD                                                        DSIN 450
C            SOLUTION IS DONE USING FACTORIZATION BY SUBROUTINE DMFSD.  DSIN 460
C                                                                       DSIN 470
C     ..................................................................DSIN 480
C                                                                       DSIN 490
      SUBROUTINE DSINV(A,N,EPS,IER)                                     DSIN 500
C                                                                       DSIN 510
C                                                                       DSIN 520
      DIMENSION A(1)                                                    DSIN 530
      DOUBLE PRECISION A,DIN,WORK                                       DSIN 540
C                                                                       DSIN 550
C        FACTORIZE GIVEN MATRIX BY MEANS OF SUBROUTINE DMFSD            DSIN 560
C        A = TRANSPOSE(T) * T                                           DSIN 570
      CALL DMFSD(A,N,EPS,IER)                                           DSIN 580
      IF(IER) 9,1,1                                                     DSIN 590
C                                                                       DSIN 600
C        INVERT UPPER TRIANGULAR MATRIX T                               DSIN 610
C        PREPARE INVERSION-LOOP                                         DSIN 620
    1 IPIV=N*(N+1)/2                                                    DSIN 630
      IND=IPIV                                                          DSIN 640
C                                                                       DSIN 650
C        INITIALIZE INVERSION-LOOP                                      DSIN 660
      DO 6 I=1,N                                                        DSIN 670
      DIN=1.D0/A(IPIV)                                                  DSIN 680
      A(IPIV)=DIN                                                       DSIN 690
      MIN=N                                                             DSIN 700
      KEND=I-1                                                          DSIN 710
      LANF=N-KEND                                                       DSIN 720
      IF(KEND) 5,5,2                                                    DSIN 730
    2 J=IND                                                             DSIN 740
C                                                                       DSIN 750
C        INITIALIZE ROW-LOOP                                            DSIN 760
      DO 4 K=1,KEND                                                     DSIN 770
      WORK=0.D0                                                         DSIN 780
      MIN=MIN-1                                                         DSIN 790
      LHOR=IPIV                                                         DSIN 800
      LVER=J                                                            DSIN 810
C                                                                       DSIN 820
C        START INNER LOOP                                               DSIN 830
      DO 3 L=LANF,MIN                                                   DSIN 840
      LVER=LVER+1                                                       DSIN 850
      LHOR=LHOR+L                                                       DSIN 860
    3 WORK=WORK+A(LVER)*A(LHOR)                                         DSIN 870
C        END OF INNER LOOP                                              DSIN 880
C                                                                       DSIN 890
      A(J)=-WORK*DIN                                                    DSIN 900
    4 J=J-MIN                                                           DSIN 910
C        END OF ROW-LOOP                                                DSIN 920
C                                                                       DSIN 930
    5 IPIV=IPIV-MIN                                                     DSIN 940
    6 IND=IND-1                                                         DSIN 950
C        END OF INVERSION-LOOP                                          DSIN 960
C                                                                       DSIN 970
C        CALCULATE INVERSE(A) BY MEANS OF INVERSE(T)                    DSIN 980
C        INVERSE(A) = INVERSE(T) * TRANSPOSE(INVERSE(T))                DSIN 990
C        INITIALIZE MULTIPLICATION-LOOP                                 DSIN1000
      DO 8 I=1,N                                                        DSIN1010
      IPIV=IPIV+I                                                       DSIN1020
      J=IPIV                                                            DSIN1030
C                                                                       DSIN1040
C        INITIALIZE ROW-LOOP                                            DSIN1050
      DO 8 K=I,N                                                        DSIN1060
      WORK=0.D0                                                         DSIN1070
      LHOR=J                                                            DSIN1080
C                                                                       DSIN1090
C        START INNER LOOP                                               DSIN1100
      DO 7 L=K,N                                                        DSIN1110
      LVER=LHOR+K-I                                                     DSIN1120
      WORK=WORK+A(LHOR)*A(LVER)                                         DSIN1130
    7 LHOR=LHOR+L                                                       DSIN1140
C        END OF INNER LOOP                                              DSIN1150
C                                                                       DSIN1160
      A(J)=WORK                                                         DSIN1170
    8 J=J+K                                                             DSIN1180
C        END OF ROW- AND MULTIPLICATION-LOOP                            DSIN1190
C                                                                       DSIN1200
    9 RETURN                                                            DSIN1210
      END                                                               DSIN1220
```

Subroutine SIMQ

```
C                                                                       SIMQ  10
C     ..................................................................SIMQ  20
C                                                                       SIMQ  30
C         SUBROUTINE SIMQ                                               SIMQ  40
C                                                                       SIMQ  50
C         PURPOSE                                                       SIMQ  60
C            OBTAIN SOLUTION OF A SET OF SIMULTANEOUS LINEAR EQUATIONS, SIMQ  70
C            AX=B                                                       SIMQ  80
C                                                                       SIMQ  90
C         USAGE                                                         SIMQ 100
C            CALL SIMQ(A,B,N,KS)                                        SIMQ 110
C                                                                       SIMQ 120
C         DESCRIPTION OF PARAMETERS                                     SIMQ 130
C            A - MATRIX OF COEFFICIENTS STORED COLUMNWISE.  THESE ARE   SIMQ 140
C                DESTROYED IN THE COMPUTATION.  THE SIZE OF MATRIX A IS SIMQ 150
C                N BY N.                                                SIMQ 160
C            B - VECTOR OF ORIGINAL CONSTANTS (LENGTH N).  THESE ARE    SIMQ 170
C                REPLACED BY FINAL SOLUTION VALUES, VECTOR X.           SIMQ 180
C            N - NUMBER OF EQUATIONS AND VARIABLES. N MUST BE .GT. ONE. SIMQ 190
C            KS - OUTPUT DIGIT                                          SIMQ 200
C                 0 FOR A NORMAL SOLUTION                               SIMQ 210
C                 1 FOR A SINGULAR SET OF EQUATIONS                     SIMQ 220
C                                                                       SIMQ 230
C         REMARKS                                                       SIMQ 240
C            MATRIX A MUST BE GENERAL.                                  SIMQ 250
C            IF MATRIX IS SINGULAR , SOLUTION VALUES ARE MEANINGLESS.   SIMQ 260
C            AN ALTERNATIVE SOLUTION MAY BE OBTAINED BY USING MATRIX    SIMQ 270
C            INVERSION (MINV) AND MATRIX PRODUCT (GMPRD).               SIMQ 280
C                                                                       SIMQ 290
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 SIMQ 300
C            NONE                                                       SIMQ 310
C                                                                       SIMQ 320
C         METHOD                                                        SIMQ 330
C            METHOD OF SOLUTION IS BY ELIMINATION USING LARGEST PIVOTAL SIMQ 340
C            DIVISOR. EACH STAGE OF ELIMINATION CONSISTS OF INTERCHANGINGSIMQ 350
C            ROWS WHEN NECESSARY TO AVOID DIVISION BY ZERO OR SMALL     SIMQ 360
C            ELEMENTS.                                                  SIMQ 370
C            THE FORWARD SOLUTION TO OBTAIN VARIABLE N IS DONE IN       SIMQ 380
C            N STAGES. THE BACK SOLUTION FOR THE OTHER VARIABLES IS     SIMQ 390
C            CALCULATED BY SUCCESSIVE SUBSTITUTIONS. FINAL SOLUTION     SIMQ 400
C            VALUES ARE DEVELOPED IN VECTOR B, WITH VARIABLE 1 IN B(1), SIMQ 410
C            VARIABLE 2 IN B(2),.....,VARIABLE N IN B(N).               SIMQ 420
C            IF NO PIVOT CAN BE FOUND EXCEEDING A TOLERANCE OF 0.0,     SIMQ 430
C            THE MATRIX IS CONSIDERED SINGULAR AND KS IS SET TO 1. THIS SIMQ 440
C            TOLERANCE CAN BE MODIFIED BY REPLACING THE FIRST STATEMENT. SIMQ 450
C                                                                       SIMQ 460
C     ..................................................................SIMQ 470
C                                                                       SIMQ 480
      SUBROUTINE SIMQ(A,B,N,KS)                                         SIMQ 490
      DIMENSION A(1),B(1)                                               SIMQ 500
C                                                                       SIMQ 510
C        FORWARD SOLUTION                                               SIMQ 520
C                                                                       SIMQ 530
      TOL=0.0                                                           SIMQ 540
      KS=0                                                              SIMQ 550
      JJ=-N                                                             SIMQ 560
      DO 65 J=1,N                                                       SIMQ 570
      JY=J+1                                                            SIMQ 580
      JJ=JJ+N+1                                                         SIMQ 590
      BIGA=0                                                            SIMQ 600
      IT=JJ-J                                                           SIMQ 610
      DO 30 I=J,N                                                       SIMQ 620
C                                                                       SIMQ 630
C        SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN                       SIMQ 640
C                                                                       SIMQ 650
      IJ=IT+I                                                           SIMQ 660
      IF(ABS(BIGA)-ABS(A(IJ))) 20,30,30                                 SIMQ 670
   20 BIGA=A(IJ)                                                        SIMQ 680
      IMAX=I                                                            SIMQ 690
   30 CONTINUE                                                          SIMQ 700
C                                                                       SIMQ 710
C        TEST FOR PIVOT LESS THAN TOLERANCE (SINGULAR MATRIX)           SIMQ 720
C                                                                       SIMQ 730
      IF(ABS(BIGA)-TOL) 35,35,40                                        SIMQ 740
   35 KS=1                                                              SIMQ 750
      RETURN                                                            SIMQ 760
C                                                                       SIMQ 770
C        INTERCHANGE ROWS IF NECESSARY                                  SIMQ 780
C                                                                       SIMQ 790
   40 I1=J+N*(J-2)                                                      SIMQ 800
      IT=IMAX-J                                                         SIMQ 810
      DO 50 K=J,N                                                       SIMQ 820
      I1=I1+N                                                           SIMQ 830
      I2=I1+IT                                                          SIMQ 840
      SAVE=A(I1)                                                        SIMQ 850
      A(I1)=A(I2)                                                       SIMQ 860
      A(I2)=SAVE                                                        SIMQ 870
C                                                                       SIMQ 880
C        DIVIDE EQUATION BY LEADING COEFFICIENT                         SIMQ 890
C                                                                       SIMQ 900
   50 A(I1)=A(I1)/BIGA                                                  SIMQ 910
      SAVE=B(IMAX)                                                      SIMQ 920
      B(IMAX)=B(J)                                                      SIMQ 930
      B(J)=SAVE/BIGA                                                    SIMQ 940
C                                                                       SIMQ 950
C        ELIMINATE NEXT VARIABLE                                        SIMQ 960
C                                                                       SIMQ 970
      IF(J-N) 55,70,55                                                  SIMQ 980
   55 IQS=N*(J-1)                                                       SIMQ 990
      DO 65 IX=JY,N                                                     SIMQ1000
      IXJ=IQS+IX                                                        SIMQ1010
      IT=J-IX                                                           SIMQ1020
      DO 60 JX=JY,N                                                     SIMQ1030
      IXJX=N*(JX-1)+IX                                                  SIMQ1040
      JJX=IXJX+IT                                                       SIMQ1050
   60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))                                   SIMQ1060
   65 B(IX)=B(IX)-(B(J)*A(IXJ))                                         SIMQ1070
C                                                                       SIMQ1080
C        BACK SOLUTION                                                  SIMQ1090
C                                                                       SIMQ1100
   70 NY=N-1                                                            SIMQ1110
      IT=N*N                                                            SIMQ1120
      DO 80 J=1,NY                                                      SIMQ1130
      IA=IT-J                                                           SIMQ1140
      IB=N-J                                                            SIMQ1150
      IC=N                                                              SIMQ1160
      DO 80 K=1,J                                                       SIMQ1170
      B(IB)=B(IB)-A(IA)*B(IC)                                           SIMQ1180
      IA=IA-N                                                           SIMQ1190
   80 IC=IC-1                                                           SIMQ1200
      RETURN                                                            SIMQ1210
      END                                                               SIMQ1220
```

Subroutines GELG and DGELG

These subroutines solve a system of general simultaneous linear equations by Gauss elimination. Consider the system of general simultaneous linear equations:

$$A * X = R \tag{1}$$

with an m by m coefficient matrix A and an m by n right-hand side matrix R both stored columnwise. Solution is done by means of Gauss elimination with complete pivoting. If matrix R is the identity matrix, solution X is the inverse of matrix A. The solution X is generated in matrix R. Thus, the computation of the solution requires no additional storage requirements.

Explicitly, the given system (1) is of the form:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & \cdots & a_{mm} \end{pmatrix} * \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{pmatrix}$$

$$= \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ r_{21} & r_{22} & \cdots & r_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ r_{m1} & r_{m2} & \cdots & r_{mn} \end{pmatrix} \tag{2}$$

The first step is to search the whole matrix A for the element of greatest absolute value, say a_{ij}, and to select it as first pivot ($p = a_{ij}$). With a_{ij}, generate the internal absolute tolerance for testing loss of significance in the following way:

$$tol = |a_{ij}| \cdot \varepsilon$$

with a given relative tolerance ε.

Suppose that pivot a_{ij} is equal to a_{11}. If it is not, interchange the first rows of matrices A and R with the i^{th}, and the first column of matrix A with the j^{th}, and save column interchange information by storing the difference (j-1) of pivot column index j and step counter k = 1 [interchanging column 1 with column j means interchanging of variables x_{11} with x_{1j} (l = 1, 2, ..., n)].

Now transform the elements of pivot rows in matrices A and R by multiplying with 1/p, and the other elements by adding $-a_{\nu 1}$ times the new first rows of these two matrices to the other ν rows, thus getting:

$$a_{11}^{(1)} = + \frac{a_{11}}{p} \quad (l = 2, 3, \ldots, m) \tag{4}$$

$$r_{11}^{(1)} = + \frac{r_{11}}{p} \quad (l = 1, 2, \ldots, n) \tag{5}$$

$$a_{\nu l}^{(1)} = a_{\nu l} - a_{\nu 1} \cdot a_{11}^{(1)} \quad \begin{matrix} (l = 2, 3, \ldots, m; \\ \nu = 2, 3, \ldots, m) \end{matrix} \tag{6}$$

$$r_{\nu l}^{(1)} = r_{\nu l} - a_{\nu 1} \cdot r_{11}^{(1)} \quad \begin{matrix} (l = 1, 2, \ldots, n; \\ \nu = 2, 3, \ldots, m) \end{matrix} \tag{7}$$

If column interchange information is saved in the first position of the main diagonal, the result of the first step is the two matrices:

$$A^{(1)} = \begin{pmatrix} (j-1) & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & \cdots & a_{2m}^{(1)} \\ 0 & a_{32}^{(1)} & a_{33}^{(1)} & \cdots & a_{3m}^{(1)} \\ & \cdots & \cdots & \cdots & \\ 0 & a_{m2}^{(1)} & a_{m3}^{(1)} & \cdots & a_{mm}^{(1)} \end{pmatrix} \text{ and}$$

$$R^{(1)} = \begin{pmatrix} r_{11}^{(1)} & r_{12}^{(1)} & \cdots & r_{1n}^{(1)} \\ r_{21}^{(1)} & r_{22}^{(1)} & \cdots & r_{2n}^{(1)} \\ \cdots & \cdots & \cdots & \cdots \\ r_{m1}^{(1)} & r_{m2}^{(1)} & \cdots & r_{mn}^{(1)} \end{pmatrix}$$

Now repeat this procedure m-2 times, starting at each step with the matrix $A^{(k)}$ of the step before

without first k rows and first k columns, and the matrix $R^{(k)}$ without first k rows. The total result after m-1 steps is the matrices:

$$A^{(m-1)} = \begin{pmatrix} (j_1\text{-}1) & a_{12}^{(1)} & a_{13}^{(1)} & \dots & a_{1m}^{(1)} \\ 0 & (j_2\text{-}2) & a_{23}^{(2)} & \dots & a_{2m}^{(2)} \\ 0 & 0 & (j_3\text{-}3) & \dots & a_{3m}^{(3)} \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & & (j_m\text{-}m) \end{pmatrix} \quad \text{and}$$

$$R^{(m-1)} = \begin{pmatrix} r_{11}^{(1)} & r_{12}^{(1)} & \dots & r_{1n}^{(1)} \\ r_{21}^{(2)} & r_{22}^{(2)} & \dots & r_{2n}^{(2)} \\ r_{31}^{(3)} & r_{32}^{(3)} & \dots & r_{3n}^{(3)} \\ \dots & \dots & \dots & \dots \\ r_{m1}^{(m)} & r_{m2}^{(m)} & \dots & r_{mn}^{(m)} \end{pmatrix}$$

Now work backward and set:

$$\left.\begin{aligned} r_{m-1,l}^{(m)} &= r_{m-1,l}^{(m-1)} - a_{m-1,m}^{(m-1)} \cdot r_{m,l}^{(m)} \quad (l = 1,2,\dots,n) \\ r_{m-2,l}^{(m)} &= r_{m-2,l}^{(m-2)} - a_{m-2,m-1}^{(m-2)} \cdot r_{m-1,l}^{(m)} \\ &\quad - a_{m-2,m}^{(m-2)} \cdot r_{m,l}^{(m)} \quad (l = 1,2,\dots,n) \\ &\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ r_{1,l}^{(m)} &= r_{1l}^{(1)} - a_{12}^{(1)} \cdot r_{2l}^{(m)} - a_{13}^{(1)} \cdot r_{3l}^{(m)} \\ &\quad - \dots - a_{1m}^{(1)} \cdot r_{ml}^{(m)} \quad (l = 1,2,\dots,n) \end{aligned}\right\} \quad (8)$$

After each step of back substitution, rows of solution matrix $X = R^{(m)}$ have to be back-interchanged according to interchange information in the corresponding main diagonal element of matrix $A^{(m-1)}$, in order to get the correct sequence of right-hand side column elements $r_{\nu l}^{(m)}$ corresponding to the sequence of left-hand side column elements $a_{j_\nu}^{(j)}$.

The only case in which the above procedure can fail to give a solution occurs when at any step all elements of the rest-matrix of $A^{(k)}$ become zero, and no pivot element can be found. In this case the procedure is bypassed, and the error message ier = -1 is given. Actually, because of rounding errors, a further check of the absolute values of pivot elements is performed by the procedure. If at elimination step k this absolute value becomes less than tol (see equation 3), it is likely that matrix A is singular too. But as this is not necessarily the case, and as this test depends highly on the choice of the relative tolerance ε+ , the procedure gives only the warning ier = k-1, indicating that there is a possible loss of significance in the results computed by the algorithm++. In case of a well scaled matrix A and an appropriate choice of the relative tolerance, warning ier = k-1 may be interpreted to mean that matrix A has the rank k-1. If there is only one equation to solve (m=1), the test on loss of significance is suppressed.

+For subroutine GELG, a relative tolerance ϵ between 10^{-6} and 10^{-7} is suggested; and for subroutine DGELG, between 10^{-14} and 10^{-16}.

++For example, $\epsilon = 10^{-5}$ and warning ier = 3 mean that there is a possible loss of about five or more significant digits in the initial values of elimination step 4, and that matrix A seems to have the rank 3.

```
C                                                                       GELG  10
C ...................................................................  GELG  20
C                                                                       GELG  30
C    SUBROUTINE GELG                                                    GELG  40
C                                                                       GELG  50
C    PURPOSE                                                            GELG  60
C       TO SOLVE A GENERAL SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS.     GELG  70
C                                                                       GELG  80
C    USAGE                                                              GELG  90
C       CALL GELG(R,A,M,N,EPS,IER)                                      GELG 100
C                                                                       GELG 110
C    DESCRIPTION OF PARAMETERS                                          GELG 120
C       R   - THE M BY N MATRIX OF RIGHT HAND SIDES.  (DESTROYED)       GELG 130
C             ON RETURN R CONTAINS THE SOLUTION OF THE EQUATIONS.       GELG 140
C       A   - THE M BY M COEFFICIENT MATRIX.  (DESTROYED)               GELG 150
C       M   - THE NUMBER OF EQUATIONS IN THE SYSTEM.                    GELG 160
C       N   - THE NUMBER OF RIGHT HAND SIDE VECTORS.                    GELG 170
C       EPS - AN INPUT CONSTANT WHICH IS USED AS RELATIVE               GELG 180
C             TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.               GELG 190
C       IER - RESULTING ERROR PARAMETER CODED AS FOLLOWS                GELG 200
C             IER=0  - NO ERROR,                                        GELG 210
C             IER=-1 - NO RESULT BECAUSE OF M LESS THAN 1 OR            GELG 220
C                      PIVOT ELEMENT AT ANY ELIMINATION STEP            GELG 230
C                      EQUAL TO 0,                                      GELG 240
C             IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-         GELG 250
C                      CANCE INDICATED AT ELIMINATION STEP K+1,         GELG 260
C                      WHERE PIVOT ELEMENT WAS LESS THAN OR             GELG 270
C                      EQUAL TO THE INTERNAL TOLERANCE EPS TIMES        GELG 280
C                      ABSOLUTELY GREATEST ELEMENT OF MATRIX A.         GELG 290
C                                                                       GELG 300
C    REMARKS                                                            GELG 310
C       INPUT MATRICES R AND A ARE ASSUMED TO BE STORED COLUMNWISE      GELG 320
C       IN MN RESP. M**2 SUCCESSIVE STORAGE LOCATIONS. ON RETURN        GELG 330
C       SOLUTION MATRIX R IS STORED COLUMNWISE TOO.                     GELG 340
C       THE PROCEDURE GIVES RESULTS IF THE NUMBER OF EQUATIONS M IS     GELG 350
C       GREATER THAN 0 AND PIVOT ELEMENTS AT ALL ELIMINATION STEPS      GELG 360
C       ARE DIFFERENT FROM 0. HOWEVER WARNING IER=K - IF GIVEN -        GELG 370
C       INDICATES POSSIBLE LOSS OF SIGNIFICANCE IN CASE OF A WELL       GELG 380
C       SCALED MATRIX A AND APPROPRIATE TOLERANCE EPS. IER=K MAY BE     GELG 390
C       INTERPRETED THAT MATRIX A HAS THE RANK K+ NO WARNING IS         GELG 400
C       GIVEN IN CASE M=1.                                              GELG 410
```

```
C                                                                       DELG  10
C   ******************************************************************* DELG  20
C                                                                       DELG  30
C       SUBROUTINE DGELG                                                DELG  40
C                                                                       DELG  50
C       PURPOSE                                                         DELG  60
C          TO SOLVE A GENERAL SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS.  DELG  70
C                                                                       DELG  80
C       USAGE                                                           DELG  90
C          CALL DGELG(R,A,M,N,EPS,IER)                                  DELG 100
C                                                                       DELG 110
C       DESCRIPTION OF PARAMETERS                                       DELG 120
C          R      - DOUBLE PRECISION M BY N RIGHT HAND SIDE MATRIX      DELG 130
C                   (DESTROYED). ON RETURN R CONTAINS THE SOLUTIONS     DELG 140
C                   OF THE EQUATIONS.                                   DELG 150
C          A      - DOUBLE PRECISION M BY M COEFFICIENT MATRIX          DELG 160
C                   (DESTROYED).                                        DELG 170
C          M      - THE NUMBER OF EQUATIONS IN THE SYSTEM.              DELG 180
C          N      - THE NUMBER OF RIGHT HAND SIDE VECTORS.              DELG 190
C          EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS    DELG 200
C                   RELATIVE TOLERANCE FOR TEST ON LOSS OF              DELG 210
C                   SIGNIFICANCE.                                       DELG 220
C          IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS          DELG 230
C                   IER=0  - NO ERROR.                                  DELG 240
C                   IER=-1 - NO RESULT BECAUSE OF M LESS THAN 1 OR      DELG 250
C                            PIVOT ELEMENT AT ANY ELIMINATION STEP      DELG 260
C                            EQUAL TO 0.                                DELG 270
C                   IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-   DELG 280
C                            CANCE INDICATED AT ELIMINATION STEP K+1,   DELG 290
C                            WHERE PIVOT ELEMENT WAS LESS THAN OR       DELG 300
C                            EQUAL TO THE INTERNAL TOLERANCE EPS TIMES  DELG 310
C                            ABSOLUTELY GREATEST ELEMENT OF MATRIX A.   DELG 320
C                                                                       DELG 330
C       REMARKS                                                         DELG 340
C          INPUT MATRICES R AND A ARE ASSUMED TO BE STORED COLUMNWISE   DELG 350
C          IN M*N RESP. M*M SUCCESSIVE STORAGE LOCATIONS. ON RETURN     DELG 360
C          SOLUTION MATRIX R IS STORED COLUMNWISE TOO.                  DELG 370
C          THE PROCEDURE GIVES RESULTS IF THE NUMBER OF EQUATIONS M IS  DELG 380
C          GREATER THAN 0 AND PIVOT ELEMENTS AT ALL ELIMINATION STEPS   DELG 390
C          ARE DIFFERENT FROM 0. HOWEVER WARNING IER=K - IF GIVEN -     DELG 400
C          INDICATES POSSIBLE LOSS OF SIGNIFICANCE. IN CASE OF A WELL   DELG 410
C          SCALED MATRIX A AND APPROPRIATE TOLERANCE EPS, IER=K MAY BE  DELG 420
C          INTERPRETED THAT MATRIX A HAS THE RANK K. NO WARNING IS      DELG 430
C          GIVEN IN CASE M=1.                                           DELG 440
C                                                                       DELG 450
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DELG 460
C          NONE                                                         DELG 470
C                                                                       DELG 480
C       METHOD                                                          DELG 490
C          SOLUTION IS DONE BY MEANS OF GAUSS-ELIMINATION WITH          DELG 500
C          COMPLETE PIVOTING.                                           DELG 510
C                                                                       DELG 520
C   ******************************************************************* DELG 530
C                                                                       DELG 540
      SUBROUTINE DGELG(R,A,M,N,EPS,IER)                                 DELG 550
C                                                                       DELG 560
C                                                                       DELG 570
      DIMENSION A(1),R(1)                                               DELG 580
      DOUBLE PRECISION R,A,PIV,TB,TOL,PIVI                              DELG 590
      IF(M)23,23,1                                                      DELG 600
C                                                                       DELG 610
C     SEARCH FOR GREATEST ELEMENT IN MATRIX A                           DELG 620
    1 IER=0                                                             DELG 630
      PIV=0.D0                                                          DELG 640
      MM=M*M                                                            DELG 650
      NM=N*M                                                            DELG 660
      DO 3 L=1,MM                                                       DELG 670
      TB=DABS(A(L))                                                     DELG 680
      IF(TB-PIV)3,3,2                                                   DELG 690
    2 PIV=TB                                                            DELG 700
      I=L                                                               DELG 710
    3 CONTINUE                                                          DELG 720
      TOL=EPS*PIV                                                       DELG 730
C     A(I) IS PIVOT ELEMENT. PIV CONTAINS THE ABSOLUTE VALUE OF A(I).   DELG 740
C                                                                       DELG 750
C                                                                       DELG 760
C     START ELIMINATION LOOP                                            DELG 770
      LST=1                                                             DELG 780
      DO 17 K=1,M                                                       DELG 790
C                                                                       DELG 800
C     TEST ON SINGULARITY                                               DELG 810
      IF(PIV)23,23,4                                                    DELG 820
    4 IF(IER)7,5,7                                                      DELG 830
    5 IF(PIV-TOL)6,6,7                                                  DELG 840
    6 IER=K-1                                                           DELG 850
    7 PIVI=1./A(I)                                                      DELG 860
      J=(I-1)/M                                                         DELG 870
      I=I-J*M+K                                                         DELG 880
      J=J+1-K                                                           DELG 890
C     I+K IS ROW-INDEX, J+K COLUMN-INDEX OF PIVOT ELEMENT               DELG 900
C                                                                       DELG 910
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN RIGHT HAND SIDE R      DELG 920
      DO 8 L=K,NM,M                                                     DELG 930
      LL=L+I                                                            DELG 940
      TB=PIVI*R(LL)                                                     DELG 950
      R(LL)=R(L)                                                        DELG 960
    8 R(L)=TB                                                           DELG 970
C                                                                       DELG 980
C     IS ELIMINATION TERMINATED                                         DELG 990
      IF(K-M)9,18,18                                                    DELG1000
C                                                                       DELG1010
C     COLUMN INTERCHANGE IN MATRIX A                                    DELG1020
    9 LEND=LST+M-K                                                      DELG1030
      IF(J)12,12,10                                                     DELG1040
   10 II=J*M                                                            DELG1050
      DO 11 L=LST,LEND                                                  DELG1060
      TB=A(L)                                                           DELG1070
      LL=L+II                                                           DELG1080
      A(L)=A(LL)                                                        DELG1090
   11 A(LL)=TB                                                          DELG1100
C                                                                       DELG1110
C     ROW INTERCHANGE AND PIVOT ROW REDUCTION IN MATRIX A               DELG1120
   12 DO 13 L=LST,MM,M                                                  DELG1130
      LL=L+I                                                            DELG1140
      TB=PIVI*A(LL)                                                     DELG1150
      A(LL)=A(L)                                                        DELG1160
   13 A(L)=TB                                                           DELG1170
C                                                                       DELG1180
C     SAVE COLUMN INTERCHANGE INFORMATION                               DELG1190
      A(LST)=J                                                          DELG1200
C                                                                       DELG1210
C     ELEMENT REDUCTION AND NEXT PIVOT SEARCH                           DELG1220
      PIV=0.D0                                                          DELG1230
      LST=LST+1                                                         DELG1240
      J=0                                                               DELG1250
      DO 16 II=LST,LEND                                                 DELG1260
      PIVI=-A(II)                                                       DELG1270
      IST=II+M                                                          DELG1280
      J=J+1                                                             DELG1290
      DO 15 L=IST,MM,M                                                  DELG1300
      LL=L-J                                                            DELG1310
      A(L)=A(L)+PIVI*A(LL)                                              DELG1320
      TB=DABS(A(L))                                                     DELG1330
      IF(TB-PIV)15,15,14                                                DELG1340
   14 PIV=TB                                                            DELG1350
      I=L                                                               DELG1360
   15 CONTINUE                                                          DELG1370
      DO 16 L=K,NM,M                                                    DELG1380
      LL=L+J                                                            DELG1390
   16 R(LL)=R(LL)+PIVI*R(L)                                             DELG1400
   17 LST=LST+M                                                         DELG1410
C     END OF ELIMINATION LOOP                                           DELG1420
C                                                                       DELG1430
C                                                                       DELG1440
C     BACK SUBSTITUTION AND BACK INTERCHANGE                            DELG1450
   18 IF(M-1)23,22,19                                                   DELG1460
   19 IST=MM+M                                                          DELG1470
      LST=M+1                                                           DELG1480
      DO 21 I=2,M                                                       DELG1490
      II=LST-I                                                          DELG1500
      IST=IST-LST                                                       DELG1510
      L=IST-M                                                           DELG1520
      L=A(L)+.5                                                         DELG1530
      DO 21 J=II,NM,M                                                   DELG1540
      TB=R(J)                                                           DELG1550
      LL=L                                                              DELG1560
      DO 20 K=IST,MM,M                                                  DELG1570
      LL=LL+1                                                           DELG1580
   20 TB=TB-A(K)*R(LL)                                                  DELG1590
      K=J+L                                                             DELG1600
      R(J)=R(K)                                                         DELG1610
   21 R(K)=TB                                                           DELG1620
   22 RETURN                                                            DELG1630
C                                                                       DELG1640
C                                                                       DELG1650
C     ERROR RETURN                                                      DELG1660
   23 IER=-1                                                            DELG1670
      RETURN                                                            DELG1680
      END                                                               DELG1690
```

```
      DO 15 L=1ST,KK,M                                                  DELG1370
      LL=L-J                                                            DELG1380
      A(L)=A(L)*PIVI*A(LL)                                              DELG1390
      TB=DABS(A(L))                                                     DELG1400
      IF(TB-PIVI)15,15,14                                               DELG1410
   14 PIV=TB                                                            DELG1420
      I=L                                                               DELG1430
   15 CONTINUE                                                          DELG1440
      DO 16 L=K,NM,M                                                    DELG1450
      LL=L+J                                                            DELG1460
   16 R(LL)=R(LL)-PIVI*R(L)                                             DELG1470
   17 1ST=1ST+M                                                         DELG1480
C     END OF ELIMINATION LOOP                                           DELG1490
C                                                                       DELG1500
C                                                                       DELG1510
C     BACK SUBSTITUTION AND BACK INTERCHANGE                            DELG1520
   18 IF(Y-1)23,22,19                                                   DELG1530
   19 1ST=NM+M                                                          DELG1540
      LST=M+1                                                           DELG1550
      DO 21 I=2,M                                                       DELG1560
      II=LST-1                                                          DELG1570
      ISF=ISF-LST                                                       DELG1580
      L=1ST-M                                                           DELG1590
      L=A(L)+.001                                                       DELG1600
      DO 21 J=II,NM,M                                                   DELG1610
      TB=R(J)                                                           DELG1620
      LL=J                                                              DELG1630
      DO 20 K=1ST,MM,M                                                  DELG1640
      LL=LL+1                                                           DELG1650
   20 TB=TB-A(K)*R(LL)                                                  DELG1660
      K=J+L                                                             DELG1670
      R(J)=R(K)                                                         DELG1680
   21 R(K)=TB                                                           DELG1690
   22 RETURN                                                            DELG1700
C                                                                       DELG1710
C                                                                       DELG1720
C     ERROR RETURN                                                      DELG1730
   23 IER=-1                                                            DELG1740
      RETURN                                                            DELG1750
      END                                                               DELG1760
```

Subroutine RSLMC

This subroutine computes an approximate solution to a system of linear equations when the coefficient matrix has been factored into a product of two triangular matrices.

1. Mathematical background

Consider a system of linear equations

$$Ax = b \tag{1}$$

having a nonsingular coefficient matrix A. There exists a permutation P such that PA = LU, where L is lower triangular with unit diagonal, and U is upper triangular. Putting c = Pb we see that (1) is equivalent to the system

$$\begin{aligned} Ux &= y \\ Ly &= c \end{aligned} \tag{2}$$

Let $x^{(p)}$ be a trial solution of the given system. It can be improved by means of the iterative process

$$\begin{aligned} r^{(p)} &= b - Ax^{(p)} \\ Ad^{(p)} &= r^{(p)} \\ x^{(p+1)} &= x^{(p)} + d^{(p)} \end{aligned} \tag{3}$$

where the correction vector $d^{(p)}$ is computed using L and U as in (2).

If A is not too ill-conditioned, this process will give a satisfactory solution, provided that $r^{(p)}$, the residual vector, is computed with sufficient accuracy.

2. Programming considerations

This routine may be used to solve a nonsingular system of linear equations whose coefficient matrix has been factored by means of subroutine FACTR.

Let $\epsilon > 0$ be a relative precision parameter (input to RSLMC). In the following discussion we use the notation $\|x\| = \Sigma |x_i|$. The process (3) is applied to the system (1) starting with $x^{(0)} = 0$, and is stopped when one of the following situations occurs:

a. *IER = 0. The components of the correction* vector $d^{(p)}$ satisfy the inequalities

$$\left| d_i^{(p)} \right| \leq \epsilon \left| x_i^{(p)} \right| \qquad i = 1, 2, \ldots, n. \tag{4}$$

Then $x = x^{(p)}$ is returned as the solution.

b. Assume that $p > 1$, for some i the inequality (4) fails and

$$\left\| d^{(k)} \right\| \leq \frac{1}{2} \left\| d^{(k-1)} \right\| \qquad k = 1, 2, \ldots, p-1$$

$$\left\| d^{(p)} \right\| > \frac{1}{2} \left\| d^{(p-1)} \right\|$$

Then:

IER = 1 if $\left\| d^{(p)} \right\| \leq \epsilon \left\| x^{(p)} \right\|$,

IER = 2 if $\left\| d^{(p)} \right\| > \epsilon \left\| x^{(p)} \right\|$.

c. IER = 3. $\left\| d^{(1)} \right\| > \frac{1}{2} \left\| d^{(0)} \right\|$. In this case the trial solution is too far from the exact solution and the process cannot converge. In general this happens when A is badly ill-conditioned.

IER = 4. U is singular.

In all cases $x = x^{(p)}$ is returned.

Note: To obtain accuracy in the computation of the residual vector, each component is computed in double-precision arithmetic.

For reference see:

(1) H. J. Bowdler, R. S. Martin, G. Peters and J. H. Wilkinson, "Solution of Real and Complex Systems of Linear Equations", Numerische Mathematik, vol. 8, no. 3, 1966.

(2) J. H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.


```
C                                                                       RSLM  10
C     ..................................................................RSLM  20
C                                                                       RSLM  30
C       SUBROUTINE RSLMC                                                RSLM  40
C                                                                       RSLM  50
C       PURPOSE                                                         RSLM  60
C          SOLUTION OF A SYSTEM OF LINEAR EQUATIONS AX=B                RSLM  70
C                                                                       RSLM  80
C       USAGE                                                           RSLM  90
C          CALL RSLMC(A,AF,B,X,N,EPSI,IER,IA,V,PER)                     RSLM 100
C                                                                       RSLM 110
C       DESCRIPTION OF PARAMETERS                                       RSLM 120
C          A       INPUT MATRIX                                         RSLM 130
C          AF      ARRAY OF THE FACTORIZATION OF THE ORIGINAL MATRIX    RSLM 140
C          B       RIGHT HAND SIDE VECTOR                               RSLM 150
C          X       VECTOR CONTAINING THE SOLUTION ON RETURN             RSLM 160
C          N       ORDER OF THE SYSTEM                                  RSLM 170
C          EPSI    RELATIVE PRECISION INDICATOR(REQUIRED INPUT)         RSLM 180
C          IER     ERROR INDICATOR                                      RSLM 190
C                     =0 IF EACH COMPONENT OF X MEETS THE PRECISION EPSIRSLM 200
C                     =1 IF ONLY THE NORM OF X MEETS THIS PRECISION     RSLM 210
C                     =2 IF THE PRECISION IN THE NORM OF THE COMPUTED   RSLM 220
C                        SOLUTION IS LOWER THAN EPSI                    RSLM 230
C                     =3 IF THE SOLUTION OBTAINED HAS NO MEANING AT ALL RSLM 240
C                     =4 IF A DIAGONAL TERM OF THE UPPER TRIANGULAR     RSLM 250
C                        FACTOR IS ZERO                                 RSLM 260
C          IA      SIZE OF THE FIRST DIMENSION ASSIGNED TO THE ARRAY A  RSLM 270
C                  IN THE CALLING PROGRAM WHEN THE MATRIX IS IN DOUBLE  RSLM 280
C                  SUBSCRIPTED DATA STORAGE MODE.  IA=N WHEN THE MATRIX RSLM 290
C                  IS IN SSP VECTOR STORAGE MODE.                       RSLM 300
C          V       WORKING STORAGE VECTOR                               RSLM 310
C                  DIMENSION OF V MUST BE GREATER THAN OR EQUAL TO N    RSLM 320
C          PER     VECTOR WHERE PERMUTATIONS OF ROWS OF THE MATRIX ARE  RSLM 330
C                  STORED                                               RSLM 340
C                  DIMENSION OF PER MUST BE GREATER THAN OR EQUAL TO N  RSLM 350
C                                                                       RSLM 360
C       REMARKS                                                         RSLM 370
C          THE MATRIX OF THE SYSTEM MAY BE FACTORIZED BY THE SUBROUTINE RSLM 380
C          FACTR IN THE ARRAY AF PRIOR TO ENTRY TO THIS SUBROUTINE.     RSLM 390
C          THE LOWER TRIANGULAR FACTOR MUST HAVE AN UNIT DIAGONAL.      RSLM 400
C          EPSI IS MODIFIED WHEN IER=2                                  RSLM 410
C                                                                       RSLM 420
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   RSLM 430
C          NONE                                                         RSLM 440
C                                                                       RSLM 450
C       METHOD                                                          RSLM 460
C          A TRIAL SOLUTION IS FIRST COMPUTED.  THEN CORRECTIONS ARE    RSLM 470
C          CALCULATED FROM RESIDUAL VECTORS.                            RSLM 480
C                                                                       RSLM 490
C       REFERENCES                                                      RSLM 500
C          J. H. WILKINSON - THE ALGEBRAIC EIGENVALUE PROBLEM -         RSLM 510
C          CLARENDON PRESS OXFORD, 1965.  H. J. BOWDLER, R. S. MARTIN,  RSLM 520
C          G. PETERS, AND J. H. WILKINSON.  'SOLUTION OF REAL AND       RSLM 530
C          COMPLEX SYSTEMS OF LINEAR EQUATIONS', NUMERISCHE MATHEMATIK, RSLM 540
C          VOL. 8, NO. 3, 1966, 217-234.                                RSLM 550
C                                                                       RSLM 560
C     ..................................................................RSLM 570
C                                                                       RSLM 580
      SUBROUTINE RSLMC (A,AF,B,X,N,EPSI,IER,IA,V,PER)                   RSLM 590
      DIMENSION A(1),AF(1),B(1),X(1),V(1),PER(1)                        RSLM 600
      DOUBLE PRECISION DP                                               RSLM 610
C                                                                       RSLM 620
C        INITIALIZATION                                                 RSLM 630
C                                                                       RSLM 640
      D0=0.                                                             RSLM 650
      IEP=0                                                             RSLM 660
      ITE=0                                                             RSLM 670
      DO 10 I=1,N                                                       RSLM 680
      V(I)=B(I)                                                         RSLM 690
   10 X(I)=0.                                                           RSLM 700
   20 ITE=ITE+1                                                         RSLM 710
C                                                                       RSLM 720
C        THE PERMUTATIONS OF ROWS OF A ARE APPLIED TO V                 RSLM 730
C                                                                       RSLM 740
      DO 30 I=1,N                                                       RSLM 750
      K=PER(I)                                                          RSLM 760
      IF (K-I)25,30,25                                                  RSLM 770
   25 D1=V(K)                                                           RSLM 780
      V(K)=V(I)                                                         RSLM 790
      V(I)=D1                                                           RSLM 800
   30 CONTINUE                                                          RSLM 810
C                                                                       RSLM 820
C        SOLUTION OF THE LOWER TRIANGULAR SYSTEM                        RSLM 830
C                                                                       RSLM 840
      DO 50 I=2,N                                                       RSLM 850
      IM1=I-1                                                           RSLM 860
      DP=V(I)                                                           RSLM 870
      IK=I                                                              RSLM 880
      DO 40 K=1,IM1                                                     RSLM 890
      DP=DP-1.D0*AF(IK)*V(K)                                            RSLM 900
   40 IK=IK+IA                                                          RSLM 910
   50 V(I)=DP                                                           RSLM 920
C                                                                       RSLM 930
C        SOLUTION OF THE UPPER TRIANGULAR SYSTEM                        RSLM 940
C                                                                       RSLM 950
      IF(AF(IK)) 58,54,58                                               RSLM 960
   54 IEP=4                                                             RSLM 970
      GO TO 82                                                          RSLM 980
   58 V(N)=DP/AF(IK)                                                    RSLM 990
      DO 70 I=2,N                                                       RSLM1000
      IM1=N-I+1                                                         RSLM1010
      INF=IM1+1                                                         RSLM1020
      DP=V(IM1)                                                         RSLM1030
      IK=(IM1-1)*IA+IM1                                                 RSLM1040
      D1=AF(IK)                                                         RSLM1050
      DO 60 K=INF,N                                                     RSLM1060
      IK=IK+IA                                                          RSLM1070
   60 DP=DP-1.D0*AF(IK)*V(K)                                            RSLM1080
   70 V(IM1)=DP/D1                                                      RSLM1090
C                                                                       RSLM1100
C        TEST OF PRECISION                                              RSLM1110
C                                                                       RSLM1120
      D1=0.                                                             RSLM1130
      D2=0.                                                             RSLM1140
      KLE=0                                                             RSLM1150
      DO 80 I=1,N                                                       RSLM1160
      D1=D1+ABS(V(I))                                                   RSLM1170
      D2=D2+ABS(X(I))                                                   RSLM1180
      IF (ABS(V(I)-EPSI*ABS(X(I)))) 80,80,75                            RSLM1190
   75 KLE=1                                                             RSLM1200
   80 CONTINUE                                                          RSLM1210
      IF (KLE)140,82,85                                                 RSLM1220
   82 RETURN                                                            RSLM1230
   85 IF (ITE-11)140,90,87                                              RSLM1240
C                                                                       RSLM1250
C        ITERATIONS ARE STOPPED WHEN THE NORM OF THE CORRECTION IS MORE RSLM1260
C        THAN HALF OF THE ONE OF THE FORMER                             RSLM1270
C                                                                       RSLM1280
   87 IF (D0-2.*D1)120,90,90                                            RSLM1290
   90 DO 95 I=1,N                                                       RSLM1300
   95 X(I)=X(I)+V(I)                                                    RSLM1310
      DO 110 I=1,N                                                      RSLM1320
      DP=B(I)                                                           RSLM1330
      IK=I                                                              RSLM1340
      DO 100 K=1,N                                                      RSLM1350
      DP=DP-1.D0*AF(IK)*X(K)                                            RSLM1360
  100 IK=IK+IA                                                          RSLM1370
  110 V(I)=DP                                                           RSLM1380
      D0=D1                                                             RSLM1390
      GO TO 20                                                          RSLM1400
  120 IF(ITE-2)130,130,125                                              RSLM1410
  125 IF (D1-EPSI*D2)127,127,130                                        RSLM1420
  127 IER=1                                                             RSLM1430
      RETURN                                                            RSLM1440
  130 IER=2                                                             RSLM1450
      EPSI=D1/D2                                                        RSLM1460
      RETURN                                                            RSLM1470
  140 IER=3                                                             RSLM1480
      RETURN                                                            RSLM1490
      END                                                               RSLM1500
```

Subroutine FACTR

This subroutine determines a decomposition of a real nonsingular matrix as a product of a lower triangular matrix with unit diagonal and an upper triangular matrix.

1. Mathematical background

Let A be a real nonsingular matrix of order n. In general, A can be factored into a product of the form A = L U, where L is lower triangular with unit diagonal and U is upper triangular.

The elements of L and U may be computed recursively as follows:

$$\bar{a}_{ip} = a_{ip} - \sum_{k=1}^{p-1} l_{ik} u_{kp} \qquad i=p, p+1, \ldots, n$$

$$l_{ip} = \bar{a}_{ip} / \bar{a}_{pp} \qquad i=p, p+1, \ldots, n$$

$$u_{pp} = \bar{a}_{pp}$$

$$u_{pj} = a_{pj} - \sum_{k=1}^{p-1} l_{pk} u_{kj} \qquad j=p+1, p+2, \ldots, n$$

Using these formulas for $p = 1, 2, \ldots, n$, the decomposition can be carried out in n stages.

2. Programming considerations

Even if A is nonsingular and well-conditioned, the above process can fail when a leading principal submatrix of A is singular; furthermore, the process is numerically unstable whenever a leading principal submatrix is ill-conditioned.

In order to avoid these inconveniences, a technique of partial pivoting combined with an equilibration of the matrix has been built into the algorithm.

Initially, the maximum norm of each row vector is computed:

$$N_p = \max_j \left| a_{pj} \right| \qquad p=1, 2, \ldots, n$$

If any $N_p = 0$, the error parameter IER is set to 3 and further calculations are bypassed. Otherwise the reciprocals $1/N_p$ are computed and stored in the vector PER.

Then, assuming that the first p-1 columns of L and p-1 rows of U have been computed, the p^{th} stage of the factorization process is:

a. Computation of the $\bar{a}_{ip}$.

$$\bar{a}_{ip} = a_{ip} - \sum_{k=1}^{p-1} l_{ik} u_{kp} \qquad i=p, p+1, \ldots, n$$

Each term $\bar{a}_{ip}$ replaces the corresponding term of A in storage.

b. Equilibrated partial pivoting.

Let m be the smallest row subscript such that

$$(1/N_p) \left| \bar{a}_{mp} \right| = \max_{i \geq p} \left\{ (1/N_i) \left| \bar{a}_{ip} \right| \right\}$$

If $\bar{a}_{mp} = 0$, the error message IER = 3 is given and further calculations are bypassed. If $\bar{a}_{mp} \neq 0$, the m^{th} and p^{th} rows of A are interchanged, PER(p) is moved to PER(m), and the number m is stored in PER(p). Thus the first p positions of PER contain the information on the permutations needed so far in the form of a transposition vector.

c. Computation of the p^{th} column of L.

$$l_{ip} = \bar{a}_{ip} / \bar{a}_{pp} \qquad i=p+1, p+2, \ldots, n$$

These terms of L replace the corresponding terms of A in storage. The diagonal terms of L, which are all equal to 1, are not stored.

d. Computation of the p^{th} row of U

$$u_{pp} = \bar{a}_{pp}$$

$$u_{pj} = a_{pj} - \sum_{k=1}^{p-1} l_{pk} u_{kj} \qquad j=p+1, \ldots, n$$

These terms replace the corresponding terms of A.

Note: Double-precision arithmetic is used to compute the inner products needed in steps (1) and (4).

For reference see:

(1) H.J. Bowdler, R.S. Martin, G. Peters, and J.H. Wilkinson, "Solution of Real and Complex Systems of Linear Equations", Numerische Mathematik, vol. 8, no. 3, 1966.

(2) J.H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.

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C                                                                       FCTR  10
C     ...................................................................FCTR  20
C                                                                       FCTR  30
C        SUBROUTINE FACTR                                               FCTR  40
C                                                                       FCTR  50
C        PURPOSE                                                        FCTR  60
C           FACTORIZATION OF THE MATRIX A INTO A PRODUCT OF A LOWER     FCTR  70
C           TRIANGULAR MATRIX L AND AN UPPER TRIANGULAR MATRIX U.  L HASFCTR  80
C           UNIT DIAGONAL WHICH IS NOT STORED.                          FCTR  90
C                                                                       FCTR 100
C        USAGE                                                          FCTR 110
C           CALL FACTR(A,PER,N,IA,IER)                                  FCTR 120
C                                                                       FCTR 130
C        DESCRIPTION OF PARAMETERS                                      FCTR 140
C           A      MATRIX A                                             FCTR 150
C           PER    ONE DIMENSIONAL ARRAY WHERE PERMUTATIONS OF ROWS OF  FCTR 160
C                  THE MATRIX ARE STORED                                FCTR 170
C                  DIMENSION OF PER MUST BE GREATER THAN OR EQUAL TO N  FCTR 180
C           N      ORDER OF THE MATRIX A                                FCTR 190
C           IA     SIZE OF THE FIRST DIMENSION ASSIGNED TO THE ARRAY A  FCTR 200
C                  IN THE CALLING PROGRAM WHEN THE MATRIX IS IN DOUBLE  FCTR 210
C                  SUBSCRIPTED DATA STORAGE MODE.  IA=N WHEN THE MATRIX FCTR 220
C                  IS IN SSP VECTOR STORAGE MODE.                       FCTR 230
C           IER    ERROR INDICATOR WHICH IS ZERO IF THERE IS NO ERROR,  FCTR 240
C                  AND IS THREE IF THE PROCEDURE FAILS.                 FCTR 250
C                                                                       FCTR 260
C        REMARKS                                                        FCTR 270
C           THE ORIGINAL MATRIX, A, IS REPLACED BY THE TRIANGULAR FACTORSFCTR 280
C                                                                       FCTR 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FCTR 300
C           NONE                                                        FCTR 310
C                                                                       FCTR 320
C        METHOD                                                         FCTR 330
C           SUCCESSIVE COMPUTATION OF THE COLUMNS OF L AND THE          FCTR 340
C           CORRESPONDING ROWS OF U.                                    FCTR 350
C                                                                       FCTR 360
C        REFERENCES                                                     FCTR 370
C           J. H. WILKINSON - THE ALGEBRAIC EIGENVALUE PROBLEM -        FCTR 380
C           CLARENDON PRESS, OXFORD, 1965. F. J. BOWDLER, R. S. MARTIN, FCTR 390
C           G. PETERS, AND J. H. WILKINSON - 'SOLUTION OF REAL AND      FCTR 400
C           COMPLEX SYSTEMS OF LINEAR EQUATIONS', NUMERISCHE MATHEMATIK,FCTR 410
C           VOL. 8, NO. 3, 1966, P. 217-234.                            FCTR 420
C                                                                       FCTR 430
C     ...................................................................FCTR 440
C                                                                       FCTR 450
      SUBROUTINE FACTR(A,PER,N,IA,IER)                                  FCTR 460
      DIMENSION A(1),PER(1)                                             FCTR 470
      DOUBLE PRECISION DP                                               FCTR 480
C                                                                       FCTR 490
C        COMPUTATION OF WEIGHTS FOR EQUILIBRATION                       FCTR 500
C                                                                       FCTR 510
      DO 2C I=1,N                                                       FCTR 520
      X=0.                                                              FCTR 530
      IJ=I                                                              FCTR 540
      DO 1C J=1,N                                                       FCTR 550
      IF (ABS(A(IJ))-X)1C,1C,5                                          FCTR 560
    5 X=ABS(A(IJ))                                                      FCTR 570
    1C IJ=IJ+IA                                                         FCTR 580
      IF (X) 11C,11C,2C                                                 FCTR 590
    2C PER(I)=1./X                                                      FCTR 600
      IC=0                                                              FCTR 610
      DO 1CC I=1,N                                                      FCTR 620
      IP1=I-1                                                           FCTR 630
      IF1=I+1                                                           FCTR 640
      IFIVCT=I                                                          FCTR 650
      X=0.                                                              FCTR 660
C                                                                       FCTR 670
C        COMPUTATION OF THE ITH COLUMN OF L                             FCTR 680
C                                                                       FCTR 690
      DO 5C K=1,N                                                       FCTR 700
      KI=IC+K                                                           FCTR 710
      DP=A(KI)                                                          FCTR 720
      IF (I-1) 11C,4C,25                                                FCTR 730
   25 KJ=K                                                              FCTR 740
      DO 3C J=1,IP1                                                     FCTR 750
      IJ=IC+J                                                           FCTR 760
      DP=DP-DBLE(A(KJ))*A(IJ)                                           FCTR 770
    3C KJ=KJ+IA                                                         FCTR 780
      A(KI)=DP                                                          FCTR 790
C                                                                       FCTR 800
C        SEARCH FOR EQUILIBRATED PIVOT                                  FCTR 810
C                                                                       FCTR 820
    4C IF (X-ABS(DP)*PER(K))45,50,50                                    FCTR 830
   45 IFIVCT=K                                                          FCTR 840
      X=ABS(DP)*PER(K)                                                  FCTR 850
   50 CONTINUE                                                          FCTR 860
      IF (X)11C,11C,55                                                  FCTR 870
C                                                                       FCTR 880
C        PERMUTATION OF ROWS IF REQUIRED                                FCTR 890
C                                                                       FCTR 900
   55 IF (IFIVCT-I) 11C,7C,57                                           FCTR 910
   57 KI=IFIVCT                                                         FCTR 920
      IJ=I                                                              FCTR 930
      DO 6C J=1,N                                                       FCTR 940
      X=A(IJ)                                                           FCTR 950
      A(IJ)=A(KI)                                                       FCTR 960
      A(KI)=X                                                           FCTR 970
      KI=KI+IA                                                          FCTR 980
    6C IJ=IJ+IA                                                        FCTR 990
      PER(IFIVCT)=PER(I)                                               FCTR1000
    7C PER(I)=IFIVCT                                                   FCTR1010
      IF (I-N) 72,1CC,1CC                                              FCTR1020
    72 IJ=IC+I                                                         FCTR1030
      X=A(IJ)                                                          FCTR1040
C                                                                      FCTR1050
C        COMPUTATION OF THE ITH ROW OF U                               FCTR1060
C                                                                      FCTR1070
      KC=IC+IA                                                         FCTR1080
      DO 9C K=IF1,N                                                    FCTR1090
      KI=IC+K                                                          FCTR1100
      A(KI)=A(KI)/X                                                    FCTR1110
      IF (I-1)11C,9C,75                                                FCTR1120
   75 IJ=I                                                             FCTR1130
      KI=KC+I                                                          FCTR1140
      DP=A(KI)                                                         FCTR1150
      DO 8C J=1,IP1                                                    FCTR1160
      KJ=KC+J                                                          FCTR1170
      DP=DP-DBLE(A(IJ))*A(KJ)                                          FCTR1180
    8C IJ=IJ+IA                                                       FCTR1190
      A(KI)=DP                                                         FCTR1200
    9C KC=KC+IA                                                        FCTR1210
  1CC IC=IC+IA                                                         FCTR1220
      IER=0                                                            FCTR1230
      RETURN                                                           FCTR1240
  11C IER=3                                                            FCTR1250
      RETURN                                                           FCTR1260
      END                                                              FCTR1270
```

Subroutines MFGR and DMFGR

The following calculations are performed for a general rectangular matrix:

1. Determine rank and linearly independent rows and columns of a given matrix.
2. Express a submatrix of maximal rank as product of triangular factors.
3. Express nonbasic rows in terms of basic ones.
4. Express basic variables in terms of free ones.

1. Theoretical background

Calculation (1) is most critical. It is not claimed that MFGR will give the correct rank in all cases, due to the intrinsic difficulty caused by performing calculations with a finite number of digits.

The rank is determined using the standard Gaussian elimination technique with complete pivoting. This implies that the rows and columns of the given m by n matrix A are interchanged at each elimination step if necessary. The interchange information is recorded in two integer permutation vectors IROW and ICOL:

The i^{th} $\left\{\begin{matrix}\text{row}\\\text{column}\end{matrix}\right\}$ of the interchanged matrix corresponds

to the $\left\{\begin{matrix}\text{IROW(I)}^{th}\ \text{row}\\\text{ICOL(I)}^{th}\ \text{column}\end{matrix}\right\}$ in the original matrix A.

Initially IROW(J) = J and ICOL(J) = J.

The notation A^i is used for the interchanged matrix implied at the i^{th} elimination step.†

a. First elimination step

Let a_{jk} be the absolutely greatest element of matrix A, which is found first in a columnwise scan. The internal tolerance TOL is set equal to $|EPS \cdot a_{jk}|$.

If $|a_{jk}| \leq TOL$, further calculation is bypassed. Otherwise rows 1 and j and columns 1 and k of matrix A are interchanged, giving A^1 . The same interchanges must be applied to IROW, interpreted as column vector, and to ICOL, interpreted as row vector.

A^1 is uniquely expressed as product $L^1 \cdot D^1 \cdot U^1$ by imposing the following conditions:

(I) U^1 is the n by n identity matrix except for the first row.

† Superscripts do not mean powers. They merely indicate the number of the elimination step at which the result is obtained.

(II) L^1 is the m by m identity matrix except for the first column. The first diagonal element has a value of one.

(III) D^1 is an m by n matrix with first diagonal element equal to one, while all remaining elements of the first row and column are equal to zero.

Partitioning of matrices A^1, L^1, D^1, U^1 leads to:

$$\begin{pmatrix} a_{11}^1 & A_{12}^1 \\ A_{21}^1 & A_{22}^1 \end{pmatrix} = \begin{pmatrix} 1 & \emptyset \\ L_{21}^1 & I \end{pmatrix} \begin{pmatrix} 1 & \emptyset \\ \emptyset & D_{22}^1 \end{pmatrix} \begin{pmatrix} u_{11}^1 & U_{12}^1 \\ \emptyset & I \end{pmatrix}^{\dagger}$$

or explicitly:

$$a_{11}^1 = u_{11}^1$$

$$A_{12}^1 = U_{12}^1$$

$$A_{21}^1 = L_{21}^1 \cdot u_{11}^1$$

$$A_{22}^1 = L_{21}^1 U_{12}^1 + D_{22}^1$$

This means:

(I) The elements of the first row of U^1 are

$$u_{11}^1 = a_{11}^1,\ u_{12}^1 = a_{12}^1, \ldots,\ u_{1n}^1 = a_{1n}^1$$

(II) The elements of the first column of L^1 are

$$l_{11}^1 = 1,\ l_{21}^1 = a_{21}^1/a_{11}, \ldots,\ l_{m1}^1 = a_{m1}^1/a_{11}^1$$

(III) The elements of submatrix D_{22}^1 of D^1 are

$$d_{ik}^1 = a_{ik}^1 - l_{i1}^1 \cdot u_{1k}^1 = a_{ik}^1 - \frac{a_{i1}^1 \quad a_{1k}^1}{a_{11}^1};$$

$i = 2, \ldots, m$
$k = 2, \ldots, n$

---

† Capital letters are used as notation for matrices or vectors throughout. $\emptyset$ means zero matrix, I means identity matrix; dimensions are implied by compatibility.

Note that it is possible to record all nontrivial entries of L^1, D^1, U^1 in the storage locations occupied by the original A, storing only:

$$\begin{pmatrix} u_{11}^1 & U_{12}^1 \\ L_{21}^1 & D_{22}^1 \end{pmatrix}$$

b. Second elimination step

Let d_{jk}^1, $j \geqq 2$, $k \geqq 2$ be the absolutely largest element of D_{22}^1. If $|d_{jk}^1| \leqq TOL$, D_{22}^1 is interpreted as being the zero matrix.

If D_{22}^1 is not zero in the above sense, it may be decomposed analogously. In the compact scheme,

$$\begin{pmatrix} u_{11}^1 & U_{12}^1 \\ L_{21}^1 & D_{22}^1 \end{pmatrix}$$

rows 2 and j and columns 2 and k are interchanged, obtaining:

$$\begin{pmatrix} u_{11}^1 & U_{12}^2 \\ L_{21}^2 & D_{22}^2 \end{pmatrix}$$

The same interchanges must be performed with IROW (interpreted as column vector), with ICOL (interpreted as row vector), and with A^1 giving result A^2:

$$A^2 = \begin{pmatrix} 1 & \emptyset \\ L_{21}^2 & I \end{pmatrix} \begin{pmatrix} 1 & \emptyset \\ \emptyset & D_{22}^2 \end{pmatrix} \begin{pmatrix} u_{11}^1 & U_{12}^2 \\ \emptyset & I \end{pmatrix}$$

Now D_{22}^2 may be expressed uniquely as the product of the form LDU, imposing conditions I, II, III. The result is:

$$D_{22}^2 = \begin{pmatrix} 1 & \emptyset \\ L_{32}^2 & I \end{pmatrix} \begin{pmatrix} 1 & \emptyset \\ \emptyset & D_{33}^2 \end{pmatrix} \begin{pmatrix} u_{22}^2 & U_{23}^2 \\ \emptyset & I \end{pmatrix}$$

It is easily seen that $A^2 = L^2 D^2 U^2$,

with:
$$L^2 = \begin{pmatrix} 1 & \emptyset & \emptyset \\ l_{21}^2 & 1 & \emptyset \\ L_{31}^2 & L_{32}^2 & I \end{pmatrix}$$

$$D^2 = \begin{pmatrix} 1 & 0 & \emptyset \\ 0 & 1 & \emptyset \\ \emptyset & \emptyset & D^2_{33} \end{pmatrix}$$

$$U^2 = \begin{pmatrix} u^1_{11} & u^2_{12} & U^2_{13} \\ 0 & u^2_{22} & U^2_{23} \\ \emptyset & \emptyset & I \end{pmatrix}$$

where $L^2_{21} = \begin{pmatrix} l^2_{21} \\ L^2_{31} \end{pmatrix}$, $U^2_{12} = (u^2_{12}, U^2_{13})$

c. Final result of elimination process

At the next elimination step D^2_{33} is factorized, and so on. Now assume that finally $D^r_{r+1,\ r+1}$ equals zero in the sense that all its elements are absolutely less than TOL. This means that A has the rank r, and the end result is the factorization $A^r = L^r D^r U^r$:

$$A^r = \begin{pmatrix} 1 & 0 & \cdots & 0 & \emptyset \\ l^2_{21} & 1 & & 0 & \emptyset \\ \vdots & \vdots & & \vdots & \vdots \\ l^r_{r1} & l^r_{r2} & \cdots & 1 & \emptyset \\ L^r_{r+1,\ 1} & L_{r+1,\ 2} & \cdots & L^r_{r+1,\ r} & I \end{pmatrix} \cdot$$

$$\begin{pmatrix} 1 & 0 \cdots 0 & \emptyset \\ 0 & 1 \cdots 0 & \emptyset \\ \vdots & \vdots & \vdots \\ 0 & 0 \cdots 1 & \emptyset \\ \emptyset & \emptyset \cdots \emptyset & D^r_{r+1,\ r+1} \end{pmatrix} \cdot$$

$$\begin{pmatrix} u^1_{11} & u^2_{12} & \cdots & u^r_{1r} & U^r_{1,\ r+1} \\ 0 & u^2_{22} & \cdots & u^r_{2r} & U^r_{2,\ r+1} \\ \vdots & & & \vdots & \vdots \\ 0 & 0 & \cdots & u^r_{rr} & U^r_{r,\ r+1} \\ \emptyset & \emptyset & \cdots & \emptyset & I \end{pmatrix}$$

Neglecting the small elements in $D^r_{r+1,\ r+1}$ this may be written more compactly as:

$$A^r = \begin{pmatrix} L \\ LR \end{pmatrix} \begin{pmatrix} U, UR \end{pmatrix}$$

with: $$L = \begin{pmatrix} 1 & 0 \cdots 0 \\ l^2_{21} & 1 \quad 0 \\ \vdots & \vdots \\ l^r_{r1} & l^r_{r2} \cdots 1 \end{pmatrix}$$

$$LR = (L^r_{r+1,\ 1},\ L^r_{r+1,\ 2}, \ldots,\ L^r_{r+1,\ r})$$

$$U = \begin{pmatrix} u^1_{11} & u^2_{12} \cdots u^r_{1r} \\ 0 & u^2_{22} \quad \vdots \\ \vdots & \quad\ddots\ \vdots \\ 0 & 0 \quad \cdots u^r_{rr} \end{pmatrix}$$

$$UR = \begin{pmatrix} U^r_{1,\ r+1} \\ U^r_{2,\ r+1} \\ \vdots \\ U^r_{r,\ r+1} \end{pmatrix}$$

L is of dimension r by r and unit lower triangular.
U is of dimension r by r and upper triangular.
LR is of dimension m - r by r; if the given matrix A is row regular (that is, m = r), LR is absent in the final factorization.
UR is of dimension r by n-r; if the given matrix A is column regular (that is, n = r), UR is absent in the final factorization.

d. Further calculations performed

The problem of matrix factorization arises in connection with the solution of systems of equations AX=R. Three different cases must be distinguished:

(1) $r = m = n$
A is nonsingular, and AX=R has a uniquely determined solution.

(2) $r < m$
A is not row regular; solutions of AX = R exist only if the linear combinations among the rows of A are also valid among the rows of R.

(3) $r < n$

A is not column regular; $AX = \emptyset$ has nontrivial solutions.

The cases (2) and (3) may occur combined.

The solution, if it exists, is uniquely determined if r = n; otherwise it contains n - r free parameters. It is quite natural to ask for the linear combinations among the rows of given matrix A and for the linear forms expressing basic variables in terms of free ones. Therefore, instead of LR and UR, matrices C and H are returned, containing linear combinations and homogeneous solutions respectively.

Observe carefully that the calculated factorization belongs to the interchanged matrix A^r. Therefore $A^r X^r = R^r$ is dealt with instead of AX = R, where $\begin{Bmatrix} X^r \\ R^r \end{Bmatrix}$ is obtained from $\begin{Bmatrix} X \\ R \end{Bmatrix}$ using the $\begin{Bmatrix} \text{ICOL(I)}^{th} \\ \text{IROW(J)}^{th} \end{Bmatrix}$ element of $\begin{Bmatrix} X \\ R \end{Bmatrix}$ as $\begin{Bmatrix} I^{th} \\ J^{th} \end{Bmatrix}$ element of $\left\{ \begin{matrix} X^r \\ R^r \end{matrix} \quad ; \quad \begin{matrix} I = 1,\ldots, n \\ J = 1,\ldots, m \end{matrix} \right\}$.

Let X^r, R^r be partitioned into $\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ and $\begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$.

Then:

$$\begin{pmatrix} L \\ LR \end{pmatrix} (U,\ UR) \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$$

or explicitly:

$$L \cdot U \cdot X_1 + L \cdot UR \cdot X_2 = R_1$$
$$LR \cdot U \cdot X_1 + LR \cdot UR \cdot X_2 = R_2$$

Since L and U are nonsingular, this implies:

$$X_1 = U^{-1} \cdot L^{-1} \cdot R_1 - U^{-1} \cdot UR \cdot X_2$$
$$LR \cdot L^{-1} R_1 = R_2$$

For the convenience of the user, LR is replaced by $LR \cdot L^{-1} = C$; UR is replaced by $-U^{-1}\ UR = H$, while L and U remain untouched. Consistency requires that $R_2 = CR_1$, and homogeneous solutions are given by $X_1 = HX_2$. In case of a consistent system of equations $A^r X^r = R^r$, the general solution is $X^r = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ with $X_1 = U^{-1} L^{-1} R_1 + HX_2$, while the values of the free variables contained in X_2 may be chosen arbitrarily.

2. Format of Results

Subroutine MFGR returns matrices L, U, C, H, D in the storage area originally occupied by the input matrix A in the compact scheme shown in Figure 9.

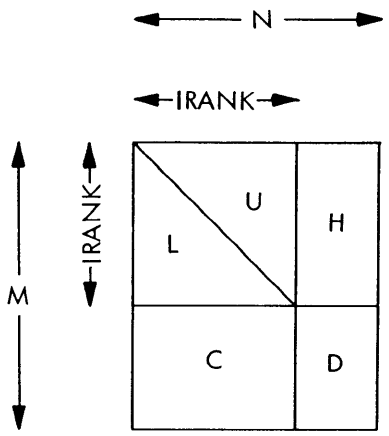

Figure 9. Format scheme (MFGR)

3. Numerical examples

a. Let $A = \begin{pmatrix} 5 & 5 \\ 1 & 1 \end{pmatrix}$, EPS = 1.0E-7

Subroutine MFGR returns as results:

L = (1), U = (5), C = (0.2), H = (-1.0)

combined in the compact scheme:

$$\begin{pmatrix} 5.0 & -1.0 \\ 0.2 & 0.6E\text{-}7 \end{pmatrix} = \left(\begin{array}{c|c} U & H \\ \hline C & D \end{array}\right)$$

IRANK = 1
ICOL = (1, 2)
IROW = (1, 2)

The value 0.6E-7 is obtained instead of the correct value 0, due to roundoff errors.

This example shows that a proper choice of EPS is somewhat greater than 10^{-d}, if d is the number of significant digits in the representation of floating point numbers.

With EPS = 0, MFGR would give the incorrect value of 2 for the rank. The choice EPS = 0 may well result in an incorrect value less than the correct rank, as shown by the following.

If the element a_{22} is slightly decreased, resulting in a matrix A of correct rank equal to 2, then subroutine MFGR gives an incorrect value of 1 for the rank with any choice of the relative tolerance EPS, even with EPS = 0.

b. Let $A = \begin{pmatrix} 1 & 3 & 5 \\ 1 & 3 & 5 \\ 1 & 3 & 1 \\ 1 & 1 & 3 \\ 1 & 3 & 5 \end{pmatrix}$, EPS = 1.0E-7

Subroutine MFGR returns as results:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0.2 & 1 & 0 \\ 0.6 & -0.3333330 & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} 5 & 3 & 1 \\ 0 & 2.4 & 0.8 \\ 0 & 0 & 0.6666664 \end{pmatrix}$$

$$C = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

combined in the compact scheme:

$$\begin{pmatrix} 5 & 3 & 1 \\ 0.2 & 2.4 & 0.8 \\ 0.6 & -0.3333330 & 0.6666664 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} U \\ L \\ C \end{pmatrix}$$

IRANK = 3
ICOL = (3, 2, 1)
IROW = (1, 3, 4, 2, 5)

Linear dependencies among rows:

row (2) = 1 · row (1) + 0 · row (3) + 0 · row (4)
row (5) = 1 · row (1) + 0 · row (3) + 0 · row (4)

$$L \cdot U = \begin{pmatrix} a_{13} & a_{12} & a_{11} \\ a_{33} & a_{32} & a_{31} \\ a_{43} & a_{42} & a_{41} \end{pmatrix} = \begin{pmatrix} 5 & 3 & 1 \\ 1 & 3 & 1 \\ 3 & 1 & 1 \end{pmatrix}$$

c. Let $A = \begin{pmatrix} 1 & 1 & 3 & 3 & 1 \\ 1 & 1 & 3 & 5 & 3 \\ 1 & 3 & 1 & 5 & 5 \end{pmatrix}$, EPS = 1.0E-7

Subroutine MFGR returns as results:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0.6 & 0.2 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 5 & 1 & 3 \\ 0 & 2 & -2 \\ 0 & 0 & 1.6 \end{pmatrix}$$

$$H = \begin{pmatrix} -0.48E-7 & -0.9999992 \\ -0.2499999 & -0.2500009 \\ -0.2499999 & 0.7499991 \end{pmatrix}$$

combined in the compact scheme:

$$\begin{pmatrix} 5 & 1 & 3 & -0.48E-7 & -0.9999992 \\ 1 & 2 & -2 & -0.2499999 & -0.2500009 \\ 0.6 & 0.2 & 1.6 & -0.2499999 & 0.7499991 \end{pmatrix} = \begin{pmatrix} U & H \\ L & \end{pmatrix}$$

IRANK = 3
ICOL = (4, 2, 3, 1, 5)
IROW = (2, 3, 1)

Homogeneous solution of A · X = 0

$$x_4 = -0.48E-7 \cdot x_1 - 0.9999992 \cdot x_5$$
$$x_2 = -0.2499999 \cdot x_1 - 0.2500009 \cdot x_5$$
$$x_3 = -0.2499999 \cdot x_1 + 0.7499991 \cdot x_5$$

x_1 and x_5 may be chosen arbitrarily.

$$L \cdot U = \begin{pmatrix} a_{24} & a_{22} & a_{23} \\ a_{34} & a_{32} & a_{33} \\ a_{14} & a_{12} & a_{13} \end{pmatrix} = \begin{pmatrix} 5 & 1 & 3 \\ 5 & 3 & 1 \\ 3 & 1 & 3 \end{pmatrix}$$

```
C                                                                       MFGR  10
C     ...................................................................MFGR  20
C                                                                       MFGR  30
C        SUBROUTINE MFGR                                                MFGR  40
C                                                                       MFGR  50
C        PURPOSE                                                        MFGR  60
C           FOR A GIVEN M BY N MATRIX THE FOLLOWING CALCULATIONS        MFGR  70
C           ARE PERFORMED                                               MFGR  80
C           (1) DETERMINE RANK AND LINEARLY INDEPENDENT ROWS AND        MFGR  90
C               COLUMNS (BASIS).                                        MFGR 100
C           (2) FACTORIZE A SUBMATRIX OF MAXIMAL RANK.                  MFGR 110
C           (3) EXPRESS NON-BASIC ROWS IN TERMS OF BASIC ONES.          MFGR 120
C           (4) EXPRESS BASIC VARIABLES IN TERMS OF FREE ONES.          MFGR 130
C                                                                       MFGR 140
C        USAGE                                                          MFGR 150
C           CALL MFGR(A,M,N,EPS,IRANK,IROW,ICOL)                        MFGR 160
C                                                                       MFGR 170
C        DESCRIPTION OF PARAMETERS                                      MFGR 180
C           A      - GIVEN MATRIX WITH M ROWS AND N COLUMNS.            MFGR 190
C                    ON RETURN A CONTAINS THE FIVE SUBMATRICES          MFGR 200
C                    L, R, H, 0, S.                                     MFGR 210
C           M      - NUMBER OF ROWS OF MATRIX A.                        MFGR 220
C           N      - NUMBER OF COLUMNS OF MATRIX A.                     MFGR 230
C           EPS    - TEST VALUE FOR ZERO AFFECTED BY ROUNDOFF NOISE.    MFGR 240
C           IRANK  - RESULTANT RANK OF GIVEN MATRIX.                    MFGR 250
C           IROW   - INTEGER VECTOR OF DIMENSION M CONTAINING THE       MFGR 260
C                    SUBSCRIPTS OF BASIC ROWS IN IROW(1),...,IROW(IRANK)MFGR 270
C           ICOL   - INTEGER VECTOR OF DIMENSION N CONTAINING THE       MFGR 280
C                    SUBSCRIPTS OF BASIC COLUMNS IN ICOL(1) UP TO       MFGR 290
C                    ICOL(IRANK).                                       MFGR 300
C                                                                       MFGR 310
C        REMARKS                                                        MFGR 320
C           THE LEFT HAND TRIANGULAR FACTOR IS NORMALIZED SUCH THAT     MFGR 330
C           THE DIAGONAL CONTAINS ALL ONES THUS ALLOWING TO STORE ONLY  MFGR 340
C           THE SUBDIAGONAL PART.                                       MFGR 350
C                                                                       MFGR 360
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MFGR 370
C           NONE                                                        MFGR 380
C                                                                       MFGR 390
C        METHOD                                                         MFGR 400
C           GAUSSIAN ELIMINATION TECHNIQUE IS USED FOR CALCULATION      MFGR 410
C           OF THE TRIANGULAR FACTORS OF A GIVEN MATRIX.                MFGR 420
C           COMPLETE PIVOTING IS BUILT IN.                              MFGR 430
C           IN CASE OF A SINGULAR MATRIX ONLY THE TRIANGULAR FACTORS    MFGR 440
C           OF A SUBMATRIX OF MAXIMAL RANK ARE RETAINED.                MFGR 450
C           THE REMAINING PARTS OF THE RESULTANT MATRIX GIVE THE        MFGR 460
C           DEPENDENCIES OF ROWS AND THE SOLUTION OF THE HOMOGENEOUS    MFGR 470
C           MATRIX EQUATION A*X=0.                                      MFGR 480
C                                                                       MFGR 490
C     ...................................................................MFGR 500
C                                                                       MFGR 510
      SUBROUTINE MFGR(A,M,N,EPS,IRANK,IROW,ICOL)                        MFGR 520
C                                                                       MFGR 530
C        DIMENSIONED DUMMY VARIABLES                                    MFGR 540
      DIMENSION A(1),IROW(1),ICOL(1)                                    MFGR 550
C                                                                       MFGR 560
C        TEST OF SPECIFIED DIMENSIONS                                   MFGR 570
      IF(M)2,2,1                                                        MFGR 580
    1 IF(N)2,2,4                                                        MFGR 590
    2 IRANK=-1                                                          MFGR 600
    3 RETURN                                                            MFGR 610
C        RETURN IN CASE OF FORMAL ERRORS                                MFGR 620
```

```
C                                                                       MFGR 630
C                                                                       MFGR 640
C         INITIALIZE COLUMN INDEX VECTOR                                MFGR 650
C         SEARCH FIRST PIVOT ELEMENT                                    MFGR 660
    4 IRANK=0                                                           MFGR 670
      PIV=0.                                                            MFGR 680
      JJ=0                                                              MFGR 690
      DO 6 J=1,N                                                        MFGR 700
      ICOL(J)=J                                                         MFGR 710
      DO 5 I=1,M                                                        MFGR 720
      JJ=JJ+1                                                           MFGR 730
      HOLD=A(JJ)                                                        MFGR 740
      IF(ABS(PIV)-ABS(HOLD))5,6,6                                       MFGR 750
    5 PIV=HOLD                                                          MFGR 760
      IR=I                                                              MFGR 770
      IC=J                                                              MFGR 780
    6 CONTINUE                                                          MFGR 790
C                                                                       MFGR 800
C         INITIALIZE ROW INDEX VECTOR                                   MFGR 810
      DO 7 I=1,M                                                        MFGR 820
    7 IROW(I)=I                                                         MFGR 830
C                                                                       MFGR 840
C         SET UP INTERNAL TOLERANCE                                     MFGR 850
      TOL=ABS(EPS*PIV)                                                  MFGR 860
C                                                                       MFGR 870
C         INITIALIZE ELIMINATION LOOP                                   MFGR 880
      NM=N*M                                                            MFGR 890
      DO 19 NCOL=M,NM,M                                                 MFGR 900
C                                                                       MFGR 910
C         TEST FOR FEASIBILITY OF PIVOT ELEMENT                         MFGR 920
    8 IF(ABS(PIV)-TOL)20,20,9                                           MFGR 930
C                                                                       MFGR 940
C         UPDATE RANK                                                   MFGR 950
    9 IRANK=IRANK+1                                                     MFGR 960
C                                                                       MFGR 970
C         INTERCHANGE ROWS IF NECESSARY                                 MFGR 980
      JJ=IR-IRANK                                                       MFGR 990
      IF(JJ)12,12,10                                                    MFGR1000
   10 DO 11 J=IRANK,NM,M                                                MFGR1010
      I=J+JJ                                                            MFGR1020
      SAVE=A(J)                                                         MFGR1030
      A(J)=A(I)                                                         MFGR1040
   11 A(I)=SAVE                                                         MFGR1050
C                                                                       MFGR1060
C         UPDATE ROW INDEX VECTOR                                       MFGR1070
      JJ=IROW(IR)                                                       MFGR1080
      IROW(IR)=IROW(IRANK)                                              MFGR1090
      IROW(IRANK)=JJ                                                    MFGR1100
C                                                                       MFGR1110
C         INTERCHANGE COLUMNS IF NECESSARY                              MFGR1120
   12 JJ=(IC-IRANK)*M                                                   MFGR1130
      IF(JJ)15,15,13                                                    MFGR1140
   13 KK=NCOL                                                           MFGR1150
      DO 14 J=1,M                                                       MFGR1160
      I=KK+JJ                                                           MFGR1170
      SAVE=A(KK)                                                        MFGR1180
      A(KK)=A(I)                                                        MFGR1190
      KK=KK-1                                                           MFGR1200
   14 A(I)=SAVE                                                         MFGR1210
C                                                                       MFGR1220
C         UPDATE COLUMN INDEX VECTOR                                    MFGR1230
      JJ=ICOL(IC)                                                       MFGR1240
      ICOL(IC)=ICOL(IRANK)                                              MFGR1250
      ICOL(IRANK)=JJ                                                    MFGR1260
   15 KK=IRANK+1                                                        MFGR1270
      MM=IRANK-M                                                        MFGR1280
      LL=NCOL+MM                                                        MFGR1290
C                                                                       MFGR1300
C         TEST FOR LAST ROW                                             MFGR1310
      IF(MM)16,25,25                                                    MFGR1320
C                                                                       MFGR1330
C         TRANSFORM CURRENT SUBMATRIX AND SEARCH NEXT PIVOT             MFGR1340
   16 JJ=LL                                                             MFGR1350
      SAVE=PIV                                                          MFGR1360
      PIV=0.                                                            MFGR1370
      DO 19 J=KK,M                                                      MFGR1380
      JJ=JJ+1                                                           MFGR1390
      HOLD=A(JJ)/SAVE                                                   MFGR1400
      A(JJ)=HOLD                                                        MFGR1410
      L=J-IRANK                                                         MFGR1420
C                                                                       MFGR1430
C         TEST FOR LAST COLUMN                                          MFGR1440
      IF(IRANK-N)17,19,19                                               MFGR1450
   17 II=JJ                                                             MFGR1460
      DO 19 I=KK,M                                                      MFGR1470
      II=II+M                                                           MFGR1480
      MM=II-L                                                           MFGR1490
      A(II)=A(II)-HOLD*A(MM)                                            MFGR1500
      IF(ABS(A(II))-ABS(PIV))19,19,18                                   MFGR1510
   18 PIV=A(II)                                                         MFGR1520
      IR=J                                                              MFGR1530
      IC=I                                                              MFGR1540
   19 CONTINUE                                                          MFGR1550
C                                                                       MFGR1560
C         SET UP MATRIX EXPRESSING ROW DEPENDENCIES                     MFGR1570
   20 IF(IRANK-1)25,25,21                                               MFGR1580
   21 IR=LL                                                             MFGR1590
      DO 24 J=2,IRANK                                                   MFGR1600
      II=J-1                                                            MFGR1610
      IR=IR-M                                                           MFGR1620
      JJ=LL                                                             MFGR1630
      DO 23 I=KK,M                                                      MFGR1640
      HOLD=0.                                                           MFGR1650
      JJ=JJ+1                                                           MFGR1660
      MM=JJ                                                             MFGR1670
      IC=IR                                                             MFGR1680
      DO 22 L=1,II                                                      MFGR1690
      HOLD=HOLD+A(MM)*A(IC)                                             MFGR1700
      IC=IC-1                                                           MFGR1710
   22 MM=MM-M                                                           MFGR1720
   23 A(MM)=A(MM)-HOLD                                                  MFGR1730
   24 CONTINUE                                                          MFGR1740
C                                                                       MFGR1750
C         TEST FOR COLUMN REGULARITY                                    MFGR1760
   25 IF(N-IRANK)3,3,2>                                                 MFGR1770
C                                                                       MFGR1780
C         SET UP MATRIX EXPRESSING BASIC VARIABLES IN TERMS OF FREE     MFGR1790
C         PARAMETERS (HOMOGENEOUS SOLUTION).                            MFGR1800
   26 IR=LL                                                             MFGR1810
      KK=LL+M                                                           MFGR1820
      DO 30 J=1,IRANK                                                   MFGR1830
      DO 29 I=KK,NM,M                                                   MFGR1840
      JJ=IR                                                             MFGR1850
      LL=I                                                              MFGR1860
      HOLD=0.                                                           MFGR1870
      II=J                                                              MFGR1880
   27 II=II-1                                                           MFGR1890
      IF(II)29,29,28                                                    MFGR1900
   28 HOLD=HOLD-A(JJ)*A(LL)                                             MFGR1910
      JJ=JJ-M                                                           MFGR1920
      LL=LL-1                                                           MFGR1930
      GOTO 27                                                           MFGR1940
   29 A(LL)=(HOLD-A(LL))/A(JJ)                                          MFGR1950
   30 IR=IR-1                                                           MFGR1960
      RETURN                                                            MFGR1970
      END                                                               MFGR1980
```

```
C                                                                       DMGR  10
C  ..................................................................   DMGR  20
C                                                                       DMGR  30
C       SUBROUTINE DMFGR                                                DMGR  40
C                                                                       DMGR  50
C       PURPOSE                                                         DMGR  60
C          FOR A GIVEN M BY N MATRIX THE FOLLOWING CALCULATIONS         DMGR  70
C          ARE PERFORMED                                                DMGR  80
C          (1) DETERMINE RANK AND LINEARLY INDEPENDENT ROWS AND         DMGR  90
C              COLUMNS (BASIS).                                         DMGR 100
C          (2) FACTORIZE A SUBMATRIX OF MAXIMAL RANK.                   DMGR 110
C          (3) EXPRESS NON-BASIC ROWS IN TERMS OF BASIC ONES.           DMGR 120
C          (4) EXPRESS BASIC VARIABLES IN TERMS OF FREE ONES.           DMGR 130
C                                                                       DMGR 140
C       USAGE                                                           DMGR 150
C          CALL DMFGR(A,M,N,EPS,IRANK,IROW,ICOL)                        DMGR 160
C                                                                       DMGR 170
C       DESCRIPTION OF PARAMETERS                                       DMGR 180
C          A      - DOUBLE PRECISION GIVEN MATRIX WITH M ROWS           DMGR 190
C                   AND N COLUMNS.                                      DMGR 200
C                   ON RETURN A CONTAINS THE TRIANGULAR FACTORS         DMGR 210
C                   OF A SUBMATRIX OF MAXIMAL RANK.                     DMGR 220
C          M      - NUMBER OF ROWS OF MATRIX A.                         DMGR 230
C          N      - NUMBER OF COLUMNS OF MATRIX A.                      DMGR 240
C          EPS    - SINGLE PRECISION TESTVALUE FOR ZERO AFFECTED BY     DMGR 250
C                   ROUNDOFF NOISE.                                     DMGR 260
C          IRANK  - RESULTANT RANK OF GIVEN MATRIX.                     DMGR 270
C          IROW   - INTEGER VECTOR OF DIMENSION M CONTAINING THE        DMGR 280
C                   SUBSCRIPTS OF BASIC ROWS IN IROW(1),...,IROW(IRANK) DMGR 290
C          ICOL   - INTEGER VECTOR OF DIMENSION N CONTAINING THE        DMGR 300
C                   SUBSCRIPTS OF BASIC COLUMNS IN ICOL(1) UP TO        DMGR 310
C                   ICOL(IRANK).                                        DMGR 320
C                                                                       DMGR 330
C       REMARKS                                                         DMGR 340
C          THE LEFT HAND TRIANGULAR FACTOR IS NORMALIZED SUCH THAT      DMGR 350
C          THE DIAGONAL CONTAINS ALL ONES THUS ALLOWING TO STORE ONLY   DMGR 360
C          THE SUBDIAGONAL PART.                                        DMGR 370
C                                                                       DMGR 380
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DMGR 390
C          NONE                                                         DMGR 400
C                                                                       DMGR 410
C       METHOD                                                          DMGR 420
C          GAUSSIAN ELIMINATION TECHNIQUE IS USED FOR CALCULATION       DMGR 430
C          OF THE TRIANGULAR FACTORS OF A GIVEN MATRIX.                 DMGR 440
C          COMPLETE PIVOTING IS BUILT IN.                               DMGR 450
C          IN CASE OF A SINGULAR MATRIX ONLY THE TRIANGULAR FACTORS     DMGR 460
C          OF A SUBMATRIX OF MAXIMAL RANK ARE RETAINED.                 DMGR 470
C          THE REMAINING PARTS OF THE RESULTANT MATRIX GIVE THE         DMGR 480
C          DEPENDENCIES OF ROWS AND THE SOLUTION OF THE HOMOGENEOUS     DMGR 490
C          MATRIX EQUATION A*X=0.                                       DMGR 500
C                                                                       DMGR 510
C  ..................................................................   DMGR 520
C                                                                       DMGR 530
      SUBROUTINE DMFGR(A,M,N,EPS,IRANK,IROW,ICOL)                       DMGR 540
C                                                                       DMGR 550
C       DIMENSIONED DUMMY VARIABLES                                     DMGR 560
      DIMENSION A(1),IROW(1),ICOL(1)                                    DMGR 570
      DOUBLE PRECISION A,PIV,HOLD,SAVE                                  DMGR 580
C                                                                       DMGR 590
C       TEST OF SPECIFIED DIMENSIONS                                    DMGR 600
      IF(M)2,2,1                                                        DMGR 610
    1 IF(N)2,2,4                                                        DMGR 620
    2 IRANK=-1                                                          DMGR 630
    3 RETURN                                                            DMGR 640
C       RETURN IN CASE OF FORMAL ERRORS                                 DMGR 650
C                                                                       DMGR 660
C                                                                       DMGR 670
C       INITIALIZE COLUMN INDEX VECTOR                                  DMGR 680
C       SEARCH FIRST PIVOT ELEMENT                                      DMGR 690
    4 IRANK=0                                                           DMGR 700
      PIV=0.D0                                                          DMGR 710
      JJ=0                                                              DMGR 720
      DO 6 J=1,N                                                        DMGR 730
      ICOL(J)=J                                                         DMGR 740
      DO 6 I=1,M                                                        DMGR 750
      JJ=JJ+1                                                           DMGR 760
      HOLD=A(JJ)                                                        DMGR 770
      IF(DABS(PIV)-DABS(HOLD))5,6,6                                     DMGR 780
    5 PIV=HOLD                                                          DMGR 790
      IR=I                                                              DMGR 800
      IC=J                                                              DMGR 810
    6 CONTINUE                                                          DMGR 820
C                                                                       DMGR 830
C       INITIALIZE ROW INDEX VECTOR                                     DMGR 840
      DO 7 I=1,M                                                        DMGR 850
    7 IROW(I)=I                                                         DMGR 860
C                                                                       DMGR 870
C       SET UP INTERNAL TOLERANCE                                       DMGR 880
      TOL=DABS(EPS*SNGL(PIV))                                           DMGR 890
C                                                                       DMGR 900
C       INITIALIZE ELIMINATION LOOP                                     DMGR 910
      NM=N*M                                                            DMGR 920
      DO 19 NCOL=M,NM,M                                                 DMGR 930
C                                                                       DMGR 940
C       TEST FOR FEASIBILITY OF PIVOT ELEMENT                           DMGR 950
    8 IF(DABS(SNGL(PIV))-TOL)20,20,9                                    DMGR 960
C                                                                       DMGR 970
C       UPDATE RANK                                                     DMGR 980
    9 IRANK=IRANK+1                                                     DMGR 990
C                                                                       DMGR1000
C       INTERCHANGE ROWS IF NECESSARY                                   DMGR1010
      JJ=IR-IRANK                                                       DMGR1020
      IF(JJ)12,12,10                                                    DMGR1030
   10 DO 11 J=IRANK,NM,M                                                DMGR1040
      I=J+JJ                                                            DMGR1050
      SAVE=A(J)                                                         DMGR1060
      A(J)=A(I)                                                         DMGR1070
   11 A(I)=SAVE                                                         DMGR1080
C                                                                       DMGR1090
C       UPDATE ROW INDEX VECTOR                                         DMGR1100
      JJ=IROW(IR)                                                       DMGR1110
      IROW(IR)=IROW(IRANK)                                              DMGR1120
      IROW(IRANK)=JJ                                                    DMGR1130
C                                                                       DMGR1140
C       INTERCHANGE COLUMNS IF NECESSARY                                DMGR1150
   12 JJ=(IC-IRANK)*M                                                   DMGR1160
```

```
      IF(JJ)15,15,13                                                    DMGR1170
   13 KK=NCOL                                                           DMGR1180
      DO 14 J=1,M                                                       DMGR1190
      I=KK+JJ                                                           DMGR1200
      SAVE=A(KK)                                                        DMGR1210
      A(KK)=A(I)                                                        DMGR1220
      A(I)=SAVE                                                         DMGR1230
   14 KK=KK-1                                                           DMGR1240
C                                                                       DMGR1250
C        UPDATE COLUMN INDEX VECTOR                                     DMGR1260
      JJ=ICOL(IC)                                                       DMGR1270
      ICOL(IC)=ICOL(IRANK)                                              DMGR1280
      ICOL(IRANK)=JJ                                                    DMGR1290
   15 KK=IRANK+1                                                        DMGR1300
      MM=IRANK-M                                                        DMGR1310
      LL=NCOL+MM                                                        DMGR1320
C                                                                       DMGR1330
C        TEST FOR LAST ROW                                              DMGR1340
      IF(MM)16,25,25                                                    DMGR1350
C                                                                       DMGR1360
C        TRANSFORM CURRENT SUBMATRIX AND SEARCH NEXT PIVOT              DMGR1370
   16 JJ=LL                                                             DMGR1380
      SAVE=PIV                                                          DMGR1390
      PIV=0.0D                                                          DMGR1400
      DO 19 J=KK,M                                                      DMGR1410
      JJ=JJ+1                                                           DMGR1420
      HOLD=A(JJ)/SAVE                                                   DMGR1430
      A(JJ)=HOLD                                                        DMGR1440
      L=J-IRANK                                                         DMGR1450
C                                                                       DMGR1460
C        TEST FOR LAST COLUMN                                           DMGR1470
      IF(IRANK-N)17,19,19                                               DMGR1480
   17 II=JJ                                                             DMGR1490
      DO 19, I=KK,N                                                     DMGR1500
      II=II+M                                                           DMGR1510
      MM=II-L                                                           DMGR1520
      A(II)=A(II)-HOLD*A(MM)                                            DMGR1530
      IF(DABS(A(II))-DABS(PIV))19,19,18                                 DMGR1540
   18 PIV=A(II)                                                         DMGR1550
      IR=I                                                              DMGR1560
      IC=I                                                              DMGR1570
   19 CONTINUE                                                          DMGR1580
C                                                                       DMGR1590
C        SET UP MATRIX EXPRESSING ROW DEPENDENCIES                      DMGR1600
   20 IF(IRANK-1)3,25,21                                                DMGR1610
   21 IR=LL                                                             DMGR1620
      DO 24 J=2,IRANK                                                   DMGR1630
      II=J-1                                                            DMGR1640
      IR=IR-M                                                           DMGR1650
      JJ=LL                                                             DMGR1660
      DO 23 I=KK,M                                                      DMGR1670
      HOLD=0.0D                                                         DMGR1680
      JJ=JJ+1                                                           DMGR1690
      MM=JJ                                                             DMGR1700
      IC=IR                                                             DMGR1710
      DO 22 L=1,II                                                      DMGR1720
      HOLD=HOLD+A(MM)*A(IC)                                             DMGR1730
      IC=IC-1                                                           DMGR1740
   22 MM=MM-M                                                           DMGR1750
   23 A(MM)=A(MM)-HOLD                                                  DMGR1760
   24 CONTINUE                                                          DMGR1770
C                                                                       DMGR1780
C        TEST FOR COLUMN REGULARITY                                     DMGR1790
   25 IF(N-IRANK)3,3,26                                                 DMGR1800
C                                                                       DMGR1810
C        SET UP MATRIX EXPRESSING BASIC VARIABLES IN TERMS OF FREE      DMGR1820
C        PARAMETERS (HOMOGENEOUS SOLUTION).                             DMGR1830
   26 IR=LL                                                             DMGR1840
      KK=LL+M                                                           DMGR1850
      DO 30 J=1,IRANK                                                   DMGR1860
      DO 29 I=KK,MM,M                                                   DMGR1870
      JJ=IR                                                             DMGR1880
      LL=I                                                              DMGR1890
      HOLD=0.0D                                                         DMGR1900
      II=J                                                              DMGR1910
   27 II=II-1                                                           DMGR1920
      IF(II)28,28,28                                                    DMGR1930
   28 HOLD=HOLD-A(JJ)*A(LL)                                             DMGR1940
      JJ=JJ-M                                                           DMGR1950
      LL=LL-1                                                           DMGR1960
      GOTO 27                                                           DMGR1970
   29 A(LL)=(HOLD-A(LL))/A(JJ)                                          DMGR1980
   30 IR=IR-1                                                           DMGR1990
      RETURN                                                            DMGR2000
      END                                                               DMGR2010
```

Subroutines GELS and DGELS

These subroutines solve a system of simultaneous linear equations with symmetric coefficient matrix by Gauss elimination. Consider the system of simultaneous linear equations

$$A * X = R \qquad (1)$$

with symmetric m by m coefficient matrix, the upper triangular part of which is stored by column in m * (m+1)/2 successive storage locations, and an m by n right-hand side matrix R stored by column in m * n successive storage locations. Solution is done by Gauss elimination with pivoting in the main diagonal of matrix A. If matrix R is the identity matrix, solution X is the inverse of matrix A. Solution matrix X is placed in positions of the right-hand side matrix R and is stored by column also. Thus, the computation of the solution requires no extra m by n array of storage. Only an auxiliary storage array named AUX with (m-1) storage locations is necessary.

Explicitly, the given system (1) is of the form:+

$$\begin{pmatrix} \underline{a_{11}} & \underline{a_{12}} & \underline{a_{13}} & \cdots & \underline{a_{1m}} \\ a_{21} & \underline{a_{22}} & \underline{a_{23}} & \cdots & \underline{a_{2m}} \\ a_{31} & a_{32} & \underline{a_{33}} & \cdots & \underline{a_{3m}} \\ a_{m1} & a_{m2} & a_{m3} & \cdots & \underline{a_{mm}} \end{pmatrix} * \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ x_{31} & x_{32} & \cdots & x_{3n} \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{pmatrix}$$

$$= \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ r_{21} & r_{22} & \cdots & r_{2n} \\ r_{31} & r_{32} & \cdots & r_{3n} \\ r_{m1} & r_{m2} & \cdots & r_{mn} \end{pmatrix} \qquad (2)$$

The first step is to search the main diagonal of matrix A for the element of greatest absolute value, say a_{jj}, and to select it as first pivot ($p = a_{jj}$). The reason for pivoting only in the main diagonal of A is that rest-matrices of $A^{(k)}$

+Note that subroutines GELS and DGELS require only the upper triangular part of matrix A; that is, the elements a_{11}; a_{12}, a_{22}; a_{13}, a_{23}, a_{33};...; a_{1m}, a_{2m},..., a_{mm}. These elements are underlined in formula (2).

$(k = 1,2,\ldots,m-1)$ must remain symmetrical during the whole algorithm. With a_{jj}, generate the internal absolute tolerance for testing usefulness of the symmetric algorithm in the following way:

$$\text{tol} = |a_{jj}| \cdot \varepsilon \qquad (3)$$

with a given relative tolerance ε .

Suppose that pivot element a_{jj} is equal to a_{11}. If it is not, interchange the first rows of matrices A and R with the j^{th} and the first column of matrix A with the j^{th}, and save column interchange information by storing the difference (j-1) of pivot column index j and step counter k = 1 [interchanging column 1 with column j means interchanging variables x_{11} with x_{1j} $(1 = 1,2,\ldots,n)$].

Now transform the elements of pivot rows in matrices A and R by division with p, and the other elements by adding $-a_{\nu 1}$ times the new first rows of these two matrices to the other ν rows, thus getting:++

$$a_{11}^{(1)} = \frac{a_{11}}{p} \quad (1 = 1,2,\ldots,m) \qquad (4)$$

$$r_{11}^{(1)} = \frac{r_{11}}{p} \quad (1 = 1,2,\ldots,n) \qquad (5)$$

$$a_{\nu 1}^{(1)} = a_{\nu 1} - a_{\nu 1} \cdot a_{11}^{(1)} \quad \begin{matrix}(1 = 2,3,\ldots,m,\\ \nu = 2,3,\ldots,m)\end{matrix} \qquad (6)$$

$$r_{\nu 1}^{(1)} = r_{\nu 1} - a_{\nu 1} \cdot r_{11}^{(1)} \quad \begin{matrix}(1 = 1,2,\ldots,n;\\ \nu = 2,3,\ldots,m)\end{matrix} \qquad (7)$$

As column interchange information is saved in the first position of the main diagonal, the result of the first step is the two matrices:

$$A^{(1)} = \begin{pmatrix} \underline{(j-1)} & a_{\underline{12}}^{(1)} & a_{\underline{13}}^{(1)} & \cdots & a_{\underline{1m}}^{(1)} \\ 0 & a_{\underline{22}}^{(1)} & a_{\underline{23}}^{(1)} & \cdots & a_{\underline{2m}}^{(1)} \\ 0 & a_{32}^{(1)} & a_{\underline{33}}^{(1)} & \cdots & a_{\underline{3m}}^{(1)} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & a_{m2}^{(1)} & a_{m3}^{(1)} & \cdots & a_{\underline{mm}}^{(1)} \end{pmatrix} \quad \text{and}$$

$$R^{(1)} = \begin{pmatrix} r_{11}^{(1)} & r_{12}^{(1)} & \cdots & r_{1n}^{(1)} \\ r_{21}^{(1)} & r_{22}^{(1)} & \cdots & r_{2n}^{(1)} \\ r_{31}^{(1)} & r_{32}^{(1)} & \cdots & r_{3n}^{(1)} \\ \cdots & \cdots & \cdots & \cdots \\ r_{m1}^{(1)} & r_{m2}^{(1)} & \cdots & r_{mn}^{(1)} \end{pmatrix}$$

It is easily seen from equations (4) - (7) that the rest of matrix $A^{(1)}$ -- that is, matrix $A^{(1)}$ without the first row and first column -- is symmetrical and that actually only the underlined elements must be calculated and stored. Therefore, the range of index 1 in formula (6) reduces to $1 = \nu, \nu+1,\ldots,m$.

Now repeat this procedure m-2 times, starting at each step with the matrix $A^{(k)}$ of the step before without the first k rows and first k columns, and the matrix $R^{(k)}$ without the first k rows. The total result after m-1 steps is the matrices:

$$A^{(m-1)} = \begin{pmatrix} (j_1-1) & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & (j_2-2) & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & (j_3-3) & \cdots & a_{3m}^{(3)} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & (j_m-m) \end{pmatrix} \quad \text{and}$$

$$R^{(m-1)} = \begin{pmatrix} r_{11}^{(1)} & r_{12}^{(1)} & \cdots & r_{1n}^{(1)} \\ r_{21}^{(2)} & r_{22}^{(2)} & \cdots & r_{2n}^{(2)} \\ r_{31}^{(3)} & r_{32}^{(3)} & \cdots & r_{3n}^{(3)} \\ \cdots & \cdots & \cdots & \cdots \\ r_{m1}^{(m)} & r_{m2}^{(m)} & \cdots & r_{mn}^{(m)} \end{pmatrix}$$

++Note that transformation of pivot row in matrix A destroys pivot column, which is, due to symmetry, stored in the same locations. As pivot column is used unchanged for transformation of rest of A and R, it has to be saved in auxiliary array AUX before transforming pivot row.

Now work backward and set:

$$
\left.
\begin{aligned}
r^{(m)}_{m-1,l} &= r^{(m-1)}_{m-1,l} - a^{(m-1)}_{m-1,m} \cdot r^{(m)}_{ml} \quad (l = 1,2,\ldots,n) \\
r^{(m)}_{m-2,l} &= r^{(m-2)}_{m-2,l} - a^{(m-2)}_{m-2,m-1} \cdot r^{(m)}_{m-1,l} \\
&\cdots\cdots\cdots \\
r^{(m)}_{1l} &= r^{(1)}_{1l} - a^{(1)}_{12} \cdot r^{(m)}_{2l} - a^{(1)}_{13} \cdot r^{(m)}_{3l} \\
&\quad - a^{(m-2)}_{m-2,m} \cdot r^{(m)}_{ml} \quad (l = 1,2,\ldots,n) \\
&\quad - \ldots - a^{(1)}_{1m} \cdot r^{(m)}_{ml} \quad (l = 1,2,\ldots,n)
\end{aligned}
\right\} \quad (8)
$$

After each step of back substitution, rows of solution matrix $X = R^{(m)}$ have to be back-interchanged according to interchange information in the corresponding main diagonal element of matrix $A^{(m-1)}$, in order to get the correct sequence of right-hand side column elements corresponding to the sequence of left-hand side row elements.

The only case in which the procedure described above can fail to give a solution occurs when at any step all elements in the main diagonal of the rest-matrix of $A^{(k)}$ become zero, and no pivot element can be found. In this case, the procedure is bypassed and the error message ier = -1 is given. This may -- but does not necessarily -- mean, that matrix A is singular. Possibly subroutines GELG or DGELG (which are working with complete pivoting) will be able to find a solution in cases where subroutines GELS or DGELS fail. Actually, because of rounding errors, a further check of the absolute values of pivot elements is performed by the procedure. If at elimination step k this absolute value becomes less than tol (see equation 3), it is likely that there was loss of significance in the computation of the diagonal elements. But as this may not necessarily be the case, and as this test depends highly on the choice of the relative tolerance ε [+], the procedure gives only the warning ier = k-1, which indicates that there is a possible loss of significance in the results computed by the algorithm.[++] But here it is also possible that subroutines GELG or DGELG will give better results. If there is only one equation to solve (m = 1), the test on loss of significance is suppressed.

[+] For subroutine GELS, a relative tolerance between 10^{-6} and 10^{-7} is suggested; and for subroutine DGELS, between 10^{-14} and 10^{-16}.

[++] For example, $\varepsilon = 10^{-5}$ and warning ier = 3 mean that there is a possible loss of about five or more significant digits in the initial values of elimination step 4.

```
C                                                                       GELS  10
C     ..................................................................GELS  20
C                                                                       GELS  30
C        SUBROUTINE GELS                                                GELS  40
C                                                                       GELS  50
C        PURPOSE                                                        GELS  60
C           TO SOLVE A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH     GELS  70
C           SYMMETRIC COEFFICIENT MATRIX UPPER TRIANGULAR PART OF WHICH GELS  80
C           IS ASSUMED TO BE STORED COLUMNWISE.                         GELS  90
C                                                                       GELS 100
C        USAGE                                                          GELS 110
C           CALL GELS(R,A,M,N,EPS,IER,AUX)                              GELS 120
C                                                                       GELS 130
C        DESCRIPTION OF PARAMETERS                                      GELS 140
C           R      - M BY N RIGHT HAND SIDE MATRIX.  (DESTROYED)        GELS 150
C                    ON RETURN R CONTAINS THE SOLUTION OF THE EQUATIONS.GELS 160
C           A      - UPPER TRIANGULAR PART OF THE SYMMETRIC             GELS 170
C                    M BY M COEFFICIENT MATRIX.  (DESTROYED)            GELS 180
C           M      - THE NUMBER OF EQUATIONS IN THE SYSTEM.             GELS 190
C           N      - THE NUMBER OF RIGHT HAND SIDE VECTORS.             GELS 200
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS RELATIVE        GELS 210
C                    TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.        GELS 220
C           IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS         GELS 230
C                    IER=0  - NO ERROR.                                 GELS 240
C                    IER=-1 - NO RESULT BECAUSE OF M LESS THAN 1 OR     GELS 250
C                             PIVOT ELEMENT AT ANY ELIMINATION STEP     GELS 260
C                             EQUAL TO 0.                               GELS 270
C                    IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-  GELS 280
C                             CANCE INDICATED AT ELIMINATION STEP K+1,  GELS 290
C                             WHERE PIVOT ELEMENT WAS LESS THAN OR      GELS 300
C                             EQUAL TO THE INTERNAL TOLERANCE EPS TIMES GELS 310
C                             ABSOLUTELY GREATEST MAIN DIAGONAL         GELS 320
C                             ELEMENT OF MATRIX A.                      GELS 330
C           AUX    - AN AUXILIARY STORAGE ARRAY WITH DIMENSION M-1.     GELS 340
C                                                                       GELS 350
C        REMARKS                                                        GELS 360
C           UPPER TRIANGULAR PART OF MATRIX A IS ASSUMED TO BE STORED   GELS 370
C           COLUMNWISE IN M*(M+1)/2 SUCCESSIVE STORAGE LOCATIONS. RIGHT GELS 380
C           HAND SIDE MATRIX R COLUMNWISE IN N*M SUCCESSIVE STORAGE     GELS 390
C           LOCATIONS. ON RETURN SOLUTION MATRIX R IS STORED COLUMNWISE GELS 400
C           TOO.                                                        GELS 410
C           THE PROCEDURE GIVES RESULTS IF THE NUMBER OF EQUATIONS M IS GELS 420
C           GREATER THAN 0 AND PIVOT ELEMENTS AT ALL ELIMINATION STEPS  GELS 430
C           ARE DIFFERENT FROM 0. HOWEVER WARNING IER=K - IF GIVEN -    GELS 440
C           INDICATES POSSIBLE LOSS OF SIGNIFICANCE. IN CASE OF A WELL  GELS 450
C           SCALED MATRIX A AND APPROPRIATE TOLERANCE EPS, IER=K MAY BE GELS 460
C           INTERPRETED THAT MATRIX A HAS THE RANK K. NO WARNING IS     GELS 470
C           GIVEN IN CASE M=1.                                          GELS 480
C           ERROR PARAMETER IER=-1 DOES NOT NECESSARILY MEAN THAT       GELS 490
C           MATRIX A IS SINGULAR, AS ONLY MAIN DIAGONAL ELEMENTS        GELS 500
C           ARE USED AS PIVOT ELEMENTS. POSSIBLY SUBROUTINE GELG (WHICH GELS 510
C           WORKS WITH TOTAL PIVOTING) WOULD BE ABLE TO FIND A SOLUTION.GELS 520
C                                                                       GELS 530
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GELS 540
C           NONE                                                        GELS 550
C                                                                       GELS 560
C        METHOD                                                         GELS 570
C           SOLUTION IS DONE BY MEANS OF GAUSS-ELIMINATION WITH         GELS 580
C           PIVOTING IN MAIN DIAGONAL, IN ORDER TO PRESERVE             GELS 590
C           SYMMETRY IN REMAINING COEFFICIENT MATRICES.                 GELS 600
C                                                                       GELS 610
C     ..................................................................GELS 620
C                                                                       GELS 630
      SUBROUTINE GELS(R,A,M,N,EPS,IER,AUX)                              GELS 640
C                                                                       GELS 650
C                                                                       GELS 660
      DIMENSION A(1),R(1),AUX(1)                                        GELS 670
      IF(M)24,24,1                                                      GELS 680
C                                                                       GELS 690
C     SEARCH FOR GREATEST MAIN DIAGONAL ELEMENT                         GELS 700
    1 IER=0                                                             GELS 710
      PIV=0.                                                            GELS 720
      L=0                                                               GELS 730
      DO 3 K=1,M                                                        GELS 740
      L=L+K                                                             GELS 750
      TB=ABS(A(L))                                                      GELS 760
      IF(TB-PIV)3,3,2                                                   GELS 770
    2 PIV=TB                                                            GELS 780
      I=L                                                               GELS 790
      J=K                                                               GELS 800
    3 CONTINUE                                                          GELS 810
      TOL=EPS*PIV                                                       GELS 820
C     MAIN DIAGONAL ELEMENT A(I)=A(J,J) IS FIRST PIVOT ELEMENT.         GELS 830
C     PIV CONTAINS THE ABSOLUTE VALUE OF A(I).                          GELS 840
C                                                                       GELS 850
C                                                                       GELS 860
C     START ELIMINATION LOOP                                            GELS 870
      LST=0                                                             GELS 880
      NM=N*M                                                            GELS 890
      LEND=M-1                                                          GELS 900
      DO 18 K=1,M                                                       GELS 910
C                                                                       GELS 920
C     TEST ON USEFULNESS OF SYMMETRIC ALGORITHM                         GELS 930
      IF(PIV)24,24,4                                                    GELS 940
    4 IF(IER)7,5,7                                                      GELS 950
    5 IF(PIV-TOL)6,6,7                                                  GELS 960
    6 IER=K-1                                                           GELS 970
    7 LI=J-K                                                            GELS 980
      LST=LST+K                                                         GELS 990
C                                                                       GELS1000
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN RIGHT HAND SIDE R      GELS1010
      PIVI=1./A(I)                                                      GELS1020
      DO 8 L=K,NM,M                                                     GELS1030
      LL=L+LI                                                           GELS1040
      TB=PIVI*R(LL)                                                     GELS1050
      R(LL)=R(L)                                                        GELS1060
    8 R(L)=TB                                                           GELS1070
C                                                                       GELS1080
C     IS ELIMINATION TERMINATED                                         GELS1090
      IF(K-M)9,19,19                                                    GELS1100
C                                                                       GELS1110
C     ROW AND COLUMN INTERCHANGE AND PIVOT ROW REDUCTION IN MATRIX A.   GELS1120
C     ELEMENTS OF PIVOT COLUMN ARE SAVED IN AUXILIARY VECTOR AUX.       GELS1130
    9 LR=LST+(LI*(K+J-1))/2                                             GELS1140
      LL=LR                                                             GELS1150
      L=LST                                                             GELS1160
      DO 14 II=K,LEND                                                   GELS1170
      L=L+II                                                            GELS1180
      LL=LL+1                                                           GELS1190
      IF(L-LR)12,10,11                                                  GELS1200
   10 A(LL)=A(LST)                                                      GELS1210
      TB=A(L)                                                           GELS1220
      GO TO 13                                                          GELS1230
   11 LL=L+LI                                                           GELS1240
   12 TB=A(LL)                                                          GELS1250
      A(LL)=A(L)                                                        GELS1260
   13 AUX(II)=TB                                                        GELS1270
   14 A(L)=PIVI*TB                                                      GELS1280
C                                                                       GELS1290
```

```
C     SAVE COLUMN INTERCHANGE INFORMATION                               GELS1330
      A(LST)=LT                                                         GELS1340
C                                                                       GELS1350
C     ELEMENT REDUCTION AND SEARCH FOR NEXT PIVOT                       GELS1360
      PIV=0.                                                            GELS1370
      LLST=LST                                                          GELS1380
      LT=0                                                              GELS1390
      DO 18 II=K,LEND                                                   GELS1400
      PIVI=-AUX(II)                                                     GELS1410
      LL=LLST                                                           GELS1420
      LT=LT+1                                                           GELS1430
      DO 15 LLD=II,LEND                                                 GELS1440
      LL=LL+LLD                                                         GELS1450
      L=LL+LT                                                           GELS1460
   15 A(L)=A(L)+PIVI*A(LL)                                              GELS1470
      LLST=LLST+II                                                      GELS1480
      LR=LLST+LT                                                        GELS1490
      TB=ABS(A(LR))                                                     GELS1500
      IF(TB-PIV)17,17,16                                                GELS1510
   16 PIV=TB                                                            GELS1520
      I=LR                                                              GELS1530
      J=II+1                                                            GELS1540
   17 DO 18 LR=K,NM,M                                                   GELS1550
      LL=LR+LT                                                          GELS1560
   18 R(LL)=R(LL)+PIVI*R(LR)                                            GELS1570
C     END OF ELIMINATION LOOP                                           GELS1580
C                                                                       GELS1590
C                                                                       GELS1600
C     BACK SUBSTITUTION AND BACK INTERCHANGE                            GELS1610
   19 IF(LEND)24,23,20                                                  GELS1620
   20 II=M                                                              GELS1630
      DO 22 I=2,M                                                       GELS1640
      LST=LST-II                                                        GELS1650
      II=II-1                                                           GELS1660
      L=A(LST)+.5                                                       GELS1670
      DO 22 J=II,NM,M                                                   GELS1680
      TB=R(J)                                                           GELS1690
      LL=J                                                              GELS1700
      K=LST                                                             GELS1710
      DO 21 LT=II,LEND                                                  GELS1720
      LL=LL+1                                                           GELS1730
      K=K+LT                                                            GELS1740
   21 TB=TB-A(K)*R(LL)                                                  GELS1750
      K=J+L                                                             GELS1760
      R(J)=R(K)                                                         GELS1770
   22 R(K)=TB                                                           GELS1780
   23 RETURN                                                            GELS1790
C                                                                       GELS1800
C                                                                       GELS1810
C     ERROR RETURN                                                      GELS1820
   24 IER=-1                                                            GELS1830
      RETURN                                                            GELS1840
      END                                                               GELS1850
```

```
C                                                                       DELS  10
C  ***************************************************************      DELS  20
C                                                                       DELS  30
C       SUBROUTINE DGELS                                                DELS  40
C                                                                       DELS  50
C       PURPOSE                                                         DELS  60
C          TO SOLVE A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH      DELS  70
C          SYMMETRIC COEFFICIENT MATRIX UPPER TRIANGULAR PART OF WHICH  DELS  80
C          IS ASSUMED TO BE STORED COLUMNWISE.                          DELS  90
C                                                                       DELS 100
C       USAGE                                                           DELS 110
C          CALL DGELS(R,A,M,N,EPS,IER,AUX)                              DELS 120
C                                                                       DELS 130
C       DESCRIPTION OF PARAMETERS                                       DELS 140
C          R      - DOUBLE PRECISION M BY N RIGHT HAND SIDE MATRIX      DELS 150
C                   (DESTROYED). ON RETURN R CONTAINS THE SOLUTION OF   DELS 160
C                   THE EQUATIONS.                                      DELS 170
C          A      - UPPER TRIANGULAR PART OF THE SYMMETRIC DOUBLE       DELS 180
C                   PRECISION M BY M COEFFICIENT MATRIX.  (DESTROYED)   DELS 190
C          M      - THE NUMBER OF EQUATIONS IN THE SYSTEM.              DELS 200
C          N      - THE NUMBER OF RIGHT HAND SIDE VECTORS.              DELS 210
C          EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS    DELS 220
C                   RELATIVE TOLERANCE FOR TEST ON LOSS OF              DELS 230
C                   SIGNIFICANCE.                                       DELS 240
C          IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS          DELS 250
C                   IER=0  - NO ERROR,                                  DELS 260
C                   IER=-1 - NO RESULT BECAUSE OF M LESS THAN 1 OR      DELS 270
C                            PIVOT ELEMENT AT ANY ELIMINATION STEP      DELS 280
C                            EQUAL TO 0,                                DELS 290
C                   IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-   DELS 300
C                            CANCE INDICATED AT ELIMINATION STEP K+1,   DELS 310
C                            WHERE PIVOT ELEMENT WAS LESS THAN OR       DELS 320
C                            EQUAL TO THE INTERNAL TOLERANCE EPS TIMES  DELS 330
C                            ABSOLUTELY GREATEST MAIN DIAGONAL          DELS 340
C                            ELEMENT OF MATRIX A.                       DELS 350
C          AUX    - DOUBLE PRECISION AUXILIARY STORAGE ARRAY            DELS 360
C                   WITH DIMENSION M-1.                                 DELS 370
C                                                                       DELS 380
C       REMARKS                                                         DELS 390
C          UPPER TRIANGULAR PART OF MATRIX A IS ASSUMED TO BE STORED    DELS 400
C          COLUMNWISE IN M*(M+1)/2 SUCCESSIVE STORAGE LOCATIONS, RIGHT  DELS 410
C          HAND SIDE MATRIX R COLUMNWISE IN N*M SUCCESSIVE STORAGE      DELS 420
C          LOCATIONS. ON RETURN SOLUTION MATRIX R IS STORED COLUMNWISE   DELS 430
C          TOO.                                                         DELS 440
C          THE PROCEDURE GIVES RESULTS IF THE NUMBER OF EQUATIONS M IS  DELS 450
C          GREATER THAN 0 AND PIVOT ELEMENTS AT ALL ELIMINATION STEPS   DELS 460
C          ARE DIFFERENT FROM 0. HOWEVER WARNING IER=K - IF GIVEN -     DELS 470
C          INDICATES POSSIBLE LOSS OF SIGNIFICANCE. IN CASE OF A WELL   DELS 480
C          SCALED MATRIX A AND APPROPRIATE TOLERANCE EPS, IER=K MAY BE  DELS 490
C          INTERPRETED THAT MATRIX A HAS THE RANK K. NO WARNING IS      DELS 500
C          GIVEN IN CASE M=1.                                           DELS 510
C          ERROR PARAMETER IER=-1 DOES NOT NECESSARILY MEAN THAT        DELS 520
C          MATRIX A IS SINGULAR, AS ONLY MAIN DIAGONAL ELEMENTS         DELS 530
C          ARE USED AS PIVOT ELEMENTS. POSSIBLY SUBROUTINE DGELG (WHICH DELS 540
C          WORKS WITH TOTAL PIVOTING) WOULD BE ABLE TO FIND A SOLUTION. DELS 550
C                                                                       DELS 560
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DELS 570
C          NONE                                                         DELS 580
C                                                                       DELS 590
C       METHOD                                                          DELS 600
C          SOLUTION IS DONE BY MEANS OF GAUSS-ELIMINATION WITH          DELS 610
C          PIVOTING IN MAIN DIAGONAL, IN ORDER TO PRESERVE              DELS 620
C          SYMMETRY IN REMAINING COEFFICIENT MATRICES.                  DELS 630
C                                                                       DELS 640
C  ***************************************************************      DELS 650
C                                                                       DELS 660
      SUBROUTINE DGELS(R,A,M,N,EPS,IER,AUX)                             DELS 670
C                                                                       DELS 680
C                                                                       DELS 690
      DIMENSION A(1),R(1),AUX(1)                                        DELS 700
      DOUBLE PRECISION R,A,AUX,PIV,TB,TOL,PIVI                          DELS 710
      IF(M)24,24,1                                                      DELS 720
C                                                                       DELS 730
C     SEARCH FOR GREATEST MAIN DIAGONAL ELEMENT                         DELS 740
    1 IER=0                                                             DELS 750
      PIV=0.D0                                                          DELS 760
      L=0                                                               DELS 770
      DO 3 K=1,M                                                        DELS 780
      L=L+K                                                             DELS 790
      TB=DABS(A(L))                                                     DELS 800
      IF(TB-PIV)3,3,2                                                   DELS 810
    2 PIV=TB                                                            DELS 820
      I=L                                                               DELS 830
      J=K                                                               DELS 840
    3 CONTINUE                                                          DELS 850
      TOL=EPS*PIV                                                       DELS 860
C     MAIN DIAGONAL ELEMENT A(I)=A(J,J) IS FIRST PIVOT ELEMENT.         DELS 870
C     PIV CONTAINS THE ABSOLUTE VALUE OF A(I).                          DELS 880
C                                                                       DELS 890
C                                                                       DELS 900
C     START ELIMINATION LOOP                                            DELS 910
      LST=0                                                             DELS 920
      NM=N*M                                                            DELS 930
      LEND=M-1                                                          DELS 940
      DO 18 K=1,M                                                       DELS 950
C                                                                       DELS 960
C     TEST ON USEFULNESS OF SYMMETRIC ALGORITHM                         DELS 970
      IF(PIV)24,24,4                                                    DELS 980
    4 IF(IER)7,5,7                                                      DELS 990
    5 IF(PIV-TOL)6,6,7                                                  DELS1000
    6 IER=K-1                                                           DELS1010
    7 LT=J-K                                                            DELS1020
      LST=LST+K                                                         DELS1030
C                                                                       DELS1040
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN RIGHT HAND SIDE R      DELS1050
      PIVI=1.D0/A(I)                                                    DELS1060
      DO 9 L=K,NM,M                                                     DELS1070
      LL=L+LT                                                           DELS1080
      TB=PIVI*R(LL)                                                     DELS1090
      R(LL)=R(L)                                                        DELS1100
    9 R(L)=TB                                                           DELS1110
C                                                                       DELS1120
C     IS ELIMINATION TERMINATED                                         DELS1130
      IF(K-M)9,19,19                                                    DELS1140
C                                                                       DELS1150
C     ROW AND COLUMN INTERCHANGE AND PIVOT ROW REDUCTION IN MATRIX A.   DELS1160
C     ELEMENTS OF PIVOT COLUMN ARE SAVED IN AUXILIARY VECTOR AUX.       DELS1170
    9 LR=LST+(LT+(K+J-1))/2                                             DELS1180
      LL=LR                                                             DELS1190
      L=LST                                                             DELS1200
      DO 14 II=K,LEND                                                   DELS1210
      L=L+II                                                            DELS1220
      LL=LL+1                                                           DELS1230
      IF(L-LR)11,10,11                                                  DELS1240
   10 A(L)=A(LST)                                                       DELS1250
      TB=A(L)                                                           DELS1260
      GO TO 13                                                          DELS1270
   11 LL=L+LT                                                           DELS1280
   12 TB=A(LL)                                                          DELS1290
      A(LL)=A(L)                                                        DELS1300
   13 AUX(II)=TB                                                        DELS1310
   14 A(L)=PIVI*TB                                                      DELS1320
C                                                                       DELS1330
C     SAVE COLUMN INTERCHANGE INFORMATION                               DELS1340
      A(LST)=LT                                                         DELS1350
C                                                                       DELS1360
C     ELEMENT REDUCTION AND SEARCH FOR NEXT PIVOT                       DELS1370
      PIV=0.D0                                                          DELS1380
      LLST=LST                                                          DELS1390
      LT=0                                                              DELS1400
      DO 18 II=K,LEND                                                   DELS1410
      PIVI=-AUX(II)                                                     DELS1420
      LL=LLST                                                           DELS1430
      LT=LT+1                                                           DELS1440
      DO 15 LLD=II,LEND                                                 DELS1450
      LL=LL+LLD                                                         DELS1460
      L=LL+LT                                                           DELS1470
   15 A(L)=A(L)+PIVI*A(LL)                                              DELS1480
      LLST=LLST+II                                                      DELS1490
      LR=LLST+LT                                                        DELS1500
      TB=DABS(A(LR))                                                    DELS1510
      IF(TB-PIV)17,17,16                                                DELS1520
   16 PIV=TB                                                            DELS1530
      I=LR                                                              DELS1540
      J=II+1                                                            DELS1550
   17 DO 18 LR=K,NM,M                                                   DELS1560
      LL=LR+LT                                                          DELS1570
   18 R(LL)=R(LL)+PIVI*R(LR)                                            DELS1580
C     END OF ELIMINATION LOOP                                           DELS1590
C                                                                       DELS1600
C                                                                       DELS1610
C     BACK SUBSTITUTION AND BACK INTERCHANGE                            DELS1620
   19 IF(LEND)24,23,20                                                  DELS1630
   20 II=M                                                              DELS1640
      DO 22 I=2,M                                                       DELS1650
      LST=LST-II                                                        DELS1660
      II=II-1                                                           DELS1670
      L=A(LST)+.5D0                                                     DELS1680
      DO 22 J=II,NM,M                                                   DELS1690
      TB=R(J)                                                           DELS1700
      LL=J                                                              DELS1710
      K=LST                                                             DELS1720
      DO 21 LT=II,LEND                                                  DELS1730
      LL=LL+1                                                           DELS1740
      K=K+LT                                                            DELS1750
   21 TB=TB-A(K)*R(LL)                                                  DELS1760
      K=J+L                                                             DELS1770
      R(J)=R(K)                                                         DELS1780
   22 R(K)=TB                                                           DELS1790
   23 RETURN                                                            DELS1800
C                                                                       DELS1810
C                                                                       DELS1820
C     ERROR RETURN                                                      DELS1830
   24 IER=-1                                                            DELS1840
      RETURN                                                            DELS1850
      END                                                               DELS1860
```

Subroutines GELB and DGELB

These subroutines solve a system of simultaneous linear equations with a coefficient matrix of band structure by Gauss elimination. Consider the system of simultaneous linear equations

$$A * X = R \qquad (1)$$

with an m by m coefficient matrix A of band structure and an m by n right-hand side matrix R. Solution is done by means of Gauss elimination with column pivoting in matrix A. If R is the identity matrix, solution X is the inverse of matrix A. Solution matrix X is placed in positions of right-hand side matrix R and is stored in the same way -- that is, columnwise in m*n successive storage locations. Thus, the computation of the solution requires no extra m by n array of storage.

As storing matrix A by row results in a much more effective inner loop than storing by column, the procedure assumes that band matrix A is stored by row in successive storage locations, the number of which is equal to the number of elements appearing in the main diagonal and upper and lower codiagonals. The elements to be handed to the procedure by the user are underlined in the following explicit writing of formula (1) in the special case of a 7 by 7 matrix A with three upper and two lower codiagonals:

$$\begin{bmatrix} \underline{a_{11}} & \underline{a_{12}} & \underline{a_{13}} & \underline{a_{14}} & 0 & 0 & 0 \\ \underline{a_{21}} & \underline{a_{22}} & \underline{a_{23}} & \underline{a_{24}} & \underline{a_{25}} & 0 & 0 \\ \underline{a_{31}} & \underline{a_{32}} & \underline{a_{33}} & \underline{a_{34}} & \underline{a_{35}} & \underline{a_{36}} & 0 \\ 0 & \underline{a_{42}} & \underline{a_{43}} & \underline{a_{44}} & \underline{a_{45}} & \underline{a_{46}} & \underline{a_{47}} \\ 0 & 0 & \underline{a_{53}} & \underline{a_{54}} & \underline{a_{55}} & \underline{a_{56}} & \underline{a_{57}} \\ 0 & 0 & 0 & \underline{a_{64}} & \underline{a_{65}} & \underline{a_{66}} & \underline{a_{67}} \\ 0 & 0 & 0 & 0 & \underline{a_{75}} & \underline{a_{76}} & \underline{a_{77}} \end{bmatrix} *$$

$$\begin{pmatrix} x_{11} & x_{12} \cdots x_{1n} \\ x_{21} & x_{22} \cdots x_{2n} \\ x_{31} & x_{32} \cdots x_{3n} \\ \cdots\cdots\cdots\cdots \\ x_{71} & x_{72} \cdots x_{7n} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{12} \cdots r_{1n} \\ r_{21} & r_{22} \cdots r_{2n} \\ r_{31} & r_{32} \cdots r_{3n} \\ \cdots\cdots\cdots\cdots \\ r_{71} & r_{72} \cdots r_{7n} \end{pmatrix} \qquad (2)$$

Immediately following the matrix elements there must be some auxiliary storage locations used by the procedure, such that in the general case of an m by m matrix A with "mud" upper and "mld" lower codiagonals the total number of storage locations of array A is:+

$$ma = m \cdot mc - \frac{(mc-mld-1)(mc-mld)}{2} \qquad (3)$$

with $mc = \min(m, 1 + mud + mld)$. (4)

That means, in the special case of formula (2), that the 33 underlined elements of matrix A must be stored by row in the first 33 successive locations of array A, which consists of 36 storage locations.

In the first part of the procedure, matrix A is searched for its absolutely greatest element, say a_{ij}, and the absolute tolerance for testing loss of significance

$$tol = \varepsilon \cdot |a_{ij}| \qquad (5)$$

is generated with a given relative tolerance ε++. Close together with this search, the elements of matrix A are moved backward, and a triangular area of zeros is inserted in the last positions of the first (mc-mud-1) rows, according to storage requirements of the Gauss algorithm for band matrices. After these manipulations, the special matrix A of formula (2) will occupy the 36 positions of array A by row as shown in Figure 10 (the underlined elements are the main diagonal elements of matrix A).

In order to make the description of the band-algorithm easier, the elements of array A are renamed according to their arrangement in Figure 10,

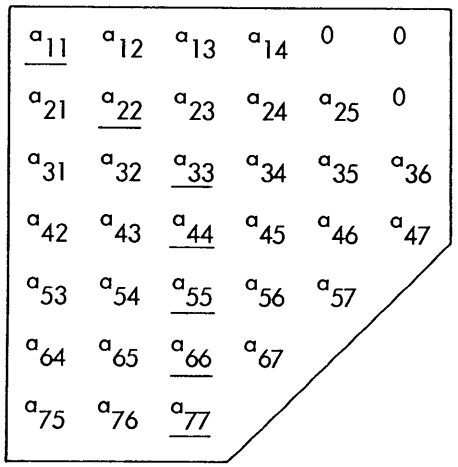

Figure 10. Array A

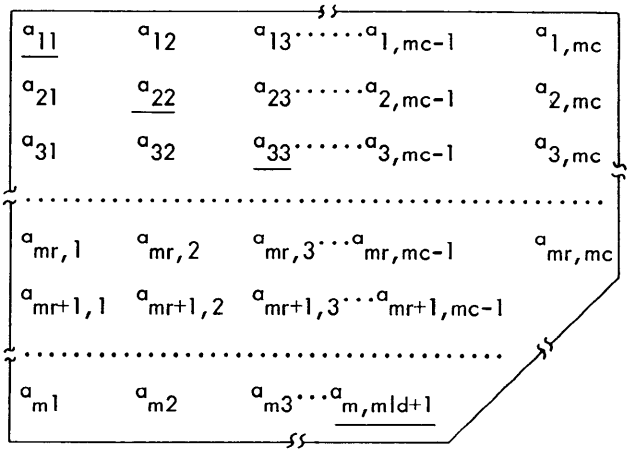

Figure 11. Array A renamed

thus generally giving the array shown in Figure 11 (main diagonal elements are underlined).

Each of the first mr = m-(mc - mld - 1) rows in this array contains mc elements; in the following rows the number of elements decreases steadily by 1 until the last row, which contains mld + 1 elements.

Now Gauss elimination can start. In the first step, search the first column of matrix A (that is, the elements of the first column of array A with row indexes from 1 up to 1 + mld) for the absolutely greatest element, say a_{j1} ($1 \le j \le 1 + mld$), and select it as pivot element ($p = a_{j1}$). Assume that j = 1. If it is not, interchange the first rows in array A and matrix R with the j^{th} rows. Now, transform the elements of the pivot rows (that is, the first rows) of array A and matrix R by division with p, and the elements of the following mld rows by adding $-a_{\nu 1}$ times the first rows to the ν^{th} rows ($\nu = 2,3,\ldots, 1 + mld$). At the same time, shift back the elements of the ν^{th} rows in array A by one position and insert a zero in the last position of each transformed row. This transformation is described by the following set of formulas:

$$a_{11}^{(1)} = \frac{a_{11}}{p} \quad (l = 1,2,\ldots, mc) \tag{6}$$

$$r_{11}^{(1)} = \frac{r_{11}}{p} \quad (l = 1,2,\ldots, n) \tag{7}$$

$$\left.\begin{aligned} a_{\nu,l-1}^{(1)} &= a_{\nu 1} - a_{\nu 1} \cdot a_{11}^{(1)} \\ &\quad (l = 2,3,\ldots, mc) \\ a_{\nu,mc}^{(1)} &= 0 \end{aligned}\right\} \quad (\nu = 2,3,\ldots, 1+mld) \tag{8}$$

$$r_{\nu 1}^{(1)} = r_{\nu 1} - a_{\nu 1} \cdot r_{11}^{(1)} \quad \begin{matrix}(l = 1,2,\ldots,n; \\ \nu = 2,3,\ldots, \\ 1+mld)\end{matrix} \tag{9}$$

Rows with row indexes greater than 1 + mld remain unchanged; nevertheless, they are marked with the superscript 1. The result of the first step is shown in Figure 12 (main diagonal elements are underlined).

$$R^{(1)} = \begin{pmatrix} r_{11}^{(1)} & r_{12}^{(1)} & \cdots & r_{1n}^{(1)} \\ r_{21}^{(1)} & r_{22}^{(1)} & \cdots & r_{2n}^{(1)} \\ r_{31}^{(1)} & r_{32}^{(1)} & \cdots & r_{3n}^{(1)} \\ \vdots & & & \\ r_{m1}^{(1)} & r_{m2}^{(1)} & \cdots & r_{mn}^{(1)} \end{pmatrix}$$

This procedure is now repeated (m-1) times, starting at the k^{th} step with array $A^{(k-1)}$ and matrix $R^{(k-1)}$.

+Note that the user must provide this number of storage locations of array A by the dimension statement in his main program.

++In case of a matrix A without lower codiagonals, tol is set equal to zero, whether ε is zero or not.

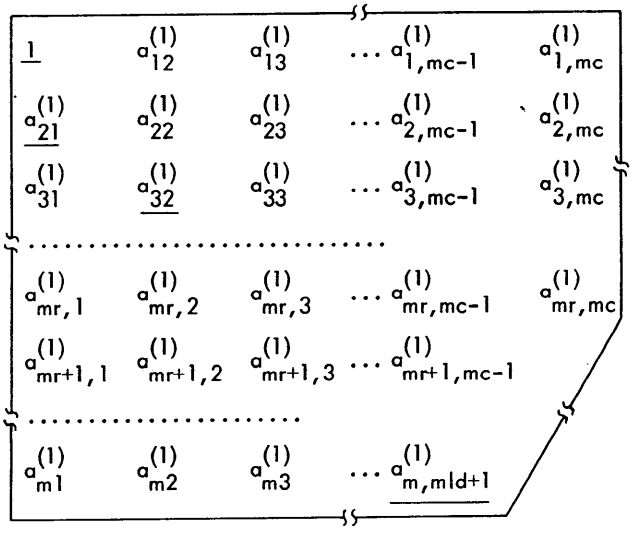

Figure 12. Array $A^{(1)}$

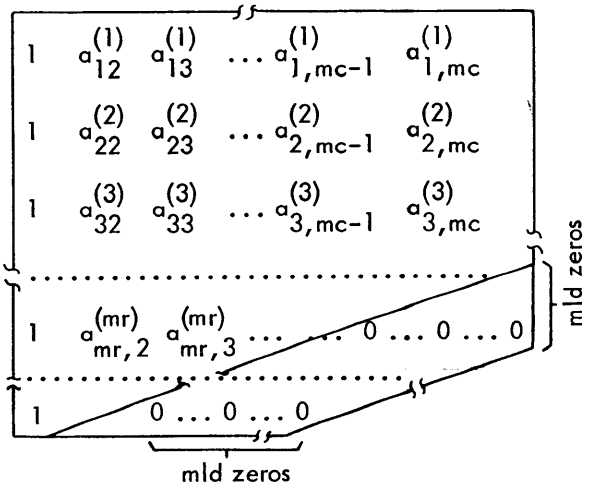

Figure 13. Array $A^{(m)}$

The rows which must be worked through at the k^{th} step are the rows with indexes i = k, k + 1,..., ilr = min (m, k + mld). As soon as ilr becomes greater than mr, the number of elements in any row of array A which have to be transformed decreases by one in each step k. The total results after m steps are shown in Figure 13.

$$R^{(m)} = \begin{bmatrix} r_{11}^{(1)} & r_{12}^{(1)} & \cdots & r_{1n}^{(1)} \\ r_{21}^{(2)} & r_{22}^{(2)} & \cdots & r_{2n}^{(2)} \\ r_{31}^{(3)} & r_{32}^{(3)} & \cdots & r_{3n}^{(3)} \\ \vdots & & & \\ r_{mr,1}^{(mr)} & r_{mr,2}^{(mr)} & \cdots & r_{mr,n}^{(mr)} \\ \vdots & & & \\ r_{m1}^{(m)} & r_{m2}^{(m)} & \cdots & r_{mn}^{(m)} \end{bmatrix}$$

Now, working backward, generate solution matrix X in the locations of right-hand side matrix R by means of the following equations:

$$\begin{aligned}
r_{m-1,l}^{(m)} &= r_{m-1,l}^{(m-1)} - a_{m-1,2}^{(m-1)} \cdot r_{m,l}^{(m)} \\
&\qquad (l = 1, 2, \ldots, n) \\
r_{m-2,l}^{(m)} &= r_{m-2,l}^{(m-2)} - a_{m-2,2}^{(m-2)} \cdot r_{m-1,l}^{(m)} \\
&\quad - a_{m-2,3}^{(m-2)} \cdot r_{m,l}^{(m)} \quad (l = 1, 2, \ldots, n) \\
&\cdots\cdots\cdots\cdots \\
r_{m-mc+1,l}^{(m)} &= r_{m-mc+1,l}^{(m-mc+1)} - a_{m-mc+1,2}^{(m-mc+1)} \\
&\quad \cdot r_{m-mc+2,l}^{(m)} - \cdots - a_{m-mc-1,mc}^{(m-mc+1)} \\
&\quad \cdot r_{m,l}^{(m)} \quad (l = 1, 2, \ldots, n) \\
r_{11}^{(m)} &= r_{11}^{(1)} - a_{12}^{(1)} \cdot r_{21}^{(m)} - a_{13}^{(1)} \cdot r_{31}^{(m)} \\
&\quad - \cdots - a_{1,mc}^{(1)} \cdot r_{mc,1}^{(m)} \quad (l = 1, 2, \ldots, n)
\end{aligned} \tag{10}$$

Note that in the first mc-1 equations of formula (10) the number of terms to be subtracted increases steadily by 1 until this number has reached mc-1. From the (mc-1)st equation up to the last equation the number of terms to be subtracted remains constant.

The only case in which the procedure described above can fail to give a solution occurs when at any step (say the k^{th} step) all elements in the k^{th} column of the transformed matrix A [that is, the elements in the first column of array A with row indexes k up to ilr = min (m, k + mld)] become zero, and no pivot element can be found. In this case, the procedure is bypassed and the error message ier = -1 is given. Actually, because of rounding errors, a further check of the absolute values of pivot elements is performed by the procedure. If at elimination step k this absolute value becomes less than tol (see equation 5 and second footnote), it is likely that matrix A is singular, too. But, as this may not necessarily be the case and as this test depends highly on the choice of the relative tolerance ϵ [+], the procedure gives only the warning ier = k-1, which indicates that there is a possible loss of significance in the results computed by the algorithm. [++] In case of a well scaled matrix A and an appropriate choice of the relative tolerance, warning ier = k-1 may be interpreted as meaning that the rank of A is less than m but not less than k - 1. If there are no lower codiagonals (mld = 0), the test on loss of significance is suppressed.

+For subroutine GELB, a relative tolerance between 10^{-6} and 10^{-7} is suggested; and for subroutine DGELB, between 10^{-14} and 10^{-16}.

++For example, $\epsilon = 10^{-5}$ and warning ier = 3 mean that there is a possible loss of about 5 or more significant digits in the initial values of elimination step 4, and that matrix A seems to have a rank less than m but not less than 3.

```
C                                                                       GELB  10
C     ...................................................................GELB  20
C                                                                       GELB  30
C        SUBROUTINE GELB                                                GELB  40
C                                                                       GELB  50
C        PURPOSE                                                        GELB  60
C           TO SOLVE A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH A   GELB  70
C           COEFFICIENT MATRIX OF BAND STRUCTURE.                       GELB  80
C                                                                       GELB  90
C        USAGE                                                          GELB 100
C           CALL GELB(R,A,M,N,MUD,MLD,EPS,IER)                          GELB 110
C                                                                       GELB 120
C        DESCRIPTION OF PARAMETERS                                      GELB 130
C           R      - M BY N RIGHT HAND SIDE MATRIX (DESTROYED).         GELB 140
C                    ON RETURN R CONTAINS THE SOLUTION OF THE EQUATIONS.GELB 150
C           A      - M BY M COEFFICIENT MATRIX WITH BAND STRUCTURE      GELB 160
C                    (DESTROYED).                                       GELB 170
C           M      - THE NUMBER OF EQUATIONS IN THE SYSTEM.             GELB 180
C           N      - THE NUMBER OF RIGHT HAND SIDE VECTORS.             GELB 190
C           MUD    - THE NUMBER OF UPPER CODIAGONALS (THAT MEANS        GELB 200
C                    CODIAGONALS ABOVE MAIN DIAGONAL).                  GELB 210
C           MLD    - THE NUMBER OF LOWER CODIAGONALS (THAT MEANS        GELB 220
C                    CODIAGONALS BELOW MAIN DIAGONAL).                  GELB 230
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS RELATIVE        GELB 240
C                    TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.        GELB 250
C           IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS         GELB 260
C                    IER=0  - NO ERROR,                                 GELB 270
C                    IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARAME-  GELB 280
C                             TERS M,MUD,MLD OR BECAUSE OF PIVOT ELEMENTGELB 290
C                             AT ANY ELIMINATION STEP EQUAL TO 0.       GELB 300
C                    IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-  GELB 310
C                             CANCE INDICATED AT ELIMINATION STEP K+1,  GELB 320
C                             WHERE PIVOT ELEMENT WAS LESS THAN OR      GELB 330
C                             EQUAL TO THE INTERNAL TOLERANCE EPS TIMES GELB 340
C                             ABSOLUTELY GREATEST ELEMENT OF MATRIX A.  GELB 350
C                                                                       GELB 360
C        REMARKS                                                        GELB 370
C           BAND MATRIX A IS ASSUMED TO BE STORED ROWWISE IN THE FIRST  GELB 380
C           MC SUCCESSIVE STORAGE LOCATIONS OF TOTALLY NEEDED MA        GELB 390
C           STORAGE LOCATIONS, WHERE                                    GELB 400
C             MA=M*MC-ML*(ML+1)/2    AND    ME=MA-MU*(MU+1)/2    WITH GELB 410
C             MC=MIN(M,1+MUD+MLD),  ML=MC-1-MLD,  MU=MC-1-MUD.          GELB 420
C           RIGHT HAND SIDE MATRIX R IS ASSUMED TO BE STORED COLUMNWISE GELB 430
C           IN N*M SUCCESSIVE STORAGE LOCATIONS. ON RETURN SOLUTION     GELB 440
C           MATRIX R IS STORED COLUMNWISE TOO.                          GELB 450
C           INPUT PARAMETERS M, MUD, MLD SHOULD SATISFY THE FOLLOWING   GELB 460
C           RESTRICTIONS      MUD NOT LESS THAN ZERO                    GELB 470
C                             MLD NOT LESS THAN ZERO                    GELB 480
C                             MUD+MLD NOT GREATER THAN 2*M-2.           GELB 490
C           NO ACTION BESIDES ERROR MESSAGE IER=-1 TAKES PLACE IF THESE GELB 500
C           RESTRICTIONS ARE NOT SATISFIED.                             GELB 510
C           THE PROCEDURE GIVES RESULTS IF THE RESTRICTIONS ON INPUT    GELB 520
C           PARAMETERS ARE SATISFIED AND IF PIVOT ELEMENTS AT ALL       GELB 530
C           ELIMINATION STEPS ARE DIFFERENT FROM 0. HOWEVER WARNING     GELB 540
C           IER=K - IF GIVEN - INDICATES POSSIBLE LOSS OF SIGNIFICANCE. GELB 550
C           IN CASE OF A WELL SCALED MATRIX A AND APPROPRIATE TOLERANCE GELB 560
C           EPS, IER=K MAY BE INTERPRETED THAT MATRIX A HAS THE RANK K. GELB 570
C           NO WARNING IS GIVEN IF MATRIX A HAS NO LOWER CODIAGONAL.    GELB 580
C                                                                       GELB 590
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GELB 600
C           NONE                                                        GELB 610
C                                                                       GELB 620
C        METHOD                                                         GELB 630
C           SOLUTION IS DONE BY MEANS OF GAUSS ELIMINATION WITH         GELB 640
C           COLUMN PIVOTING ONLY, IN ORDER TO PRESERVE BAND STRUCTURE   GELB 650
C           IN REMAINING COEFFICIENT MATRICES.                          GELB 660
C                                                                       GELB 670
C     ...................................................................GELB 680
C                                                                       GELB 690
      SUBROUTINE GELB(R,A,M,N,MUD,MLD,EPS,IER)                          GELB 700
C                                                                       GELB 710
C                                                                       GELB 720
      DIMENSION R(1),A(1)                                               GELB 730
C                                                                       GELB 740
C     TEST ON WRONG INPUT PARAMETERS                                    GELB 750
      IF(MLD)47,1,1                                                     GELB 760
    1 IF(MUD)47,2,2                                                     GELB 770
    2 MC=1+MLD+MUD                                                      GELB 780
      IF(MC+1-M-M)3,3,47                                                GELB 790
C                                                                       GELB 800
C     PREPARE INTEGER PARAMETERS                                        GELB 810
C        MC=NUMBER OF COLUMNS IN MATRIX A                               GELB 820
C        MU=NUMBER OF ZEROS TO BE INSERTED IN FIRST ROW OF MATRIX A     GELB 830
C        ML=NUMBER OF MISSING ELEMENTS IN LAST ROW OF MATRIX A          GELB 840
C        MR=INDEX OF LAST ROW IN MATRIX A WITH MC ELEMENTS              GELB 850
C        MZ=TOTAL NUMBER OF ZEROS TO BE INSERTED IN MATRIX A            GELB 860
C        MA=TOTAL NUMBER OF STORAGE LOCATIONS NECESSARY FOR MATRIX A    GELB 870
C        NM=NUMBER OF ELEMENTS IN MATRIX R                              GELB 880
    3 IF(MC-M)5,5,4                                                     GELB 890
    4 MC=M                                                              GELB 900
    5 MU=MC-MUD-1                                                       GELB 910
      ML=MC-MLD-1                                                       GELB 920
      MR=M-ML                                                           GELB 930
      MZ=(MU*(MU+1))/2                                                  GELB 940
      MA=M*MC-(ML*(ML+1))/2                                             GELB 950
      NM=N*M                                                            GELB 960
C                                                                       GELB 970
C     MOVE ELEMENTS BACKWARD AND SEARCH FOR ABSOLUTELY GREATEST ELEMENT  GELB 980
C     (NOT NECESSARY IN CASE OF A MATRIX WITHOUT LOWER CODIAGONALS)      GELB 990
      IER=0                                                             GELB1000
      PIV=0.                                                            GELB1010
      IF(MLD)14,14,6                                                    GELB1020
    6 JJ=MA                                                             GELB1030
      J=MA-MZ                                                           GELB1040
      KST=J                                                             GELB1050
      DO 9 K=1,KST                                                      GELB1060
      TB=A(J)                                                           GELB1070
      A(JJ)=TB                                                          GELB1080
      TB=ABS(TB)                                                        GELB1090
      IF(TB-PIV)8,8,7                                                   GELB1100
    7 PIV=TB                                                            GELB1110
    8 J=J-1                                                             GELB1120
    9 JJ=JJ-1                                                           GELB1130
C                                                                       GELB1140
C     INSERT ZEROS IN FIRST MU ROWS (NOT NECESSARY IN CASE MZ=0)        GELB1150
      IF(MZ)14,14,10                                                    GELB1160
   10 JJ=1                                                              GELB1170
      J=1+MZ                                                            GELB1180
      IC=1+MUD                                                          GELB1190
      DO 13 I=1,MU                                                      GELB1200
      DO 12 K=1,MC                                                      GELB1210
      A(JJ)=0.                                                          GELB1220
      IF(K-IC)11,11,12                                                  GELB1230
   11 A(JJ)=A(J)                                                        GELB1240
      J=J+1                                                             GELB1250
   12 JJ=JJ+1                                                           GELB1260
   13 IC=IC+1                                                           GELB1270
C                                                                       GELB1280
```

```
C     GENERATE TEST VALUE FOR SINGULARITY                              GELB1290
   14 TOL=EPS*PIV                                                      GELB1300
C                                                                      GELB1310
C                                                                      GELB1320
C     START DECOMPOSITION LOOP                                         GELB1330
      KST=1                                                            GELB1340
      IDST=MC                                                          GELB1350
      IC=MC-1                                                          GELB1360
      DO 38 K=1,M                                                      GELB1370
      IF(K-MA-1)16,16,15                                               GELB1380
   15 IDST=IDST-1                                                      GELB1390
   16 ID=IDST                                                          GELB1400
      ILR=K+MLD                                                        GELB1410
      IF(ILR-M)18,18,17                                                GELB1420
   17 ILR=M                                                            GELB1430
   18 II=KST                                                           GELB1440
C                                                                      GELB1450
C     PIVOT SEARCH IN FIRST COLUMN (ROW INDEXES FROM I=K UP TO I=ILR)  GELB1460
      PIV=0.                                                           GELB1470
      DO 22 I=K,ILR                                                    GELB1480
      TB=ABS(A(II))                                                    GELB1490
      IF(TB-PIV)20,20,19                                               GELB1500
   19 PIV=TB                                                           GELB1510
      J=I                                                              GELB1520
      JJ=II                                                            GELB1530
   20 IF(I-MR)22,22,21                                                 GELB1540
   21 ID=ID-1                                                          GELB1550
   22 II=II+ID                                                         GELB1560
C                                                                      GELB1570
C     TEST ON SINGULARITY                                              GELB1580
      IF(PIV)47,47,23                                                  GELB1590
   23 IF(IER)26,24,26                                                  GELB1600
   24 IF(PIV-TOL)25,25,26                                              GELB1610
   25 IER=K-1                                                          GELB1620
   26 PIV=1./A(JJ)                                                     GELB1630
C                                                                      GELB1640
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN RIGHT HAND SIDE R     GELB1650
      ID=J-K                                                           GELB1660
      DO 27 I=K,NM,M                                                   GELB1670
      II=I+ID                                                          GELB1680
      TB=PIV*R(II)                                                     GELB1690
      R(II)=R(I)                                                       GELB1700
   27 R(I)=TB                                                          GELB1710
C                                                                      GELB1720
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN COEFFICIENT MATRIX A  GELB1730
      II=KST                                                           GELB1740
      JJ=JJ+IC                                                         GELB1750
      DO 29 I=JJ,J                                                     GELB1760
      TB=PIV*A(II)                                                     GELB1770
      A(II)=A(I)                                                       GELB1780
      A(I)=TB                                                          GELB1790
   28 II=II+1                                                          GELB1800
C                                                                      GELB1810
C     ELEMENT REDUCTION                                                GELB1820
      IF(K-ILR)29,34,34                                                GELB1830
   29 ID=KST                                                           GELB1840
      II=K+1                                                           GELB1850
      MU=KST+1                                                         GELB1860
      MZ=KST+IC                                                        GELB1870
      DO 33 I=II,ILR                                                   GELB1880
C                                                                      GELB1890
C     IN MATRIX A                                                      GELB1900
      ID=ID+MC                                                         GELB1910
      JJ=I-MR-1                                                        GELB1920
      IF(JJ)31,31,30                                                   GELB1930
   30 ID=ID-JJ                                                         GELB1940
   31 PIV=-A(ID)                                                       GELB1950
      J=ID+1                                                           GELB1960
      DO 32 JJ=MU,MZ                                                   GELB1970
      A(J-1)=A(J)+PIV*A(JJ)                                            GELB1980
   32 J=J+1                                                            GELB1990
      A(J-1)=0.                                                        GELB2000
C                                                                      GELB2010
C     IN MATRIX R                                                      GELB2020
      J=K                                                              GELB2030
      DO 33 JJ=I,NM,M                                                  GELB2040
      R(JJ)=R(JJ)+PIV*R(J)                                             GELB2050
   33 J=J+M                                                            GELB2060
   34 KST=KST+MC                                                       GELB2070
      IF(ILR-MR)36,35,35                                               GELB2080
   35 IC=IC-1                                                          GELB2090
   36 ID=K-MR                                                          GELB2100
      IF(ID)38,38,37                                                   GELB2110
   37 KST=KST-ID                                                       GELB2120
   38 CONTINUE                                                         GELB2130
C     END OF DECOMPOSITION LOOP                                        GELB2140
C                                                                      GELB2150
C                                                                      GELB2160
C     BACK SUBSTITUTION                                                GELB2170
      IF(MC-1)40,40,39                                                 GELB2180
   39 IC=2                                                             GELB2190
      KST=MA+ML-ML*2                                                   GELB2200
      II=M                                                             GELB2210
      DO 45 I=2,M                                                      GELB2220
      KST=KST-MC                                                       GELB2230
      II=II-1                                                          GELB2240
      J=II-MR                                                          GELB2250
      IF(J)41,41,40                                                    GELB2260
   40 KST=KST+J                                                        GELB2270
   41 DO 43 J=II,NM,M                                                  GELB2280
      TB=R(J)                                                          GELB2290
      MZ=KST+IC-2                                                      GELB2300
      ID=J                                                             GELB2310
      DO 42 JJ=KST,MZ                                                  GELB2320
      ID=ID+1                                                          GELB2330
   42 TB=TB-A(JJ)*R(ID)                                                GELB2340
   43 R(J)=TB                                                          GELB2350
      IF(IC-MC)44,45,45                                                GELB2360
   44 IC=IC+1                                                          GELB2370
   45 CONTINUE                                                         GELB2380
   46 RETURN                                                           GELB2390
C                                                                      GELB2400
C                                                                      GELB2410
C     ERROR RETURN                                                     GELB2420
   47 IER=-1                                                           GELB2430
      RETURN                                                           GELB2440
      END                                                              GELB2450
```

```
C                                                                      DELB  10
C     ******************************************************************DELB  20
C                                                                      DELB  30
      SUBROUTINE DGELB                                                 DELB  40
C                                                                      DELB  50
C     PURPOSE                                                          DELB  60
C        TO SOLVE A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH A     DELB  70
C        COEFFICIENT MATRIX OF BAND STRUCTURE.                         DELB  80
C                                                                      DELB  90
C     USAGE                                                            DELB 100
C        CALL DGELB(R,A,M,N,MUD,MLD,EPS,IER)                           DELB 110
C                                                                      DELB 120
C     DESCRIPTION OF PARAMETERS                                        DELB 130
C        R    - DOUBLE PRECISION M BY N RIGHT HAND SIDE MATRIX         DELB 140
C               (DESTROYED). ON RETURN R CONTAINS THE SOLUTION         DELB 150
C               OF THE EQUATIONS.                                      DELB 160
C        A    - DOUBLE PRECISION M BY M COEFFICIENT MATRIX WITH        DELB 170
C               BAND STRUCTURE (DESTROYED).                            DELB 180
C        M    - THE NUMBER OF EQUATIONS IN THE SYSTEM.                 DELB 190
C        N    - THE NUMBER OF RIGHT HAND SIDE VECTORS.                 DELB 200
C        MUD  - THE NUMBER OF UPPER CODIAGONALS (THAT MEANS            DELB 210
C               CODIAGONALS ABOVE MAIN DIAGONAL).                      DELB 220
C        MLD  - THE NUMBER OF LOWER CODIAGONALS (THAT MEANS            DELB 230
C               CODIAGONALS BELOW MAIN DIAGONAL).                      DELB 240
C        EPS  - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS       DELB 250
C               RELATIVE TOLERANCE FOR TEST ON LOSS OF                 DELB 260
C               SIGNIFICANCE.                                          DELB 270
C        IER  - RESULTING ERROR PARAMETER CODED AS FOLLOWS             DELB 280
C               IER=0  - NO ERROR,                                     DELB 290
C               IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARAME-      DELB 300
C                        TERS M,MUD,MLD OR BECAUSE OF PIVOT ELEMENT    DELB 310
C                        AT ANY ELIMINATION STEP EQUAL TO C,           DELB 320
C               IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-      DELB 330
C                        CANCE INDICATED AT ELIMINATION STEP K+1,      DELB 340
C                        WHERE PIVOT ELEMENT WAS LESS THAN OR          DELB 350
C                        EQUAL TO THE INTERNAL TOLERANCE EPS TIMES     DELB 360
C                        ABSOLUTELY GREATEST ELEMENT OF MATRIX A.      DELB 370
C                                                                      DELB 380
C     REMARKS                                                          DELB 390
C        BAND MATRIX A IS ASSUMED TO BE STORED ROWWISE IN THE FIRST    DELB 400
C        ME SUCCESSIVE STORAGE LOCATIONS OF TOTALLY NEEDED MA          DELB 410
C        STORAGE LOCATIONS, WHERE                                      DELB 420
C          MA=M*MC-ML*(ML+1)/2     AND     ME=MA-MU*(MU+1)/2    WITH DELB 430
C          MC=MIN(K+1+MUD+MLD),  ML=MC-1-MLD,  MU=MC-1-MUD.           DELB 440
C        RIGHT HAND SIDE MATRIX R IS ASSUMED TO BE STORED COLUMNWISE   DELB 450
C        IN N*M SUCCESSIVE STORAGE LOCATIONS. ON RETURN SOLUTION       DELB 460
C        MATRIX R IS STORED COLUMNWISE TOO.                            DELB 470
C        INPUT PARAMETERS M, MUD, MLD SHOULD SATISFY THE FOLLOWING     DELB 480
C        RESTRICTIONS      MUD NOT LESS THAN ZERO                      DELB 490
C                          MLD NOT LESS THAN ZERO                      DELB 500
C                          MUD+MLD NOT GREATER THAN 2*M-2.             DELB 510
C        NO ACTION BESIDES ERROR MESSAGE IER=-1 TAKES PLACE IF THESE   DELB 520
C        RESTRICTIONS ARE NOT SATISFIED.                               DELB 530
C        THE PROCEDURE GIVES RESULTS IF THE RESTRICTIONS ON INPUT      DELB 540
C        PARAMETERS ARE SATISFIED AND IF PIVOT ELEMENTS AT ALL         DELB 550
C        ELIMINATION STEPS ARE DIFFERENT FROM C. HOWEVER WARNING       DELB 560
C        IER=K - IF GIVEN - INDICATES POSSIBLE LOSS OF SIGNIFICANCE.   DELB 570
C        IN CASE OF A WELL SCALED MATRIX A AND APPROPRIATE TOLERANCE   DELB 580
C        EPS, IER=K MAY BE INTERPRETED THAT MATRIX A HAS THE RANK K.   DELB 590
C        NO WARNING IS GIVEN IF MATRIX A HAS NO LOWER CODIAGONAL.      DELB 600
C                                                                      DELB 610
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                    DELB 620
C        NONE                                                          DELB 630
C                                                                      DELB 640
C     METHOD                                                           DELB 650
C        SOLUTION IS DONE BY MEANS OF GAUSS ELIMINATION WITH           DELB 660
C        COLUMN PIVOTING ONLY, IN ORDER TO PRESERVE BAND STRUCTURE     DELB 670
C        IN REMAINING COEFFICIENT MATRICES.                            DELB 680
C                                                                      DELB 690
C     ******************************************************************DELB 700
C                                                                      DELB 710
      SUBROUTINE DGELB(R,A,M,N,MUD,MLD,EPS,IER)                        DELB 720
C                                                                      DELB 730
C                                                                      DELB 740
      DIMENSION R(1),A(1)                                              DELB 750
      DOUBLE PRECISION R,A,PIV,TB,TOL                                  DELB 760
C                                                                      DELB 770
C     TEST ON WRONG INPUT PARAMETERS                                   DELB 780
      IF(MLD)47,1,1                                                    DELB 790
    1 IF(MUD)47,2,2                                                    DELB 800
    2 MC=1+MLD+MUD                                                     DELB 810
      IF(MC+1-M-M)3,3,47                                               DELB 820
C                                                                      DELB 830
C     PREPARE INTEGER PARAMETERS                                       DELB 840
C        MC=NUMBER OF COLUMNS IN MATRIX A                              DELB 850
C        MU=NUMBER OF ZEROS TO BE INSERTED IN FIRST ROW OF MATRIX A    DELB 860
C        ML=NUMBER OF MISSING ELEMENTS IN LAST ROW OF MATRIX A         DELB 870
C        MR=INDEX OF LAST ROW IN MATRIX A WITH MC ELEMENTS             DELB 880
C        MZ=TOTAL NUMBER OF ZEROS TO BE INSERTED IN MATRIX A           DELB 890
C        MA=TOTAL NUMBER OF STORAGE LOCATIONS NECESSARY FOR MATRIX A   DELB 900
C        NM=NUMBER OF ELEMENTS IN MATRIX R                             DELB 910
    3 IF(MC-4)5,5,4                                                    DELB 920
    4 MC=M                                                             DELB 930
    5 MU=MC-MUD-1                                                      DELB 940
      ML=MC-MLD-1                                                      DELB 950
      MR=M-ML                                                          DELB 960
      MZ=(MU*(MU+1))/2                                                 DELB 970
      MA=M*MC-(ML*(ML+1))/2                                            DELB 980
      NM=N*M                                                           DELB 990
C                                                                      DELB1000
C     MOVE ELEMENTS BACKWARD AND SEARCH FOR ABSOLUTELY GREATEST ELEMENT DELB1010
C     (NOT NECESSARY IN CASE OF A MATRIX WITHOUT LOWER CODIAGONALS)    DELB1020
      IER=0                                                            DELB1030
      PIV=0.D0                                                         DELB1040
      IF(MLD)14,14,6                                                   DELB1050
    6 JJ=MA                                                            DELB1060
      J=MA-MZ                                                          DELB1070
      KST=J                                                            DELB1080
      DO 9 K=1,KST                                                     DELB1090
      TB=A(J)                                                          DELB1100
      A(JJ)=TB                                                         DELB1110
      TB=DABS(TB)                                                      DELB1120
      IF(TB-PIV)9,8,7                                                  DELB1130
    7 PIV=TB                                                           DELB1140
    8 J=J-1                                                            DELB1150
    9 JJ=JJ-1                                                          DELB1160
C                                                                      DELB1170
C     INSERT ZEROS IN FIRST MU ROWS (NOT NECESSARY IN CASE MZ=0)       DELB1180
      IF(MZ)14,14,10                                                   DELB1190
   10 JJ=1                                                             DELB1200
      J=1+MZ                                                           DELB1210
      IC=1+MUD                                                         DELB1220
      DO 13 I=1,MU                                                     DELB1230
      DO 12 K=1,MC                                                     DELB1240
      A(JJ)=0.D0                                                       DELB1250
      IF(K-IC)11,11,12                                                 DELB1260
   11 A(JJ)=A(J)                                                       DELB1270
      J=J+1                                                            DELB1280
   12 JJ=JJ+1                                                          DELB1290
```

```
   13 IC=IC+1
C
C     GENERATE TEST VALUE FOR SINGULARITY
   14 TOL=EPS*PIV
C
C
C     START DECOMPOSITION LOOP
      KST=1
      IDST=MC
      IC=MC-1
      DO 38 K=1,M
      IF(K-MA-1)16,15,15
   15 IDST=IDST-1
   16 ID=ID+T
      ILR=K+MLO
      IF(ILR-M)18,18,17
   17 ILR=M
   18 II=KST
C
C     PIVOT SEARCH IN FIRST COLUMN (ROW INDEXES FROM I=K UP TO I=ILR)
      PIV=0.0E
      DO 22 I=K,ILR
      TB=DABS(A(II))
      IF(TB-PIV)20,20,19
   19 PIV=TB
      J=I
      JJ=II
   20 IF(I-MA)22,22,21
   21 ID=ID-1
   22 II=II+ID
C
C     TEST ON SINGULARITY
      IF(PIV)47,47,23
   23 IF(IER)26,24,26
   24 IF(PIV-TOL)25,25,26
   25 IER=K-1
   26 PIV=1.0E/A(JJ)
C
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN RIGHT HAND SIDE R
      ID=J-K
      DO 27 I=K,NM,M
      II=I+ID
      TB=PIV*R(II)
      R(II)=R(I)
   27 R(I)=TB
C
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN COEFFICIENT MATRIX A
      II=KST
      J=JJ+IC
      DO 28 I=JJ,J
      TB=PIV*A(II)
      A(II)=A(I)
      A(I)=TB
   28 II=II+1
C
C     ELEMENT REDUCTION
      IF(K-ILR)29,34,34
   29 ID=KST
      II=K+1
      MU=KST+1
      MZ=KST+IC
      DO 33 I=II,ILR
C
C     IN MATRIX A
      IC=ID+MC
      JJ=I-MA-1
      IF(JJ)31,31,30
   30 ID=ID-JJ
   31 PIV=-A(II)
      J=ID+1
      DO 32 JJ=MU,MZ
      A(J-1)=A(J)+PIV*A(JJ)
   32 J=J+1
      A(J-1)=0.0
C
C     IN MATRIX R
      J=K
      DO 33 JJ=1,NM,M
      R(JJ)=R(JJ)+PIV*R(J)
   33 J=J+M
   34 KST=KST+MC
      IF(ILR-MA)36,35,35
   35 IC=IC-1
   36 ID=K-MA
      IF(ID)38,38,37
   37 KST=KST-ID
   38 CONTINUE
C     END OF DECOMPOSITION LOOP
C
C
C     BACK SUBSTITUTION
      IF(MC-1)46,46,39
   39 IC=2
      KST=MA*ML-MC+2
      II=M
      DO 45 I=2,M
      KST=KST-MC
      II=II-1
      J=II-MA
      IF(J)41,41,40
   40 KST=KST+J
   41 DO 43 J=II,NM,M
      TB=R(J)
      MZ=KST+IC-2
      ID=J
      DO 42 JJ=KST,MZ
      ID=ID+1
   42 TB=TB-A(JJ)*R(ID)
   43 R(J)=TB
      IF(IC-MC)44,45,45
   44 IC=IC+1
   45 CONTINUE
   46 RETURN
C
C
C     ERROR RETURN
   47 IER=-1
      RETURN
      END
```

Subroutines MTDS and DMTDS

Given a general matrix A and a nonsingular upper triangular matrix T, these subroutines will perform one of the following six operations, depending on the value of an input parameter IOP:

IOP = 1: A is replaced by $T^{-1}A$.
IOP = -1: A is replaced by AT^{-1}.
IOP = 2: A is replaced by $(T^{-1})\,{}^{T}A$.
IOP = -2: A is replaced by $A(T^{-1})^{T}$.
IOP = 3: A is replaced by $(T^{T}T)^{-1}A$.
IOP = -3: A is replaced by $A(T^{T}T)^{-1}$.

1. Mathematical background

a. Calculation of $X = T^{-1}A$ is done using backward substitution to obtain X from $TX = A$.

b. Calculation of $Y = (T^{-1})\,{}^{T}A$ is done using forward substitution to obtain Y from $T^{T}Y = A$.

c. Calculation of $Z = (T^{T}T)^{-1}A$ is done by first solving $T^{T}Y = A$ and then solving $TZ = Y$.

The remaining three operations are reducible to the above three.

2. Applications

Subroutines MTDS and DMTDS may be used to compute the solution of a system of equations $BX = A$ with symmetric positive definite coefficient matrix B. The first step towards the solution is the triangular factorization of B by means of subroutine MFSD or DMFSD. The second step, which may be repeated for different sets of right-hand sides A, is the calculation of $(T^{T}T)^{-1}A$ by means of MTDS or DMTDS with IOP = 3. Another useful application is the computation of the product $A^{T}B^{-1}A$ with symmetric positive definite B and arbitrary A in only three steps and without additional storage requirements:

a. Replace B by T where $B = T^{T}T$.
b. Replace A by $C = (T^{T})^{-1}A$.
c. Replace B by $C^{T}C$.

```
C                                                                       MTDS  10
C     ..................................................................MTDS  20
C                                                                       MTDS  30
C        SUBROUTINE MTDS                                                MTDS  40
C                                                                       MTDS  50
C        PURPOSE                                                        MTDS  60
C           MULTIPLY A GENERAL MATRIX A ON THE LEFT OF RIGHT BY         MTDS  70
C           INVERSE(T),INVERSE(TRANSPOSE(T)) OR INVERSE(TRANSPOSE(T*T)) MTDS  80
C           THE TRIANGULAR MATRIX T IS STORED COLUMNWISE IN COMPRESSED  MTDS  90
C           FORM, I.E. UPPER TRIANGULAR PART ONLY.                      MTDS 100
C                                                                       MTDS 110
C        USAGE                                                          MTDS 120
C           CALL MTDS(A,M,N,T,IOP,IER)                                  MTDS 130
C                                                                       MTDS 140
C        DESCRIPTION OF PARAMETERS                                      MTDS 150
C           A      - GIVEN GENERAL MATRIX WHITH M ROWS AND N COLUMNS.   MTDS 160
C           M      - NUMBER OF ROWS OF MATRIX A                         MTDS 170
C           N      - NUMBER OF COLUMNS OF MATRIX A                      MTDS 180
C           T      - GIVEN TRIANGULAR MATRIX STORED COLUMNWISE UPPER    MTDS 190
C                    TRIANGULAR PART ONLY. ITS NUMBER OF ROWS AND       MTDS 200
C                    COLUMNS K IS IMPLIED BY COMPATIBILITY.             MTDS 210
C                    K = M IF IOP IS POSITIVE,                          MTDS 220
C                    K = N IF IOP IS NEGATIVE.                          MTDS 230
C                    T OCCUPIES K*(K+1)/2 STORAGE POSITIONS.            MTDS 240
C           IOP    - INPUT VARIABLE FOR SELECTION OF OPERATION          MTDS 250
C                    IOP = 1 - A IS REPLACED BY INVERSE(T)*A            MTDS 260
C                    IOP =-1 - A IS REPLACED BY A*INVERSE(T)            MTDS 270
C                    IOP = 2 - A IS REPLACED BY INVERSE(TRANSPOSE(T))*A MTDS 280
C                    IOP =-2 - A IS REPLACED BY A*INVERSE(TRANSPOSE(T)) MTDS 290
C                    IOP = 3 - A IS REPLACED BY INVERSE(TRANSPOSE(T)*T)*AMTDS 300
C                    IOP =-3 - A IS REPLACED BY A*INVERSE(TRANSPOSE(T)*T)MTDS 310
C           IER    - RESULTING ERROR PARAMETER                          MTDS 320
C                    IER =-1 MEANS M AND N ARE NOT BOTH POSITIVE        MTDS 330
C                            AND/OR IOP IS ILLEGAL                      MTDS 340
C                    IER = 0 MEANS OPERATION WAS SUCCESSFUL             MTDS 350
C                    IER = 1 MEANS TRIANGULAR MATRIX T IS SINGULAR      MTDS 360
C                                                                       MTDS 370
C        REMARKS                                                        MTDS 380
C           SUBROUTINE MTDS MAY BE USED TO CALCULATE THE SOLUTION OF    MTDS 390
C           A SYSTEM OF EQUATIONS WITH SYMMETRIC POSITIVE DEFINITE      MTDS 400
C           COEFFICIENT MATRIX. THE FIRST STEP TOWARDS THE SOLUTION     MTDS 410
C           IS TRIANGULAR FACTORIZATION BY MEANS OF MFSD. THE SECOND    MTDS 420
C           STEP IS APPLICATION OF MTDS.                                MTDS 430
C           SUBROUTINES MFSD AND MTDS MAY BE USED IN ORDER TO CALCULATE MTDS 440
C           THE PRODUCT TRANSPOSE(A)*INVERSE(B)*A WITH GIVEN SYMMETRIC  MTDS 450
C           POSITIVE DEFINITE B AND GIVEN A EFFICIENTLY IN THREE STEPS  MTDS 460
C           1) TRIANGULAR FACTORIZATION OF B (B=TRANSPOSE(T)*T)         MTDS 470
C           2) MULTIPLICATION OF A ON THE LEFT BY INVERSE(TRANSPOSE(T)) MTDS 480
C              A IS REPLACED BY C=INVERSE(TRANSPOSE(T))*A               MTDS 490
C           3) CALCULATION OF THE RESULT FORMING TRANSPOSE(C)*C         MTDS 500
C                                                                       MTDS 510
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MTDS 520
C           NONE                                                        MTDS 530
C                                                                       MTDS 540
C        METHOD                                                         MTDS 550
C           CALCULATION OF X = INVERSE(T)*A IS DONE USING BACKWARD      MTDS 560
C           SUBSTITUTION TO OBTAIN X FROM T*X = A.                      MTDS 570
C           CALCULATION OF Y = INVERSE(TRANSPOSE(T))*A IS DONE USING    MTDS 580
C           FORWARD SUBSTITUTION TO OBTAIN Y FROM TRANSPOSE(T)*Y = A.   MTDS 590
C           CALCULATION OF Z = INVERSE(TRANSPOSE(T)*T)*Z IS DONE        MTDS 600
C           SOLVING FIRST TRANSPOSE(T)*Y = A AND THEN T*Z = Y, I.E.     MTDS 610
C           USING THE ABOVE TWO STEPS IN REVERSE ORDER                  MTDS 620
C                                                                       MTDS 630
C     ..................................................................MTDS 640
C                                                                       MTDS 650
      SUBROUTINE MTDS(A,M,N,T,IOP,IER)                                  MTDS 660
C                                                                       MTDS 670
C                                                                       MTDS 680
      DIMENSION A(1),T(1)                                               MTDS 690
      DOUBLE PRECISION DSUM                                             MTDS 700
C                                                                       MTDS 710
C        TEST OF DIMENSION                                              MTDS 720
      IF(M)2,2,1                                                        MTDS 730
    1 IF(N)2,2,3                                                        MTDS 740
C                                                                       MTDS 750
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSIONS                     MTDS 760
    2 IER=-1                                                            MTDS 770
      RETURN                                                            MTDS 780
C                                                                       MTDS 790
C        ERROR RETURN IN CASE OF SINGULAR MATRIX T                      MTDS 800
    3 IER=1                                                             MTDS 810
      RETURN                                                            MTDS 820
C                                                                       MTDS 830
C        INITIALIZE DIVISION PROCESS                                    MTDS 840
    4 MN=M*N                                                            MTDS 850
      MM=M*(M+1)/2                                                      MTDS 860
      MM1=M-1                                                           MTDS 870
      IER=0                                                             MTDS 880
      ICS=M                                                             MTDS 890
      IRS=1                                                             MTDS 900
      IMEND=M                                                           MTDS 910
C                                                                       MTDS 920
C        TEST SPECIFIED OPERATION                                       MTDS 930
      IF(IOP)5,7,4                                                      MTDS 940
    5 MM=N*(N+1)/2                                                      MTDS 950
      MM1=N-1                                                           MTDS 960
      IRS=M                                                             MTDS 970
      ICS=1                                                             MTDS 980
      IMEND=MN-M+1                                                      MTDS 990
      MN=M                                                              MTDS1000
    6 IOP=-MOD(IOP+3,3)                                                 MTDS1010
      IF(IABS(IOP)-3)7,7,2                                              MTDS1020
    7 IF(IOP+1)8,18,9                                                   MTDS1030
C                                                                       MTDS1040
C        INITIALIZE SOLUTION OF TRANSPOSE(T)*X = A                      MTDS1050
    8 MEND=1                                                            MTDS1060
      LLD=IRS                                                           MTDS1070
      MSTA=1                                                            MTDS1080
      MDEL=1                                                            MTDS1090
      MX=1                                                              MTDS1100
      LD=1                                                              MTDS1110
      LX=0                                                              MTDS1120
C                                                                       MTDS1130
C        TEST FOR NUMERICAL DIAGONAL TERM IN T                          MTDS1140
    9 IF(T(MSTA))10,3,10                                                MTDS1150
   10 DO 11 I=MEND,MN,ICS                                               MTDS1160
   11 A(I)=A(I)/T(LD+MSTA)                                              MTDS1170
C                                                                       MTDS1180
C        IS M EQUAL 1                                                   MTDS1190
      IF(MM)12,15,12                                                    MTDS1200
   12 DO 14 J=1,MM1                                                     MTDS1210
      MSTA=MSTA+MDEL                                                    MTDS1220
      MDEL=MDEL+MX                                                      MTDS1230
      DO 14 I=MEND,MN,ICS                                               MTDS1240
      DSUM=0.D0                                                         MTDS1250
      L=MSTA                                                            MTDS1260
      LDX=LD                                                            MTDS1270
      LL=I                                                              MTDS1280
      DO 13 K=1,J                                                       MTDS1290
      DSUM=DSUM+T(L)*A(LL)                                              MTDS1300
      LL=LL+LLD                                                         MTDS1310
      L=L+LDX                                                           MTDS1320
   13 LDX=LDX+LX                                                        MTDS1330
      IF(T(L))14,3,14                                                   MTDS1340
   14 A(LL)=(A(LL)-DSUM)*A(L))/T(L)                                     MTDS1350
C                                                                       MTDS1360
C        TEST KIND OF OPERATION                                         MTDS1370
   15 IF(IOP)16,17,16                                                   MTDS1380
   16 IER=0                                                             MTDS1390
      RETURN                                                            MTDS1400
   17 IF(IOP)13,18,16                                                   MTDS1410
C                                                                       MTDS1420
C        INITIALIZE SOLUTION OF T*X = A                                 MTDS1430
   18 IER=1                                                             MTDS1440
      MEND=IMEND                                                        MTDS1450
      MN=M*N                                                            MTDS1460
      LLD=-IRS                                                          MTDS1470
      MSTA=MM                                                           MTDS1480
      MDEL=-1                                                           MTDS1490
      MX=0                                                              MTDS1500
      LD=-MM1                                                           MTDS1510
      LX=1                                                              MTDS1520
      GOTO 9                                                            MTDS1530
      END                                                               MTDS1540
```

```
C                                                                       DMTD  10
C     ..................................................................DMTD  20
C                                                                       DMTD  30
C        SUBROUTINE DMTDS                                               DMTD  40
C                                                                       DMTD  50
C        PURPOSE                                                        DMTD  60
C           MULTIPLY A GENERAL MATRIX A ON THE LEFT OF RIGHT BY         DMTD  70
C           INVERSE(T),INVERSE(TRANSPOSE(T)) OR INVERSE(TRANSPOSE(T*T)) DMTD  80
C           THE TRIANGULAR MATRIX T IS STORED COLUMNWISE IN COMPRESSED  DMTD  90
C           FORM, I.E. UPPER TRIANGULAR PART ONLY.                      DMTD 100
C                                                                       DMTD 110
C        USAGE                                                          DMTD 120
C           CALL DMTDS(A,M,N,T,IOP,IER)                                 DMTD 130
C                                                                       DMTD 140
C        DESCRIPTION OF PARAMETERS                                      DMTD 150
C           A      - GIVEN GENERAL MATRIX WITH  M ROWS AND N COLUMNS.   DMTD 160
C                    A MUST BE OF DOUBLE PRECISION                      DMTD 170
C           M      - NUMBER OF ROWS OF MATRIX A                         DMTD 180
C           N      - NUMBER OF COLUMNS OF MATRIX A                      DMTD 190
C           T      - GIVEN TRIANGULAR MATRIX STORED COLUMNWISE UPPER    DMTD 200
C                    TRIANGULAR PART ONLY. ITS NUMBER OF ROWS AND       DMTD 210
C                    COLUMNS K IS IMPLIED BY COMPATIBILITY.             DMTD 220
C                    K = M IF IOP IS POSITIVE,                          DMTD 230
C                    K = N IF IOP IS NEGATIVE.                          DMTD 240
C                    T OCCUPIES K*(K+1)/2 STORAGE POSITIONS.            DMTD 250
C                    T MUST BE OF DOUBLE PRECISION                      DMTD 260
C           IOP    - INPUT VARIABLE FOR SELECTION OF OPERATION          DMTD 270
C                    IOP = 1 - A IS REPLACED BY INVERSE(T)*A            DMTD 280
C                    IOP =-1 - A IS REPLACED BY A*INVERSE(T)            DMTD 290
C                    IOP = 2 - A IS REPLACED BY INVERSE(TRANSPOSE(T))*A DMTD 300
C                    IOP =-2 - A IS REPLACED BY A*INVERSE(TRANSPOSE(T)) DMTD 310
C                    IOP = 3 - A IS REPLACED BY INVERSE(TRANSPOSE(T)*T)*ADMTD 320
C                    IOP =-3 - A IS REPLACED BY A*INVERSE(TRANSPOSE(T)*T)DMTD 330
C           IER    - RESULTING ERROR PARAMETER                          DMTD 340
C                    IER =-1 MEANS M AND N ARE NOT BOTH POSITIVE        DMTD 350
C                            AND/OR IOP IS ILLEGAL                      DMTD 360
C                    IER = 0 MEANS OPERATION WAS SUCCESSFUL             DMTD 370
C                    IER = 1 MEANS TRIANGULAR MATRIX T IS SINGULAR      DMTD 380
C                                                                       DMTD 390
C        REMARKS                                                        DMTD 400
C           SUBROUTINE DMTDS MAY BE USED TO CALCULATE THE SOLUTION OF   DMTD 410
C           A SYSTEM OF EQUATIONS WITH SYMMETRIC POSITIVE DEFINITE      DMTD 420
C           COEFFICIENT MATRIX. THE FIRST STEP TOWARDS THE SOLUTION     DMTD 430
C           IS TRIANGULAR FACTORIZATION BY MEANS OF DMFSD. THE SECOND   DMTD 440
C           STEP IS APPLICATION OF DMTDS.                               DMTD 450
C           SUBROUTINES DMFSD AND DMTDS MAY BE USED IN ORDER TO         DMTD 460
C           CALCULATE THE PRODUCT TRANSPOSE(A)*INVERSE(B)*A WITH GIVEN  DMTD 470
C           SYMMETRIC POSITIVE DEFINITE B AND GIVEN A IN THREE STEPS    DMTD 480
C           1) TRIANGULAR FACTORIZATION OF B (B=TRANSPOSE(T)*T)         DMTD 490
C           2) MULTIPLICATION OF A ON THE LEFT BY INVERSE(TRANSPOSE(T)) DMTD 500
C              A IS REPLACED BY C=INVERSE(TRANSPOSE(T))*A               DMTD 510
C           3) CALCULATION OF THE RESULT FORMING TRANSPOSE(C)*C         DMTD 520
C                                                                       DMTD 530
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DMTD 540
C           NONE                                                        DMTD 550
C                                                                       DMTD 560
C        METHOD                                                         DMTD 570
C           CALCULATION OF X = INVERSE(T)*A IS DONE USING BACKWARD      DMTD 580
C           SUBSTITUTION TO OBTAIN X FROM T*X = A.                      DMTD 590
C           CALCULATION OF Y = INVERSE(TRANSPOSE(T))*A IS DONE USING    DMTD 600
C           FORWARD SUBSTITUTION TO OBTAIN Y FROM TRANSPOSE(T)*Y = A.   DMTD 610
C           CALCULATION OF Z = INVERSE(TRANSPOSE(T)*T)*Z IS DONE        DMTD 620
C           SOLVING FIRST TRANSPOSE(T)*Y = A AND THEN T*Z = Y, I.E.     DMTD 630
C           USING THE ABOVE TWO STEPS IN REVERSE ORDER                  DMTD 640
C                                                                       DMTD 650
```

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C     ..................................................................DMTD 660
C                                                                      DMTD 670
      SUBROUTINE DMTDS(A,M,N,T,IOP,IER)                                DMTD 680
C                                                                      DMTD 690
C                                                                      DMTD 700
      DIMENSION A(1),T(1)                                              DMTD 710
      DOUBLE PRECISION DSUM,A,T                                        DMTD 720
C                                                                      DMTD 730
C        TEST OF DIMENSION                                             DMTD 740
      IF(M)2,2,1                                                       DMTD 750
    1 IF(N)2,2,4                                                       DMTD 760
C                                                                      DMTD 770
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSIONS                    DMTD 780
    2 IER=-1                                                           DMTD 790
      RETURN                                                           DMTD 800
C                                                                      DMTD 810
C        ERROR RETURN IN CASE OF SINGULAR MATRIX T                     DMTD 820
    3 IER=1                                                            DMTD 830
      RETURN                                                           DMTD 840
C                                                                      DMTD 850
C        INITIALIZE DIVISION PROCESS                                   DMTD 860
    4 MN=M*N                                                           DMTD 870
      MM=M*(M+1)/2                                                     DMTD 880
      MM1=M-1                                                          DMTD 890
      IER=0                                                            DMTD 900
      ICS=M                                                            DMTD 910
      IRS=1                                                            DMTD 920
      IMEND=M                                                          DMTD 930
C                                                                      DMTD 940
C        TEST SPECIFIED OPERATION                                      DMTD 950
      IF(IOP)5,2,6                                                     DMTD 960
    5 MM=N*(N+1)/2                                                     DMTD 970
      MM1=N-1                                                          DMTD 980
      IRS=M                                                            DMTD 990
      ICS=1                                                            DMTD1000
      IMEND=MN-M+1                                                     DMTD1010
      MN=M                                                             DMTD1020
    6 IOPE=MOD(IOP+3,3)                                                DMTD1030
      IF(IABS(IOP)-3)7,7,2                                             DMTD1040
    7 IF(IOPE-1)8,18,8                                                 DMTD1050
C                                                                      DMTD1060
C        INITIALIZE SOLUTION OF TRANSPOSE(T)*X = A                     DMTD1070
    8 MEND=1                                                           DMTD1080
      LLD=IRS                                                          DMTD1090
      MSTA=1                                                           DMTD1100
      MDEL=1                                                           DMTD1110
      MX=1                                                             DMTD1120
      LD=1                                                             DMTD1130
      LX=0                                                             DMTD1140
C                                                                      DMTD1150
C        TEST FOR NONZERO DIAGONAL TERM IN T                           DMTD1160
    9 IF(T(MSTA))10,3,10                                               DMTD1170
   10 DO 11 I=MEND,MN,ICS                                              DMTD1180
   11 A(I)=A(I)/T(MSTA)                                                DMTD1190
C                                                                      DMTD1200
C        IS M EQUAL 1                                                  DMTD1210
      IF(MM1)2,15,12                                                   DMTD1220
   12 DO 14 J=1,MM1                                                    DMTD1230
      MSTA=MSTA+MDEL                                                   DMTD1240
      MDEL=MDEL+MX                                                     DMTD1250
      DO 14 I=MEND,MN,ICS                                              DMTD1260
      DSUM=0.D0                                                        DMTD1270
      L=MSTA                                                           DMTD1280
      LDX=LD                                                           DMTD1290
      LL=I                                                             DMTD1300
      DO 13 K=1,J                                                      DMTD1310
      DSUM=DSUM-T(L)*A(LL)                                             DMTD1320
      LL=LL+LLD                                                        DMTD1330
      L=L+LDX                                                          DMTD1340
   13 LDX=LDX+LX                                                       DMTD1350
      IF(T(L))14,3,14                                                  DMTD1360
   14 A(LL)=(DSUM+A(LL))/T(L)                                          DMTD1370
C                                                                      DMTD1380
C        TEST END OF OPERATION                                         DMTD1390
   15 IF(IER)16,17,16                                                  DMTD1400
   16 IER=0                                                            DMTD1410
      RETURN                                                           DMTD1420
   17 IF(IOPE)18,18,16                                                 DMTD1430
C                                                                      DMTD1440
C        INITIALIZE SOLUTION OF T*X = A                                DMTD1450
   18 IER=1                                                            DMTD1460
      MEND=IMEND                                                       DMTD1470
      MN=M*N                                                           DMTD1480
      LLD=-IRS                                                         DMTD1490
      MSTA=MM                                                          DMTD1500
      MDEL=-1                                                          DMTD1510
      MX=0                                                             DMTD1520
      LD=-MM1                                                          DMTD1530
      LX=1                                                             DMTD1540
      GOTO 9                                                           DMTD1550
      END                                                              DMTD1560
```

Subroutines MLSS and DMLSS

These subroutines will compute the least-squares solution of minimal length of a system of linear equations

$$AX = R \tag{1}$$

with symmetric positive semidefinite coefficient matrix A. That is, they will determine that vector X of smallest Euclidean length $\|X\|$ for which $\|AX - R\|$ = minimum.

The matrix A is not used directly as input. Instead, MLSS expects the matrices U, T, and T_u and the permutation P that would be obtained if subroutine MFSS were used with A as input matrix (for details see MFSS under "Final result of elimination").

The given vector R is replaced by the solution vector X.

1. Mathematical background

Instead of (1), solve the system of equations:

$$(PAP^T)PX = PR \tag{2}$$

Any solution PX of (2) determines the solution P^{-1} (PX) of (1); therefore it suffices to consider (2).

Using the decomposition:

$$PAP^T = \begin{bmatrix} I & O \\ U^T & I \end{bmatrix} \begin{bmatrix} A_S & O \\ O & O \end{bmatrix} \begin{bmatrix} I & U \\ O & I \end{bmatrix} \tag{3}$$

where $A_S = (T)^T T$ (see MFSS), it is easy to see that (2) is equivalent to the system:

$$A_S(X_1 + UX_2) = R_1 \tag{4}$$

$$OX_2 = R_2 - U^T R_1$$

where $PX = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$ and $PR = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}$. If rank(A) = n, formula (3) reduces to $PAP^T = A_S$, and (4) is

$$A_S X = R \tag{4'}$$

In solving (2), or equivalently (4), three cases must be distinguished:

a. Rank(A) = n. Then the unique solution PX is given by $PX = A_S^{-1} R$, which is computed easily using the triangular decomposition $A_S = (T)^T T$.

b. Rank(A) = r < n and $R_2 = U^T R_1$ (a compatible system). Then the solution of minimal length is:

$$X_1 = (I + UU^T)^{-1} T^{-1(T^{-1})} T R_1$$

$$X_2 = U^T X_1$$

Using the identity $(I + UU^T)^{-1} = I - U(I + U^T U)^{-1} U^T$ and the triangular factorization of $(I + U^T U) = T_u^T T_u$, X_1 may be computed by the following sequence of operations:

$$X_1 = T^{-1}(T^T)^{-1} R_1$$

$$X_2 = T_u^{-1}(T_u^{-1})^T U^T X_1$$

$$X_1 = X_1 - UX_2$$

c. Rank(A) = r< n and $R_2 \neq U^T R_1$ (an incompatible system). Then the least-squares solution of minimal length is:

$$X_1 = (I + UU^T)^{-1} T^{-1} (T^T)^{-1} (I + UU^T)^{-1} (R_1 + UR_2)$$

$$X_2 = U^T X_1$$

X_1 may be computed using the following sequence of operations:

$$X_1 = R_1 + UR_2$$

$$X_2 = -T_u^{-1}(T_u^{-1})^T U^T X_1$$

$$X_1 = T^{-1}(T^T)^{-1}(X_1 + UX_2)$$

$$X_2 = -T_u^{-1}(T_u^{-1})^T U^T X_1$$

$$X_1 = X_1 + UX_2$$

2. Programming considerations

Cases a, b and c above are easily combined into one sequence of operations:

(1) X = PR (interchange given right-hand side)
(2) $X_1 = X_1 + U X_2$
(3) $X_2 = -U^T X_1$
(4) $X_2 = (T_u)^{-1} ((T_u)^T)^{-1} X_2$
(5) $X_1 = X_1 + U X_2$
(6) $X_1 = T^{-1}(T^T)^{-1} X_1$
(7) $X_2 = -U^T X_1$
(8) $X_2 = (T_u)^{-1} ((T_u)^T)^{-1} X_2$
(9) $X_1 = X_1 + U X_2$
(10) $X_2 = (U^T) X_1$
(11) $X = P^{-1} X$ (reinterchange calculated solution)

In case a, the only steps performed are (1), (6), (11).
In case b, only steps (1) and (6) up to (11) are performed.
In case c, all steps are performed.

```
C                                                                       MLSS  10
C     ***************************************************************MLSS  20
C                                                                       MLSS  30
C        SUBROUTINE MLSS                                                MLSS  40
C                                                                       MLSS  50
C        PURPOSE                                                        MLSS  60
C           SUBROUTINE MLSS IS THE SECOND STEP IN THE PROCEDURE FOR     MLSS  70
C           CALCULATING THE LEAST SQUARES SOLUTION OF MINIMAL LENGTH    MLSS  80
C           OF A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH SYMMETRIC MLSS  90
C           POSITIVE SEMI-DEFINITE COEFFICIENT MATRIX.                  MLSS 100
C                                                                       MLSS 110
C        USAGE                                                          MLSS 120
C           CALL MLSS(A,N,IRANK,TRAC,INC,RHS,IER)                       MLSS 130
C                                                                       MLSS 140
C        DESCRIPTION OF PARAMETERS                                      MLSS 150
C           A      - COEFFICIENT MATRIX IN FACTORED FORM AS GENERATED   MLSS 160
C                    BY SUBROUTINE MFSS FROM INITIALLY GIVEN SYMMETRIC  MLSS 170
C                    COEFFICIENT MATRIX A STORED IN N*(N+1)/2 LOCATIONS MLSS 180
C                    A REMAINS UNCHANGED                                MLSS 190
C           N      - DIMENSION OF COEFFICIENT MATRIX                    MLSS 200
C           IRANK  - RANK OF COEFFICIENT MATRIX, CALCULATED BY MEANS OF MLSS 210
C                    SUBROUTINE MFSS                                    MLSS 220
C           TRAC   - VECTOR OF DIMENSION N CONTAINING THE               MLSS 230
C                    SUBSCRIPTS OF PIVOT ROWS AND COLUMNS, I.E. THE     MLSS 240
C                    PRODUCT REPRESENTATION IN TRANSPOSITIONS OF THE    MLSS 250
C                    PERMUTATION WHICH WAS APPLIED TO ROWS AND COLUMNS  MLSS 260
C                    OF A IN THE FACTORIZATION PROCESS                  MLSS 270
C                    TRAC IS A RESULTANT ARRAY OF SUBROUTINE MFSS       MLSS 280
C           INC    - INPUT VARIABLE WHICH SHOULD CONTAIN THE VALUE ZERO MLSS 290
C                    IF THE SYSTEM OF SIMULTANEOUS EQUATIONS IS KNOWN   MLSS 300
C                    TO BE COMPATIBLE AND A NONZERO VALUE OTHERWISE     MLSS 310
C           RHS    - VECTOR OF DIMENSION N CONTAINING THE RIGHT HAND SIDEMLSS 320
C                    ON RETURN RHS CONTAINS THE MINIMAL LENGTH SOLUTION MLSS 330
C           IER    - RESULTANT ERROR PARAMETER                          MLSS 340
C                    IER = 0 MEANS NO ERRORS                            MLSS 350
C                    IER =-1 MEANS N AND/OR IRANK IS NOT POSITIVE AND/OR MLSS 360
C                            IRANK IS GREATER THAN N                    MLSS 370
C                    IER = 1 MEANS THE FACTORIZATION CONTAINED IN A HAS MLSS 380
C                            ZERO DIVISORS AND/OR TRAC CONTAINS         MLSS 390
C                            VALUES OUTSIDE THE FEASIBLE RANGE 1 UP TO N MLSS 400
C                                                                       MLSS 410
C        REMARKS                                                        MLSS 420
C           THE MINIMAL LENGTH SOLUTION IS PRODUCED IN THE STORAGE      MLSS 430
C           LOCATIONS OCCUPIED BY THE RIGHT HAND SIDE.                  MLSS 440
C           SUBROUTINE MLSS DOES TAKE CARE OF THE PERMUTATION           MLSS 450
C           WHICH WAS APPLIED TO ROWS AND COLUMNS OF A.                 MLSS 460
C           OPERATION IS BYPASSED IN CASE OF A NON POSITIVE VALUE       MLSS 470
C           OF IRANK                                                    MLSS 480
C                                                                       MLSS 490
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MLSS 500
C           NONE                                                        MLSS 510
C                                                                       MLSS 520
C        METHOD                                                         MLSS 530
C           LET T, U, TU BE THE COMPONENTS OF THE FACTORIZATION OF A,   MLSS 540
C           AND LET THE RIGHT HAND SIDE B BE PARTITIONED INTO A FIRST   MLSS 550
C           PART X1 OF DIMENSION IRANK AND A SECOND PART X2 OF DIMENSIONMLSS 560
C           N-IRANK. THEN THE FOLLOWING OPERATIONS ARE APPLIED IN       MLSS 570
C           SEQUENCE                                                    MLSS 580
C           (1) INTERCHANGE RIGHT HAND SIDE                             MLSS 590
C           (2) X1 = X1 * U * X2                                        MLSS 600
C           (3) X2 =-TRANSPOSE(U) * X1                                  MLSS 610
C           (4) X2 = INVERSE(TU) * INVERSE(TRANSPOSE(TU)) * X2          MLSS 620
C           (5) X1 = X1 * U * X2                                        MLSS 630
C           (6) X1 = INVERSE(T) * INVERSE(TRANSPOSE(T)) * X1            MLSS 640
C           (7) X2 =-TRANSPOSE(U) * X1                                  MLSS 650
C           (8) X2 = INVERSE(TU) * INVERSE(TRANSPOSE(TU)) * X2          MLSS 660
C           (9) X1 = X1 * U * X2                                        MLSS 670
C           (10)X2 = TRANSPOSE(U) * X1                                  MLSS 680
C           (11) REINTERCHANGE CALCULATED SOLUTION                      MLSS 690
C           IF THE SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS IS SPECIFIED MLSS 700
C           TO BE COMPATIBLE THEN STEPS (2), (3), (4) AND (5) ARE       MLSS 710
C           CANCELLED.                                                  MLSS 720
C           IF THE COEFFICIENT MATRIX HAS RANK N, THEN THE ONLY STEPS   MLSS 730
C           PERFORMED ARE (1), (6) AND (11).                            MLSS 740
C                                                                       MLSS 750
C     ***************************************************************MLSS 760
C                                                                       MLSS 770
      SUBROUTINE MLSS(A,N,IRANK,TRAC,INC,RHS,IER)                       MLSS 780
C                                                                       MLSS 790
C                                                                       MLSS 800
C        DIMENSIONED DUMMY VARIABLES                                    MLSS 810
      DIMENSION A(1),TRAC(1),RHS(1)                                     MLSS 820
      DOUBLE PRECISION SUM                                              MLSS 830
C                                                                       MLSS 840
C        TEST OF SPECIFIED DIMENSIONS                                   MLSS 850
      IDEF=N-IRANK                                                      MLSS 860
      IF(N)33,33,1                                                      MLSS 870
    1 IF(IRANK)33,33,2                                                  MLSS 880
    2 IF(IDEF)33,3,3                                                    MLSS 890
C                                                                       MLSS 900
C        CALCULATE AUXILIARY VALUES                                     MLSS 910
    3 ITE=IRANK*(IRANK+1)/2                                             MLSS 920
      IX2=IRANK+1                                                       MLSS 930
      NP1=N+1                                                           MLSS 940
      IER=0                                                             MLSS 950
C                                                                       MLSS 960
C        INTERCHANGE RIGHT HAND SIDE                                    MLSS 970
      JJ=1                                                              MLSS 980
      II=1                                                              MLSS 990
    4 DO 6 I=1,N                                                        MLSS1000
      J=TRAC(II)                                                        MLSS1010
      IF(J)31,31,5                                                      MLSS1020
    5 HOLD=RHS(II)                                                      MLSS1030
      RHS(II)=RHS(J)                                                    MLSS1040
      RHS(J)=HOLD                                                       MLSS1050
    6 II=II+JJ                                                          MLSS1060
      IF(JJ)32,7,7                                                      MLSS1070
C                                                                       MLSS1080
C        PERFORM STEP 2 IF NECESSARY                                    MLSS1090
    7 ISW=1                                                             MLSS1100
      IF(INC*IDEF)9,28,8                                                MLSS1110
C                                                                       MLSS1120
C        CALCULATE X1 = X1 + U * X2                                     MLSS1130
    8 ISTA=ITE                                                          MLSS1140
      DO 10 I=1,IRANK                                                   MLSS1150
      ISTA=ISTA+1                                                       MLSS1160
      JJ=ISTA                                                           MLSS1170
      SUM=0.00                                                          MLSS1180
      DO 9 J=IX2,N                                                      MLSS1190
      SUM=SUM+A(JJ)*RHS(J)                                              MLSS1200
    9 JJ=JJ+J                                                           MLSS1210
   10 RHS(I)=RHS(I)+SUM                                                 MLSS1220
      GOTO(11,28,11),ISW                                                MLSS1230
C                                                                       MLSS1240
C        CALCULATE X2 = TRANSPOSE(U) * X1                               MLSS1250
   11 ISTA=ITE                                                          MLSS1260
      DO 15 I=IX2,N                                                     MLSS1270
      JJ=ISTA                                                           MLSS1280
      SUM=0.00                                                          MLSS1290
      DO 12 J=1,IRANK                                                   MLSS1300
      JJ=JJ+1                                                           MLSS1310
   12 SUM=SUM+A(JJ)*RHS(J)                                              MLSS1320
      GOTO(13,13,14),ISW                                                MLSS1330
   13 SUM=-SUM                                                          MLSS1340
   14 RHS(I)=SUM                                                        MLSS1350
   15 ISTA=ISTA+I                                                       MLSS1360
      GOTO(16,29,30),ISW                                                MLSS1370
C                                                                       MLSS1380
C        INITIALIZE STEP (4) OR STEP (6)                                MLSS1390
   16 ISTA=IX2                                                          MLSS1400
      IEND=N                                                            MLSS1410
      JJ=ITE+ISTA                                                       MLSS1420
C                                                                       MLSS1430
C        DIVISION OF X1 BY TRANSPOSE OF TRIANGULAR MATRIX               MLSS1440
   17 SUM=0.00                                                          MLSS1450
      DO 20 I=ISTA,IEND                                                 MLSS1460
      IF(A(JJ))18,31,18                                                 MLSS1470
   18 RHS(I)=(RHS(I)-SUM)/A(JJ)                                         MLSS1480
      IF(I-IEND)19,21,21                                                MLSS1490
   19 JJ=JJ+ISTA                                                        MLSS1500
      SUM=0.00                                                          MLSS1510
      DO 20 J=ISTA,I                                                    MLSS1520
      SUM=SUM+A(JJ)*RHS(J)                                              MLSS1530
   20 JJ=JJ+1                                                           MLSS1540
C                                                                       MLSS1550
C        DIVISION OF X1 BY TRIANGULAR MATRIX                            MLSS1560
   21 SUM=0.00                                                          MLSS1570
      II=IEND                                                           MLSS1580
      DO 24 I=ISTA,IEND                                                 MLSS1590
      RHS(II)=(RHS(II)-SUM)/A(JJ)                                       MLSS1600
      IF(II-ISTA)25,25,22                                               MLSS1610
   22 KK=JJ-1                                                           MLSS1620
      SUM=0.00                                                          MLSS1630
      DO 23 J=II,IEND                                                   MLSS1640
      SUM=SUM+A(KK)*RHS(J)                                              MLSS1650
   23 KK=KK+J                                                           MLSS1660
      JJ=JJ-II                                                          MLSS1670
   24 II=II-1                                                           MLSS1680
   25 IF(IDEF)26,30,26                                                  MLSS1690
   26 GOTO(27,11,6),ISW                                                 MLSS1700
C                                                                       MLSS1710
C        PERFORM STEP (5)                                               MLSS1720
   27 ISW=2                                                             MLSS1730
      GOTO 8                                                            MLSS1740
C                                                                       MLSS1750
C        PERFORM STEP (6)                                               MLSS1760
   28 ISTA=1                                                            MLSS1770
      IEND=IRANK                                                        MLSS1780
      JJ=1                                                              MLSS1790
      ISW=2                                                             MLSS1800
      GOTO 17                                                           MLSS1810
C                                                                       MLSS1820
C        PERFORM STEP (8)                                               MLSS1830
   29 ISW=3                                                             MLSS1840
      GOTO 16                                                           MLSS1850
C                                                                       MLSS1860
C        REINTERCHANGE CALCULATED SOLUTION                              MLSS1870
   30 II=N                                                              MLSS1880
      JJ=-1                                                             MLSS1890
      GOTO 4                                                            MLSS1900
C                                                                       MLSS1910
C        ERROR RETURN IN CASE OF ZERO DIVISOR                           MLSS1920
   31 IER=1                                                             MLSS1930
   32 RETURN                                                            MLSS1940
C                                                                       MLSS1950
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSION                      MLSS1960
   33 IER=-1                                                            MLSS1970
      RETURN                                                            MLSS1980
      END                                                               MLSS1990
```

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C                                                                       DMLS  10
C     ***************************************************************DMLS  20
C                                                                       DMLS  30
C        SUBROUTINE DMLSS                                               DMLS  40
C                                                                       DMLS  50
C        PURPOSE                                                        DMLS  60
C           SUBROUTINE DMLSS IS THE SECOND STEP IN THE PROCEDURE FOR    DMLS  70
C           CALCULATING THE LEAST SQUARES SOLUTION OF MINIMAL LENGTH    DMLS  80
C           OF A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH SYMMETRIC DMLS  90
C           POSITIVE SEMI-DEFINITE COEFFICIENT MATRIX.                  DMLS 100
C                                                                       DMLS 110
C        USAGE                                                          DMLS 120
C           CALL DMLSS(A,N,IRANK,TRAC,INC,RHS,IER)                      DMLS 130
C                                                                       DMLS 140
C        DESCRIPTION OF PARAMETERS                                      DMLS 150
C           A      - COEFFICIENT MATRIX IN FACTORED FORM AS GENERATED   DMLS 160
C                    BY SUBROUTINE MFSS FROM INITIALLY GIVEN SYMMETRIC  DMLS 170
C                    COEFFICIENT MATRIX A STORED IN N*(N+1)/2 LOCATIONS DMLS 180
C                    A REMAINS UNCHANGED                                DMLS 190
C                    A MUST BE OF DOUBLE PRECISION                      DMLS 200
C           N      - DIMENSION OF COEFFICIENT MATRIX                    DMLS 210
C           IRANK  - RANK OF COEFFICIENT MATRIX, CALCULATED BY MEANS OF DMLS 220
C                    SUBROUTINE DMFSS                                   DMLS 230
C           TRAC   - VECTOR OF DIMENSION N CONTAINING THE               DMLS 240
C                    SUBSCRIPTS OF PIVOT ROWS AND COLUMNS, I.E. THE     DMLS 250
C                    PRODUCT REPRESENTATION IN TRANSPOSITIONS OF THE    DMLS 260
C                    PERMUTATION WHICH WAS APPLIED TO ROWS AND COLUMNS  DMLS 270
C                    OF A IN THE FACTORIZATION PROCESS                  DMLS 280
C                    TRAC IS A RESULTANT ARRAY OF SUBROUTINE MFSS       DMLS 290
C                    TRAC MUST BE OF DOUBLE PRECISION                   DMLS 300
C           INC    - INPUT VARIABLE WHICH SHOULD CONTAIN THE VALUE ZERO DMLS 310
C                    IF THE SYSTEM OF SIMULTANEOUS EQUATIONS IS KNOWN   DMLS 320
C                    TO BE COMPATIBLE AND A NONZERO VALUE OTHERWISE     DMLS 330
C           RHS    - VECTOR OF DIMENSION N CONTAINING THE RIGHT HAND SIDEDMLS 340
C                    ON RETURN RHS CONTAINS THE MINIMAL LENGTH SOLUTION DMLS 350
C                    RHS MUST BE OF DOUBLE PRECISION                    DMLS 360
C           IER    - RESULTANT ERROR PARAMETER                          DMLS 370
C                    IER = 0 MEANS NO ERRORS                            DMLS 380
C                    IER =-1 MEANS N AND/OR IRANK IS NOT POSITIVE AND/OR DMLS 390
C                            IRANK IS GREATER THAN N                    DMLS 400
C                    IER = 1 MEANS THE FACTORIZATION CONTAINED IN A HAS DMLS 410
C                            ZERO DIVISORS AND/OR TRAC CONTAINS         DMLS 420
C                            VALUES OUTSIDE THE FEASIBLE RANGE 1 UP TO N DMLS 430
C                                                                       DMLS 440
C        REMARKS                                                        DMLS 450
C           THE MINIMAL LENGTH SOLUTION IS PRODUCED IN THE STORAGE      DMLS 460
C           LOCATIONS OCCUPIED BY THE RIGHT HAND SIDE.                  DMLS 470
C           SUBROUTINE DMLSS DOES TAKE CARE OF THE PERMUTATION          DMLS 480
C           WHICH WAS APPLIED TO ROWS AND COLUMNS OF A.                 DMLS 490
C           OPERATION IS BYPASSED IN CASE OF A NON POSITIVE VALUE       DMLS 500
C           OF IRANK                                                    DMLS 510
C                                                                       DMLS 520
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DMLS 530
C           NONE                                                        DMLS 540
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C                                                                       DMLS 550
C       METHOD                                                          DMLS 560
C          LET T, U, TU BE THE COMPONENTS OF THE FACTORIZATION OF A,    DMLS 570
C          AND LET THE RIGHT HAND SIDE BE PARTITIONED INTO A FIRST      DMLS 580
C          PART X1 OF DIMENSION IRANK AND A SECOND PART X2 OF DIMENSIONDMLS 590
C          N-IRANK. THEN THE FOLLOWING OPERATIONS ARE APPLIED IN        DMLS 600
C          SEQUENCE                                                     DMLS 610
C          (1) INTERCHANGE RIGHT HAND SIDE                              DMLS 620
C          (2) X1 = X1 + U * X2                                         DMLS 630
C          (3) X2 =-TRANSPOSE(U) * X1                                   DMLS 640
C          (4) X2 = INVERSE(TU) * INVERSE(TRANSPOSE(TU)) * X2           DMLS 650
C          (5) X1 = X1 + U * X2                                         DMLS 660
C          (6) X1 = INVERSE(T) * INVERSE(TRANSPOSE(T)) * X1             DMLS 670
C          (7) X2 =-TRANSPOSE(U) * X1                                   DMLS 680
C          (8) X2 = INVERSE(TU) * INVERSE(TRANSPOSE(TU)) * X2           DMLS 690
C          (9) X1 = X1 + U * X2                                         DMLS 700
C          (10)X2 = TRANSPOSE(U) * X1                                   DMLS 710
C          (11) REINTERCHANGE CALCULATED SOLUTION                       DMLS 720
C          IF THE SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS IS SPECIFIED  DMLS 730
C          TO BE COMPATIBLE THEN STEPS (2), (3), (4) AND (5) ARE        DMLS 740
C          CANCELLED.                                                   DMLS 750
C          IF THE COEFFICIENT MATRIX HAS RANK N, THEN THE ONLY STEPS    DMLS 760
C          PERFORMED ARE (1), (6) AND (11).                             DMLS 770
C                                                                       DMLS 780
C     ****************************************************************DMLS 790
C                                                                       DMLS 800
      SUBROUTINE DMLSS(A,N,IRANK,TRAC,INC,RHS,IER)                      DMLS 810
C                                                                       DMLS 820
C                                                                       DMLS 830
C        DIMENSIONED DUMMY VARIABLES                                    DMLS 840
      DIMENSION A(1),TRAC(1),RHS(1)                                     DMLS 850
      DOUBLE PRECISION SUM,A,RHS,TRAC,HOLD                              DMLS 860
C                                                                       DMLS 870
C        TEST OF SPECIFIED DIMENSIONS                                   DMLS 880
      IDEF=N-IRANK                                                      DMLS 890
      IF(N)33,33,1                                                      DMLS 900
    1 IF(IRANK)33,33,2                                                  DMLS 910
    2 IF(IDEF)33,3,3                                                    DMLS 920
C                                                                       DMLS 930
C        CALCULATE AUXILIARY VALUES                                     DMLS 940
    3 ITF=IRANK*(IRANK+1)/2                                             DMLS 950
      IX2=IRANK+1                                                       DMLS 960
      NP1=N+1                                                           DMLS 970
      IER=0                                                             DMLS 980
C                                                                       DMLS 990
C        INTERCHANGE RIGHT HAND SIDE                                    DMLS1000
      JJ=1                                                              DMLS1010
      II=1                                                              DMLS1020
    4 DO 6 I=1,N                                                        DMLS1030
      J=TRAC(II)                                                        DMLS1040
      IF(J)31,31,5                                                      DMLS1050
    5 HOLD=RHS(II)                                                      DMLS1060
      RHS(II)=RHS(J)                                                    DMLS1070
      RHS(J)=HOLD                                                       DMLS1080
    6 II=II+JJ                                                          DMLS1090
      IF(JJ)32,7,7                                                      DMLS1100
C                                                                       DMLS1110
C        PERFORM STEP 2 IF NECESSARY                                    DMLS1120
    7 ISW=1                                                             DMLS1130
      IF(INC*IDEF)8,28,8                                                DMLS1140
C                                                                       DMLS1150
C        CALCULATE X1 = X1 + U * X2                                     DMLS1160
    8 ISTA=ITF                                                          DMLS1170
      DO 10 I=1,IRANK                                                   DMLS1180
      ISTA=ISTA+1                                                       DMLS1190
      JJ=ISTA                                                           DMLS1200
      SUM=0.D0                                                          DMLS1210
      DO 9 J=IX2,N                                                      DMLS1220
      SUM=SUM+A(JJ)*RHS(J)                                              DMLS1230
    9 JJ=JJ+J                                                           DMLS1240
   10 RHS(I)=RHS(I)+SUM                                                 DMLS1250
      GOTO(11,29,11),ISW                                                DMLS1260
C                                                                       DMLS1270
C        CALCULATE X2 = TRANSPOSE(U) * X1                               DMLS1280
   11 ISTA=ITF                                                          DMLS1290
      DO 15 I=IX2,N                                                     DMLS1300
      JJ=ISTA                                                           DMLS1310
      SUM=0.D0                                                          DMLS1320
      DO 12 J=1,IRANK                                                   DMLS1330
      JJ=JJ+1                                                           DMLS1340
   12 SUM=SUM+A(JJ)*RHS(J)                                              DMLS1350
      GOTO(13,13,14),ISW                                                DMLS1360
   13 SUM=-SUM                                                          DMLS1370
   14 RHS(I)=SUM                                                        DMLS1380
   15 ISTA=ISTA+I                                                       DMLS1390
      GOTO(16,29,30),ISW                                                DMLS1400
C                                                                       DMLS1410
C        INITIALIZE STEP (4) OR STEP (8)                                DMLS1420
   16 ISTA=IX2                                                          DMLS1430
      IEND=N                                                            DMLS1440
      JJ=ITF+ISTA                                                       DMLS1450
C                                                                       DMLS1460
C        DIVISION OF X1 BY TRANSPOSE OF TRIANGULAR MATRIX               DMLS1470
   17 SUM=0.D0                                                          DMLS1480
      DO 20 I=ISTA,IEND                                                 DMLS1490
      IF(A(JJ))18,31,18                                                 DMLS1500
   18 RHS(I)=(RHS(I)-SUM)/A(JJ)                                         DMLS1510
      IF(I-IEND)19,21,21                                                DMLS1520
   19 JJ=JJ+ISTA                                                        DMLS1530
      SUM=0.D0                                                          DMLS1540
      DO 20 J=ISTA,I                                                    DMLS1550
      SUM=SUM+A(JJ)*RHS(J)                                              DMLS1560
   20 JJ=JJ+1                                                           DMLS1570
C                                                                       DMLS1580
C        DIVISION OF X1 BY TRIANGULAR MATRIX                            DMLS1590
   21 SUM=0.D0                                                          DMLS1600
      II=IEND                                                           DMLS1610
      DO 24 I=ISTA,IEND                                                 DMLS1620
      RHS(II)=(RHS(II)-SUM)/A(JJ)                                       DMLS1630
      IF(II-ISTA)25,25,22                                               DMLS1640
   22 KK=JJ-1                                                           DMLS1650
      SUM=0.D0                                                          DMLS1660
      DO 23 J=II,IEND                                                   DMLS1670
      SUM=SUM+A(KK)*RHS(J)                                              DMLS1680
   23 KK=KK+J                                                           DMLS1690
      JJ=JJ-II                                                          DMLS1700
   24 II=II-1                                                           DMLS1710
   25 IF(IDEF)26,30,26                                                  DMLS1720
   26 GOTO(27,11,8),ISW                                                 DMLS1730
C                                                                       DMLS1740
C        PERFORM STEP (5)                                               DMLS1750
   27 ISW=2                                                             DMLS1760
      GOTO 8                                                            DMLS1770
C                                                                       DMLS1780
C        PERFORM STEP (6)                                               DMLS1790
   28 ISTA=1                                                            DMLS1800
      IEND=IRANK                                                        DMLS1810
      JJ=1                                                              DMLS1820
      ISW=2                                                             DMLS1830
      GOTO 17                                                           DMLS1840
C                                                                       DMLS1850
C        PERFORM STEP (8)                                               DMLS1860
   29 ISW=3                                                             DMLS1870
      GOTO 16                                                           DMLS1880
C                                                                       DMLS1890
C        REINTERCHANGE CALCULATED SOLUTION                              DMLS1900
   30 II=N                                                              DMLS1910
      JJ=-1                                                             DMLS1920
      GOTO 4                                                            DMLS1930
C                                                                       DMLS1940
C        ERROR RETURN IN CASE OF ZERO DIVISOR                           DMLS1950
   31 IER=1                                                             DMLS1960
   32 RETURN                                                            DMLS1970
C                                                                       DMLS1980
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSION                      DMLS1990
   33 IER=-1                                                            DMLS2000
      RETURN                                                            DMLS2010
      END                                                               DMLS2020
```

Subroutines MCHB and DMCHB

These subroutines will compute a triangular factorization

$$A = (T_u)^T T_u \tag{1}$$

of an m by m symmetric positive definite band matrix A. They may also be used to replace a given m by n matrix R by $A^{-1}R$, $T_u^{-1}R$, or $(T_u^{-1})^T R$, depending on the value of an input parameter IOP, as shown in Table 3.

1. Mathematical background

The upper triangular matrix T_u is computed using the following recursive formulas:

$$t_{kj} = (1/t_{kk})\left(a_{kj} - \sum_{i=1}^{k-1} t_{ik}t_{ij}\right) \quad \begin{matrix} k = 1, \ldots, m \\ j = k, k+1, \ldots, m \end{matrix} \tag{2}$$

(Any symbol $\sum_{i=j}^{k} x_i$ is to be interpreted as zero if $j > k$.)

In the special case $j = k$, equation (2) may be written:

$$t_{kk} = \sqrt{a_{kk} - \sum_{i=1}^{k-1} t_{ik}^2}, \quad k = 1, 2, \ldots, m \tag{3}$$

When A is a symmetric band matrix with mud upper codiagonals, all elements a_{kj} are equal to zero if $j > k + mud$. From formulas (2) and (3) it is easy to see that the same is true for t_{kj}:

$$t_{kj} = 0 \text{ if } j > k + mud \tag{4}$$

Therefore formulas (2) and (3) reduce to:

$$t_{kj} = (1/t_{kk})\left(a_{kj} - \sum_{i=i_o}^{k-1} t_{ik}t_{ij}\right) \quad \begin{matrix} k = 1, 2, \ldots, m \\ j = k+1, \ldots, \min(m, k+mud) \end{matrix} \tag{5}$$

$$i_o = \max(1, j-mud)$$

$$t_{kk} = \sqrt{a_{kk} - \sum_{i=i_o}^{k-1} t_{ik}^2} \quad k = 1, 2, \ldots, m \tag{6}$$

$$i_o = \max(1, k-mud)$$

Computing $(T_u^{-1})^T$ is equivalent to solving for Y in the system of equations:

$$T_u^T Y = R \tag{7}$$

The solution of (7) is computed using the following recursive scheme:

$$y_{kj} = (1/t_{kk})\left(r_{kj} - \sum_{i=i_o}^{k-1} t_{ik}y_{ij}\right) \quad \begin{matrix} k = 1, 2, \ldots, m \\ j = 1, 2, \ldots, n \end{matrix} \tag{8}$$

$$i_o = \max(1, k-mud)$$

After each y_{kj} is computed, it may be stored in the location of r_{kj}.

Analogously, computing $T_u^{-1} R$ is the same as solving for X in the system of equations:

$$T_u X = R \tag{9}$$

The solution of (9) is given using a similar recursive scheme:

$$x_{kj} = (1/t_{kk})\left(r_{kj} - \sum_{i=k+1}^{i_o} t_{ki}x_{ij}\right) \quad \begin{matrix} k = m, m-1, \ldots, 1 \\ j = 1, 2, \ldots, n \end{matrix} \tag{10}$$

$$i_o = \min(m, k+mud)$$

$A^{-1}R$ is computed by first computing $S = (T_u^T)^{-1}R$ in the locations of R, and then computing $T_u^{-1}S$, again in the locations of R. If $R = I$, this process replaces R with the inverse A^{-1} of A. Note that in general A^{-1} is no longer a band matrix.

2. Programming considerations

The input matrix A is assumed to be stored in compressed form, that is, main diagonal and mud upper codiagonals rowwise in successive storage locations. Therefore, the total storage requirement for matrix A is $m + mud\,(2m-mud-1)/2$ storage locations. The general m by n matrix R is assumed to be stored columnwise in nm successive storage locations.

The operations performed by the subroutines depend on the actual value of the decision parameter IOP.

Table 3 shows input and output depending on the value of IOP.

Table 3. Dependence of Input and Output on IOP

	IOP	0	1	-1	2	-2	3	-3
INPUT	A in compressed form	A	A	T_u	A	T_u	A	T_u
	R column-wise	irrelevant	R	R	R	R	R	R
OUTPUT	A in compressed form	T_u	T_u	T_u	T_u	T_u	T_u	T_u
	R column-wise	unchanged	$A^{-1}R$	$A^{-1}R$	$T_u^{-1}R$	$T_u^{-1}R$	$(T_u^{-1})^T R$	$(T_u^{-1})^T R$

If IOP is not equal to one of the values listed in Table 3, no action except error message IER = -1 takes place. In this case A and R remain unchanged. The same is true if mud (the number of upper codiagonals of A) is negative or if m (the number of rows of A) is less than 1+mud.

There is one way in which the factorization described above may fail to give a solution, which is easily seen from equation (6). If at any step the radicand of equation (6) is not positive, the procedure is bypassed, and the error message IER = -1 is given. The interpretation may be that matrix A is not positive-definite; however, failure is also possible due to roundoff errors.

Backsubstitutions may fail too, as is easily seen from equations (8) and (10). If any main diagonal element of T_u is equal to zero (this is only possible if T_u is given by input), the procedure is bypassed, and the error message IER = -1 is given.

A further test on possible loss of significance in the factorization part is performed by the subroutines. If at the kth factorization step the radicand of equation (6) is not greater than $|\ EPS.a_{kk}\ |$, with the relative tolerance EPS given by input, the subroutines give the message IER = k-1.

For subroutine MCHB a relative tolerance between 10^{-6} and 10^{-7} is suggested, and for subroutine DMCHB, between 10^{-14} and 10^{-16}. The message IER = k-1, in case EPS = 10^{-D}, means that there are about D or more significant digits lost in the computation of the radicand in formula (6) at the kth factorization step. The interpretation may be that there is loss of significance in the factorized matrix from the kth row on, while the results of rows 1 up to k-1 may be better. Loss of significance in the lower part of the factorized matrix may affect the results of matrix divisions.

For reference see H. Rutishauser, "Algorithmus 1 - Lineares Gleichungs-system mit symmetrischer positiv-definiter Bandmatrix nach Cholesky-Computing," Archives for Electronic Computing, vol. 1, iss. 1 (1966), pp. 77-78.

```
C                                                                       MCHB  10
C  ....................................................................MCHB  20
C                                                                       MCHB  30
C     SUBROUTINE MCHB                                                   MCHB  40
C                                                                       MCHB  50
C     PURPOSE                                                           MCHB  60
C        FOR A GIVEN POSITIVE-DEFINITE N BY M MATRIX A WITH SYMMETRIC   MCHB  70
C        BAND STRUCTURE AND - IF NECESSARY - A GIVEN GENERAL M BY N     MCHB  80
C        MATRIX R, THE FOLLOWING CALCULATIONS (DEPENDENT ON THE         MCHB  90
C        VALUE OF THE DECISION PARAMETER IOP) ARE PERFORMED             MCHB 100
C        (1) MATRIX A IS FACTORIZED (IF IOP IS NOT NEGATIVE), THAT      MCHB 110
C            MEANS BAND MATRIX TU WITH UPPER CODIAGONALS ONLY IS        MCHB 120
C            GENERATED ON THE LOCATIONS OF A SUCH THAT                  MCHB 130
C            TRANSPOSE(TU)*TU=A.                                        MCHB 140
C        (2) MATRIX R IS MULTIPLIED ON THE LEFT BY INVERSE(TU)          MCHB 150
C            AND/OR INVERSE(TRANSPOSE(TU)) AND THE RESULT IS STORED     MCHB 160
C            IN THE LOCATIONS OF R.                                     MCHB 170
C        THIS SUBROUTINE ESPECIALLY CAN BE USED TO SOLVE THE SYSTEM     MCHB 180
C        OF SIMULTANEOUS LINEAR EQUATIONS A*X=R WITH POSITIVE-          MCHB 190
C        DEFINITE COEFFICIENT MATRIX A OF SYMMETRIC BAND STRUCTURE.     MCHB 200
C                                                                       MCHB 210
C     USAGE                                                             MCHB 220
C        CALL MCHB (R,A,M,N,MUD,IOP,EPS,IER)                            MCHB 230
C                                                                       MCHB 240
C     DESCRIPTION OF PARAMETERS                                         MCHB 250
C        R   - INPUT IN CASES IOP=-3,-2,-1,1,2,3  M BY N RIGHT          MCHB 260
C                 HAND SIDE MATRIX,                                     MCHB 270
C                 IN CASE IOP=0  IRRELEVANT.                            MCHB 280
C              OUTPUT IN CASES IOP=1,-1  INVERSE(A)*R,                  MCHB 290
C                      IN CASES IOP=2,-2  INVERSE(TU)*R,                MCHB 300
C                      IN CASES IOP=3,-3  INVERSE(TRANSPOSE(TU))*R,     MCHB 310
C                      IN CASE  IOP=0     UNCHANGED.                    MCHB 320
C        A   - INPUT IN CASES IOP=0,1,2,3 M BY M POSITIVE-DEFINITE      MCHB 330
C                 COEFFICIENT MATRIX OF SYMMETRIC BAND STRUC-           MCHB 340
C                 TURE STORED IN COMPRESSED FORM (SEE REMARKS),         MCHB 350
C                 IN CASES IOP=-1,-2,-3  M BY M BAND MATRIX TU          MCHB 360
C                 WITH UPPER CODIAGONALS ONLY, STORED IN                MCHB 370
C                 COMPRESSED FORM (SEE REMARKS).                        MCHB 380
C              OUTPUT IN ALL CASES  BAND MATRIX TU WITH UPPER           MCHB 390
C                      CODIAGONALS ONLY, STORED IN COMPRESSED FORM      MCHB 400
C                      (THAT MEANS UNCHANGED IF IOP=-1,-2,-3).          MCHB 410
C        M   - INPUT VALUE SPECIFYING THE NUMBER OF ROWS AND            MCHB 420
C              COLUMNS OF A AND THE NUMBER OF ROWS OF R.                MCHB 430
C        N   - INPUT VALUE SPECIFYING THE NUMBER OF COLUMNS OF R        MCHB 440
C              (IRRELEVANT IN CASE IOP=0).                              MCHB 450
C        MUD - INPUT VALUE SPECIFYING THE NUMBER OF UPPER               MCHB 460
C              CODIAGONALS OF A.                                        MCHB 470
C        IOP - ONE OF THE VALUES -3,-2,-1,0,1,2,3 GIVEN AS INPUT        MCHB 480
C              AND USED AS DECISION PARAMETER.                          MCHB 490
C        EPS - INPUT VALUE USED AS RELATIVE TOLERANCE FOR TEST ON       MCHB 500
C              LOSS OF SIGNIFICANT DIGITS.                              MCHB 510
C        IER - RESULTING ERROR PARAMETER CODED AS FOLLOWS               MCHB 520
C                 IER=0  - NO ERROR,                                    MCHB 530
C                 IER=-1 - NO RESULT BECAUSE OF WRONG INPUT             MCHB 540
C                          PARAMETERS M,MUD,IOP (SEE REMARKS),          MCHB 550
C                          OR BECAUSE OF A NONPOSITIVE RADICAND AT      MCHB 560
C                          SOME FACTORIZATION STEP,                     MCHB 570
C                          OR BECAUSE OF A ZERO DIAGONAL ELEMENT        MCHB 580
C                          AT SOME DIVISION STEP.                       MCHB 590
C                 IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-     MCHB 600
C                          CANCE INDICATED AT FACTORIZATION STEP K+1    MCHB 610
C                          WHERE RADICAND WAS NO LONGER GREATER         MCHB 620
C                          THAN EPS*A(K+1,K+1).                         MCHB 630
C                                                                       MCHB 640
C     REMARKS                                                           MCHB 650
C        UPPER PART OF SYMMETRIC BAND MATRIX A CONSISTING OF MAIN       MCHB 660
C        DIAGONAL AND MUD UPPER CODIAGONALS (RESP. BAND MATRIX TU       MCHB 670
C        CONSISTING OF MAIN DIAGONAL AND MUD UPPER CODIAGONALS)         MCHB 680
C        IS ASSUMED TO BE STORED IN COMPRESSED FORM, I.E. ROWWISE       MCHB 690
C        IN TOTALLY NEEDED M*MUD*(2M-MUD-1)/2 SUCCESSIVE STORAGE        MCHB 700
C        LOCATIONS. ON RETURN UPPER BAND FACTOR TU (ON THE LOCATIONS     MCHB 710
C        OF A) IS STORED IN THE SAME WAY.                               MCHB 720
C        RIGHT HAND SIDE MATRIX R IS ASSUMED TO BE STORED COLUMNWISE    MCHB 730
C        IN NM SUCCESSIVE STORAGE LOCATIONS. ON RETURN RESULT MATRIX    MCHB 740
C        INVERSE(A)*R OR INVERSE(TU)*R OR INVERSE(TRANSPOSE(TU))*R      MCHB 750
C        IS STORED COLUMNWISE TOO IN THE LOCATIONS OF R.                MCHB 760
C        INPUT PARAMETERS M, MUD, IOP SHOULD SATISFY THE FOLLOWING      MCHB 770
C        RESTRICTIONS        MUD NOT LESS THAN ZERO,                    MCHB 780
C                            M+MUD NOT GREATER THAN M,                  MCHB 790
C                            ABS(IOP) NOT GREATER THAN 3.               MCHB 800
C        NO ACTION BESIDES ERROR MESSAGE IER=-1 TAKES PLACE IF THESE    MCHB 810
C        RESTRICTIONS ARE NOT SATISFIED.                                MCHB 820
C        THE PROCEDURE GIVES RESULTS IF THE RESTRICTIONS ON INPUT       MCHB 830
C        PARAMETERS ARE SATISFIED, IF RADICANDS AT ALL FACTORIZATION    MCHB 840
C        STEPS ARE POSITIVE AND/OR IF ALL DIAGONAL ELEMENTS OF          MCHB 850
C        UPPER BAND FACTOR TU ARE NONZERO.                              MCHB 860
C                                                                       MCHB 870
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     MCHB 880
C        NONE                                                           MCHB 890
C                                                                       MCHB 900
C     METHOD                                                            MCHB 910
C        FACTORIZATION IS DONE USING CHOLESKY-S SQUARE-ROOT METHOD,     MCHB 920
C        WHICH GENERATES THE UPPER BAND MATRIX TU SUCH THAT             MCHB 930
C        TRANSPOSE(TU)*TU=A. TU IS RETURNED AS RESULT ON THE            MCHB 940
C        LOCATIONS OF A. FURTHER, DEPENDENT ON THE ACTUAL VALUE OF      MCHB 950
C        IOP, DIVISION OF R BY TRANSPOSE(TU) AND/OR TU IS PERFORMED     MCHB 960
C        AND THE RESULT IS RETURNED ON THE LOCATIONS OF R.              MCHB 970
C        FOR REFERENCE, SEE H. RUTISHAUSER, ALGORITHMUS 1 - LINEARES    MCHB 980
C        GLEICHUNGSSYSTEM MIT SYMMETRISCHER POSITIV-DEFINITER           MCHB 990
C        BANDMATRIX NACH CHOLESKY - , COMPUTING (ARCHIVES FOR           MCHB1000
C        ELECTRONIC COMPUTING), VOL.1, ISS.1 (1966), PP.77-78.          MCHB1010
C                                                                       MCHB1020
C  ....................................................................MCHB1030
C                                                                       MCHB1040
      SUBROUTINE MCHER(A,M,N,MUD,IOP,EPS,IER)                           MCHB1050
C                                                                       MCHB1060
C                                                                       MCHB1070
      DIMENSION R(1),A(1)                                               MCHB1080
      DOUBLE PRECISION TOL,SUM,PIV                                      MCHB1090
C                                                                       MCHB1100
C        TEST ON WRONG INPUT PARAMETERS                                 MCHB1110
      IF(IABS(IOP)-3)1,1,43                                             MCHB1120
    1 IF(MUD)43,2,2                                                     MCHB1130
    2 MC=MUD+1                                                          MCHB1140
      IF(M-MC)43,3,3                                                    MCHB1150
    3 MR=M-MUD                                                          MCHB1160
      IER=0                                                             MCHB1170
C                                                                       MCHB1180
C        MC IS THE MAXIMUM NUMBER OF ELEMENTS IN THE ROWS OF ARRAY A    MCHB1190
C        MR IS THE INDEX OF THE LAST ROW IN ARRAY A WITH MC ELEMENTS     MCHB1200
C                                                                       MCHB1210
C  ********************************************************************MCHB1220
C                                                                       MCHB1230
C        START FACTORIZATION OF MATRIX A                                MCHB1240
      IF(IOP)24,4,4                                                     MCHB1250
    4 IEND=0                                                            MCHB1260
      LLOST=MUD                                                         MCHB1270
      DO 23 K=1,M                                                       MCHB1280
      IST=IEND+1                                                        MCHB1290
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```
      IEND=IST+MUD                                                      MCHR1300
      J=K-MR                                                            MCHR1310
      IF(J)6,4,5                                                        MCHR1320
    5 IEND=IEND-J                                                       MCHR1330
    6 IF(J-1)4,4,7                                                      MCHR1340
    7 LLDST=LLDST-1                                                     MCHR1350
    8 LMAX=MUD                                                          MCHR1360
      J=MC-K                                                            MCHR1370
      IF(J)10,10,9                                                      MCHR1380
    9 LMAX=LMAX-J                                                       MCHR1390
   10 ID=0                                                              MCHR1400
      TOL=A(IST)*EPS                                                    MCHR1410
C                                                                       MCHR1420
C        START FACTORIZATION-LOOP OVER K-TH ROW                         MCHR1430
      DO 23 I=IST,IEND                                                  MCHR1440
      SUM=0.D0                                                          MCHR1450
      IF(LMAX)14,14,11                                                  MCHR1460
C                                                                       MCHR1470
C        PREPARE INNER LOOP                                             MCHR1480
   11 LL=IST                                                            MCHR1490
      LLD=LLDST                                                         MCHR1500
C                                                                       MCHR1510
C        START INNER LOOP                                               MCHR1520
      DO 13 L=1,LMAX                                                    MCHR1530
      LL=LL-LLD                                                         MCHR1540
      LLL=LL+ID                                                         MCHR1550
      SUM=SUM+A(LL)*A(LLL)                                              MCHR1560
      IF(LLD-MUD)12,13,13                                               MCHR1570
   12 LLD=LLD+1                                                         MCHR1580
   13 CONTINUE                                                          MCHR1590
C        END OF INNER LOOP                                              MCHR1600
C                                                                       MCHR1610
C        TRANSFORM ELEMENT A(I)                                         MCHR1620
   14 SUM=DBLE(A(I))-SUM                                                MCHR1630
      IF(I-IST)15,15,20                                                 MCHR1640
C                                                                       MCHR1650
C        A(I) IS DIAGONAL ELEMENT, ERROR TEST.                          MCHR1660
   15 IF(SUM)43,43,16                                                   MCHR1670
C                                                                       MCHR1680
C        TEST ON LOSS OF SIGNIFICANT DIGITS AND MARKING                 MCHR1690
   16 IF(SUM-TOL)17,17,19                                               MCHR1700
   17 IF(IER)18,18,19                                                   MCHR1710
   18 IER=-K-1                                                          MCHR1720
C                                                                       MCHR1730
C        COMPUTATION OF PIVOT ELEMENT                                   MCHR1740
   19 PIV=DSQRT(SUM)                                                    MCHR1750
      A(I)=PIV                                                          MCHR1760
      PIV=1.D0/PIV                                                      MCHR1770
      GO TO 21                                                          MCHR1780
C                                                                       MCHR1790
C        A(I) IS NOT DIAGONAL ELEMENT                                   MCHR1800
   20 A(I)=SUM*PIV                                                      MCHR1810
C                                                                       MCHR1820
C        UPDATE ID AND LMAX                                             MCHR1830
   21 ID=ID+1                                                           MCHR1840
      IF(ID-J)22,22,23                                                  MCHR1850
   22 LMAX=LMAX+1                                                       MCHR1860
   23 CONTINUE                                                          MCHR1870
C        END OF FACTORIZATION-LOOP OVER K-TH ROW                        MCHR1880
C        END OF FACTORIZATION OF MATRIX A                               MCHR1890
C                                                                       MCHR1900
C     ****************************************************************MCHR1910
C                                                                       MCHR1920
C        PREPARE MATRIX DIVISIONS                                       MCHR1930
      IF(IDP)26,44,24                                                   MCHR1940
   24 ID=M*M                                                            MCHR1950
      IEND=IABS(IDP)-2                                                  MCHR1960
      IF(IEND)25,35,25                                                  MCHR1970
C                                                                       MCHR1980
C     ****************************************************************MCHR1990
C                                                                       MCHR2000
C        START DIVISION BY TRANSPOSE OF MATRIX TU (TU IS STORED IN      MCHR2010
C        LOCATIONS OF A)                                                MCHR2020
   25 IST=1                                                             MCHR2030
      LMAX=0                                                            MCHR2040
      J=-MR                                                             MCHR2050
      LLDST=MUD                                                         MCHR2060
      DO 34 K=1,N                                                       MCHR2070
      PIV=A(IST)                                                        MCHR2080
      IF(PIV)26,43,26                                                   MCHR2090
   26 PIV=1.D0/PIV                                                      MCHR2100
C                                                                       MCHR2110
C        START BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R           MCHR2120
      DO 30 I=K,ID,M                                                    MCHR2130
      SUM=0.D0                                                          MCHR2140
      IF(LMAX)30,30,27                                                  MCHR2150
C                                                                       MCHR2160
C        PREPARE INNER LOOP                                             MCHR2170
   27 LL=IST                                                            MCHR2180
      LLL=I                                                             MCHR2190
      LLD=LLDST                                                         MCHR2200
C                                                                       MCHR2210
C        START INNER LOOP                                               MCHR2220
      DO 29 L=1,LMAX                                                    MCHR2230
      LL=LL-LLD                                                         MCHR2240
      LLL=LLL-1                                                         MCHR2250
      SUM=SUM+A(LL)*R(LLL)                                              MCHR2260
      IF(LLD-MUD)28,29,29                                               MCHR2270
   28 LLD=LLD+1                                                         MCHR2280
   29 CONTINUE                                                          MCHR2290
C        END OF INNER LOOP                                              MCHR2300
C                                                                       MCHR2310
C        TRANSFORM ELEMENT R(I)                                         MCHR2320
   30 R(I)=PIV*(DBLE(R(I))-SUM)                                         MCHR2330
C        END OF BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R          MCHR2340
C                                                                       MCHR2350
C        UPDATE PARAMETERS LMAX, IST AND LLDST                          MCHR2360
      IF(MC-K)32,32,31                                                  MCHR2370
   31 LMAX=K                                                            MCHR2380
   32 IST=IST+MC                                                        MCHR2390
      J=J+1                                                             MCHR2400
      IF(J)34,34,33                                                     MCHR2410
   33 IST=IST-J                                                         MCHR2420
      LLDST=LLDST-1                                                     MCHR2430
   34 CONTINUE                                                          MCHR2440
C                                                                       MCHR2450
C        END OF DIVISION BY TRANSPOSE OF MATRIX TU                      MCHR2460
C                                                                       MCHR2470
C     ****************************************************************MCHR2480
C                                                                       MCHR2490
C        START DIVISION BY MATRIX TU (TU IS STORED ON LOCATIONS OF A)   MCHR2500
      IF(IEND)35,35,44                                                  MCHR2510
   35 IST=M*(MUD*(M+M-MC))/2+1                                          MCHR2520
      LMAX=0                                                            MCHR2530
      K=M                                                               MCHR2540
   36 IEND=IST-1                                                        MCHR2550
      IST=IEND-LMAX                                                     MCHR2560
      PIV=A(IST)                                                        MCHR2570
      IF(PIV)37,43,37                                                   MCHR2580
   37 PIV=1.D0/PIV                                                      MCHR2590
      L=IST+1                                                           MCHR2600
C                                                                       MCHR2610
C        START BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R           MCHR2620
      DO 40 I=K,ID,M                                                    MCHR2630
      SUM=0.D0                                                          MCHR2640
      IF(LMAX)40,40,38                                                  MCHR2650
   38 LLL=I                                                             MCHR2660
C                                                                       MCHR2670
C        START INNER LOOP                                               MCHR2680
      DO 39 LL=L,IEND                                                   MCHR2690
      LLL=LLL+1                                                         MCHR2700
   39 SUM=SUM+A(LL)*R(LLL)                                              MCHR2710
C        END OF INNER LOOP                                              MCHR2720
C                                                                       MCHR2730
C                                                                       MCHR2740
C        TRANSFORM ELEMENT R(I)                                         MCHR2750
   40 R(I)=PIV*(DBLE(R(I))-SUM)                                         MCHR2760
C        END OF BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R          MCHR2770
C                                                                       MCHR2780
C        UPDATE PARAMETERS LMAX AND K                                   MCHR2790
      IF(K-MU)42,42,41                                                  MCHR2800
   41 LMAX=LMAX+1                                                       MCHR2810
   42 K=K-1                                                             MCHR2820
      IF(K)44,44,36                                                     MCHR2830
C                                                                       MCHR2840
C        END OF DIVISION BY MATRIX TU                                   MCHR2850
C                                                                       MCHR2860
C     ****************************************************************MCHR2870
C                                                                       MCHR2880
C        ERROR EXIT IN CASE OF WRONG INPUT PARAMETERS OR PIVOT ELEMENT  MCHR2890
C        LESS THAN OR EQUAL TO ZERO                                     MCHR2900
   43 IER=-I                                                            MCHR2910
   44 RETURN                                                            MCHR2920
      END                                                               MCHR2930
                                                                        MCHR2940
```

```
C                                                                       DMCH  10
C     ****************************************************************DMCH  20
C                                                                       DMCH  30
C        SUBROUTINE DMCHE                                               DMCH  40
C                                                                       DMCH  50
C        PURPOSE                                                        DMCH  60
C           FOR A GIVEN POSITIVE-DEFINITE M BY M MATRIX A WITH SYMMETRIC DMCH  70
C           BAND STRUCTURE AND - IF NECESSARY - A GIVEN GENERAL M BY N  DMCH  80
C           MATRIX R, THE FOLLOWING CALCULATIONS (DEPENDENT ON THE      DMCH  90
C           VALUE OF THE DECISION PARAMETER IDP) ARE PERFORMED          DMCH 100
C           (1) MATRIX A IS FACTORIZED (IF IDP IS NOT NEGATIVE), THAT   DMCH 110
C               MEANS BAND MATRIX TU WITH UPPER CODIAGONALS ONLY IS     DMCH 120
C               GENERATED ON THE LOCATIONS OF A SUCH THAT               DMCH 130
C               TRANSPOSE(TU)*TU=A.                                     DMCH 140
C           (2) MATRIX R IS MULTIPLIED ON THE LEFT BY INVERSE(TU)       DMCH 150
C               AND/OR INVERSE(TRANSPOSE(TU)) AND THE RESULT IS STORED  DMCH 160
C               IN THE LOCATIONS OF R.                                  DMCH 170
C           THIS SUBROUTINE ESPECIALLY CAN BE USED TO SOLVE THE SYSTEM  DMCH 180
C           OF SIMULTANEOUS LINEAR EQUATIONS A*X=R WITH POSITIVE-       DMCH 190
C           DEFINITE COEFFICIENT MATRIX A OF SYMMETRIC BAND STRUCTURE.  DMCH 200
C                                                                       DMCH 210
C        USAGE                                                          DMCH 220
C           CALL DMCHE (R,A,M,N,MUD,IDP,EPS,IER)                        DMCH 230
C                                                                       DMCH 240
C        DESCRIPTION OF PARAMETERS                                      DMCH 250
C           R      - INPUT IN CASES IDP=-3,-2,-1,1,2,3  DOUBLE PRECISIONDMCH 260
C                    M BY N RIGHT HAND SIDE MATRIX,                     DMCH 270
C                    IN CASE IDP=0  IRRELEVANT.                         DMCH 280
C                  OUTPUT IN CASES IDP=1,-1  INVERSE(A)*R,              DMCH 290
C                    IN CASES IDP=2,-2  INVERSE(TU)*R,                  DMCH 300
C                    IN CASES IDP=3,-3  INVERSE(TRANSPOSE(TU))*R,       DMCH 310
C                    IN CASE  IDP=0     UNCHANGED.                      DMCH 320
C           A      - INPUT IN CASES IDP=0,1,2,3  DOUBLE PRECISION M BY MDMCH 330
C                    POSITIVE-DEFINITE COEFFICIENT MATRIX OF            DMCH 340
C                    SYMMETRIC BAND STRUCTURE STORED IN                 DMCH 350
C                    COMPRESSED FORM (SEE REMARKS),                     DMCH 360
C                    IN CASES IDP=-1,-2,-3 DOUBLE PRECISION M BY MDMCH 370
C                    BAND MATRIX TU WITH UPPER CODIAGONALS ONLY,        DMCH 380
C                    STORED IN COMPRESSED FORM (SEE REMARKS).           DMCH 390
C                  OUTPUT IN ALL CASES  BAND MATRIX TU WITH UPPER       DMCH 400
C                    CODIAGONALS ONLY, STORED IN COMPRESSED FORM DMCH 410
C                    (THAT MEANS UNCHANGED IF IDP=-1,-2,-3).            DMCH 420
C           M      - INPUT VALUE SPECIFYING THE NUMBER OF ROWS AND      DMCH 430
C                    COLUMNS OF A AND THE NUMBER OF ROWS OF R.          DMCH 440
C           N      - INPUT VALUE SPECIFYING THE NUMBER OF COLUMNS OF R  DMCH 450
C                    (IRRELEVANT IF CASE IDP=0).                        DMCH 460
C           MUD    - INPUT VALUE SPECIFYING THE NUMBER OF UPPER         DMCH 470
C                    CODIAGONALS OF A.                                  DMCH 480
C           IDP    - ONE OF THE VALUES -3,-2,-1,0,1,2,3 GIVEN AS INPUT  DMCH 490
C                    AND USED AS DECISION PARAMETER.                    DMCH 500
C           EPS    - SINGLE PRECISION INPUT VALUE USED AS RELATIVE      DMCH 510
C                    TOLERANCE FOR TEST ON LOSS OF SIGNIFICANT DIGITS.  DMCH 520
C           IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS         DMCH 530
C                    IER=0  - NO ERROR,                                 DMCH 540
C                    IER=-1 - NO RESULT BECAUSE OF WRONG INPUT          DMCH 550
C                             PARAMETERS N,MUD,IDP (SEE REMARKS),       DMCH 560
C                             OR BECAUSE OF A NONPOSITIVE RADICAND AT   DMCH 570
C                             SOME FACTORIZATION STEP,                  DMCH 580
C                             OR BECAUSE OF A ZERO DIAGONAL ELEMENT     DMCH 590
C                             AT SOME DIVISION STEP.                    DMCH 600
C                    IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-  DMCH 610
C                             CANCE INDICATED AT FACTORIZATION STEP K+1,DMCH 620
C                             WHERE RADICAND WAS NOT LONGER GREATER     DMCH 630
C                             THAN EPS*A(K+1,K+1).                      DMCH 640
C                                                                       DMCH 650
C        REMARKS                                                        DMCH 660
C           UPPER PART OF SYMMETRIC BAND MATRIX A CONSISTING OF MAIN    DMCH 670
C           DIAGONAL AND MUD UPPER CODIAGONALS (RESP. BAND MATRIX TU    DMCH 680
C           CONSISTING OF MAIN DIAGONAL AND MUD UPPER CODIAGONALS)      DMCH 690
C           IS ASSUMED TO BE STORED IN COMPRESSED FORM, I.E. ONLY       DMCH 700
C           IN TOTALLY NEEDED M*MUD+(2M-MUD-1)/2 SUCCESSIVE STORAGE     DMCH 710
C           LOCATIONS. ON RETURN UPPER BAND FACTOR TU (IN THE LOCATIONS DMCH 720
C           OF A) IS STORED IN THE SAME WAY.                            DMCH 730
C           RIGHT HAND SIDE MATRIX R IS ASSUMED TO BE STORED COLUMNWISE DMCH 740
C           IN NEW SUCCESSIVE STORAGE LOCATIONS. ON RETURN RESULT MATRIXDMCH 750
C           INVERSE(A)*R OR INVERSE(TU)*R OR INVERSE(TRANSPOSE(TU))*R   DMCH 760
C           IS STORED COLUMNWISE TOO IN THE LOCATIONS OF R.             DMCH 770
C           INPUT PARAMETERS M, MUD, IDP SHOULD SATISFY THE FOLLOWING   DMCH 780
C           RESTRICTIONS      MUD NOT LESS THAN ZERO,                   DMCH 790
C                             1+MUD NOT GREATER THAN M,                 DMCH 800
C                             ABS(IDP) NOT GREATER THAN 3.              DMCH 810
C           NO ACTION BESIDES ERROR MESSAGE IER=-1 TAKES PLACE IF THESE DMCH 820
C           RESTRICTIONS ARE NOT SATISFIED.                             DMCH 830
C           THE PROCEDURE GIVES RESULTS IF THE RESTRICTIONS ON INPUT    DMCH 840
C           PARAMETERS ARE SATISFIED, IF RADICANDS AT ALL FACTORIZATION DMCH 850
C           STEPS ARE POSITIVE AND/OR IF ALL DIAGONAL ELEMENTS OF       DMCH 860
C           UPPER BAND FACTOR TU ARE NONZERO.                           DMCH 870
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```
C                                                                       DMCH 880
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DMCH 890
C          NONE                                                         DMCH 900
C                                                                       DMCH 910
C       METHOD                                                          DMCH 920
C          FACTORIZATION IS DONE USING CHOLESKY-S SQUARE-ROOT METHOD,    DMCH 930
C          WHICH GENERATES THE UPPER BAND MATRIX TU SUCH THAT           DMCH 940
C          TRANSPOSE(TU)*TU=A. TU IS STORED AS RESULT ON THE            DMCH 950
C          LOCATIONS OF A. FURTHER, DEPENDENT ON THE ACTUAL VALUE OF    DMCH 960
C          IOP, DIVISION OF R BY TRANSPOSE(TU) AND/OR TU IS PERFORMED   DMCH 970
C          AND THE RESULT IS RETURNED ON THE LOCATIONS OF R.            DMCH 980
C          FOR REFERENCE, SEE H. RUTISHAUSER, ALGORITHMUS 1 -,LINEARES  DMCH 990
C          GLEICHUNGSSYSTEM MIT SYMMETRISCHER POSITIV-DEFINITER         DMCH1000
C          BANDMATRIX NACH CHOLESKY - , COMPUTING (ARCHIVES FOR         DMCH1010
C          ELECTRONIC COMPUTING), VOL.1, ISS.1 (1966), PP.77-78.        DMCH1020
C                                                                       DMCH1030
C     ******************************************************************DMCH1040
C                                                                       DMCH1050
      SUBROUTINE DMCHSER(R,A,M,N,MUD,IOP,EPS,IER)                       DMCH1060
C                                                                       DMCH1070
C                                                                       DMCH1080
      DIMENSION R(1),A(1)                                               DMCH1090
      DOUBLE PRECISION TOL,SUM,PIV,R,A                                  DMCH1100
C                                                                       DMCH1110
C        TEST ON WRONG INPUT PARAMETERS                                 DMCH1120
      IF(IABS(IOP)-3)1,1,43                                             DMCH1130
    1 IF(MUD)43,2,2                                                     DMCH1140
    2 MC=MUD+1                                                          DMCH1150
      IF(M-MC)43,3,3                                                    DMCH1160
    3 MR=M-MUD                                                          DMCH1170
      IER=0                                                             DMCH1180
C                                                                       DMCH1190
C        MC IS THE MAXIMUM NUMBER OF ELEMENTS IN THE ROWS OF ARRAY A    DMCH1200
C        MR IS THE INDEX OF THE LAST ROW IN ARRAY A WITH MC ELEMENTS    DMCH1210
C                                                                       DMCH1220
C     ******************************************************************DMCH1230
C                                                                       DMCH1240
C        START FACTORIZATION OF MATRIX A                                DMCH1250
      IF(IOP)24,4,4                                                     DMCH1260
    4 IEND=0                                                            DMCH1270
      LLDST=MUD                                                         DMCH1280
      DO 21 K=1,M                                                       DMCH1290
      IST=IEND+1                                                        DMCH1300
      IEND=IST+MUD                                                      DMCH1310
      J=K-MR                                                            DMCH1320
      IF(J)6,6,5                                                        DMCH1330
    5 IEND=IEND-J                                                       DMCH1340
    6 IF(J-1)8,8,7                                                      DMCH1350
    7 LLDST=LLDST-1                                                     DMCH1360
    8 LMAX=MUD                                                          DMCH1370
      J=MC-K                                                            DMCH1380
      IF(J)10,10,9                                                      DMCH1390
    9 LMAX=LMAX-J                                                       DMCH1400
   10 ID=0                                                              DMCH1410
      TOL=A(IST)*EPS                                                    DMCH1420
C                                                                       DMCH1430
C        START FACTORIZATION-LOOP OVER K-TH ROW                         DMCH1440
      DO 23 I=IST,IEND                                                  DMCH1450
      SUM=0.D0                                                          DMCH1460
      IF(LMAX)14,14,11                                                  DMCH1470
C                                                                       DMCH1480
C        PREPARE INNER LOOP                                             DMCH1490
   11 LL=IST                                                            DMCH1500
      LLD=LLDST                                                         DMCH1510
C                                                                       DMCH1520
C        START INNER LOOP                                               DMCH1530
      DO 13 L=1,LMAX                                                    DMCH1540
      LL=LL-LLD                                                         DMCH1550
      LLL=LL+ID                                                         DMCH1560
      SUM=SUM+A(LL)*A(LLL)                                              DMCH1570
      IF(LLD-MUD)12,13,13                                               DMCH1580
   12 LLD=LLD+1                                                         DMCH1590
   13 CONTINUE                                                          DMCH1600
C        END OF INNER LOOP                                              DMCH1610
C                                                                       DMCH1620
C        TRANSFORM ELEMENT A(I)                                         DMCH1630
   14 SUM=A(I)-SUM                                                      DMCH1640
      IF(I-IST)15,15,20                                                 DMCH1650
C                                                                       DMCH1660
C        A(I) IS DIAGONAL ELEMENT. ERROR TEST.                          DMCH1670
   15 IF(SUM)43,43,16                                                   DMCH1680
C                                                                       DMCH1690
C        TEST ON LOSS OF SIGNIFICANT DIGITS AND WARNING                 DMCH1700
   16 IF(SUM-TOL)17,17,19                                               DMCH1710
   17 IF(IER)18,18,19                                                   DMCH1720
   18 IER=K-1                                                           DMCH1730
C                                                                       DMCH1740
C        COMPUTATION OF PIVOT ELEMENT                                   DMCH1750
   19 PIV=DSQRT(SUM)                                                    DMCH1760
      A(I)=PIV                                                          DMCH1770
      PIV=1.D0/PIV                                                      DMCH1780
      GO TO 21                                                          DMCH1790
C                                                                       DMCH1800
C        A(I) IS NOT DIAGONAL ELEMENT                                   DMCH1810
   20 A(I)=SUM*PIV                                                      DMCH1820
C                                                                       DMCH1830
C        UPDATE ID AND LMAX                                             DMCH1840
   21 ID=ID+1                                                           DMCH1850
      IF(ID-J)23,23,22                                                  DMCH1860
   22 LMAX=LMAX-1                                                       DMCH1870
   23 CONTINUE                                                          DMCH1880
C                                                                       DMCH1890
C        END OF FACTORIZATION-LOOP OVER K-TH ROW                        DMCH1900
C        END OF FACTORIZATION OF MATRIX A                               DMCH1910
C                                                                       DMCH1920
C     ******************************************************************DMCH1930
C                                                                       DMCH1940
C        PREPARE MATRIX DIVISIONS                                       DMCH1950
      IF(IOP)24,44,24                                                   DMCH1960
   24 ID=N*M                                                            DMCH1970
      IEND=IABS(IOP)-2                                                  DMCH1980
      IF(IEND)25,35,25                                                  DMCH1990
C                                                                       DMCH2000
C     ******************************************************************DMCH2010
C                                                                       DMCH2020
C        START DIVISION BY TRANSPOSE OF MATRIX TU (TU IS STORED IN      DMCH2030
C        LOCATIONS OF A)                                                DMCH2040
   25 IST=1                                                             DMCH2050
      LMAX=0                                                            DMCH2060
      J=-MR                                                             DMCH2070
      LLDST=MUD                                                         DMCH2080
      DO 34 K=1,M                                                       DMCH2090
      PIV=A(IST)                                                        DMCH2100
      IF(PIV)26,43,26                                                   DMCH2110
   26 PIV=1.D0/PIV                                                      DMCH2120
C                                                                       DMCH2130
C        STA-T BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R           DMCH2140
      DO 30 I=K,ID,M                                                    DMCH2150
      SUM=0.D0                                                          DMCH2160
      IF(LMAX)30,30,27                                                  DMCH2170
C                                                                       DMCH2180
C        PREPARE INNER LOOP                                             DMCH2190
   27 LL=IST                                                            DMCH2200
      LLL=I                                                             DMCH2210
      LLD=LLDST                                                         DMCH2220
C                                                                       DMCH2230
C        START INNER LOOP                                               DMCH2240
      DO 29 L=1,LMAX                                                    DMCH2250
      LL=LL-LLD                                                         DMCH2260
      LLL=LLL-1                                                         DMCH2270
      SUM=SUM+A(LL)*R(LLL)                                              DMCH2280
      IF(LLD-MUD)28,29,29                                               DMCH2290
   28 LLD=LLD+1                                                         DMCH2300
   29 CONTINUE                                                          DMCH2310
C        END OF INNER LOOP                                              DMCH2320
C                                                                       DMCH2330
C        TRANSFORM ELEMENT R(I)                                         DMCH2340
   30 R(I)=PIV*(R(I)-SUM)                                               DMCH2350
C        END OF BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R          DMCH2360
C                                                                       DMCH2370
C        UPDATE PARAMETERS LMAX, IST AND LLDST                          DMCH2380
      IF(MC-K)32,32,31                                                  DMCH2390
   31 LMAX=K                                                            DMCH2400
   32 IST=IST+MC                                                        DMCH2410
      J=J+1                                                             DMCH2420
      IF(J)34,34,33                                                     DMCH2430
   33 IST=IST-J                                                         DMCH2440
      LLDST=LLDST-1                                                     DMCH2450
   34 CONTINUE                                                          DMCH2460
C                                                                       DMCH2470
C        END OF DIVISION BY TRANSPOSE OF MATRIX TU                      DMCH2480
C                                                                       DMCH2490
C     ******************************************************************DMCH2500
C                                                                       DMCH2510
C        START DIVISION BY MATRIX TU (TU IS STORED ON LOCATIONS OF A)   DMCH2520
      IF(IEND)35,35,44                                                  DMCH2530
   35 IST=M+(MUD*(M+M-MC))/2+1                                          DMCH2540
      LMAX=0                                                            DMCH2550
      K=M                                                               DMCH2560
   36 IEND=IST-1                                                        DMCH2570
      IST=IEND-LMAX                                                     DMCH2580
      PIV=A(IST)                                                        DMCH2590
      IF(PIV)37,43,37                                                   DMCH2600
   37 PIV=1.D0/PIV                                                      DMCH2610
      L=IST+1                                                           DMCH2620
C                                                                       DMCH2630
C        START BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R           DMCH2640
      DO 40 I=K,ID,M                                                    DMCH2650
      SUM=0.D0                                                          DMCH2660
      IF(LMAX)40,40,38                                                  DMCH2670
   38 LLL=I                                                             DMCH2680
C                                                                       DMCH2690
C        START INNER LOOP                                               DMCH2700
      DO 39 LL=1,IEND                                                   DMCH2710
      LLL=LLL+1                                                         DMCH2720
   39 SUM=SUM+A(LL)*R(LLL)                                              DMCH2730
C        END OF INNER LOOP                                              DMCH2740
C                                                                       DMCH2750
C        TRANSFORM ELEMENT R(I)                                         DMCH2760
   40 R(I)=PIV*(R(I)-SUM)                                               DMCH2770
C        END OF BACKSUBSTITUTION-LOOP FOR K-TH ROW OF MATRIX R          DMCH2780
C                                                                       DMCH2790
C        UPDATE PARAMETERS LMAX AND K                                   DMCH2800
      IF(K-MR)42,42,41                                                  DMCH2810
   41 LMAX=LMAX+1                                                       DMCH2820
   42 K=K-1                                                             DMCH2830
      IF(K)44,44,36                                                     DMCH2840
C                                                                       DMCH2850
C        END OF DIVISION BY MATRIX TU                                   DMCH2860
C                                                                       DMCH2870
C     ******************************************************************DMCH2880
C                                                                       DMCH2890
C        ERROR EXIT IN CASE OF WRONG INPUT PARAMETERS OR PIVOT ELEMENT  DMCH2900
C        LESS THAN OR EQUAL TO ZERO                                     DMCH2910
   43 IER=-1                                                            DMCH2920
   44 RETURN                                                            DMCH2930
      END                                                               DMCH2940
```

Subroutine MFSS and DMFSS

Given a symmetric positive semidefinite matrix A, MFSS will:

(1) Determine the rank and linearly independent rows (and columns)

(2) Compute a triangular factorization of a symmetric submatrix of maximal rank

(3) Express nonbasic rows (and columns) in terms of basic ones and express nonbasic variables in terms of free ones.

1. Mathematical background

The rank is determined using the method of Cholesky (square root method) with pivoting along the main diagonal. Pivoting on diagonal elements means that the same permutation is applied to the rows and columns of A, thereby preserving symmetry. The interchange information is recorded in the auxiliary vector TRAC. The notation A^m is used for the interchanged matrix determined during the mth step. The given matrix A is assumed to be stored column-wise in compressed form, that is, upper triangular part only.

$$A = \begin{bmatrix} a_{11} & a_{12} \cdots & a_{1n} \\ & a_{22} \cdots & a_{2n} \\ & & a_{nn} \end{bmatrix}$$

To allow for easy pivoting, the diagonal terms of A are moved into vector TRAC.

The following two facts will be used repeatedly:

(I) If $S=(s_{ik})$ is symmetric with $s_{11} > 0$, then S admits the unique decomposition:

$$S = \begin{bmatrix} t & 0 \\ V^T & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & D \end{bmatrix} \begin{bmatrix} t & V \\ 0 & I \end{bmatrix} = \tag{1}$$

$$\begin{bmatrix} s_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$$

where $t = \sqrt{s_{11}}$, $V = (1/t)S_{12}$ and $D = S_{22} - V^TV$.

(II) If S is symmetric positive semidefinite:

$$s_{jj} \geq 0 \text{ for all } j \text{ and } |s_{ik}| \leq \max_j(s_{jj}) \text{ for all } i,k \tag{2}$$

a. First step

Let $a_{jj} = \max_i(a_{ii})$. If $a_{jj} = 0$, formula (2) implies $A = 0$, and further calculations are bypassed. Assuming $a_{jj} > 0$, rows 1 and $k_1 = j$ and columns 1 and k_1 of A are interchanged, obtaining A^1. TRAC(k_1) is replaced by TRAC(1), and k_1 is stored in TRAC(1). Decomposition of A^1 gives:

$$A^1 = \begin{bmatrix} A^1_{11} & A^1_{12} \\ A^1_{21} & A^1_{22} \end{bmatrix} = \begin{bmatrix} t^1_{11} & 0 \\ (V^1)^T & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & D^1 \end{bmatrix} \begin{bmatrix} t^1_{11} & V^1 \\ 0 & I \end{bmatrix}$$

where $t^1_{11} = \sqrt{a^1_{11}}$, $V^1 = (1/t^1_{11})A^1_{12}$ and $D^1 = A^1_{22} - (V^1)^TV^1$. D^1 is not calculated explicitly, only its diagonal terms are computed and stored in locations TRAC(2) through TRAC(n).

The first row of A^1 is replaced by t^1_{11}, V^1. The compressed storage scheme now looks like this:

$$\begin{matrix} t^1_{11} & V^1 \\ & A^1_{22} \end{matrix}$$

b. General step

Suppose that after m steps ($1 \leq m < n$) we have determined a transposition vector ($k_1, k_2, \ldots, k_m$), an m by m nonsingular upper triangular matrix:

$$T^m = \begin{bmatrix} t^1_{11} & t^2_{12} \cdots & t^m_{1m} \\ & t^2_{22} \cdots & t^m_{2m} \\ & & t^m_{mm} \end{bmatrix}$$

an m by (n-m) matrix:

$$V^m = \begin{bmatrix} V^m_1 \\ V^m_2 \\ \cdot \\ \cdot \\ \cdot \\ V^m_m \end{bmatrix}$$

and an (n-m) by (n-m) matrix D^m such that:

$$A^m = \begin{bmatrix} A^m_{11} & A^m_{12} \\ A^m_{21} & A^m_{22} \end{bmatrix} = \begin{bmatrix} (T^m)^T & 0 \\ (V^m)^T & I \end{bmatrix} \cdot \begin{bmatrix} I & 0 \\ 0 & D^m \end{bmatrix} \cdot \begin{bmatrix} T^m & V^m \\ 0 & I \end{bmatrix} \quad (3)$$

where $A^m = P^m A (P^m)^T$, and P^m is the permutation matrix associated with the transposition vector $(k_1,\ldots,k_m)$. Again, D^m is not known explicitly, but is computable from:

$$D^m = A^m_{22} - (V^m)^T V^m \quad (4)$$

T^m, V^m and A^m_{22} are assumed to be stored in the following way:

T^m V^m

A^m_{22}

If $A^m_{22} = 0$, it follows from (4) and the fact that D^m is positive semidefinite that $D^m = 0$. Then (3) is the desired factorization, and the process terminates. If $A^m_{22} \neq 0$, there is at least one positive diagonal term a^m_{kk}, and we may compute:

$$t = d^m_{jj}/a^m_{jj} = \max_k \left\{ d^m_{kk}/a^m_{kk} \;\middle|\; a^m_{kk} > 0 \right\}$$

From (4) and (2), $\max_{i,k} \left| d^m_{ik} \right| \leq t \max_{i,k} \left| a^m_{ik} \right|$.

If $t \leq \epsilon$, the norm of D^m is small compared to the norm of A^m_{22}, and we interpret this as $D^m = 0$. Assuming $t > \epsilon$, rows m+1 and $k_{m+1} = m+j$ and columns m+1 and k_{m+1} are interchanged in the compressed storage areas, obtaining

T^m V'^m

A'^m_{22}

TRAC(k_{m+1}) is replaced by TRAC(m+1), and k_{m+1} is stored in TRAC(m+1). As a result of these interchanges:

$$QA^mQ = \begin{bmatrix} (T^m)^T & 0 \\ (V'^m)^T & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & D'^m \end{bmatrix} \begin{bmatrix} T^m & V'^m \\ 0 & I \end{bmatrix} \quad (5)$$

where $D'^m = A'^m_{22} - (V'^m)^T V'^m$, and Q is the permutation matrix associated with the transposition $(m+1, k_{m+1})$. Now decompose D'^m:

$$D'^m = \begin{bmatrix} t^{m+1}_{m+1,m+1} & 0 \\ (V^{m+1}_{m+1})^T & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & D^{m+1} \end{bmatrix} \begin{bmatrix} t^{m+1}_{m+1,m+1} & V^{m+1}_{m+1} \\ 0 & I \end{bmatrix}$$

and store $t^{m+1}_{m+1,m+1}$, V^{m+1}_{m+1} in the first row of A'^m_{22}. Let A^{m+1}_{22} denote the remaining rows and columns of A'^m_{22}, and rename the elements of V'^m as follows:

$$V'^m = \begin{bmatrix} t^{m+1}_{1,m+1} & V^{m+1}_1 \\ t^{m+1}_{m,m+1} & V^{m+1}_m \end{bmatrix}$$

The storage area now looks like this:

T^m $t^{m+1}_{1,m+1}$ V^{m+1}_1

$t^{m+1}_{m+1,m+1}$ V^{m+1}_{m+1}

A^{m+1}_{22}

Let T^{m+1} be the enlarged triangular t-array indicated above, (that is, add the column of t's to T^m), and let V^{m+1} be the V-array. An easy calculation shows that we are back in the situation (3), (4) with m replaced by m+1. This completes step m+1.

c. Final result of elimination

The above process is continued until for some m=r, say, $D^r = 0$ (in the sense mentioned above) or until m=n whichever comes first. In the case r < n, the result is the factorization:

$$A^r = P^r A (P^r)^T = \begin{bmatrix} (T^r)^T & 0 \\ (V^r)^T & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} T^r & V^r \\ 0 & I \end{bmatrix}$$

where P^r is the permutation matrix associated with the permutation:

$$P^r = (r,k_r)(r-1,k_{r-1})..(1,k_1)$$

T^r is nonsingular, and we may compute $U^r = (T^r)^{-1}V^r$ in the same storage locations occupied by V^r. An easy calculation shows:

$$A^r = \begin{bmatrix} I & 0 \\ (U^r)^T & I \end{bmatrix} \begin{bmatrix} A_s & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I & U^r \\ 0 & I \end{bmatrix}$$

where $A_s = (T^r)^T T^r$. We also compute $I + (U^r)^T U^r$ and store it in the last n-r rows and columns of A, producing the storage scheme:

$$\begin{matrix} T^r & U^r \\ I + (U^r)^T U^r \end{matrix}$$

We now operate on $I + (U^r)^T U^r$ in the same way that we operated on A. Whenever it is necessary to interchange two columns of this matrix, we also interchange the same columns of U^r in the storage area. Interchange information is recorded in TRAC (r+1) up to TRAC(n). The foregoing proof establishes a permutation matrix Q and an (n-r) by (n-r) nonsingular upper triangular T_u such that:

$$(T_u)^T T_u = Q(I + (U^r)^T U^r)Q^T = I + (U^r Q^T)^T (U^r Q^T)$$

Let $T = T^r$, $U = U^r Q^T$ and $P^{n-r} = \begin{bmatrix} I & 0 \\ 0 & Q \end{bmatrix}$. An easy calculation then gives the final results:

$$A^n = PAP^T = \begin{bmatrix} I & 0 \\ U^T & I \end{bmatrix} \begin{bmatrix} A_s & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I & U \\ 0 & I \end{bmatrix} \quad (6)$$

$$(T_u)^T T_u = I + U^T U \quad (7)$$

where $P = P^{n-r}P^r$. The final storage scheme is

$$\begin{matrix} T & U \\ & T_u \end{matrix}$$

TRAC contains the permutation P^T in the form of a transposition vector $(k_1, k_2, \ldots, k_n)$.

d. Dependencies among rows and columns

The basic rows of A^n are $A_b = A_s [I, U]$. The nonbasic rows are then $U^T A_b$. Of course basic columns are $(A_b)^T$, and nonbasic columns are $(A_b)^T U$.

e. Systems of equations

Subroutines MFSS and DMFSS may be used to solve systems of equations

$$AX = R$$

with positive semidefinite coefficient matrix A. Using the permutation P, this system is transformed into the system

$$A^n X^n = R^n \quad (8)$$

where $X^n = PX$ and $R^n = PR$. If A has rank r=n, equation (8) is

$$A_s X^n = R^n$$

which is easily solved since $A_s^{-1} = T^{-1}(T^{-1})^T$.

Assuming $r < n$, the vectors X^n, R^n are partitioned as follows:

$$X^n = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \text{ and } R^n = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix},$$

where X_1 consists of the first r elements of X^n, etc. Using the decomposition (6), it is easy to see that (8) is equivalent to:

$$\begin{aligned} A_s(X_1 + UX_2) &= R_1 \\ 0X_2 &= -U^T R_1 + R_2 \end{aligned} \quad (9)$$

(By equivalent systems we mean they have the same solutions.)
If $R_2 = U^T R_1$ (a compatible system), equation (9) has the n-r parameter family of solutions:

$$\begin{aligned} X_1 &= A_s^{-1} R_1 - UX_2 \\ X_2 &= \text{arbitrary} \end{aligned} \quad (10)$$

If $R_2 \neq U^T R_1$ (an incompatible system), it is natural to ask for a least-squares solution of (8), that is a vector X^n such that $\|A^n X^n - R^n\|^2 = \text{minimum}$. This problem leads to the system of equations:

$$(A^n)^2 X^n = A^n R^n \tag{11}$$

Given the factorization (6) of A^n, it is easy to show that $B^n = (A^n)^2$ admits the factorization:

$$B^n = \begin{bmatrix} I & 0 \\ U^T & I \end{bmatrix} \begin{bmatrix} B_s & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I & U \\ 0 & I \end{bmatrix}$$

where $B_s = A_s(I+UU^T)A_s$. Using this fact, (11) is equivalent to:

$$\begin{aligned} B_s(X_1 + UX_2) &= A_s(R_1 + UR_2) \\ 0 \cdot X_2 &= 0 \cdot R_2 \end{aligned} \tag{12}$$

which is clearly a compatible system. Therefore (12) has the solutions:

$$\begin{aligned} X_1 &= B_s^{-1}A_s(R_1 + UR_2) - UX_2 \\ X_2 &= \text{arbitrary} \end{aligned} \tag{13}$$

Now the identity $(I + UU^T)^{-1} = I - U(I + U^TU)^{-1}U^T$ shows that it suffices to know $(I + U^TU)^{-1}$ in order to compute B_s^{-1}. But by (7):

$$(I + U^TU)^{-1} = T_u^{-1}(T_u^{-1})^T$$

and T_u^{-1} is easy to compute, since T_u is upper triangular.

f. Solutions of minimal length

The solutions (10) or (13) contain n-r free parameters X_2, and it is possible to choose them so that X^n has minimal Euclidean length, that is so that $\|X^n\| = \min$. Some easy calculations show that in the compatible case (10), X^n is given by:

$$X_1 = (I + UU^T)^{-1}A_s^{-1}R_1$$

$$X_2 = U^TX_1$$

and in the incompatible case (13), X^n is:

$$X_1 = (I + UU^T)^{-1}A_s^{-1}(I + UU^T)^{-1}(R_1+UR_2)$$

$$X_2 = U^TX_1$$

g. Accuracy

Determining the rank of a matrix on a computer is a difficult matter, and it is not claimed that MFSS will compute the correct rank in all cases. This is an intrinsic difficulty due to the fact that we work with finite arithmetic.

h. Error returns

Normally IRANK contains the computed rank r. A nonpositive value returned in IRANK means:

IRANK = 0 A has no positive diagonal element, or $|\epsilon| \geq 1$.

IRANK = -1 A nonpositive dimension of A was specified.

IRANK = -2 $I + U^TU$ is ill-conditioned and/or the relative tolerance ϵ was specified incorrectly.

```
C                                                                       MFSS  10
C .....................................................................MFSS  20
C                                                                       MFSS  30
C     SUBROUTINE MFSS                                                   MFSS  40
C                                                                       MFSS  50
C     PURPOSE                                                           MFSS  60
C        GIVEN A SYMMETRIC POSITIVE SEMI DEFINITE MATRIX , MFSS WILL    MFSS  70
C        (1) DETERMINE THE RANK AND LINEARLY INDEPENDENT ROWS AND       MFSS  80
C            COLUMNS                                                    MFSS  90
C        (2) FACTOR A SYMMETRIC SUBMATRIX OF MAXIMAL RANK               MFSS 100
C        (3) EXPRESS NONBASIC ROWS IN TERMS OF BASIC ONES.              MFSS 110
C            EXPRESS NONBASIC COLUMNS IN TERMS OF BASIC ONES            MFSS 120
C            EXPRESS BASIC VARIABLES IN TERMS OF FREE ONES              MFSS 130
C        SUBROUTINE MFSS MAY BE USED AS A PREPARATORY STEP FOR THE      MFSS 140
C        CALCULATION OF THE LEAST SQUARES SOLUTION OF MINIMAL           MFSS 150
C        LENGTH OF A SYSTEM OF LINEAR EQUATIONS WITH SYMMETRIC          MFSS 160
C        POSITIVE SEMI-DEFINITE COEFFICIENT MATRIX                      MFSS 170
C                                                                       MFSS 180
C     USAGE                                                             MFSS 190
C        CALL MFSS(A,N,EPS,IRANK,TRAC)                                  MFSS 200
C                                                                       MFSS 210
C     DESCRIPTION OF PARAMETERS                                         MFSS 220
C        A      - UPPER TRIANGULAR PART OF GIVEN SYMMETRIC SEMI-        MFSS 230
C                 DEFINITE MATRIX STORED COLUMNWISE IN COMPRESSED FORM MFSS 240
C                 ON RETURN A CONTAINS THE MATRIX T AND, IF IRANK IS    MFSS 250
C                 LESS THAN N, THE MATRICES U AND TU                    MFSS 260
C        N      - DIMENSION OF GIVEN MATRIX A                          MFSS 270
C        EPS    - TESTVALUE FOR ZERO AFFECTED BY ROUND-OFF NOISE       MFSS 280
C        IRANK  - RESULTANT VARIABLE, CONTAINING THE RANK OF GIVEN     MFSS 290
C                 MATRIX A IF A IS SEMI-DEFINITE                        MFSS 300
C                 IRANK = 0 MEANS A HAS NO POSITIVE DIAGONAL ELEMENT    MFSS 310
C                           AND/OR EPS IS NOT ABSOLUTELY LESS THAN ONE  MFSS 320
C                 IRANK =-1 MEANS DIMENSION N IS NOT POSITIVE           MFSS 330
C                 IRANK =-2 MEANS COMPLETE FAILURE, POSSIBLY DUE TO     MFSS 340
C                           INADEQUATE RELATIVE TOLERANCE EPS           MFSS 350
C        TRAC   - VECTOR OF DIMENSION N CONTAINING THE                 MFSS 360
C                 SOURCE INDEX OF THE I-TH PIVOT ROW IN ITS I-TH        MFSS 370
C                 LOCATION, THIS MEANS THAT TRAC CONTAINS THE           MFSS 380
C                 PRODUCT REPRESENTATION OF THE PERMUTATION WHICH       MFSS 390
C                 IS APPLIED TO ROWS AND COLUMNS OF A IN TERMS OF       MFSS 400
C                 TRANSPOSITIONS                                        MFSS 410
C                                                                       MFSS 420
C     REMARKS                                                           MFSS 430
C        EPS MUST BE ABSOLUTELY LESS THAN ONE. A SENSIBLE VALUE IS      MFSS 440
C        SOMEWHERE IN BETWEEN 10**(-4) AND 10**(-6)                     MFSS 450
C        THE ABSOLUTE VALUE OF INPUT PARAMETER EPS IS USED AS           MFSS 460
C        RELATIVE TOLERANCE.                                            MFSS 470
C        IN ORDER TO PRESERVE SYMMETRY ONLY PIVOTING ALONG THE          MFSS 480
C        DIAGONAL IS BUILT IN.                                          MFSS 490
C        ALL PIVOTELEMENTS MUST BE GREATER THAN THE ABSOLUTE VALUE      MFSS 500
C        OF EPS TIMES ORIGINAL DIAGONAL ELEMENT                         MFSS 510
C        OTHERWISE THEY ARE TREATED AS IF THEY WERE ZERO                MFSS 520
C        MATRIX A REMAINS UNCHANGED IF THE RESULTANT VALUE IRANK        MFSS 530
C        EQUALS ZERO                                                    MFSS 540
C                                                                       MFSS 550
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     MFSS 560
C        NONE                                                           MFSS 570
C                                                                       MFSS 580
C     METHOD                                                            MFSS 590
C        THE SQUARE ROOT METHOD WITH DIAGONAL PIVOTING IS USED FOR      MFSS 600
C        CALCULATION OF THE RIGHT HAND TRIANGULAR FACTOR.               MFSS 610
C        IN CASE OF AN ONLY SEMI-DEFINITE MATRIX THE SUBROUTINE         MFSS 620
C        RETURNS THE IRANK X IRANK UPPER TRIANGULAR FACTOR T OF A       MFSS 630
C        SUBMATRIX OF MAXIMAL RANK, THE IRANK X (N-IRANK) MATRIX U      MFSS 640
C        AND THE (N-IRANK) X (N-IRANK) UPPER TRIANGULAR TU SUCH         MFSS 650
C        THAT TRANSPOSE(TU)*TU=I+TRANSPOSE(U)*U                         MFSS 660
C                                                                       MFSS 670
C .....................................................................MFSS 680
C                                                                       MFSS 690
      SUBROUTINE MFSS(A,N,EPS,IRANK,TRAC)                               MFSS 700
C                                                                       MFSS 710
C                                                                       MFSS 720
C        DIMENSIONED DUMMY VARIABLES                                    MFSS 730
      DIMENSION A(1),TRAC(1)                                            MFSS 740
      DOUBLE PRECISION SUM                                              MFSS 750
C                                                                       MFSS 760
C        TEST OF SPECIFIED DIMENSION                                    MFSS 770
      IF(N)36,36,1                                                      MFSS 780
```

```
C
C          INITIALIZE TRIANGULAR FACTORIZATION
    1 IRANK=0
      ISUB=0
      KPIV=0
      J=0
      PIV=0.
C
C          SEARCH FIRST PIVOT ELEMENT
      DO 3 K=1,N
      J=J+K
      TRAC(K)=A(J)
      IF(A(J)-PIV)3,3,2
    2 PIV=A(J)
      KSUB=J
      KPIV=K
    3 CONTINUE
C
C          START LOOP OVER ALL ROWS OF A
      DO 32 I=1,N
      ISUB=ISUB+I
      IMI=I-1
    4 KMI=KPIV-I
      IF(KMI)35,9,5
C
C          PERFORM PARTIAL COLUMN INTERCHANGE
    5 JI=KSUB-KMI
      IDC=JI-ISUB
      JJ=ISUB-IMI
      DO 6 K=JJ,ISUB
      KK=K+IDC
      HOLD=A(K)
      A(K)=A(KK)
    6 A(KK)=HOLD
C
C          PERFORM PARTIAL ROW INTERCHANGE
      KK=KSUB
      DO 7 K=KPIV,N
      II=KK-KMI
      HOLD=A(KK)
      A(KK)=A(II)
      A(II)=HOLD
    7 KK=KK+K
C
C          PERFORM REMAINING INTERCHANGE
      JJ=KPIV-1
      II=ISUB
      DO 8 K=1,JJ
      HOLD=A(II)
      A(II)=A(JI)
      A(JI)=HOLD
      II=II+K
    8 JI=JI+1
    9 IF(IRANK)22,10,10
C
C          RECORD INTERCHANGE IN TRANSPOSITION VECTOR
   10 TRAC(KPIV)=TRAC(I)
      TRAC(I)=KPIV
C
C          MODIFY CURRENT PIVOT ROW
      KK=IMI-IRANK
      KMI=ISUB-KK
      PIV=0.
      IDC=IRANK+1
      JI=ISUB-1
      JK=KMI
      JJ=ISUB-I
      DO 19 K=I,N
      SUM=0.D0
C
C          BUILD UP SCALAR PRODUCT IF NECESSARY
      IF(KK)13,13,11
   11 DO 12 J=KMI,JI
      SUM=SUM-A(J)*A(JK)
   12 JK=JK+1
   13 JJ=JJ+K
      IF(K-I)14,14,16
   14 SUM=A(ISUB)+SUM
C
C          TEST RADICAND FOR LOSS OF SIGNIFICANCE
      IF(SUM-ABS(A(ISUB)*EPS))20,20,15
   15 A(ISUB)=DSQRT(SUM)
      KPIV=I+1
      GOTO 19
   16 SUM=(A(JK)+SUM)/A(ISUB)
      A(JK)=SUM
C
C          SEARCH FOR NEXT PIVOT ROW
      IF(A(JJ))19,19,17
   17 TRAC(K)=TRAC(K)-SUM*SUM
      HOLD=TRAC(K)/A(JJ)
      IF(PIV-HOLD)18,19,19
   18 PIV=HOLD
      KPIV=K
      KSUB=JJ
   19 JK=JJ+IDC
      GOTO 32
C
C          CALCULATE MATRIX OF DEPENDENCIES U
   20 IF(IRANK)21,21,37
   21 IRANK=-1
      GOTO 4
   22 IRANK=IMI
      II=ISUB-IRANK
      JI=II
      DO 26 K=1,IRANK
      JI=JI-1
      JK=ISUB-1
      JJ=K-1
      DO 26 J=1,N
      IDC=IRANK
      SUM=0.D0
      KMI=JI
      KK=JK
      IF(JJ)25,25,23
   23 DO 24 L=1,JJ
      IDC=IDC-1
      SUM=SUM-A(KMI)*A(KK)
      KMI=KMI-IDC
   24 KK=KK-1
   25 A(KK)=(SUM+A(KK))/A(KMI)
   26 JK=JK+J
C
C          CALCULATE I+TRANSPOSE(U)*U
      JJ=ISUB-I
      PIV=0.
      KK=ISUB-1
      DO 31 K=I,N
      JJ=JJ+K
      IDC=0
      DO 28 J=K,N
      SUM=0.D0
      KMI=JJ+IDC
      DO 27 L=II,KK
      JK=L+IDC
   27 SUM=SUM+A(L)*A(JK)
      A(KMI)=SUM
   28 IDC=IDC+J
      A(JJ)=A(JJ)+1.D0
      TRAC(K)=A(JJ)
C
C          SEARCH NEXT DIAGONAL ELEMENT
      IF(PIV-A(JJ))29,30,30
   29 KPIV=K
      KSUB=JJ
      PIV=A(JJ)
   30 II=II+K
      KK=KK+K
   31 CONTINUE
      GOTO 4
   32 CONTINUE
   33 IF(IRANK)35,34,35
   34 IRANK=N
   35 RETURN
C
C          ERROR RETURNS
C
C          RETURN IN CASE OF ILLEGAL DIMENSION
   36 IRANK=-1
      RETURN
C
C          INSTABLE FACTORIZATION OF I+TRANSPOSE(U)*U
   37 IRANK=-2
      RETURN
      END
```

MFSS 790 … MFSS2430

```
C                                                                       DMSS  10
C  ..................................................................   DMSS  20
C                                                                       DMSS  30
C     SUBROUTINE DMFSS                                                  DMSS  40
C                                                                       DMSS  50
C     PURPOSE                                                           DMSS  60
C        GIVEN A SYMMETRIC POSITIVE SEMI DEFINITE MATRIX, DMFSS WILL    DMSS  70
C        (1) DETERMINE THE RANK AND LINEARLY INDEPENDENT ROWS AND       DMSS  80
C            COLUMNS                                                    DMSS  90
C        (2) FACTOR A SYMMETRIC SUBMATRIX OF MAXIMAL RANK               DMSS 100
C        (3) EXPRESS NONBASIC ROWS IN TERMS OF BASIC ONES,              DMSS 110
C            EXPRESS NONBASIC COLUMNS IN TERMS OF BASIC ONES            DMSS 120
C            EXPRESS BASIC VARIABLES IN TERMS OF FREE ONES              DMSS 130
C        SUBROUTINE DMFSS MAY BE USED AS A PREPARATORY STEP FOR THE     DMSS 140
C        CALCULATION OF THE LEAST SQUARES SOLUTION OF MINIMAL           DMSS 150
C        LENGTH OF A SYSTEM OF LINEAR EQUATIONS WITH SYMMETRIC          DMSS 160
C        POSITIVE SEMI-DEFINITE COEFFICIENT MATRIX                      DMSS 170
C                                                                       DMSS 180
C     USAGE                                                             DMSS 190
C        CALL DMFSSIA,N,EPS,IRANK,TRAC)                                 DMSS 200
C                                                                       DMSS 210
C     DESCRIPTION OF PARAMETERS                                         DMSS 220
C        A      - UPPER TRIANGULAR PART OF GIVEN SYMMETRIC SEMI-        DMSS 230
C                 DEFINITE MATRIX STORED COLUMNWISE IN COMPRESSED FORM  DMSS 240
C                 ON RETURN A CONTAINS THE MATRIX T AND, IF IRANK IS    DMSS 250
C                 LESS THAN N, THE MATRICES U AND TU                    DMSS 260
C                 A MUST BE OF DOUBLE PRECISION                         DMSS 270
C        N      - DIMENSION OF GIVEN MATRIX A                          DMSS 280
C        EPS    - TESTVALUE FOR ZERO AFFECTED BY ROUND-OFF NOISE       DMSS 290
C        IRANK  - RESULTANT VARIABLE, CONTAINING THE RANK OF GIVEN     DMSS 300
C                 MATRIX A IF A IS SEMI-DEFINITE                        DMSS 310
C                 IRANK = 0 MEANS A HAS NO POSITIVE DIAGONAL ELEMENT    DMSS 320
C                           AND/OR EPS IS NOT ABSOLUTELY LESS THAN ONE  DMSS 330
C                 IRANK =-1 MEANS DIMENSION N IS NOT POSITIVE           DMSS 340
C                 IRANK =-2 MEANS COMPLETE FAILURE, POSSIBLY DUE TO     DMSS 350
C                           INADEQUATE RELATIVE TOLERANCE EPS           DMSS 360
C        TRAC   - VECTOR OF DIMENSION N CONTAINING THE                 DMSS 370
C                 SOURCE INDEX OF THE I-TH PIVOT ROW IN ITS I-TH        DMSS 380
C                 LOCATION, THIS MEANS THAT TRAC CONTAINS THE           DMSS 390
C                 PRODUCT REPRESENTATION OF THE PERMUTATION WHICH       DMSS 400
C                 IS APPLIED TO ROWS AND COLUMNS OF A IN TERMS OF       DMSS 410
C                 TRANSPOSITIONS                                        DMSS 420
C                 TRAC MUST BE OF DOUBLE PRECISION                      DMSS 430
C                                                                       DMSS 440
C     REMARKS                                                           DMSS 450
C        EPS MUST BE ABSOLUTELY LESS THAN ONE. A SENSIBLE VALUE IS      DMSS 460
C        SOMEWHERE IN BETWEEN 10**(-4) AND 10**(-6)                     DMSS 470
C        THE ABSOLUTE VALUE OF INPUT PARAMETER EPS IS USED AS           DMSS 480
C        RELATIVE TOLERANCE.                                            DMSS 490
C        IN ORDER TO PRESERVE SYMMETRY ONLY PIVOTING ALONG THE          DMSS 500
C        DIAGONAL IS BUILT IN.                                          DMSS 510
C        ALL PIVOTELEMENTS MUST BE GREATER THAN THE ABSOLUTE VALUE      DMSS 520
C        OF EPS TIMES ORIGINAL DIAGONAL ELEMENT                         DMSS 530
C        OTHERWISE THEY ARE TREATED AS IF THEY WERE ZERO                DMSS 540
C        MATRIX A REMAINS UNCHANGED IF THE RESULTANT VALUE IRANK        DMSS 550
C        EQUALS ZERO                                                    DMSS 560
C                                                                       DMSS 570
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DMSS 580
C        NONE                                                           DMSS 590
C                                                                       DMSS 600
C     METHOD                                                            DMSS 610
C        THE SQUARE ROOT METHOD WITH DIAGONAL PIVOTING IS USED FOR      DMSS 620
C        CALCULATION OF THE RIGHT HAND TRIANGULAR FACTOR T.             DMSS 630
C        IN CASE OF AN ONLY SEMI-DEFINITE MATRIX THE SUBROUTINE         DMSS 640
C        RETURNS THE IRANK X IRANK UPPER TRIANGULAR FACTOR T OF A       DMSS 650
C        SUBMATRIX OF MAXIMAL RANK, THE IRANK X (N-IRANK) MATRIX U      DMSS 660
C        AND THE (N-IRANK) X (N-IRANK) UPPER TRIANGULAR TU SUCH         DMSS 670
C        THAT TRANSPOSE(T)*T=I+TRANSPOSE(U)*U                           DMSS 680
C                                                                       DMSS 690
C  ..................................................................   DMSS 700
      SUBROUTINE DMFSS(A,N,EPS,IRANK,TRAC)                              DMSS 710
C                                                                       DMSS 720
C                                                                       DMSS 730
C        DIMENSIONED DUMMY VARIABLES                                    DMSS 740
      DIMENSION A(1),TRAC(1)                                            DMSS 750
      DOUBLE PRECISION SUM,A,TRAC,PIV,HOLD                              DMSS 760
C                                                                       DMSS 770
C        TEST OF SPECIFIED DIMENSION                                    DMSS 780
      IF(N)36,36,1                                                      DMSS 790
C                                                                       DMSS 800
C        INITIALIZE TRIANGULAR FACTORIZATION                            DMSS 810
    1 IRANK=0                                                           DMSS 820
      ISUB=0                                                            DMSS 830
                                                                        DMSS 840
```

MFSS2080 … MFSS2430

```
      KPIV=0
      J=0
      PIV=0.00
C
C        SEARCH FIRST PIVOT ELEMENT
C
      DO 3 K=1,N
      J=J+K
      TRAC(K)=A(J)
      IF(A(J)-PIV)3,3,2
    2 PIV=A(J)
      KSUB=J
      KPIV=K
    3 CONTINUE
C
C        START LOOP OVER ALL ROWS OF A
C
      DO 32 I=1,N
      ISUB=ISUB+I
      IM1=I-1
    4 KMI=KPIV-I
      IF(KMI)35,9,5
C
C        PERFORM PARTIAL COLUMN INTERCHANGE
C
    5 JI=KSUB-KMI
      IDC=JI-ISUB
      JJ=ISUB-IM1
      DO 6 K=JJ,ISUB
      KK=K+IDC
      HOLD=A(K)
      A(K)=A(KK)
    6 A(KK)=HOLD
C
C        PERFORM PARTIAL ROW INTERCHANGE
C
      KK=KSUB
      DO 7 K=KPIV,N
      II=KK-KMI
      HOLD=A(KK)
      A(KK)=A(II)
      A(II)=HOLD
    7 KK=KK+K
C
C        PERFORM REMAINING INTERCHANGE
C
      JJ=KPIV-1
      II=ISUB
      DO 8 K=1,JJ
      HOLD=A(II)
      A(II)=A(JI)
      A(JI)=HOLD
      II=II+K
    8 JI=JI+1
    9 IF(IRANK)22,10,10
C
C        RECORD INTERCHANGE IN TRANSPOSITION VECTOR
C
   10 TRAC(KPIV)=TRAC(I)
      TRAC(I)=KPIV
C
C        MODIFY CURRENT PIVOT ROW
C
      KK=IM1-IRANK
      KMI=ISUB-KK
      PIV=0.00
      IDC=IRANK+1
      JI=ISUB-I
      JK=KMI
      JJ=ISUB-I
      DO 19 K=I,N
      SUM=0.00
C
C        BUILD UP SCALAR PRODUCT IF NECESSARY
C
      IF(KK)13,13,11
   11 DO 12 J=KMI,JI
      SUM=SUM-A(J)*A(JK)
   12 JK=JK+1
   13 JJ=JJ+K
      IF(K-I)14,14,15
   14 SUM=A(ISUB)+SUM
C
C        TEST RADICAND FOR LOSS OF SIGNIFICANCE
C
      IF(SUM-DABS(A(ISUB)*DBLE(EPS)))20,22,15
   15 A(ISUB)=DSQRT(SUM)
      KPIV=I+1
      GOTO 19
   16 SUM=(A(JK)+SUM)/A(ISUB)
      A(JK)=SUM
C
C        SEARCH FOR NEXT PIVOT ROW
C
      IF(A(JJ))19,19,17
   17 TRAC(K)=TRAC(K)-SUM*SUM
      HOLD=TRAC(K)/A(JJ)
      IF(PIV-HOLD)18,19,19
   18 PIV=HOLD
      KPIV=K
      KSUB=JJ
   19 JK=JJ+IDC
      GOTO 32
C
C        CALCULATE MATRIX OF DEPENDENCIES U
C
   20 IF(IRANK)21,21,37
   21 IRANK=-1
      GOTO 4
   22 IRANK=IM1
      II=ISUB-IRANK
      JI=II
      DO 26 K=1,IRANK
      JI=JI-1
      JK=ISUB-1
      JJ=K-1
      DO 26 J=1,N
      IDC=IRANK
      SUM=0.00
      KMI=JI
      KK=JK
      IF(JJ)25,25,23
   23 DO 24 L=1,JJ
      IDC=IDC-1
      SUM=SUM-A(KMI)*A(KK)
      KMI=KMI-IDC
   24 KK=KK-1
   25 A(KK)=(SUM+A(KK))/A(KMI)
   26 JK=JK+J
C
C        CALCULATE I+TRANSPOSE(U)*U
C
      JJ=ISUB-I
      PIV=0.00
      KK=ISUB-I
      DO 31 K=I,N
      JJ=JJ+K
      IDC=0
      DO 28 J=K,N
      SUM=0.00
      KMI=JJ+IDC
      DO 27 L=II,KK
      JK=L+IDC
   27 SUM=SUM+A(L)*A(JK)
      A(KMI)=SUM
   28 IDC=IDC+J
      A(JJ)=A(JJ)+1.00
      TRAC(K)=A(JJ)
C
C        SEARCH NEXT DIAGONAL ELEMENT
C
      IF(PIV-A(JJ))29,30,30
   29 KPIV=K
      KSUB=JJ
      PIV=A(JJ)
   30 II=II+K
      KK=KK+K
   31 CONTINUE
      GOTO 4
   32 CONTINUE
   33 IF(IRANK)35,34,35
   34 IRANK=N
   35 RETURN
C
C        ERROR RETURNS
C
C        RETURN IN CASE OF ILLEGAL DIMENSION
C
   36 IRANK=-1
      RETURN
C
C        INSTABLE FACTORIZATION OF I+TRANSPOSE(U)*U
C
   37 IRANK=-2
      RETURN
      END
```

Subroutines MFSD and DMFSD

These subroutines will compute a triangular factorization of a symmetric positive definite matrix using the square root method of Cholesky.

1. Mathematical background

Given an n by n symmetric positive definite matrix A, we compute an upper triangular matrix R such that

$$A = R^T R$$

The elements r_{ik} of R are computed using the following recursive formulas:

$$r_{1k} = a_{1k}/r_{11} \qquad k=1,\ 2,\ 3,\ \ldots\ ,\ n$$

$$r_{jk} = (1/r_{jj})\left(a_{jk} - \sum_{i=1}^{j-1} r_{ij}r_{ik}\right) \qquad j=2,\ 3,\ \ldots\ ,\ n$$

$$k=j,\ j+1,\ \ldots\ ,\ n$$

Note: The determinant of A is $\det(A) = \left(\prod_{i=1}^{n} r_{ii}\right)^2$.

2. Programming considerations

The given matrix A is assumed stored columnwise in compressed form, that is upper triangular part only. MFSD stores the solution R in the same locations as A.

If any calculated radicand r_{kk}^2 $(k=1,\ 2,\ \ldots,n)$ is not positive, further calculation is bypassed, and the error parameter IER is set to -1. This means that A is not positive definite, possibly due to roundoff errors. IER is also set to -1 if the input parameter n is less than 1.

Let all radicands be positive and let r_{kk}^2 be the first radicand which is no longer greater than the internal tolerance TOL = $|\text{EPS } a_{kk}|$. The subroutine then gives the warning IER = k-1; however, calculation is continued. The warning indicates that there may be loss of significance at factorization step k due to loss of significant digits in the calculation of r_{kk}^2.

```
C                                                                       MFSD  10
C     ...................................................................MFSD  20
C                                                                       MFSD  30
C        SUBROUTINE MFSD                                                MFSD  40
C                                                                       MFSD  50
C        PURPOSE                                                        MFSD  60
C           FACTOR A GIVEN SYMMETRIC POSITIVE DEFINITE MATRIX           MFSD  70
C                                                                       MFSD  80
C        USAGE                                                          MFSD  90
C           CALL MFSD(A,N,EPS,IER)                                      MFSD 100
C                                                                       MFSD 110
C        DESCRIPTION OF PARAMETERS                                      MFSD 120
C           A      - UPPER TRIANGULAR PART OF THE GIVEN SYMMETRIC       MFSD 130
C                    POSITIVE DEFINITE N BY N COEFFICIENT MATRIX.       MFSD 140
C                    ON RETURN A CONTAINS THE RESULTANT UPPER           MFSD 150
C                    TRIANGULAR MATRIX.                                 MFSD 160
C           N      - THE NUMBER OF ROWS (COLUMNS) IN GIVEN MATRIX.      MFSD 170
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS RELATIVE        MFSD 180
C                    TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.        MFSD 190
C           IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS         MFSD 200
C                    IER=0  - NO ERROR                                  MFSD 210
C                    IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARAME-  MFSD 220
C                             TER N OR BECAUSE SOME RADICAND IS NON-    MFSD 230
C                             POSITIVE (MATRIX A IS NOT POSITIVE        MFSD 240
C                             DEFINITE, POSSIBLY DUE TO LOSS OF SIGNI-  MFSD 250
C                             FICANCE)                                  MFSD 260
C                    IER=K  - WARNING WHICH INDICATES LOSS OF SIGNIFI-  MFSD 270
C                             CANCE. THE RADICAND FORMED AT FACTORIZA-  MFSD 280
C                             TION STEP K+1 WAS STILL POSITIVE BUT NO   MFSD 290
C                             LONGER GREATER THAN ABS(EPS*A(K+1,K+1)).  MFSD 300
C                                                                       MFSD 310
C        REMARKS                                                        MFSD 320
C           THE UPPER TRIANGULAR PART OF GIVEN MATRIX IS ASSUMED TO BE  MFSD 330
C           STORED COLUMNWISE IN N*(N+1)/2 SUCCESSIVE STORAGE LOCATIONS.MFSD 340
C           IN THE SAME STORAGE LOCATIONS THE RESULTING UPPER TRIANGU-   MFSD 350
C           LAR MATRIX IS STORED COLUMNWISE TOO.                        MFSD 360
C           THE PROCEDURE GIVES RESULTS IF N IS GREATER THAN 0 AND ALL  MFSD 370
C           CALCULATED RADICANDS ARE POSITIVE.                          MFSD 380
C           THE PRODUCT OF RETURNED DIAGONAL TERMS IS EQUAL TO THE      MFSD 390
C           SQUARE-ROOT OF THE DETERMINANT OF THE GIVEN MATRIX.         MFSD 400
C                                                                       MFSD 410
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MFSD 420
C           NONE                                                        MFSD 430
C                                                                       MFSD 440
C        METHOD                                                         MFSD 450
C           SOLUTION IS DONE USING THE SQUARE-ROOT METHOD OF CHOLESKY.  MFSD 460
C           THE GIVEN MATRIX IS REPRESENTED AS PRODUCT OF TWO TRIANGULARMFSD 470
C           MATRICES, WHERE THE LEFT HAND FACTOR IS THE TRANSPOSE OF    MFSD 480
C           THE RETURNED RIGHT HAND FACTOR.                             MFSD 490
C                                                                       MFSD 500
C     ...................................................................MFSD 510
C                                                                       MFSD 520
      SUBROUTINE MFSD(A,N,EPS,IER)                                      MFSD 530
C                                                                       MFSD 540
C                                                                       MFSD 550
      DIMENSION A(1)                                                    MFSD 560
      DOUBLE PRECISION DPIV,DSUM                                        MFSD 570
C                                                                       MFSD 580
C        TEST ON WRONG INPUT PARAMETER N                                MFSD 590
      IF(N-1) 12,1,1                                                    MFSD 600
    1 IER=0                                                             MFSD 610
C                                                                       MFSD 620
C        INITIALIZE DIAGONAL-LOOP                                       MFSD 630
      KPIV=0                                                            MFSD 640
      DO 11 K=1,N                                                       MFSD 650
      KPIV=KPIV+K                                                       MFSD 660
      IND=KPIV                                                          MFSD 670
      LEND=K-1                                                          MFSD 680
C                                                                       MFSD 690
C        CALCULATE TOLERANCE                                            MFSD 700
      TOL=ABS(EPS*A(KPIV))                                              MFSD 710
C                                                                       MFSD 720
C        START FACTORIZATION-LOOP OVER K-TH ROW                         MFSD 730
      DO 11 I=K,N                                                       MFSD 740
      DSUM=0.D0                                                         MFSD 750
      IF(LEND) 2,4,2                                                    MFSD 760
C                                                                       MFSD 770
C        START INNER LOOP                                               MFSD 780
    2 DO 3 L=1,LEND                                                     MFSD 790
      LANF=KPIV-L                                                       MFSD 800
      LIND=IND-L                                                        MFSD 810
    3 DSUM=DSUM+DBLE(A(LANF)*A(LIND))                                   MFSD 820
C        END OF INNER LOOP                                              MFSD 830
C                                                                       MFSD 840
C        TRANSFORM ELEMENT A(IND)                                       MFSD 850
    4 DSUM=DBLE(A(IND))-DSUM                                            MFSD 860
      IF(I-K) 10,5,10                                                   MFSD 870
C                                                                       MFSD 880
C        TEST FOR NEGATIVE PIVOT ELEMENT AND FOR LOSS OF SIGNIFICANCE   MFSD 890
    5 IF(SNGL(DSUM)-TOL) 6,6,9                                          MFSD 900
    6 IF(DSUM) 12,12,7                                                  MFSD 910
    7 IF(IER) 8,8,9                                                     MFSD 920
    8 IER=K-1                                                           MFSD 930
C                                                                       MFSD 940
C        COMPUTE PIVOT ELEMENT                                          MFSD 950
    9 DPIV=DSQRT(DSUM)                                                  MFSD 960
      A(KPIV)=DPIV                                                      MFSD 970
      DPIV=1.D0/DPIV                                                    MFSD 980
      GO TO 11                                                          MFSD 990
C                                                                       MFSD1000
C        CALCULATE TERMS IN ROW                                         MFSD1010
   10 A(IND)=DSUM*DPIV                                                  MFSD1020
   11 IND=IND+I                                                         MFSD1030
C                                                                       MFSD1040
C        END OF DIAGONAL-LOOP                                           MFSD1050
      RETURN                                                            MFSD1060
   12 IER=-1                                                            MFSD1070
      RETURN                                                            MFSD1080
      END                                                               MFSD1090
```

```
C                                                                       DMSD  10
C     ***************************************************************.DMSD  20
C                                                                       DMSD  30
      SUBROUTINE DMFSD                                                  DMSD  40
C                                                                       DMSD  50
C     PURPOSE                                                           DMSD  60
C        FACTOR A GIVEN SYMMETRIC POSITIVE DEFINITE MATRIX A            DMSD  70
C                                                                       DMSD  80
C     USAGE                                                             DMSD  90
C        CALL DMFSD(A,N,EPS,IER)                                        DMSD 100
C                                                                       DMSD 110
C     DESCRIPTION OF PARAMETERS                                         DMSD 120
C        A      - DOUBLE PRECISION UPPER TRIANGULAR PART OF GIVEN       DMSD 130
C                 SYMMETRIC POSITIVE DEFINITE N BY N COEFFICIENT       DMSD 140
C                 MATRIX.                                              DMSD 150
C                 ON RETURN A CONTAINS THE RESULTANT UPPER             DMSD 160
C                 TRIANGULAR MATRIX IN DOUBLE PRECISION.               DMSD 170
C        N      - THE NUMBER OF ROWS (COLUMNS) IN GIVEN MATRIX.        DMSD 180
C        EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED        DMSD 190
C                 AS RELATIVE TOLERANCE FOR TEST ON LOSS OF            DMSD 200
C                 SIGNIFICANCE.                                        DMSD 210
C        IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS           DMSD 220
C                 IER=0  - NO ERROR                                    DMSD 230
C                 IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARAME-    DMSD 240
C                          TER N OR BECAUSE SOME RADICAND IS NON-      DMSD 250
C                          POSITIVE (MATRIX A IS NOT POSITIVE          DMSD 260
C                          DEFINITE, POSSIBLY DUE TO LOSS OF SIGNI-    DMSD 270
C                          FICANCE)                                    DMSD 280
C                 IER=K  - WARNING WHICH INDICATES LOSS OF SIGNIFI-    DMSD 290
C                          CANCE. THE RADICAND FORMED AT FACTORIZA-    DMSD 300
C                          TION STEP K+1 WAS STILL POSITIVE BUT NO     DMSD 310
C                          LONGER GREATER THAN ABS(EPS*A(K+1,K+1)).    DMSD 320
C                                                                       DMSD 330
C     REMARKS                                                           DMSD 340
C        THE UPPER TRIANGULAR PART OF GIVEN MATRIX IS ASSUMED TO BE     DMSD 350
C        STORED COLUMNWISE IN N*(N+1)/2 SUCCESSIVE STORAGE LOCATIONS.   DMSD 360
C        IN THE SAME STORAGE LOCATIONS THE RESULTING UPPER TRIANGU-      DMSD 370
C        LAR MATRIX IS STORED COLUMNWISE TOO.                           DMSD 380
C        THE PROCEDURE GIVES RESULTS IF N IS GREATER THAN 0 AND ALL     DMSD 390
C        CALCULATED RADICANDS ARE POSITIVE.                             DMSD 400
C        THE PRODUCT OF RETURNED DIAGONAL TERMS IS EQUAL TO THE         DMSD 410
C        SQUARE-ROOT OF THE DETERMINANT OF THE GIVEN MATRIX.            DMSD 420
C                                                                       DMSD 430
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DMSD 440
C        NONE                                                           DMSD 450
C                                                                       DMSD 460
C     METHOD                                                            DMSD 470
C        SOLUTION IS DONE USING THE SQUARE-ROOT METHOD OF CHOLESKY.     DMSD 480
C        THE GIVEN MATRIX IS REPRESENTED AS PRODUCT OF TWO TRIANGULAR   DMSD 490
C        MATRICES, WHERE THE LEFT HAND FACTOR IS THE TRANSPOSE OF       DMSD 500
C        THE RETURNED RIGHT HAND FACTOR.                                DMSD 510
C                                                                       DMSD 520
C     ***************************************************************.DMSD 530
C                                                                       DMSD 540
      SUBROUTINE DMFSD(A,N,EPS,IER)                                     DMSD 550
C                                                                       DMSD 560
C                                                                       DMSD 570
      DIMENSION A(1)                                                    DMSD 580
      DOUBLE PRECISION DPIV,DSUM,A                                      DMSD 590
C                                                                       DMSD 600
C        TEST ON WRONG INPUT PARAMETER N                                DMSD 610
      IF(N-1) 12,1,1                                                    DMSD 620
    1 IER=0                                                             DMSD 630
C                                                                       DMSD 640
C        INITIALIZE DIAGONAL-LOOP                                       DMSD 650
      KPIV=0                                                            DMSD 660
      DO 11 K=1,N                                                       DMSD 670
      KPIV=KPIV+K                                                       DMSD 680
      IND=KPIV                                                          DMSD 690
      LEND=K-1                                                          DMSD 700
C                                                                       DMSD 710
C        CALCULATE TOLERANCE                                            DMSD 720
      TOL=ABS(EPS*SNGL(A(KPIV)))                                        DMSD 730
C                                                                       DMSD 740
C        START FACTORIZATION-LOOP OVER K-TH ROW                         DMSD 750
      DO 11 I=K,N                                                       DMSD 760
      DSUM=0.D0                                                         DMSD 770
      IF(LEND) 2,4,2                                                    DMSD 780
C                                                                       DMSD 790
C        START INNER LOOP                                               DMSD 800
    2 DO 3 L=1,LEND                                                     DMSD 810
      LANF=KPIV-L                                                       DMSD 820
      LIND=IND-L                                                        DMSD 830
    3 DSUM=DSUM+A(LANF)*A(LIND)                                         DMSD 840
C        END OF INNER LOOP                                              DMSD 850
C                                                                       DMSD 860
C        TRANSFORM ELEMENT A(IND)                                       DMSD 870
    4 DSUM=A(IND)-DSUM                                                  DMSD 880
      IF(I-K) 10,5,10                                                   DMSD 890
C                                                                       DMSD 900
C        TEST FOR NEGATIVE PIVOT ELEMENT AND FOR LOSS OF SIGNIFICANCE   DMSD 910
    5 IF(SNGL(DSUM)-TOL) 6,6,9                                          DMSD 920
    6 IF(DSUM) 12,12,7                                                  DMSD 930
    7 IF(IER) 8,8,9                                                     DMSD 940
    8 IER=K-1                                                           DMSD 950
C                                                                       DMSD 960
C        COMPUTE PIVOT ELEMENT                                          DMSD 970
    9 DPIV=DSQRT(DSUM)                                                  DMSD 980
      A(KPIV)=DPIV                                                      DMSC 990
      DPIV=1.D0/DPIV                                                    DMSD1000
      GO TO 11                                                          DMSD1010
C                                                                       DMSD1020
C        CALCULATE TERMS IN ROW                                         DMSD1030
   10 A(IND)=DSUM*DPIV                                                  DMSD1040
   11 IND=IND+I                                                         DMSD1050
C        END OF DIAGONAL-LOOP                                           DMSD1060
C                                                                       DMSD1070
      RETURN                                                            DMSD1080
   12 IER=-1                                                            DMSD1090
      RETURN                                                            DMSD1100
      END                                                               DMSD1110
```

Subroutines LLSQ and DLLSQ

These subroutines obtain the solution of linear least-squares problems. Consider a real m by n matrix A of rank n ($m \geq n$) with elements a_{ik} ($i = 1,2,\ldots,m$; $k = 1,2,\ldots,n$) and l right-hand side column vectors B_j ($j = 1,2,\ldots,l$) of dimension m, written as an m by l right-hand side matrix B with elements b_{ik} ($i = 1,2,\ldots,m$; $k = 1,2,\ldots,l$). The problem is to determine l column vectors X_j ($j = 1,2,\ldots,l$) of dimension n -- written as an n by l matrix X with elements x_{ik} ($i = 1,2,\ldots,n$; $k = 1,2,\ldots,l$)-- such that:

$$\| B_j - A * X_j \| = \min_j \quad (j = 1,2,\ldots,l) \qquad (1)$$

where $\| R \|$ indicates the Euclidean norm of any column vector R with elements r_i ($i = 1,2,\ldots,m$); that is:

$$\| R \| = \sqrt{\sum_{i=1}^{m} r_i^2} \qquad (2)$$

In the special case m = n, solution of the linear least-squares problem means solution of the system of simultaneous linear equations:

$$A * X = B \qquad (3)$$

Solution of the given problem is based on the well known principle that transformation of any column vector R by an orthogonal matrix Q does not change its norm $\|R\|$; that is:

$$\| Q * R \| = \| R \| \qquad (4)$$

Writing the given problem in the following form:

$$\begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1l} \\ b_{21} & b_{22} & \cdots & b_{2l} \\ b_{31} & b_{32} & \cdots & b_{3l} \\ \vdots & \vdots & & \vdots \\ b_{m1} & b_{m2} & \cdots & b_{ml} \end{pmatrix} - \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ a_{31} & a_{32} & \cdots & a_{3n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix} \cdot$$

$$\begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1l} \\ x_{21} & x_{22} & \cdots & x_{2l} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nl} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1l} \\ r_{21} & r_{22} & \cdots & r_{2l} \\ r_{31} & r_{32} & \cdots & r_{3l} \\ \vdots & \vdots & & \vdots \\ r_{m1} & r_{m2} & \cdots & r_{ml} \end{pmatrix} \qquad (5)$$

the orthogonal transformation matrix Q is determined so that matrix A is transformed to upper triangular form; that is, all elements a_{ik} with $i > k$ are transformed to zero. An effective way to realize this decomposition is via Householder transformations. The algorithm is a recursive n-step procedure defined by the following recursion formulas:

$$A^{(1)} = A \qquad (6)$$

$$A^{(k+1)} = P^{(k)} * A^{(k)} \quad (k = 1,2,\ldots,n) \qquad (7)$$

In order to get an upper triangular matrix $A^{(n+1)}$, every matrix $P^{(k)}$ ($k = 1,2,\ldots,n$) should be defined so that it is symmetric and orthogonal, and so that it transforms all elements of the k^{th} column of $A^{(k)}$ below the main diagonal to zero. All these restrictions to $P^{(k)}$ are satisfied, setting:

$$p^{(k)} = I - \beta_k * U^{(k)} * U^{(k)^T} \qquad (8)$$

with

$$\beta_k = \frac{1}{\sigma_k \, (\sigma_k + a_{kk}^{(k)})} \qquad (9)$$

and

$$\sigma_k = \pm \sqrt{\sum_{i=k}^{m} (a_{ik}^{(k)})^2} \quad \text{with} \begin{cases} + \text{ for } a_{kk}^{(k)} \geq 0 \\ - \text{ for } a_{kk}^{(k)} < 0 \end{cases} \qquad (10)$$

where I is the identity matrix.

$U^{(k)T}$ denotes the transpose of column vector $U^{(k)}$, the m components of which are defined as follows:

$$u_i^{(k)} = 0 \quad \text{for } i < k \tag{11}$$

$$u_k^{(k)} = \sigma_k + a_{kk}^{(k)} \tag{12}$$

$$u_i^{(k)} = a_{ik}^{(k)} \quad \text{for } i > k \tag{13}$$

Neither matrices $P^{(k)}$ $(k = 1,2,\ldots,n)$ nor matrix $Q = P^{(n)} * P^{(n-1)} * \ldots * P^{(1)}$ are computed explicitly, since from (7) and (8):

$$A^{(k+1)} = A^{(k)} - U^{(k)} * Y^{(k)T} \tag{14}$$

with

$$Y^{(k)T} = \beta_k * U^{(k)T} * A^{(k)} \tag{15}$$

Writing the components of row vector $Y^{(k)T}$ explicitly:

$$y_j^{(k)} = 0 \quad \text{for } j < k \tag{16}$$

$$y_k^{(k)} = 1 \tag{17}$$

$$y_j^{(k)} = \beta_k \sum_{i=k}^{m} u_i^{(k)} \cdot a_{ij}^{(k)} \quad \text{for } j > k \tag{18}$$

Using (14), (16), (17), and (18), the explicit transformation formulas for matrix $A^{(k)}$ appear as follows:

$$a_{kk}^{(k+1)} = -\sigma_k \tag{19}$$

$$a_{ik}^{(k+1)} = 0 \qquad (i = k+1, k+2, \ldots, m) \tag{20}$$

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - u_i^{(k)} \cdot y_j^{(k)}$$

$(j = k+1, k+2, \ldots, n$ and for fixed j, $i = k, k+1, \ldots, m)$ (21)

All other elements of matrix $A^{(k)}$ do not change. Naturally, the same transformation is performed on matrix B.

Using (6) and (7):

$$B^{(1)} = B \tag{22}$$

$$B^{(k+1)} = P^{(k)} * B^{(k)} \qquad (k = 1,2,\ldots,n) \tag{23}$$

Using (8) and (23):

$$B^{(k+1)} = B^{(k)} - U^{(k)} * Z^{(k)T} \tag{24}$$

with

$$Z^{(k)T} = \beta_k * U^{(k)T} * B^{(k)} \tag{25}$$

or explicitly:

$$b_{ij}^{(k+1)} = b_{ij}^{(k)} - u_i^{(k)} \cdot z_j^{(k)} \qquad \begin{matrix}(j = 1,2,\ldots,l;\\ i = 1,2,\ldots,m)\end{matrix} \tag{26}$$

with

$$z_j^{(k)} = \beta_k \sum_{i=k}^{m} u_i^{(k)} \cdot b_{ij}^{(k)} \qquad (j = 1,2,\ldots,l) \tag{27}$$

In order to keep roundoff errors as small as possible, column interchange is performed in such a way that, at the k^{th} stage, the column of $A^{(k)}$ is chosen to be reduced next, which will maximize $\left|a_{kk}^{(k+1)}\right|$. Using (19) and (10), the index of this column is determined by giving the maximum overall j of:

$$s_j^{(k)} = \sum_{i=k}^{m} (a_{ij}^{(k)})^2 \qquad (j = k, k+1, \ldots, n) \tag{28}$$

After $A^{(k+1)}$ has been computed, it is possible to compute $s_j^{(k+1)}$ as follows:

$$s_j^{(k+1)} = s_j^{(k)} - (a_{kj}^{(k+1)})^2 \qquad (j = k+1, k+2, \ldots, n) \tag{29}$$

since the orthogonal transformations leave the column lengths invariant.

After having computed matrices $A^{(n+1)}$ (upper triangular matrix) and $B^{(n+1)}$, the computation of the n by l solution matrix X is performed by back substitution according to the following formulas:

$$x_{ni} = \frac{1}{a_{nn}^{(n+1)}} \cdot b_{ni}^{(n+1)} \qquad (i = 1, 2, \ldots, l) \tag{30}$$

$$x_{ki} = \frac{1}{a_{kk}^{(n+1)}} \left(b_{ki}^{(n+1)} - a_{k,k+1}^{(n+1)} \cdot x_{k+1,i} \right.$$

$$- a_{k,k+2}^{(n+1)} \cdot x_{k+2,i} - \ldots - a_{k,n-1}^{(n+1)} \cdot x_{n-1,i}$$

$$\left. - a_{kn}^{(n+1)} \cdot x_{ni} \right)$$

$$(k = n-j+1;\ j = 2, 3, \ldots, n \text{ and}$$
$$i = 1, 2, \ldots, l \text{ for fixed } j) \tag{31}$$

After any row of matrix X has been computed, back interchange of rows is performed according to column interchanges in matrices $A^{(k)}$ in order to get the correct sequence of components in the solution vectors X_j.

Finally, the vector of linear least squares with components

$$lsq_j = \sum_{i=n+1}^{m} (b_{ij}^{(n+1)})^2 \qquad (j = 1, 2, \ldots, l) \tag{32}$$

is computed, which gives the squares of the minimized Euclidean norms $\|B_j - A * X_j\|$ for all right-hand side column vectors B_j $(j = 1, 2, \ldots, l)$.

The only case in which the whole procedure can fail occurs when, at any stage k, no column with nonzero parameter σ_k can be found; that is, no nonzero main diagonal element can be generated. In this case, the rank of matrix A is less than n. With respect to roundoff errors, the test is made in the following way.

At first, all elements $s_j^{(1)}$ are computed according to (28) and the maximum overall j (that is, σ_1^2) is determined. With the relative tolerance ε given by input, the following absolute tolerance is generated:

$$tol = \sigma_1 \cdot \varepsilon \tag{33}$$

If at any stage k $(= 1, 2, \ldots, n+1)$ the square root of the maximum overall $j = k+1, \ldots, n$ of $s_j^{(k+1)}$, say piv, is not greater than tol, the rank of matrix A is declared to be $k < n$, and the procedure returns an error message to the calling program, thus indicating that no solution could be found. In this case, the last n - k elements of vector IPIV denote the useless columns of matrix A; the remaining useful columns form a base of matrix A.

For reference see G. Golub, "Numerical Method for Solving Linear Least Squares Problems", Numerische Mathematik, vol. 7, no. 3 (1965), pp. 206 - 216.

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C                                                                       LLSQ  10
C     ...................................................................LLSQ  20
C                                                                       LLSQ  30
C        SUBROUTINE LLSQ                                                LLSQ  40
C                                                                       LLSQ  50
C        PURPOSE                                                        LLSQ  60
C           TO SOLVE LINEAR LEAST SQUARES PROBLEMS, I.E. TO MINIMIZE    LLSQ  70
C           THE EUCLIDEAN NORM OF B-A*X, WHERE A IS A M BY N MATRIX     LLSQ  80
C           WITH M NOT LESS THAN N. IN THE SPECIAL CASE M=N SYSTEMS OF  LLSQ  90
C           LINEAR EQUATIONS MAY BE SOLVED.                             LLSQ 100
C                                                                       LLSQ 110
C        USAGE                                                          LLSQ 120
C           CALL LLSQ (A,B,M,N,L,X,IPIV,EPS,IER,AUX)                    LLSQ 130
C                                                                       LLSQ 140
C        DESCRIPTION OF PARAMETERS                                      LLSQ 150
C           A      - M BY N COEFFICIENT MATRIX (DESTROYED).             LLSQ 160
C           B      - M BY L RIGHT HAND SIDE MATRIX (DESTROYED).         LLSQ 170
C           M      - ROW NUMBER OF MATRICES A AND B.                    LLSQ 180
C           N      - COLUMN NUMBER OF MATRIX A, ROW NUMBER OF MATRIX X. LLSQ 190
C           L      - COLUMN NUMBER OF MATRICES B AND X.                 LLSQ 200
C           X      - N BY L SOLUTION MATRIX.                            LLSQ 210
C           IPIV   - INTEGER OUTPUT VECTOR OF DIMENSION N WHICH         LLSQ 220
C                    CONTAINS INFORMATIONS ON COLUMN INTERCHANGES        LLSQ 230
C                    IN MATRIX A. (SEE REMARK NO.3).                    LLSQ 240
C           EPS    - INPUT PARAMETER WHICH SPECIFIES A RELATIVE          LLSQ 250
C                    TOLERANCE FOR DETERMINATION OF RANK OF MATRIX A.    LLSQ 260
C           IER    - A RESULTING ERROR PARAMETER.                       LLSQ 270
C           AUX    - AUXILIARY STORAGE ARRAY OF DIMENSION MAX(2*N,L).   LLSQ 280
C                    ON RETURN FIRST L LOCATIONS OF AUX CONTAIN THE      LLSQ 290
C                    RESULTING LEAST SQUARES.                           LLSQ 300
C                                                                       LLSQ 310
C        REMARKS                                                        LLSQ 320
C           (1) NO ACTION BESIDES ERROR MESSAGE IER=-2 IN CASE          LLSQ 330
C               M LESS THAN N.                                          LLSQ 340
C           (2) NO ACTION BESIDES ERROR MESSAGE IER=-1 IN CASE          LLSQ 350
C               OF A ZERO-MATRIX A.                                     LLSQ 360
C           (3) IF RANK K OF MATRIX A IS FOUND TO BE LESS THAN N BUT    LLSQ 370
C               GREATER THAN 0, THE PROCEDURE RETURNS WITH ERROR CODE   LLSQ 380
C               IER=K INTO CALLING PROGRAM. THE LAST N-K ELEMENTS OF    LLSQ 390
C               VECTOR IPIV DENOTE THE USELESS COLUMNS IN MATRIX A.     LLSQ 400
C               THE REMAINING USEFUL COLUMNS FORM A BASE OF MATRIX A.   LLSQ 410
C           (4) IF THE PROCEDURE WAS SUCCESSFUL, ERROR PARAMETER IER    LLSQ 420
C               IS SET TO 0.                                            LLSQ 430
C                                                                       LLSQ 440
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  LLSQ 450
C           NONE                                                        LLSQ 460
C                                                                       LLSQ 470
C        METHOD                                                         LLSQ 480
C           HOUSEHOLDER TRANSFORMATIONS ARE USED TO TRANSFORM MATRIX A  LLSQ 490
C           TO UPPER TRIANGULAR FORM. AFTER HAVING APPLIED THE SAME     LLSQ 500
C           TRANSFORMATION TO THE RIGHT HAND SIDE MATRIX B, AN          LLSQ 510
C           APPROXIMATE SOLUTION OF THE PROBLEM IS COMPUTED BY          LLSQ 520
C           BACK SUBSTITUTION. FOR REFERENCE, SEE                       LLSQ 530
C           G. GOLUB, NUMERICAL METHODS FOR SOLVING LINEAR LEAST        LLSQ 540
C           SQUARES PROBLEMS, NUMERISCHE MATHEMATIK, VOL.7,             LLSQ 550
C           ISS.3 (1965), PP.206-216.                                   LLSQ 560
C                                                                       LLSQ 570
C     ...................................................................LLSQ 580
C                                                                       LLSQ 590
      SUBROUTINE LLSQ(A,B,M,N,L,X,IPIV,EPS,IER,AUX)                     LLSQ 600
C                                                                       LLSQ 610
      DIMENSION A(1),B(1),X(1),IPIV(1),AUX(1)                           LLSQ 620
C                                                                       LLSQ 630
C     ERROR TEST                                                        LLSQ 640
      IF(M-N)30,1,1                                                     LLSQ 650
C                                                                       LLSQ 660
C     GENERATION OF INITIAL VECTOR S(K) (K=1,2,...,N) IN STORAGE        LLSQ 670
C     LOCATIONS AUX(K) (K=1,2,...,N)                                    LLSQ 680
    1 PIV=0.                                                            LLSQ 690
      IEND=0                                                            LLSQ 700
      DO 4 K=1,N                                                        LLSQ 710
      IPIV(K)=K                                                         LLSQ 720
      H=0.                                                              LLSQ 730
      IST=IEND+1                                                        LLSQ 740
      IEND=IEND+M                                                       LLSQ 750
      DO 2 I=IST,IEND                                                   LLSQ 760
    2 H=H+A(I)*A(I)                                                     LLSQ 770
      AUX(K)=H                                                          LLSQ 780
      IF(H-PIV)4,4,3                                                    LLSQ 790
    3 PIV=H                                                             LLSQ 800
      KPIV=K                                                            LLSQ 810
    4 CONTINUE                                                          LLSQ 820
C                                                                       LLSQ 830
C     ERROR TEST                                                        LLSQ 840
      IF(PIV)31,31,5                                                    LLSQ 850
C                                                                       LLSQ 860
C     DEFINE TOLERANCE FOR CHECKING RANK OF A                           LLSQ 870
    5 SIG=SQRT(PIV)                                                     LLSQ 880
      TOL=SIG*ABS(EPS)                                                  LLSQ 890
C                                                                       LLSQ 900
C                                                                       LLSQ 910
C     DECOMPOSITION LOOP                                                LLSQ 920
      LM=L*M                                                            LLSQ 930
      IST=M                                                             LLSQ 940
      DO 21 K=1,N                                                       LLSQ 950
      IST=IST+M+1                                                       LLSQ 960
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      IEND=IST+M-K                                                      LLSQ 970
      I=KPIV-K                                                          LLSQ 980
      IF(I)5,8,6                                                        LLSQ 990
C                                                                       LLSQ1000
C     INTERCHANGE K-TH COLUMN OF A WITH KPIV-TH IN CASE KPIV.GT.K       LLSQ1010
    6 H=AUX(K)                                                          LLSQ1020
      AUX(K)=AUX(KPIV)                                                  LLSQ1030
      AUX(KPIV)=H                                                       LLSQ1040
      ID=I*M                                                            LLSQ1050
      DO 7 I=IST,IEND                                                   LLSQ1060
      J=I+ID                                                            LLSQ1070
      H=A(I)                                                            LLSQ1080
      A(I)=A(J)                                                         LLSQ1090
    7 A(J)=H                                                            LLSQ1100
C                                                                       LLSQ1110
C     COMPUTATION OF PARAMETER SIG                                      LLSQ1120
    8 IF(K-1)11,11,9                                                    LLSQ1130
    9 SIG=0.                                                            LLSQ1140
      DO 10 I=IST,IEND                                                  LLSQ1150
   10 SIG=SIG+A(I)*A(I)                                                 LLSQ1160
      SIG=SQRT(SIG)                                                     LLSQ1170
C                                                                       LLSQ1180
C     TEST ON SINGULARITY                                               LLSQ1190
      IF(SIG-TOL)32,32,11                                               LLSQ1200
C                                                                       LLSQ1210
C     GENERATE CORRECT SIGN OF PARAMETER SIG                            LLSQ1220
   11 H=A(IST)                                                          LLSQ1230
      IF(H)12,13,13                                                     LLSQ1240
   12 SIG=-SIG                                                          LLSQ1250
C                                                                       LLSQ1260
C     SAVE INTERCHANGE INFORMATION                                      LLSQ1270
   13 IPIV(KPIV)=IPIV(K)                                                LLSQ1280
      IPIV(K)=KPIV                                                      LLSQ1290
C                                                                       LLSQ1300
C     GENERATION OF VECTOR UK IN K-TH COLUMN OF MATRIX A AND OF         LLSQ1310
C     PARAMETER BETA                                                    LLSQ1320
      BETA=H*SIG                                                        LLSQ1330
      A(IST)=BETA                                                       LLSQ1340
      BETA=1./(SIG*BETA)                                                LLSQ1350
      J=N*K                                                             LLSQ1360
      AUX(J)=-SIG                                                       LLSQ1370
      IF(K-N)14,19,19                                                   LLSQ1380
C                                                                       LLSQ1390
C     TRANSFORMATION OF MATRIX A                                        LLSQ1400
   14 PIV=0.                                                            LLSQ1410
      ID=0                                                              LLSQ1420
      JST=K+1                                                           LLSQ1430
      KPIV=JST                                                          LLSQ1440
      DO 18 J=JST,N                                                     LLSQ1450
      ID=ID+M                                                           LLSQ1460
      H=0.                                                              LLSQ1470
      DO 15 I=IST,IEND                                                  LLSQ1480
      II=I+ID                                                           LLSQ1490
   15 H=H+A(I)*A(II)                                                    LLSQ1500
      H=BETA*H                                                          LLSQ1510
      DO 16 I=IST,IEND                                                  LLSQ1520
      II=I+ID                                                           LLSQ1530
   16 A(II)=A(II)-A(I)*H                                                LLSQ1540
C                                                                       LLSQ1550
C     UPDATING OF ELEMENT S(J) STORED IN LOCATION AUX(J)                LLSQ1560
      II=IST+ID                                                         LLSQ1570
      H=AUX(J)-A(II)*A(II)                                              LLSQ1580
      AUX(J)=H                                                          LLSQ1590
      IF(H-PIV)16,18,18                                                 LLSQ1600
   17 PIV=H                                                             LLSQ1610
      KPIV=J                                                            LLSQ1620
   18 CONTINUE                                                          LLSQ1630
C                                                                       LLSQ1640
C     TRANSFORMATION OF RIGHT HAND SIDE MATRIX B                        LLSQ1650
   19 DO 21 J=K,LM,M                                                    LLSQ1660
      H=0.                                                              LLSQ1670
      I=N+J-K                                                           LLSQ1680
      II=IST                                                            LLSQ1690
      DO 20 I=J,IEND                                                    LLSQ1700
      H=H+A(II)*B(I)                                                    LLSQ1710
   20 II=II+1                                                           LLSQ1720
      H=BETA*H                                                          LLSQ1730
      II=IST                                                            LLSQ1740
      DO 21 I=J,IEND                                                    LLSQ1750
      B(I)=B(I)-A(II)*H                                                 LLSQ1760
   21 II=II+1                                                           LLSQ1770
C     END OF DECOMPOSITION LOOP                                         LLSQ1780
C                                                                       LLSQ1790
C                                                                       LLSQ1800
C     BACK SUBSTITUTION AND BACK INTERCHANGE                            LLSQ1810
      IER=0                                                             LLSQ1820
      I=N                                                               LLSQ1830
      LN=L*N                                                            LLSQ1840
      PIV=1./AUX(2*N)                                                   LLSQ1850
      DO 22 K=N,LN,N                                                    LLSQ1860
      X(K)=PIV*B(I)                                                     LLSQ1870
   22 I=I+M                                                             LLSQ1880
      IF(N-1)25,26,23                                                   LLSQ1890
   23 JST=(N-1)*M+N                                                     LLSQ1900
      DO 25 J=2,N                                                       LLSQ1910
      JST=JST-M-1                                                       LLSQ1920
      K=N+N+1-J                                                         LLSQ1930
      PIV=1./AUX(K)                                                     LLSQ1940
      KST=K-N                                                           LLSQ1950
      ID=IPIV(KST)-KST                                                  LLSQ1960
      IST=J-1                                                           LLSQ1970
      DO 25 K=1,L                                                       LLSQ1980
      H=B(KST)                                                          LLSQ1990
      IST=IST+N                                                         LLSQ2000
      IEND=IST+J-2                                                      LLSQ2010
      II=JST                                                            LLSQ2020
      DO 24 I=IST,IEND                                                  LLSQ2030
      II=II+M                                                           LLSQ2040
   24 H=H-A(II)*X(I)                                                    LLSQ2050
      I=IST-1                                                           LLSQ2060
      II=I+ID                                                           LLSQ2070
      X(I)=X(II)                                                        LLSQ2080
      X(II)=PIV*H                                                       LLSQ2090
   25 KST=KST+M                                                         LLSQ2100
C                                                                       LLSQ2110
C                                                                       LLSQ2120
C     COMPUTATION OF LEAST SQUARES                                      LLSQ2130
   26 IST=N+1                                                           LLSQ2140
      IEND=0                                                            LLSQ2150
      DO 29 J=1,L                                                       LLSQ2160
      IEND=IEND+M                                                       LLSQ2170
      H=0.                                                              LLSQ2180
      IF(M-N)29,29,27                                                   LLSQ2190
   27 DO 28 I=IST,IEND                                                  LLSQ2200
   28 H=H+B(I)*B(I)                                                     LLSQ2210
      IST=IST+M                                                         LLSQ2220
   29 AUX(J)=H                                                          LLSQ2230
      RETURN                                                            LLSQ2240
C                                                                       LLSQ2250
C     ERROR RETURN IN CASE M LESS THAN N                                LLSQ2260
   30 IER=-2                                                            LLSQ2270
      RETURN                                                            LLSQ2280
C                                                                       LLSQ2290
C     ERROR RETURN IN CASE OF ZERO-MATRIX A                             LLSQ2300
   31 IER=-1                                                            LLSQ2310
      RETURN                                                            LLSQ2320
C                                                                       LLSQ2330
C     ERROR RETURN IN CASE OF RANK OF MATRIX A LESS THAN N              LLSQ2340
   32 IER=K-1                                                           LLSQ2350
      RETURN                                                            LLSQ2360
      END                                                               LLSQ2370
```

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C                                                                       DLLS  10
C     ..................................................................DLLS  20
C                                                                       DLLS  30
C        SUBROUTINE DLLSQ                                               DLLS  40
C                                                                       DLLS  50
C        PURPOSE                                                        DLLS  60
C           TO SOLVE LINEAR LEAST SQUARES PROBLEMS, I.E. TO MINIMIZE    DLLS  70
C           THE EUCLIDEAN NORM OF B-A*X, WHERE A IS A M BY N MATRIX     DLLS  80
C           WITH M NOT LESS THAN N. IN THE SPECIAL CASE M=N SYSTEMS OF  DLLS  90
C           LINEAR EQUATIONS MAY BE SOLVED.                             DLLS 100
C                                                                       DLLS 110
C        USAGE                                                          DLLS 120
C           CALL DLLSQ (A,B,M,N,L,X,IPIV,EPS,IER,AUX)                   DLLS 130
C                                                                       DLLS 140
C        DESCRIPTION OF PARAMETERS                                      DLLS 150
C           A      - DOUBLE PRECISION M BY N COEFFICIENT MATRIX         DLLS 160
C                    (DESTROYED).                                       DLLS 170
C           B      - DOUBLE PRECISION M BY L RIGHT HAND SIDE MATRIX     DLLS 180
C                    (DESTROYED).                                       DLLS 190
C           M      - ROW NUMBER OF MATRICES A AND B.                    DLLS 200
C           N      - COLUMN NUMBER OF MATRIX A, ROW NUMBER OF MATRIX X. DLLS 210
C           L      - COLUMN NUMBER OF MATRICES B AND X.                 DLLS 220
C           X      - DOUBLE PRECISION N BY L SOLUTION MATRIX.           DLLS 230
C           IPIV   - INTEGER OUTPUT VECTOR OF DIMENSION N WHICH         DLLS 240
C                    CONTAINS INFORMATIONS ON COLUMN INTERCHANGES        DLLS 250
C                    IN MATRIX A. (SEE REMARK NO.3).                    DLLS 260
C           EPS    - SINGLE PRECISION INPUT PARAMETER WHICH SPECIFIES    DLLS 270
C                    A RELATIVE TOLERANCE FOR DETERMINATION OF RANK OF  DLLS 280
C                    MATRIX A.                                          DLLS 290
C           IER    - A RESULTING ERROR PARAMETER.                       DLLS 300
C           AUX    - A DOUBLE PRECISION AUXILIARY STORAGE ARRAY OF      DLLS 310
C                    DIMENSION MAX(2*N,L). ON RETURN FIRST L LOCATIONS  DLLS 320
C                    OF AUX CONTAIN THE RESULTING LEAST SQUARES.        DLLS 330
C                                                                       DLLS 340
C        REMARKS                                                        DLLS 350
C           (1) NO ACTION BESIDES ERROR MESSAGE IER=-2 IN CASE          DLLS 360
C               M LESS THAN N.                                          DLLS 370
C           (2) NO ACTION BESIDES ERROR MESSAGE IER=-1 IN CASE          DLLS 380
C               OF A ZERO-MATRIX A.                                     DLLS 390
C           (3) IF RANK K OF MATRIX A IS FOUND TO BE LESS THAN N BUT    DLLS 400
C               GREATER THAN 0, THE PROCEDURE RETURNS WITH ERROR CODE   DLLS 410
C               IER=K INTO CALLING PROGRAM. THE LAST N-K ELEMENTS OF    DLLS 420
C               VECTOR IPIV DENOTE THE USELESS COLUMNS IN MATRIX A.     DLLS 430
C               THE REMAINING USEFUL COLUMNS FORM A BASE OF MATRIX A.   DLLS 440
C           (4) IF THE PROCEDURE WAS SUCCESSFUL, ERROR PARAMETER IER    DLLS 450
C               IS SET TO 0.                                            DLLS 460
C                                                                       DLLS 470
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DLLS 480
C           NONE                                                        DLLS 490
C                                                                       DLLS 500
C        METHOD                                                         DLLS 510
C           HOUSEHOLDER TRANSFORMATIONS ARE USED TO TRANSFORM MATRIX A  DLLS 520
C           TO UPPER TRIANGULAR FORM. AFTER HAVING APPLIED THE SAME     DLLS 530
C           TRANSFORMATION TO THE RIGHT HAND SIDE MATRIX B, AN          DLLS 540
C           APPROXIMATE SOLUTION OF THE PROBLEM IS COMPUTED BY          DLLS 550
C           BACK SUBSTITUTION. FOR REFERENCE, SEE                       DLLS 560
C           G. GOLUB, NUMERICAL METHODS FOR SOLVING LINEAR LEAST        DLLS 570
C           SQUARES PROBLEMS, NUMERISCHE MATHEMATIK, VOL.7,             DLLS 580
C           183.3 (1965), PP.206-216.                                   DLLS 590
C                                                                       DLLS 600
C     ..................................................................DLLS 610
C                                                                       DLLS 620
      SUBROUTINE DLLSQ(A,B,M,N,L,X,IPIV,EPS,IER,AUX)                    DLLS 630
C                                                                       DLLS 640
      DIMENSION A(1),B(1),X(1),IPIV(1),AUX(1)                           DLLS 650
      DOUBLE PRECISION A,B,X,AUX,PIV,H,SIG,BETA,TOL                     DLLS 660
C                                                                       DLLS 670
C     ERROR TEST                                                        DLLS 680
      IF(M-N)30,1,1                                                     DLLS 690
C                                                                       DLLS 700
C     GENERATION OF INITIAL VECTOR S(K) (K=1,2,...,N) IN STORAGE        DLLS 710
C     LOCATIONS AUX(K) (K=1,2,...,N)                                    DLLS 720
    1 PIV=0.D0                                                          DLLS 730
      IEND=0                                                            DLLS 740
      DO 4 K=1,N                                                        DLLS 750
      IPIV(K)=K                                                         DLLS 760
      H=0.D0                                                            DLLS 770
      IST=IEND+1                                                        DLLS 780
      IEND=IEND+M                                                       DLLS 790
      DO 2 I=IST,IEND                                                   DLLS 800
    2 H=H+A(I)*A(I)                                                     DLLS 810
      AUX(K)=H                                                          DLLS 820
      IF(H-PIV)4,4,3                                                    DLLS 830
    3 PIV=H                                                             DLLS 840
      KPIV=K                                                            DLLS 850
    4 CONTINUE                                                          DLLS 860
C                                                                       DLLS 870
C     ERROR TEST                                                        DLLS 880
      IF(PIV)31,31,5                                                    DLLS 890
C                                                                       DLLS 900
C     DEFINE TOLERANCE FOR CHECKING RANK OF A                           DLLS 910
    5 SIG=DSQRT(PIV)                                                    DLLS 920
      TOL=SIG*DABS(EPS)                                                 DLLS 930
C                                                                       DLLS 940
C                                                                       DLLS 950
C     DECOMPOSITION LOOP                                                DLLS 960
      LM=L*M                                                            DLLS 970
      IST=-M                                                            DLLS 980
      DO 27 K=1,N                                                       DLLS 990
      IST=IST+M+1                                                       DLLS1000
      IEND=IST+M-K                                                      DLLS1010
      I=KPIV-K                                                          DLLS1020
      IF(I)8,8,6                                                        DLLS1030
C                                                                       DLLS1040
C     INTERCHANGE K-TH COLUMN OF A WITH KPIV-TH IN CASE KPIV.GT.K       DLLS1050
    6 H=AUX(K)                                                          DLLS1060
      AUX(K)=AUX(KPIV)                                                  DLLS1070
      AUX(KPIV)=H                                                       DLLS1080
      ID=I*M                                                            DLLS1090
      DO 7 I=IST,IEND                                                   DLLS1100
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```
      J=I+ID
      H=A(I)
      A(I)=A(J)
    7 A(J)=H
C
C     COMPUTATION OF PARAMETER SIG
    8 IF(K-1)11,11,9
    9 SIG=0.0D
      DO 10 I=IST,IEND
   10 SIG=SIG+A(I)*A(I)
      SIG=DSQRT(SIG)
C
C     TEST ON SINGULARITY
      IF(SIG-TOL)32,32,11
C
C     GENERATE CORRECT SIGN OF PARAMETER SIG
   11 H=A(IST)
      IF(H)12,13,13
   12 SIG=-SIG
C
C     SAVE INTERCHANGE INFORMATION
   13 IPIV(KPIV)=IPIV(K)
      IPIV(K)=KPIV
C
C     GENERATION OF VECTOR UK IN K-TH COLUMN OF MATRIX A AND OF
C     PARAMETER BETA
      BETA=H*SIG
      A(IST)=BETA
      BETA=1.0D/(SIG*BETA)
      J=N+K
      AUX(J)=-SIG
      IF(K-N)14,19,19
C
C     TRANSFORMATION OF MATRIX A
   14 PIV=0.0D
      ID=0
      JST=K+1
      KPIV=JST
      DO 18 J=JST,N
      ID=ID+M
      H=0.0D
      DO 15 I=IST,IEND
      II=I+ID
   15 H=H+A(I)*A(II)
      H=BETA*H
      DO 16 I=IST,IEND
      II=I+ID
   16 A(II)=A(II)-A(I)*H
C
C     UPDATING OF ELEMENT S(J) STORED IN LOCATION AUX(J)
      II=IST+ID
      H=AUX(J)-A(II)*A(II)
      AUX(J)=H
      IF(H-PIV)18,18,17
   17 PIV=H
      KPIV=J
   18 CONTINUE
C
C     TRANSFORMATION OF RIGHT HAND SIDE MATRIX B
   19 DO 21 J=K,L,M
      H=0.0D
      IEND=J+M-K
      II=IST
      DO 20 I=J,IEND
      H=H+A(II)*B(I)
   20 II=II+1
      H=BETA*H
      II=IST
      DO 21 I=J,IEND
      B(I)=B(I)-A(II)*H
   21 II=II+1
C     END OF DECOMPOSITION LOOP
C
C
C     BACK SUBSTITUTION AND BACK INTERCHANGE
      IER=0
      I=N
      LN=L*N
      PIV=1.0D/AUX(2*N)
      DO 22 K=N,LN,N
      X(K)=PIV*B(I)
   22 I=I+M
      IF(N-1)25,25,23
   23 JST=(N-1)*M+N
      DO 25 J=2,N
      JST=JST-M-1
      K=N+N+1-J
      PIV=1.0D/AUX(K)
      KST=K-N
      ID=IPIV(KST)-KST
      IST=2-J
      DO 25 K=1,L
      H=B(KST)
      IST=IST+N
      IEND=IST+J-2
      II=JST
      DO 24 I=IST,IEND
      II=II+M
   24 H=H-A(II)*X(I)
      I=IST-1
      II=I+ID
      X(I)=X(II)
      X(II)=PIV*H
   25 KST=KST+M
C
C
C     COMPUTATION OF LEAST SQUARES
   26 IST=N+1
      IEND=0
      DO 29 J=1,L
      IEND=IEND+M
      H=0.0D
      IF(M-N)29,29,27
   27 DO 28 I=IST,IEND
   28 H=H+B(I)*B(I)
      IST=IST+M
   29 AUX(J)=H
      RETURN
C
C     ERROR RETURN IN CASE M LESS THAN N
   30 IER=-2
      RETURN
C
C     ERROR RETURN IN CASE OF ZERO-MATRIX A
   31 IER=-1
      RETURN
C
C     ERROR RETURN IN CASE OF RANK OF MATRIX A LESS THAN N
   32 IER=K-1
      RETURN
      END
```

```
DLLS1120
DLLS1130
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Matrices: Eigenanalysis and Related Topics

Subroutine EIGEN

This subroutine computes the eigenvalues and eigenvectors of a real symmetric matrix.

Given a symmetric matrix A of order N, eigenvalues are to be developed in the diagonal elements of the matrix. A matrix of eigenvectors R is also to be generated.

An identity matrix is used as a first approximation of R.

The initial off-diagonal norm is computed:

$$\nu_I = \left\{ \sum_{i<k} 2A_{ik}^2 \right\}^{1/2} \qquad (1)$$

ν_I = initial norm

A = input matrix (symmetric)

This norm is divided by N at each stage to produce the threshold.

The final norm is computed:

$$\nu_F = \frac{\nu_I \times 10^{-6}}{N} \qquad (2)$$

This final norm is set sufficiently small that the requirement that any off-diagonal element A_{lm} shall be smaller than ν_F in absolute magnitude defines the convergence of the process.

An indicator is initialized. This indicator is later used to determine whether any off-diagonal elements have been found that are greater than the present threshold.

Each off-diagonal element is selected in turn and a transformation is performed to annihilate the off-diagonal (pivotal) element, as shown by the following equations:

$$\lambda = -A_{lm} \qquad (3)$$

$$\mu = 1/2\,(A_{11} - A_{mm}) \qquad (4)$$

$$\omega = \text{sign}\,(\mu)\,\frac{\lambda}{\sqrt{\lambda^2 + \mu^2}} \qquad (5)$$

$$\sin\theta = \frac{\omega}{\sqrt{2\,(1+\sqrt{1-\omega^2})}} \qquad (6)$$

$$\cos\theta = \sqrt{1-\sin^2\theta} \qquad (7)$$

$$B = A_{il} \cos\theta - A_{im} \sin\theta \quad (8)$$

$$A_{im} = A_{il} \sin\theta + A_{im} \cos\theta \quad (9)$$

$$A_{il} = B \quad (10)$$

$$B = R_{il} \cos\theta - R_{im} \sin\theta \quad (11)$$

$$R_{im} = R_{il} \sin\theta + R_{im} \cos\theta \quad (12)$$

$$R_{il} = B \quad (13)$$

$$A_{ll} = A_{11}\cos^2\theta + A_{mm} \sin^2\theta - 2A_{lm} \sin\theta \cos\theta \quad (14)$$

$$A_{mm} = A_{ll} \sin^2\theta + A_{mm} \cos^2\theta + 2A_{lm} \sin\theta \cos\theta \quad (15)$$

$$A_{lm} = (A_{ll} - A_{mm}) \sin\theta \cos\theta + A_{lm} (\cos^2\theta - \sin^2\theta) \quad (16)$$

The above calculations are repeated until all of the pivotal elements are less than the threshold.

```
C                                                                       EIGE  10
C     ..................................................................EIGE  20
C                                                                       EIGE  30
C        SUBROUTINE EIGEN                                               EIGE  40
C                                                                       EIGE  50
C        PURPOSE                                                        EIGE  60
C           COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC    EIGE  70
C           MATRIX                                                      EIGE  80
C                                                                       EIGE  90
C        USAGE                                                          EIGE 100
C           CALL EIGEN(A,R,N,MV)                                        EIGE 110
C                                                                       EIGE 120
C        DESCRIPTION OF PARAMETERS                                      EIGE 130
C           A - ORIGINAL MATRIX (SYMMETRIC), DESTROYED IN COMPUTATION.  EIGE 140
C               RESULTANT EIGENVALUES ARE DEVELOPED IN DIAGONAL OF      EIGE 150
C               MATRIX A IN DESCENDING ORDER.                           EIGE 160
C           R - RESULTANT MATRIX OF EIGENVECTORS (STORED COLUMNWISE,     EIGE 170
C               IN SAME SEQUENCE AS EIGENVALUES)                        EIGE 180
C           N - ORDER OF MATRICES A AND R                               EIGE 190
C           MV- INPUT CODE                                              EIGE 200
C                     0   COMPUTE EIGENVALUES AND EIGENVECTORS         EIGE 210
C                     1   COMPUTE EIGENVALUES ONLY (R NEED NOT BE      EIGE 220
C                         DIMENSIONED BUT MUST STILL APPEAR IN CALLING EIGE 230
C                         SEQUENCE)                                     EIGE 240
C                                                                       EIGE 250
C        REMARKS                                                        EIGE 260
C           ORIGINAL MATRIX A MUST BE REAL SYMMETRIC (STORAGE MODE=1)   EIGE 270
C           MATRIX A CANNOT BE IN THE SAME LOCATION AS MATRIX R         EIGE 280
C                                                                       EIGE 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  EIGE 300
C           NONE                                                        EIGE 310
C                                                                       EIGE 320
C        METHOD                                                         EIGE 330
C           DIAGONALIZATION METHOD ORIGINATED BY JACOBI AND ADAPTED     EIGE 340
C           BY VON NEUMANN FOR LARGE COMPUTERS AS FOUND IN 'MATHEMATICALEIGE 350
C           METHODS FOR DIGITAL COMPUTERS', EDITED BY A. RALSTON AND    EIGE 360
C           H.S. WILF, JOHN WILEY AND SONS, NEW YORK, 1962, CHAPTER 7   EIGE 370
C                                                                       EIGE 380
C     ..................................................................EIGE 390
C                                                                       EIGE 400
      SUBROUTINE EIGEN(A,R,N,MV)                                        EIGE 410
      DIMENSION A(1),R(1)                                               EIGE 420
C                                                                       EIGE 430
C     ..................................................................EIGE 440
C                                                                       EIGE 450
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  EIGE 460
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      EIGE 470
C        STATEMENT WHICH FOLLOWS.                                       EIGE 480
C                                                                       EIGE 490
C     DOUBLE PRECISION A,R,ANORM,ANRMX,THR,X,Y,SINX,SINX2,COSX,         EIGE 500
C    1                 COSX2,SINCS,RANGE                                EIGE 510
C                                                                       EIGE 520
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    EIGE 530
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      EIGE 540
C        ROUTINE.                                                       EIGE 550
C                                                                       EIGE 560
C        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      EIGE 570
C        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENTSEIGE 580
C        40, 68, 75, AND 78 MUST BE CHANGED TO DSQRT.  ABS IN STATEMENT EIGE 590
C        62 MUST BE CHANGED TO DABS. THE CONSTANT IN STATEMENT 5 SHOULD EIGE 600
C        BE CHANGED TO 1.0D-12.                                         EIGE 610
C                                                                       EIGE 620
C     ..................................................................EIGE 630
C                                                                       EIGE 640
C        GENERATE IDENTITY MATRIX                                       EIGE 650
C                                                                       EIGE 660
    5 RANGE=1.0E-6                                                      EIGE 670
      IF(MV-1) 10,25,10                                                 EIGE 680
   10 IQ=-N                                                             EIGE 690
      DO 20 J=1,N                                                       EIGE 700
      IQ=IQ+N                                                           EIGE 710
      DO 20 I=1,N                                                       EIGE 720
      IJ=IQ+I                                                           EIGE 730
      R(IJ)=0.0                                                         EIGE 740
      IF(I-J) 20,15,20                                                  EIGE 750
   15 R(IJ)=1.0                                                         EIGE 760
   20 CONTINUE                                                          EIGE 770
C                                                                       EIGE 780
C        COMPUTE INITIAL AND FINAL NORMS (ANORM AND ANORMX)             EIGE 790
C                                                                       EIGE 800
   25 ANORM=0.0                                                         EIGE 810
      DO 35 I=1,N                                                       EIGE 820
      DO 35 J=I,N                                                       EIGE 830
      IF(I-J) 30,35,30                                                  EIGE 840
   30 IA=I+(J*J-J)/2                                                    EIGE 850
      ANORM=ANORM+A(IA)*A(IA)                                           EIGE 860
   35 CONTINUE                                                          EIGE 870
      IF(ANORM) 165,165,40                                              EIGE 880
   40 ANORM=1.414*SQRT(ANORM)                                           EIGE 890
      ANRMX=ANORM*RANGE/FLOAT(N)                                        EIGE 900
C                                                                       EIGE 910
C        INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR               EIGE 920
C                                                                       EIGE 930
      IND=0                                                             EIGE 940
      THR=ANORM                                                         EIGE 950
   45 THR=THR/FLOAT(N)                                                  EIGE 960
   50 L=1                                                               EIGE 970
   55 M=L+1                                                             EIGE 980
C                                                                       EIGE 990
C        COMPUTE SIN AND COS                                            EIGE1000
C                                                                       EIGE1010
   60 MQ=(M*M-M)/2                                                      EIGE1020
      LQ=(L*L-L)/2                                                      EIGE1030
      LM=L+MQ                                                           EIGE1040
   62 IF( ABS(A(LM))-THR) 130,65,65                                     EIGE1050
   65 IND=1                                                             EIGE1060
      LL=L+LQ                                                           EIGE1070
      MM=M+MQ                                                           EIGE1080
      X=0.5*(A(LL)-A(MM))                                               EIGE1090
   68 Y=-A(LM)/ SQRT(A(LM)*A(LM)+X*X)                                   EIGE1100
      IF(X) 70,75,75                                                    EIGE1110
   70 Y=-Y                                                              EIGE1120
   75 SINX=Y/ SQRT(2.0*(1.0+( SQRT(1.0-Y*Y))))                          EIGE1130
      SINX2=SINX*SINX                                                   EIGE1140
   78 COSX= SQRT(1.0-SINX2)                                             EIGE1150
      COSX2=COSX*COSX                                                   EIGE1160
      SINCS =SINX*COSX                                                  EIGE1170
C                                                                       EIGE1180
C        ROTATE L AND M COLUMNS                                         EIGE1190
C                                                                       EIGE1200
      ILQ=N*(L-1)                                                       EIGE1210
      IMQ=N*(M-1)                                                       EIGE1220
      DO 125 I=1,N                                                      EIGE1230
      IQ=(I*I-I)/2                                                      EIGE1240
      IF(I-L) 80,115,80                                                 EIGE1250
   80 IF(I-M) 85,115,90                                                 EIGE1260
   85 IM=I+MQ                                                           EIGE1270
      GO TO 95                                                          EIGE1280
   90 IM=M+IQ                                                           EIGE1290
   95 IF(I-L) 100,105,105                                               EIGE1300
  100 IL=I+LQ                                                           EIGE1310
      GO TO 110                                                         EIGE1320
  105 IL=L+IQ                                                           EIGE1330
  110 X=A(IL)*COSX-A(IM)*SINX                                           EIGE1340
      A(IM)=A(IL)*SINX+A(IM)*COSX                                       EIGE1350
      A(IL)=X                                                           EIGE1360
  115 IF(MV-1) 120,125,120                                              EIGE1370
  120 ILR=ILQ+I                                                         EIGE1380
      IMR=IMQ+I                                                         EIGE1390
      X=R(ILR)*COSX-R(IMR)*SINX                                         EIGE1400
      R(IMR)=R(ILR)*SINX+R(IMR)*COSX                                    EIGE1410
      R(ILR)=X                                                          EIGE1420
  125 CONTINUE                                                          EIGE1430
      X=2.0*A(LM)*SINCS                                                 EIGE1440
      Y=A(LL)*COSX2+A(MM)*SINX2-X                                       EIGE1450
      X=A(LL)*SINX2+A(MM)*COSX2+X                                       EIGE1460
      A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)                     EIGE1470
      A(LL)=Y                                                           EIGE1480
      A(MM)=X                                                           EIGE1490
C                                                                       EIGE1500
C        TESTS FOR COMPLETION                                           EIGE1510
C                                                                       EIGE1520
C        TEST FOR M = LAST COLUMN                                       EIGE1530
C                                                                       EIGE1540
  130 IF(M-N) 135,140,135                                               EIGE1550
  135 M=M+1                                                             EIGE1560
      GO TO 60                                                          EIGE1570
C                                                                       EIGE1580
C        TEST FOR L = SECOND FROM LAST COLUMN                           EIGE1590
C                                                                       EIGE1600
  140 IF(L-(N-1)) 145,150,145                                           EIGE1610
  145 L=L+1                                                             EIGE1620
      GO TO 55                                                          EIGE1630
  150 IF(IND-1) 160,155,160                                             EIGE1640
  155 IND=0                                                             EIGE1650
      GO TO 50                                                          EIGE1660
C                                                                       EIGE1670
C        COMPARE THRESHOLD WITH FINAL NORM                              EIGE1680
C                                                                       EIGE1690
  160 IF(THR-ANRMX) 165,165,45                                          EIGE1700
C                                                                       EIGE1710
C        SORT EIGENVALUES AND EIGENVECTORS                              EIGE1720
C                                                                       EIGE1730
  165 IQ=-N                                                             EIGE1740
      DO 185 I=1,N                                                      EIGE1750
      IQ=IQ+N                                                           EIGE1760
      LL=I+((I*I-I)/2                                                   EIGE1770
      JQ=N*(I-2)                                                        EIGE1780
      DO 185 J=I,N                                                      EIGE1790
      JQ=JQ+N                                                           EIGE1800
      MM=J+(J*J-J)/2                                                    EIGE1810
      IF(A(LL)-A(MM)) 170,185,185                                       EIGE1820
  170 X=A(LL)                                                           EIGE1830
      A(LL)=A(MM)                                                       EIGE1840
      A(MM)=X                                                           EIGE1850
      IF(MV-1) 175,185,175                                              EIGE1860
  175 DO 180 K=1,N                                                      EIGE1870
      ILR=IQ+K                                                          EIGE1880
      IMR=JQ+K                                                          EIGE1890
      X=R(ILR)                                                          EIGE1900
      R(ILR)=R(IMR)                                                     EIGE1910
  180 R(IMR)=X                                                          EIGE1920
  185 CONTINUE                                                          EIGE1930
      RETURN                                                            EIGE1940
      END                                                               EIGE1950
```

Subroutine NROOT

This subroutine calculates the eigenvalues, λ_i, and the matrix of eigenvectors, V, of a real square non-symmetric matrix of the special form $B^{-1}A$, where both B and A are real symmetric matrices and B is positive-definite. This subroutine is normally called by the subroutine CANOR in performing a canonical correlation analysis. The computational steps are as follows.

A symmetric matrix (storage mode 1) is formed by using the upper triangle elements of the square matrix B. Then the eigenvalues, h_i, and the matrix of eigenvectors, H, of the symmetric matrix are calculated by the subroutine EIGEN.

The reciprocal of square root of each eigenvalue is formed as follows:

$$\mu_i = \frac{1}{\sqrt{h_i}} \qquad (1)$$

where i = 1, 2, ..., m

m = order of matrix B

The matrix $B^{-1/2}$ is formed by multiplying the j^{th} column vector of H by μ_j, where j = 1, 2, ..., m.

The symmetric matrix $S = (B^{-1/2})' AB^{-1/2}$ is formed in the following two matrix multiplications:

$$Q = (B^{-1/2})' A \qquad (2)$$

$$S = QB^{-1/2} \qquad (3)$$

and eigenvalues, λ_i, and the matrix of eigenvectors, M, of S are calculated by the subroutine EIGEN.

The matrix $W = B^{-1/2}M$ is formed, and the vectors in W are normalized to form the matrix of eigenvectors, V, by the following equation:

$$V_{ij} = \frac{W_{ij}}{\sqrt{SUMV_j}} \qquad (4)$$

where i = 1, 2, ..., m

j = 1, 2, ..., m

$$SUMV_j = \sum_{i=1}^{m} W_{ij}^2 \qquad (5)$$

```
C
C     ..................................................................NROO  10
C                                                                      NROO  20
C                                                                      NROO  30
C       SUBROUTINE NROOT                                               NROO  40
C                                                                      NROO  50
C       PURPOSE                                                        NROO  60
C          COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL NONSYMMETRIC NROO  70
C          MATRIX OF THE FORM B-INVERSE TIMES A.  THIS SUBROUTINE IS   NROO  80
C          NORMALLY CALLED BY SUBROUTINE CANOR IN PERFORMING A         NROO  90
C          CANONICAL CORRELATION ANALYSIS.                             NROO 100
C                                                                      NROO 110
C       USAGE                                                          NROO 120
C          CALL NROOT (M,A,B,XL,X)                                     NROO 130
C                                                                      NROO 140
C       DESCRIPTION OF PARAMETERS                                      NROO 150
C          M  - ORDER OF SQUARE MATRICES A, B, AND X.                  NROO 160
C          A  - INPUT MATRIX (M X M).                                  NROO 170
C          B  - INPUT MATRIX (M X M).                                  NROO 180
C          XL - OUTPUT VECTOR OF LENGTH M CONTAINING EIGENVALUES OF    NROO 190
C               B-INVERSE TIMES A.                                     NROO 200
C          X  - OUTPUT MATRIX (M X M) CONTAINING EIGENVECTORS COLUMN-  NROO 210
C               WISE.                                                  NROO 220
C                                                                      NROO 230
C       REMARKS                                                        NROO 240
C          NONE                                                        NROO 250
C                                                                      NROO 260
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  NROO 270
C          EIGEN                                                       NROO 280
C                                                                      NROO 290
C       METHOD                                                         NROO 300
C          REFER TO W. W. COOLEY AND P. R. LOHNES, 'MULTIVARIATE PRO-  NROO 310
C          CEDURES FOR THE BEHAVIORAL SCIENCES', JOHN WILEY AND SONS,  NROO 320
C          1962, CHAPTER 3.                                            NROO 330
C                                                                      NROO 340
C     ..................................................................NROO 350
      SUBROUTINE NROOT (M,A,B,XL,X)                                    NROO 360
      DIMENSION A(1),B(1),XL(1),X(1)                                   NROO 370
C                                                                      NROO 380
C     ..................................................................NROO 390
C                                                                      NROO 400
C       IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  NROO 410
C       C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      NROO 420
C       STATEMENT WHICH FOLLOWS.                                       NROO 430
C                                                                      NROO 440
C     DOUBLE PRECISION A,B,XL,X,SUMV                                   NROO 450
C                                                                      NROO 460
C       THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    NROO 470
C       APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      NROO 480
C       ROUTINE.                                                       NROO 490
C                                                                      NROO 500
C       THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO      NROO 510
C       CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENTSNROO 520
C       110 AND 175 MUST BE CHANGED TO DSQRT.  ABS IN STATEMENT 110    NROO 530
C       MUST BE CHANGED TO DABS.                                       NROO 540
C                                                                      NROO 550
C     ..................................................................NROO 560
C                                                                      NROO 570
C     COMPUTE EIGENVALUES AND EIGENVECTORS OF B                        NROO 580
C                                                                      NROO 590
      K=1                                                              NROO 600
      DO 100 J=2,M                                                     NROO 610
      L=M*(J-1)                                                        NROO 620
      DO 100 I=1,J                                                     NROO 630
      L=L+1                                                            NROO 640
      K=K+1                                                            NROO 650
  100 B(K)=B(L)                                                        NROO 660
C                                                                      NROO 670
C       THE MATRIX B IS A REAL SYMMETRIC MATRIX.                       NROO 680
C                                                                      NROO 690
      MV=0                                                             NROO 700
      CALL EIGEN (B,X,M,MV)                                            NROO 710
C                                                                      NROO 720
C     FORM RECIPROCALS OF SQUARE ROOT OF EIGENVALUES.  THE RESULTS     NROO 730
C     ARE PREMULTIPLIED BY THE ASSOCIATED EIGENVECTORS.                NROO 740
C                                                                      NROO 750
      L=0                                                              NROO 760
      DO 110 J=1,M                                                     NROO 770
      L=L+J                                                            NROO 780
  110 XL(J)=1.0/ SQRT( ABS(B(L)))                                      NROO 790
      K=0                                                              NROO 800
      DO 115 J=1,M                                                     NROO 810
      DO 115 I=1,M                                                     NROO 820
      K=K+1                                                            NROO 830
  115 B(K)=X(K)*XL(J)                                                  NROO 840
C                                                                      NROO 850
C     FORM (B**(-1/2))PRIME * A * (B**(-1/2))                          NROO 860
C                                                                      NROO 870
      DO 120 I=1,M                                                     NROO 880
      N2=0                                                             NROO 890
      DO 120 J=1,M                                                     NROO 900
      N1=M*(I-1)                                                       NROO 910
      L=M*(J-1)+I                                                      NROO 920
      X(L)=0.0                                                         NROO 930
      DO 120 K=1,M                                                     NROO 940
      N1=N1+1                                                          NROO 950
      N2=N2+1                                                          NROO 960
  120 X(L)=X(L)+B(N1)*A(N2)                                            NROO 970
      L=0                                                              NROO 980
      DO 130 J=1,M                                                     NROO 990
      DO 130 I=1,J                                                     NROO1000
      N1=I-M                                                           NROO1010
      N2=M*(J-1)                                                       NROO1020
      L=L+1                                                            NROO1030
      A(L)=0.0                                                         NROO1040
      DO 130 K=1,M                                                     NROO1050
      N1=N1+M                                                          NROO1060
      N2=N2+1                                                          NROO1070
  130 A(L)=A(L)+X(N1)*B(N2)                                            NROO1080
C                                                                      NROO1090
C     COMPUTE EIGENVALUES AND EIGENVECTORS OF A                        NROO1100
C                                                                      NROO1110
      CALL EIGEN (A,X,M,MV)                                            NROO1120
      L=0                                                              NROO1130
      DO 140 I=1,M                                                     NROO1140
      L=L+I                                                            NROO1150
  140 XL(I)=A(L)                                                       NROO1160
C                                                                      NROO1170
C     COMPUTE THE NORMALIZED EIGENVECTORS                              NROO1180
C                                                                      NROO1190
      DO 150 I=1,M                                                     NROO1200
      N2=0                                                             NROO1210
      DO 150 J=1,M                                                     NROO1220
      N1=I-M                                                           NROO1230
      L=M*(J-1)+I                                                      NROO1240
      A(L)=0.0                                                         NROO1250
      DO 150 K=1,M                                                     NROO1260
      N1=N1+M                                                          NROO1270
      N2=N2+1                                                          NROO1280
  150 A(L)=A(L)+B(N1)*X(N2)                                            NROO1290
      L=0                                                              NROO1300
      K=0                                                              NROO1310
      DO 180 J=1,M                                                     NROO1320
      SUMV=0.0                                                         NROO1330
      DO 170 I=1,M                                                     NROO1340
      L=L+1                                                            NROO1350
  170 SUMV=SUMV+A(L)*A(L)                                              NROO1360
  175 SUMV= SQRT(SUMV)                                                 NROO1370
      DO 180 I=1,M                                                     NROO1380
      K=K+1                                                            NROO1390
  180 X(K)=A(K)/SUMV                                                   NROO1400
      RETURN                                                           NROO1410
      END                                                              NROO1420
                                                                       NROO1430
```

Subroutine ATEIG

This subroutine computes the eigenvalues of a real upper almost-triangular matrix (Hessenberg form -- see subroutine HSBG) using the double QR iteration of J. G. F. Francis.

1. Mathematical background

a. Definition of the QR iteration

Let A be a real or complex nonsingular matrix of order n. Then a decomposition of A exists of the form

$$A = Q\,R$$

where Q is unitary and R is upper triangular. If the diagonal elements of R are real and positive, Q is unique. Consider now the sequence of matrices $A^{(p)}$ defined recursively by

$$A^{(o)} = A,\ A^{(p)} = Q^{(p)}\,R^{(p)},\ A^{(p+1)} = R^{(p)}\,Q^{(p)}\ p \geq 0.$$

Note that $A^{(p+1)} = Q^{(p)*}\,A^{(p)}\,Q^{(p)}$ for $p \geq 0$; hence it follows that $A^{(p)}$ is similar to A for all p.

Furthermore, if A satisfies certain conditions, it can be proved that $A^{(p)}$ tends to an upper triangular matrix as $p \to \infty$; thus the eigenvalues of A are the diagonal elements of this limit matrix.

b. Convergence

If the moduli of the eigenvalues are distinct, the elements $a^{(p)}_{ij}$ below the main diagonal of $A^{(p)}$ tend to zero, as $d^{o}|\lambda_i|^p/|\lambda_j|^p$, the eigenvalues being subscripted so that $|\lambda_i| > |\lambda_{i+1}|$.

Thus, in general, the eigenvalues appear on the main diagonal, starting from the last position, in increasing order of moduli.

So, when the smallest eigenvalue λ_n has been found, we can reduce the order of the matrix by neglecting the last row and column and find λ_{n-1} by the same process, without any special deflation.

Note that the speed of convergence is considerably improved when the origin of the eigenvalues is shifted close to λ_n.

Such a shift, say $s^{(p)}$, can be introduced before an iteration and the opposite one afterwards. Then the iteration can be written as:

$$A^{(p)} - s^{(p)}\,I = Q^{(p)}\,R^{(p)}$$

$$A^{(p+1)} = R^{(p)}\,Q^{(p)} + s^{(p)}\,I$$

In general, $A^{(p)}_{n,n}$, for p large enough, can provide an efficient value for $s^{(p)}$.

c. Use of the Hessenberg form

The Hessenberg form is preserved under the QR iteration. Thus, a reduction of the initial matrix to the Hessenberg form can give a significant saving of computation in each iteration for the QR decomposition, the lower part of the matrix consisting only of the codiagonal terms.

Before each iteration, the codiagonal terms will be inspected. If some of these are zero, the matrix will be split according to this occurrence, and the iteration will be applied to the lower main submatrix only.

d. The double QR iteration

Let A be a diagonalizable real upper Hessenberg matrix. Such a matrix must be expected to have complex conjugate pairs of eigenvalues. If these pairs are the only eigenvalues of equal modulus, it can be shown that they will appear as the latent roots of main submatrices of order 2. In this case, if a shift is close to one of these roots, it will be complex, and we will have to deal with complex matrices, although the initial one is real. The use of the double QR iteration avoids this inconvenience.

Taking $s^{(p+1)} = \bar{s}^{(p)}$, consider the transformation giving $A^{(p+2)}$ from $A^{(p)}$:

$$A^{(p+2)} = Q^{(p+1)*}\,Q^{(p)*}\,A^{(p)}\,Q^{(p)}\,Q^{(p+1)}$$

It can be proved that the product $Q^{(p)}Q^{(p+1)}$ derives from the QR decomposition of the matrix $M = (A^{(p)} - s^{(p)}\,I)\,(A^{(p)} - s^{(p+1)}I)$, which is real.

In fact, Francis (1961, 1962) showed that only the first column m_1 of M is necessary for determining the transformation which gives $A^{(p+2)}$ from $A^{(p)}$, if they both have the Hessenberg form.

Practically, the first part of the double iteration consists of the application of an initial transformation $N_1^*\,A^{(p)}\,N_1$ where N_1 is unitary and such that $N_1^*\,m_1 = \pm\,\|m_1\|\,e_1$. This leads to a matrix which no longer has the Hessenberg form.

Thus, the remaining part of the iteration will involve the application of (n-1) successive transformations, which have the same form as the initial one whose matrices N_i are such that the resulting matrix $A^{(p+2)}$ has the Hessenberg form.

This process can fail when a subdiagonal term of the given matrix is zero. In this case, the matrix can be split, and the iteration is performed on the lower main submatrix only.

In the subroutine, N_i are Householder's matrices.

2. Programming considerations

At each iteration, the latent roots x_1 and x_2 of the lower main submatrix of order 2 are computed. Then, the following situations can occur:

a. The term $a_{n-1,n-2}$ can be taken as zero. Then, x_1 and x_2 are eigenvalues of the original matrix, and the order of the matrix is reduced by 2. IANA(N) and IANA(N-1) are set to 0 and 2 respectively.

b. The term $a_{n,n-1}$ can be taken as zero. In this case, $a_{n,n}$ is an eigenvalue of the original matrix, and the order of the matrix is reduced by 1. IANA(N) is set to 1.

c. One of the last two subdiagonal terms is stable through one iteration. Then the smaller one is considered as zero. The corresponding components of IANA are set to 0, 1, or 2, according to a. or b.

d. The maximum number of iterations is reached. In this case, the smaller of the last two subdiagonal elements is taken as zero. The corresponding components of IANA are set to 0, 1, or 2, according to a. or b.

The user can check the results by inspecting the subdiagonal terms of the matrix on return from the subroutine, according to the vector IANA, in the following way:

If for each IANA(I) containing 1 or 2, $2 \le I \le M$,

$$\left|A(I,I-1)\right| \le 10^{-7}\left(\left|RR(I)\right|+\left|RI(I)\right|\right),$$

then RR(I) and RI(I) were computed with a satisfactory accuracy.

For reference see:

(1) J. G. F. Francis, Computer Journal. October, 1961 4-3, January, 1962 4-4.

(2) J. H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.


```
C                                                                       ATEI  10
C     ...................................................................ATEI  20
C                                                                       ATEI  30
C        SUBROUTINE ATEIG                                               ATEI  40
C                                                                       ATEI  50
C        PURPOSE                                                        ATEI  60
C           COMPUTE THE EIGENVALUES OF A REAL ALMOST TRIANGULAR MATRIX  ATEI  70
C                                                                       ATEI  80
C        USAGE                                                          ATEI  90
C           CALL ATEIG(M,A,RR,RI,IANA,IA)                               ATEI 100
C                                                                       ATEI 110
C        DESCRIPTION OF THE PARAMETERS                                  ATEI 120
C           M       ORDER OF THE MATRIX                                 ATEI 130
C           A       THE INPUT MATRIX, M BY M                            ATEI 140
C           RR      VECTOR CONTAINING THE REAL PARTS OF THE EIGENVALUES ATEI 150
C                   ON RETURN                                           ATEI 160
C           RI      VECTOR CONTAINING THE IMAGINARY PARTS OF THE EIGEN- ATEI 170
C                   VALUES ON RETURN                                    ATEI 180
C           IANA    VECTOR WHOSE DIMENSION MUST BE GREATER THAN OR EQUAL ATEI 190
C                   TO M, CONTAINING ON RETURN INDICATIONS ABOUT THE WAY ATEI 200
C                   THE EIGENVALUES APPEARED (SEE MATH. DESCRIPTION)    ATEI 210
C           IA      SIZE OF THE FIRST DIMENSION ASSIGNED TO THE ARRAY A ATEI 220
C                   IN THE CALLING PROGRAM WHEN THE MATRIX IS IN DOUBLE ATEI 230
C                   SUBSCRIPTED DATA STORAGE MODE.                      ATEI 240
C                   IA=M WHEN THE MATRIX IS IN SSP VECTOR STORAGE MODE. ATEI 250
C                                                                       ATEI 260
C        REMARKS                                                        ATEI 270
C           THE ORIGINAL MATRIX IS DESTROYED                            ATEI 280
C           THE DIMENSION OF RR AND RI MUST BE GREATER OR EQUAL TO M    ATEI 290
C                                                                       ATEI 300
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ATEI 310
C           NONE                                                        ATEI 320
C                                                                       ATEI 330
C        METHOD                                                         ATEI 340
C           QR DOUBLE ITERATION                                         ATEI 350
C                                                                       ATEI 360
C        REFERENCES                                                     ATEI 370
C           J.G.F. FRANCIS - THE QR TRANSFORMATION---THE COMPUTER       ATEI 380
C           JOURNAL, VOL. 4, NO. 3, OCTOBER 1961, VOL. 4, NO. 4, JANUARYATEI 390
C           1962.  J. H. WILKINSON - THE ALGEBRAIC EIGENVALUE PROBLEM - ATEI 400
C           CLARENDON PRESS, OXFORD, 1965.                              ATEI 410
C                                                                       ATEI 420
C     ...................................................................ATEI 430
C                                                                       ATEI 440
      SUBROUTINE ATEIG(M,A,RR,RI,IANA,IA)                               ATEI 450
      DIMENSION A(1),RR(1),RI(1),PRR(2),PRI(2),IANA(1)                  ATEI 460
      INTEGER P,Q,C                                                     ATEI 470
C                                                                       ATEI 480
      E7=1.E-8                                                          ATEI 490
      E6=1.E-6                                                          ATEI 500
      E1C=1.E-1C                                                        ATEI 510
      DELTA=0.5                                                         ATEI 520
      MAXIT=3C                                                          ATEI 530
C                                                                       ATEI 540
C        INITIALIZATION                                                 ATEI 550
C                                                                       ATEI 560
      N=M                                                               ATEI 570
   2C N1=N-1                                                            ATEI 580
      IN=N1*IA                                                          ATEI 590
      NN=IN+N                                                           ATEI 600
      IF(N1) 3C,13CC,3C                                                 ATEI 610
   3C NP=N+1                                                            ATEI 620
C                                                                       ATEI 630
C        ITERATION COUNTER                                              ATEI 640
C                                                                       ATEI 650
      IT=C                                                              ATEI 660
C                                                                       ATEI 670
C        ACCTS OF THE 2ND ORDER MAIN SUBMATRIX AT THE PREVIOUS          ATEI 680
C        ITERATION                                                      ATEI 690
C                                                                       ATEI 700
      DO 4C I=1,2                                                       ATEI 710
      PRR(I)=C.C                                                        ATEI 720
   4C PRI(I)=C.C                                                        ATEI 730
C                                                                       ATEI 740
C        LAST TWO SUBDIAGONAL ELEMENTS AT THE PREVIOUS ITERATION        ATEI 750
C                                                                       ATEI 760
      PAN=C.C                                                           ATEI 770
      PAN1=C.C                                                          ATEI 780
C                                                                       ATEI 790
C        ORIGIN SHIFT                                                   ATEI 800
C                                                                       ATEI 810
      P=C.C                                                             ATEI 820
      S=C.C                                                             ATEI 830
C                                                                       ATEI 840
C        ACCTS OF THE LOWER MAIN 2 BY 2 SUBMATRIX                       ATEI 850
C                                                                       ATEI 860
      N2=N1-1                                                           ATEI 870
      IN1=IN-IA                                                         ATEI 880
      NN1=IN1+N                                                         ATEI 890
      N1N=IN+N1                                                         ATEI 900
      N1N1=IN1+N1                                                       ATEI 910
   6C T=A(N1N1)-A(NN)                                                   ATEI 920
      L=T*T                                                             ATEI 930
      W=4.C*A(N1N)*A(NN1)                                               ATEI 940
      IF(ABS(W)-L*E7) 1CC,1CC,65                                        ATEI 950
   65 T=L+W                                                             ATEI 960
      IF(ABS(T)-AMAX1(L,ABS(W))*E6) 67,67,6E                            ATEI 970
   67 T=C.C                                                             ATEI 980
   6E L=(A(N1N1)+A(NN))/2.C                                             ATEI 990
      W=SQRT(ABS(T))/2.C                                                ATEI1000
      IF(T)14C,7C,7C                                                    ATEI1010
   7C IF(L) 8C,75,75                                                    ATEI1020
   75 RR(N1)=L+W                                                        ATEI1030
      RR(N)=L-W                                                         ATEI1040
      GO TO 13C                                                         ATEI1050
   8C RR(N1)=L-W                                                        ATEI1060
      RR(N)=L+W                                                         ATEI1070
      GO TO 13C                                                         ATEI1080
  1CC IF(T)12C,11C,11C                                                  ATEI1090
  11C RR(N1)=A(N1N1)                                                    ATEI1100
      RR(N)=A(NN)                                                       ATEI1110
      GO TO 13C                                                         ATEI1120
  12C RR(N1)=A(NN)                                                      ATEI1130
      RR(N)=A(N1N1)                                                     ATEI1140
  13C RI(N)=C.C                                                         ATEI1150
      RI(N1)=C.C                                                        ATEI1160
      GO TO 16C                                                         ATEI1170
  14C RR(N1)=L                                                          ATEI1180
      RR(N)=L                                                           ATEI1190
      RI(N1)=W                                                          ATEI1200
      RI(N)=-W                                                          ATEI1210
  16C IF(N2)128C,128C,18C                                               ATEI1220
C                                                                       ATEI1230
C        TESTS OF CONVERGENCE                                           ATEI1240
C                                                                       ATEI1250
  18C N1N2=N1N1-IA                                                      ATEI1260
      APCC=ABS(A(N1N1))+ABS(RR(N1)+RI(N1))+ABS(RR(N1))                  ATEI1270
      EPS=E1C*SQRT(APCC)                                                ATEI1280
      IF(ABS(A(N1N2))-EPS)122C,122C,24C                                 ATEI1290
  24C IF(ABS(A(NN1))-E1C*ABS(A(NN))) 13CC,13CC,250                      ATEI1300
  25C IF(ABS(PAN1-A(N1N2))-ABS(A(N1N2))*E6) 124C,124C,26C               ATEI1310
  26C IF(ABS(PAN-A(NN1))-ABS(A(NN1))*EE)124C,1240,30C                   ATEI1320
  30C IF(IT-MAXIT) 32C,124C,124C                                        ATEI1330
C                                                                       ATEI1340
C        COMPUTE THE SHIFT                                              ATEI1350
C                                                                       ATEI1360
  32C J=1                                                               ATEI1370
      DO 36C I=1,2                                                      ATEI1380
      K=NP-I                                                            ATEI1390
      IF(ABS(PRR(K)-PRR(I))+ABS(PRI(K)-PRI(I))-DELTA*(ABS(RR(K))        ATEI1400
     1    +ABS(RI(K))) 34C,34C,36C                                      ATEI1410
  34C J=J+I                                                             ATEI1420
  36C CONTINUE                                                          ATEI1430
      GO TO (44C,46C,46C,46C),J                                         ATEI1440
  44C P=C.C                                                             ATEI1450
      S=C.C                                                             ATEI1460
      GO TO 5CC                                                         ATEI1470
  46C J=N+2-J                                                           ATEI1480
      P=RR(J)+RR(J)                                                     ATEI1490
      S=RR(J)*RR(J)                                                     ATEI1500
      GO TO 5CC                                                         ATEI1510
  48C H=RR(N)*RR(N1)-RI(N1)*RI(N1)                                      ATEI1520
      S=RR(N)+RR(N1)                                                    ATEI1530
C                                                                       ATEI1540
C        SAVE THE LAST TWO SUBDIAGONAL TERMS AND THE ACCTS OF THE       ATEI1550
C        SUBMATRIX BEFORE ITERATION                                     ATEI1560
C                                                                       ATEI1570
  5CC PAN=A(NN1)                                                        ATEI1580
      PAN1=A(N1N2)                                                      ATEI1590
      DO 52C I=1,2                                                      ATEI1600
      K=NP-I                                                            ATEI1610
      PRR(I)=RR(K)                                                      ATEI1620
   52C PRI(I)=RI(K)                                                     ATEI1630
C                                                                       ATEI1640
C        SEARCH FOR A PARTITION OF THE MATRIX, DEFINED BY P AND Q       ATEI1650
C                                                                       ATEI1660
      F=N2                                                              ATEI1670
      IF (N-3)6CC,6CC,525                                               ATEI1675
  525 IPI=N1N2                                                          ATEI1680
      DO 58C J=2,N2                                                     ATEI1690
      IFI=IPI-IA-1                                                      ATEI1700
      IF(ABS(A(IPI))-EPS) 6CC,6CC,53C                                   ATEI1710
```

```
   53C IPIF=IFI+IA                                                    ATEI1720
       IFIF2=IFIF+IA                                                  ATEI1730
       E=A(IPIF)*(A(IPIP)-S)+A(IPIP2)*A(IPIP+1)+R                     ATEI1740
       IF(E)54C,56C,54C                                               ATEI1750
   54C IF(ABS(A(IPI)*A(IPIP+1))*(ABS(A(IPIP)+A(IPIP2+1)-S)+ABS(A(IPIP2+2)ATEI1760
      1 ))-ABS(E)*EPS) 62C,62C,56C                                    ATEI1770
   56C F=N1-J                                                         ATEI1780
   58C CONTINUE                                                       ATEI1790
   60C G=P                                                            ATEI1800
       GO TO 66C                                                      ATEI1810
   62C F1=F-1                                                         ATEI1820
       G=F1                                                           ATEI1830
       IF (F1-1) 68C,66C,65C                                          ATEI1835
   65C DO 66C I=2, F1                                                 ATEI1840
       IFI=IPI-IA-I                                                   ATEI1850
       IF(ABS(A(IFI))-EPS)66C,68C,66C                                 ATEI1860
   66C G=G-1                                                          ATEI1870
C                                                                     ATEI1880
C        OR DOUBLE ITERATION                                          ATEI1890
C                                                                     ATEI1900
   68C II=(P-1)*IA+P                                                  ATEI1910
       DO 122C I=P,N1                                                 ATEI1920
       III=II-IA                                                      ATEI1930
       IIP=II+IA                                                      ATEI1940
       IF(I-P)72C,70C,72C                                             ATEI1950
   70C IFI=II+1                                                       ATEI1960
       IFIP=IIP+1                                                     ATEI1970
C                                                                     ATEI1980
C        INITIALIZATION OF THE TRANSFORMATION                         ATEI1990
C                                                                     ATEI2000
       G1=A(II)*(A(II)-S)+A(IIP)*A(IPI)+R                             ATEI2010
       G2=A(IFI)*(A(IPIF)+A(III)-S)                                   ATEI2020
       G3=A(IFI)*A(IPIF+1)                                            ATEI2030
       A(IFI+1)=0.0                                                   ATEI2040
       GO TO 76C                                                      ATEI2050
   72C G1=A(III)                                                      ATEI2060
       G2=A(III+1)                                                    ATEI2070
       IF(I-N2)74C,74C,76C                                            ATEI2080
   74C G3=A(III+2)                                                    ATEI2090
       GO TO 78C                                                      ATEI2100
   76C G3=0.0                                                         ATEI2110
   78C CAP=SQRT(G1*G1+G2*G2+G3*G3)                                    ATEI2120
       IF(CAP)80C,80C,80C                                             ATEI2130
   80C IF(G1)82C,84C,84C                                              ATEI2140
   82C CAP=-CAP                                                       ATEI2150
   84C T=G1+CAP                                                       ATEI2160
       PSI1=G2/T                                                      ATEI2170
       PSI2=G3/T                                                      ATEI2180
       ALPHA=2.0/(1.0+PSI1*PSI1+PSI2*PSI2)                            ATEI2190
       GO TO 88C                                                      ATEI2200
   86C ALPHA=2.0                                                      ATEI2210
       PSI1=0.0                                                       ATEI2220
       PSI2=0.0                                                       ATEI2230
   88C IF(I-P)90C,96C,90C                                             ATEI2240
   90C IF(I-P1)92C,94C,92C                                            ATEI2250
   92C A(III)=-CAP                                                    ATEI2260
       GO TO 96C                                                      ATEI2270
   94C A(III)=-A(III)                                                 ATEI2280
C                                                                     ATEI2290
C        ROW OPERATION                                                ATEI2300
C                                                                     ATEI2310
   96C IJ=II                                                          ATEI2320
       DO 104C J=I,N                                                  ATEI2330
       T=PSI1*A(IJ+1)                                                 ATEI2340
       IF(I-N1)98C,100C,100C                                          ATEI2350
   98C IP2J=IJ+2                                                      ATEI2360
       T=T+PSI2*A(IP2J)                                               ATEI2370
  100C ETA=ALPHA*(T+A(IJ))                                            ATEI2380
       A(IJ)=A(IJ)-ETA                                                ATEI2390
       A(IJ+1)=A(IJ+1)-PSI1*ETA                                       ATEI2400
       IF(I-N1)102C,104C,104C                                         ATEI2410
  102C A(IP2J)=A(IP2J)-PSI2*ETA                                       ATEI2420
  104C IJ=IJ+IA                                                       ATEI2430
C                                                                     ATEI2440
C        COLUMN OPERATION                                             ATEI2450
C                                                                     ATEI2460
       IF(I-N1)106C,106C,106C                                         ATEI2470
  106C K=N                                                            ATEI2480
       GO TO 110C                                                     ATEI2490
  108C K=I+2                                                          ATEI2500
  110C IF=IIF-I                                                       ATEI2510
       DO 118C J=G,K                                                  ATEI2520
       JIF=IP+J                                                       ATEI2530
       JI=JIF-IA                                                      ATEI2540
       T=PSI1*A(JIP)                                                  ATEI2550
       IF(I-N1)112C,114C,114C                                         ATEI2560
  112C JIF2=JIF+IA                                                    ATEI2570
       T=T+PSI2*A(JIP2)                                               ATEI2580
  114C ETA=ALPHA*(T+A(JI))                                            ATEI2590
       A(JI)=A(JI)-ETA                                                ATEI2600
       A(JIF)=A(JIF)-ETA*PSI1                                         ATEI2610
       IF(I-N1)116C,116C,116C                                         ATEI2620
  116C A(JIF2)=A(JIP2)-ETA*PSI2                                       ATEI2630
  118C CONTINUE                                                       ATEI2640
       IF(I-N2)120C,122C,122C                                         ATEI2650
  120C JI=II+3                                                        ATEI2660
       JIP=JI+IA                                                      ATEI2670
       JIF2=JIF+IA                                                    ATEI2680
       ETA=ALPHA*PSI2*A(JIP2)                                         ATEI2690
       A(JI)=-ETA                                                     ATEI2700
       A(JIF)=-ETA*PSI1                                               ATEI2710
       A(JIF2)=A(JIF2)-ETA*PSI2                                       ATEI2720
  122C II=IIF+1                                                       ATEI2730
       IT=IT+1                                                        ATEI2740
       GO TO 60                                                       ATEI2750
C                                                                     ATEI2760
C        END OF ITERATION                                             ATEI2770
C                                                                     ATEI2780
  124C IF(ABS(A(NN1))-ABS(A(NN2))) 130C,128C,128C                     ATEI2790
C                                                                     ATEI2800
C        TWO EIGENVALUES HAVE BEEN FOUND                              ATEI2810
C                                                                     ATEI2820
  126C IAMA(N)=0                                                      ATEI2830
       IAMA(N1)=2                                                     ATEI2840
       N=N2                                                           ATEI2850
       IF(N2)114C0,114C0,2C                                           ATEI2860
C                                                                     ATEI2870
C        ONE EIGENVALUE HAS BEEN FOUND                                ATEI2880
C                                                                     ATEI2890
  130C WR(N)=A(NN)                                                    ATEI2900
       WI(N)=0.0                                                      ATEI2910
       IAMA(N)=1                                                      ATEI2920
       IF(N)114C0,114C0,132C                                          ATEI2930
  132C N=N1                                                           ATEI2940
       GO TO 2C                                                       ATEI2950
  140C RETURN                                                         ATEI2960
       END                                                            ATEI2970
```

Subroutine HSBG

This subroutine reduces an n by n real matrix A by a similarity transformation to upper almost-triangular (Hessenberg) form. Each row is reduced in turn, starting from the last one, by applying a suitable right elimination matrix, and similarity is achieved by also applying the left inverse transformation. Thus the eigenvalues of A are preserved.

1. Mathematical background

Let $A^{(p)}$ denote the matrix obtained from $A^{(o)} = A$ after reducing rows $n, n-1, \ldots, n-p+1$. The similarity which transforms $A^{(p)}$ to $A^{(p+1)}$ is as follows:

a. First we determine a pivot element $a^{(p)}_{n-p,k}$ whose column subscript k is such that

$$\left| a^{(p)}_{n-p,k} \right| = \max_i \left| a^{(p)}_{n-p,i} \right| , i = 1, 2, \ldots, n-p-1$$

b. If the pivot element $a^{(p)}_{n-p,k} = 0$, no transformations are necessary; that is, the (p+1)th similarity is the identity transformation. Otherwise, if it is necessary ($k \neq n-p-1$), we interchange the kth and (n-p-1)th columns so that the pivot element is in the subdiagonal position. The same interchange is applied to the rows of $A^{(p)}$. The resulting matrix is similar to $A^{(p)}$, and, to ease the notation, we denote it by $A^{(p)}$.

c. Define multipliers

$$b^{(p)}_j = a^{(p)}_{n-p,j} / a^{(p)}_{n-p,n-p-1} \quad j=1,2,\ldots,n-p-2$$

Then the (p+1)th similarity is given by the following.

Right elimination:

$$\bar{a}^{(p)}_{ij} = a^{(p)}_{ij} - b^{(p)}_j \, a^{(p)}_{i,n-p-1}$$

$i=1,2,\ldots,n-p$
$j=1,2,\ldots,n-p-2$

$$\bar{a}^{(p)}_{ij} = a^{(p)}_{ij} \qquad \text{other indices}$$

Left inverse transformation:

$$a^{(p+1)}_{n-p-1,j} = \bar{a}^{(p)}_{n-p-1,j} + \sum_{i=1}^{n-p-2} b^{(p)}_i \, \bar{a}^{(p)}_{ij}$$

$$a_{ij}^{(p+1)} = \bar{a}_{ij}^{(p)} \qquad i \neq n-p-1$$

Finally, $A^{(n-2)}$ will have the upper almost-triangular form.

For reference see J. H. Wilkinson, The Algebraic Eigenvalue Problem. Clarendon Press, Oxford, 1965.

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C                                                                       HSBG  10
C     ..................................................................HSBG  20
C                                                                       HSBG  30
C        SUBROUTINE HSBG                                                HSBG  40
C                                                                       HSBG  50
C        PURPOSE                                                        HSBG  60
C           TO REDUCE A REAL MATRIX INTO UPPER ALMOST TRIANGULAR FORM   HSBG  70
C                                                                       HSBG  80
C        USAGE                                                          HSBG  90
C           CALL HSBG(N,A,IA)                                           HSBG 100
C                                                                       HSBG 110
C        DESCRIPTION OF THE PARAMETERS                                  HSBG 120
C           N       ORDER OF THE MATRIX                                 HSBG 130
C           A       THE INPUT MATRIX, N BY N                            HSBG 140
C           IA      SIZE OF THE FIRST DIMENSION ASSIGNED TO THE ARRAY   HSBG 150
C                   A IN THE CALLING PROGRAM WHEN THE MATRIX IS IN      HSBG 160
C                   DOUBLE SUBSCRIPTED DATA STORAGE MODE.  IA=N WHEN    HSBG 170
C                   THE MATRIX IS IN SSP VECTOR STORAGE MODE.           HSBG 180
C                                                                       HSBG 190
C        REMARKS                                                        HSBG 200
C           THE HESSENBERG FORM REPLACES THE ORIGINAL MATRIX IN THE      HSBG 210
C           ARRAY A.                                                    HSBG 220
C                                                                       HSBG 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  HSBG 240
C           NONE                                                        HSBG 250
C                                                                       HSBG 260
C        METHOD                                                         HSBG 270
C           SIMILARITY TRANSFORMATIONS USING ELEMENTARY ELIMINATION     HSBG 280
C           MATRICES, WITH PARTIAL PIVOTING.                            HSBG 290
C                                                                       HSBG 300
C        REFERENCES                                                     HSBG 310
C           J.H. WILKINSON - THE ALGEBRAIC EIGENVALUE PROBLEM -         HSBG 320
C           CLARENDON PRESS, OXFORD, 1965.                              HSBG 330
C                                                                       HSBG 340
C     ..................................................................HSBG 350
C                                                                       HSBG 360
      SUBROUTINE HSBG(N,A,IA)                                           HSBG 370
      DIMENSION A(1)                                                    HSBG 380
      DOUBLE PRECISION S                                                HSBG 390
      L=N                                                               HSBG 400
      NIA=L*IA                                                          HSBG 410
      LIA=NIA-IA                                                        HSBG 420
C                                                                       HSBG 430
C        L IS THE ROW INDEX OF THE ELIMINATION                          HSBG 440
C                                                                       HSBG 450
   20 IF(L-3) 360,40,40                                                 HSBG 460
   40 LIA=LIA-IA                                                        HSBG 470
      L1=L-1                                                            HSBG 480
      L2=L1-1                                                           HSBG 490
C                                                                       HSBG 500
C        SEARCH FOR THE PIVOTAL ELEMENT IN THE LTH ROW                  HSBG 510
C                                                                       HSBG 520
      ISUB=LIA+L                                                        HSBG 530
      IPIV=ISUB-IA                                                      HSBG 540
      PIV=ABS(A(IPIV))                                                  HSBG 550
      IF(L-3) 90,90,50                                                  HSBG 560
   50 M=IPIV-IA                                                         HSBG 570
      DO 90 I=L,M,IA                                                    HSBG 580
      T=ABS(A(I))                                                       HSBG 590
      IF(T-PIV) 80,80,60                                                HSBG 600
   60 IPIV=I                                                            HSBG 610
      PIV=T                                                             HSBG 620
   80 CONTINUE                                                          HSBG 630
   90 IF(PIV) 100,320,100                                               HSBG 640
  100 IF(PIV-ABS(A(ISUB))) 180,180,120                                  HSBG 650
C                                                                       HSBG 660
C        INTERCHANGE THE COLUMNS                                        HSBG 670
C                                                                       HSBG 680
  120 M=IPIV-L                                                          HSBG 690
      DO 140 I=1,L                                                      HSBG 700
      J=M+I                                                             HSBG 710
      T=A(J)                                                            HSBG 720
      K=LIA+I                                                           HSBG 730
      A(J)=A(K)                                                         HSBG 740
  140 A(K)=T                                                            HSBG 750
C                                                                       HSBG 760
C        INTERCHANGE THE ROWS                                           HSBG 770
C                                                                       HSBG 780
      M=L2-M/IA                                                         HSBG 790
      DO 160 I=L1,NIA,IA                                                HSBG 800
      T=A(I)                                                            HSBG 810
      J=I-M                                                             HSBG 820
      A(I)=A(J)                                                         HSBG 830
  160 A(J)=T                                                            HSBG 840
C                                                                       HSBG 850
C        TERMS OF THE ELEMENTARY TRANSFORMATION                         HSBG 860
C                                                                       HSBG 870
  180 DO 200 I=L,LIA,IA                                                 HSBG 880
  200 A(I)=A(I)/A(ISUB)                                                 HSBG 890
C                                                                       HSBG 900
C        RIGHT TRANSFORMATION                                           HSBG 910
C                                                                       HSBG 920
      J=-IA                                                             HSBG 930
      DO 240 I=1,L2                                                     HSBG 940
      J=J+IA                                                            HSBG 950
      LJ=L+J                                                            HSBG 960
      DO 220 K=1,L1                                                     HSBG 970
      KJ=K+J                                                            HSBG 980
      KL=K+LIA                                                          HSBG 990
  220 A(KJ)=A(KJ)-A(LJ)*A(KL)                                           HSBG1000
  240 CONTINUE                                                          HSBG1010
C                                                                       HSBG1020
C        LEFT TRANSFORMATION                                            HSBG1030
C                                                                       HSBG1040
      K=-IA                                                             HSBG1050
      DO 300 I=1,N                                                      HSBG1060
      K=K+IA                                                            HSBG1070
      LK=K+L1                                                           HSBG1080
      S=A(LK)                                                           HSBG1090
      LJ=L-IA                                                           HSBG1100
      DO 280 J=1,L2                                                     HSBG1110
      JK=K+J                                                            HSBG1120
      LJ=LJ+IA                                                          HSBG1130
  280 S=S+A(LJ)*A(JK)*1.000                                             HSBG1140
  300 A(LK)=S                                                           HSBG1150
C                                                                       HSBG1160
C        SET THE LOWER PART OF THE MATRIX TO ZERO                       HSBG1170
C                                                                       HSBG1180
      DO 310 I=L,LIA,IA                                                 HSBG1190
  310 A(I)=0.0                                                          HSBG1200
  320 L=L1                                                              HSBG1210
      GO TO 20                                                          HSBG1220
  360 RETURN                                                            HSBG1230
      END                                                               HSBG1240
```

Subroutine PADD

```
C                                                                       PADD  10
C     ...................................................................PADD  20
C                                                                       PADD  30
C        SUBROUTINE PADD                                                PADD  40
C                                                                       PADD  50
C        PURPOSE                                                        PADD  60
C           ADD TWO POLYNOMIALS                                         PADD  70
C                                                                       PADD  80
C        USAGE                                                          PADD  90
C           CALL PADD(Z,IDIMZ,X,IDIMX,Y,IDIMY)                          PADD 100
C                                                                       PADD 110
C        DESCRIPTION OF PARAMETERS                                      PADD 120
C           Z      - VECTOR OF RESULTANT COEFFICIENTS, ORDERED FROM     PADD 130
C                    SMALLEST TO LARGEST POWER                          PADD 140
C           IDIMZ - DIMENSION OF Z (CALCULATED)                        PADD 150
C           X      - VECTOR OF COEFFICIENTS FOR FIRST POLYNOMIAL, ORDEREDPADD 160
C                    FROM SMALLEST TO LARGEST POWER                     PADD 170
C           IDIMX - DIMENSION OF X (DEGREE IS IDIMX-1)                 PADD 180
C           Y      - VECTOR OF COEFFICIENTS FOR SECOND POLYNOMIAL,      PADD 190
C                    ORDERED FROM SMALLEST TO LARGEST POWER             PADD 200
C           IDIMY - DIMENSION OF Y (DEGREE IS IDIMY-1)                 PADD 210
C                                                                       PADD 220
C        REMARKS                                                        PADD 230
C           VECTOR Z MAY BE IN SAME LOCATION AS EITHER VECTOR X OR      PADD 240
C           VECTOR Y ONLY IF THE DIMENSION OF THAT VECTOR IS NOT LESS   PADD 250
C           THAN THE OTHER INPUT VECTOR                                PADD 260
C           THE RESULTANT POLYNOMIAL MAY HAVE TRAILING ZERO COEFFICIENTSPADD 270
C                                                                       PADD 280
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PADD 290
C           NONE                                                        PADD 300
C                                                                       PADD 310
C        METHOD                                                         PADD 320
C           DIMENSION OF RESULTANT VECTOR IDIMZ IS CALCULATED AS THE    PADD 330
C           LARGER OF THE TWO INPUT VECTOR DIMENSIONS. CORRESPONDING    PADD 340
C           COEFFICIENTS ARE THEN ADDED TO FORM Z.                      PADD 350
C                                                                       PADD 360
C     ...................................................................PADD 370
C                                                                       PADD 380
      SUBROUTINE PADD(Z,IDIMZ,X,IDIMX,Y,IDIMY)                          PADD 390
      DIMENSION Z(1),X(1),Y(1)                                          PADD 400
C                                                                       PADD 410
C     TEST DIMENSIONS OF SUMMANDS                                       PADD 420
C                                                                       PADD 430
      NDIM=IDIMX                                                        PADD 440
      IF (IDIMX-IDIMY) 10,20,20                                         PADD 450
   10 NDIM=IDIMY                                                        PADD 460
   20 IF(NDIM) 90,90,30                                                 PADD 470
   30 DO 80 I=1,NDIM                                                    PADD 480
      IF(I-IDIMX) 40,40,60                                              PADD 490
   40 IF(I-IDIMY) 50,50,70                                              PADD 500
   50 Z(I)=X(I)+Y(I)                                                    PADD 510
      GO TO 80                                                          PADD 520
   60 Z(I)=Y(I)                                                         PADD 530
      GO TO 80                                                          PADD 540
   70 Z(I)=X(I)                                                         PADD 550
   80 CONTINUE                                                          PADD 560
   90 IDIMZ=NDIM                                                        PADD 570
      RETURN                                                            PADD 580
      END                                                               PADD 590
```

Subroutine PSUB

```
C                                                                       PSUB  10
C     ...................................................................PSUB  20
C                                                                       PSUB  30
C        SUBROUTINE PSUB                                                PSUB  40
C                                                                       PSUB  50
C        PURPOSE                                                        PSUB  60
C           SUBTRACT ONE POLYNOMIAL FROM ANOTHER                        PSUB  70
C                                                                       PSUB  80
C        USAGE                                                          PSUB  90
C           CALL PSUB(Z,IDIMZ,X,IDIMX,Y,IDIMY)                          PSUB 100
C                                                                       PSUB 110
C        DESCRIPTION OF PARAMETERS                                      PSUB 120
C           Z      - VECTOR OF RESULTANT COEFFICIENTS, ORDERED FROM     PSUB 130
C                    SMALLEST TO LARGEST POWER                          PSUB 140
C           IDIMZ - DIMENSION OF Z (CALCULATED)                        PSUB 150
C           X      - VECTOR OF COEFFICIENTS FOR FIRST POLYNOMIAL, ORDEREDPSUB 160
C                    FROM SMALLEST TO LARGEST POWER                     PSUB 170
C           IDIMX - DIMENSION OF X (DEGREE IS IDIMX-1)                 PSUB 180
C           Y      - VECTOR OF COEFFICIENTS FOR SECOND POLYNOMIAL,      PSUB 190
C                    ORDERED FROM SMALLEST TO LARGEST POWER             PSUB 200
C           IDIMY - DIMENSION OF Y (DEGREE IS IDIMY-1)                 PSUB 210
C                                                                       PSUB 220
C        REMARKS                                                        PSUB 230
C           VECTOR Z MAY BE IN SAME LOCATION AS EITHER VECTOR X OR      PSUB 240
C           VECTOR Y ONLY IF THE DIMENSION OF THAT VECTOR IS NOT LESS   PSUB 250
C           THAN THE OTHER INPUT VECTOR                                PSUB 260
C           THE RESULTANT POLYNOMIAL MAY HAVE TRAILING ZERO COEFFICIENTSPSUB 270
C                                                                       PSUB 280
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PSUB 290
C           NONE                                                        PSUB 300
C                                                                       PSUB 310
C        METHOD                                                         PSUB 320
C           DIMENSION OF RESULTANT VECTOR IDIMZ IS CALCULATED AS THE    PSUB 330
C           LARGER OF THE TWO INPUT VECTOR DIMENSIONS. COEFFICIENTS IN  PSUB 340
C           VECTOR Y ARE THEN SUBTRACTED FROM CORRESPONDING COEFFICIENTSPSUB 350
C           IN VECTOR X.                                               PSUB 360
C                                                                       PSUB 370
C     ...................................................................PSUB 380
C                                                                       PSUB 390
      SUBROUTINE PSUB(Z,IDIMZ,X,IDIMX,Y,IDIMY)                          PSUB 400
      DIMENSION Z(1),X(1),Y(1)                                          PSUB 410
C                                                                       PSUB 420
C     TEST DIMENSIONS OF SUMMANDS                                       PSUB 430
C                                                                       PSUB 440
      NDIM=IDIMX                                                        PSUB 450
      IF (IDIMX-IDIMY) 10,20,20                                         PSUB 460
   10 NDIM=IDIMY                                                        PSUB 470
   20 IF (NDIM) 90,90,30                                                PSUB 480
   30 DO 80 I=1,NDIM                                                    PSUB 490
      IF (I-IDIMX) 40,40,60                                             PSUB 500
   40 IF (I-IDIMY) 50,50,70                                             PSUB 510
   50 Z(I)=X(I)-Y(I)                                                    PSUB 520
      GO TO 80                                                          PSUB 530
   60 Z(I)=-Y(I)                                                        PSUB 540
      GO TO 80                                                          PSUB 550
   70 Z(I)=X(I)                                                         PSUB 560
   80 CONTINUE                                                          PSUB 570
   90 IDIMZ=NDIM                                                        PSUB 580
      RETURN                                                            PSUB 590
      END                                                               PSUB 600
```

Subroutine PMPY

```
C                                                                       PMPY  10
C     ...................................................................PMPY  20
C                                                                       PMPY  30
C        SUBROUTINE PMPY                                                PMPY  40
C                                                                       PMPY  50
C        PURPOSE                                                        PMPY  60
C           MULTIPLY TWO POLYNOMIALS                                    PMPY  70
C                                                                       PMPY  80
C        USAGE                                                          PMPY  90
C           CALL PMPY(Z,IDIMZ,X,IDIMX,Y,IDIMY)                          PMPY 100
C                                                                       PMPY 110
C        DESCRIPTION OF PARAMETERS                                      PMPY 120
C           Z      - VECTOR OF RESULTANT COEFFICIENTS, ORDERED FROM     PMPY 130
C                    SMALLEST TO LARGEST POWER                          PMPY 140
C           IDIMZ - DIMENSION OF Z (CALCULATED)                        PMPY 150
C           X      - VECTOR OF COEFFICIENTS FOR FIRST POLYNOMIAL, ORDEREDPMPY 160
C                    FROM SMALLEST TO LARGEST POWER                     PMPY 170
C           IDIMX - DIMENSION OF X (DEGREE IS IDIMX-1)                 PMPY 180
C           Y      - VECTOR OF COEFFICIENTS FOR SECOND POLYNOMIAL,      PMPY 190
C                    ORDERED FROM SMALLEST TO LARGEST POWER             PMPY 200
C           IDIMY - DIMENSION OF Y (DEGREE IS IDIMY-1)                 PMPY 210
C                                                                       PMPY 220
C        REMARKS                                                        PMPY 230
C           Z CANNOT BE IN THE SAME LOCATION AS X                       PMPY 240
C           Z CANNOT BE IN THE SAME LOCATION AS Y                       PMPY 250
C                                                                       PMPY 260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PMPY 270
C           NONE                                                        PMPY 280
C                                                                       PMPY 290
C        METHOD                                                         PMPY 300
C           DIMENSION OF Z IS CALCULATED AS IDIMX+IDIMY-1               PMPY 310
C           THE COEFFICIENTS OF Z ARE CALCULATED AS SUM OF PRODUCTS     PMPY 320
C           OF COEFFICIENTS OF X AND Y , WHOSE EXPONENTS ADD UP TO THE  PMPY 330
C           CORRESPONDING EXPONENT OF Z.                                PMPY 340
C                                                                       PMPY 350
C     ...................................................................PMPY 360
C                                                                       PMPY 370
      SUBROUTINE PMPY(Z,IDIMZ,X,IDIMX,Y,IDIMY)                          PMPY 380
      DIMENSION Z(1),X(1),Y(1)                                          PMPY 390
C                                                                       PMPY 400
      IF(IDIMX*IDIMY)10,10,20                                           PMPY 410
   10 IDIMZ=0                                                           PMPY 420
      GO TO 50                                                          PMPY 430
   20 IDIMZ=IDIMX+IDIMY-1                                               PMPY 440
      DO 30 I=1,IDIMZ                                                   PMPY 450
   30 Z(I)=0.                                                           PMPY 460
      DO 40 I=1,IDIMX                                                   PMPY 470
      DO 40 J=1,IDIMY                                                   PMPY 480
      K=I+J-1                                                           PMPY 490
   40 Z(K)=X(I)*Y(J)+Z(K)                                               PMPY 500
   50 RETURN                                                            PMPY 510
      END                                                               PMPY 520
```

Subroutine PDIV

```
C                                                                       PDIV  10
C     ...................................................................PDIV  20
C                                                                       PDIV  30
C        SUBROUTINE PDIV                                                PDIV  40
C                                                                       PDIV  50
C        PURPOSE                                                        PDIV  60
C           DIVIDE ONE POLYNOMIAL BY ANOTHER                            PDIV  70
C                                                                       PDIV  80
C        USAGE                                                          PDIV  90
C           CALL PDIV(P,IDIMP,X,IDIMX,Y,IDIMY,TOL,IER)                  PDIV 100
C                                                                       PDIV 110
C        DESCRIPTION OF PARAMETERS                                      PDIV 120
C           P      - RESULTANT VECTOR OF INTEGRAL PART                  PDIV 130
C           IDIMP - DIMENSION OF P                                      PDIV 140
C           X      - VECTOR OF COEFFICIENTS FOR DIVIDENO POLYNOMIAL,    PDIV 150
C                    ORDERED FROM SMALLEST TO LARGEST POWER. IT IS      PDIV 160
C                    REPLACED BY REMAINDER AFTER DIVISION.              PDIV 170
C           IDIMX - DIMENSION OF X                                      PDIV 180
C           Y      - VECTOR OF COEFFICIENTS FOR DIVISOR POLYNOMIAL,     PDIV 190
C                    ORDERED FROM SMALLEST TO LARGEST POWER             PDIV 200
C           IDIMY - DIMENSION OF Y                                      PDIV 210
C           TOL    - TOLERANCE VALUE BELOW WHICH COEFFICIENTS ARE       PDIV 220
C                    ELIMINATED DURING NORMALIZATION                    PDIV 230
C           IER    - ERROR CODE. 0 IS NORMAL, 1 IS FOR ZERO DIVISOR     PDIV 240
C                                                                       PDIV 250
C        REMARKS                                                        PDIV 260
C           THE REMAINDER R REPLACES X.                                 PDIV 270
C           THE DIVISOR Y REMAINS UNCHANGED.                            PDIV 280
C           IF DIMENSION OF Y EXCEEDS DIMENSION OF X, IDIMP IS SET TO   PDIV 290
C           ZERO AND CALCULATION IS BYPASSED                            PDIV 300
C                                                                       PDIV 310
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PDIV 320
C           PNORM                                                       PDIV 330
C                                                                       PDIV 340
C        METHOD                                                         PDIV 350
C           POLYNOMIAL X IS DIVIDED BY POLYNOMIAL Y GIVING INTEGER PART PDIV 360
C           P AND REMAINDER R SUCH THAT X = P*Y + R.                    PDIV 370
C           DIVISOR Y AND REMAINDER  VECTOR GET NORMALIZED.             PDIV 380
C                                                                       PDIV 390
C     ...................................................................PDIV 400
C                                                                       PDIV 410
      SUBROUTINE PDIV(P,IDIMP,X,IDIMX,Y,IDIMY,TOL,IER)                  PDIV 420
      DIMENSION P(1),X(1),Y(1)                                          PDIV 430
C                                                                       PDIV 440
      CALL PNORM (Y,IDIMY,TOL)                                          PDIV 450
      IF(IDIMY) 50,50,10                                                PDIV 460
   10 IDIMP=IDIMX-IDIMY+1                                               PDIV 470
      IF(IDIMP) 20,30,60                                                PDIV 480
C                                                                       PDIV 490
C     DEGREE OF DIVISOR WAS GREATER THAN DEGREE OF DIVIDENO             PDIV 500
C                                                                       PDIV 510
   20 IDIMP=0                                                           PDIV 520
   30 IER=0                                                             PDIV 530
   40 RETURN                                                            PDIV 540
C                                                                       PDIV 550
C     Y IS ZERO POLYNOMIAL                                              PDIV 560
C                                                                       PDIV 570
   50 IER=1                                                             PDIV 580
      GO TO 40                                                          PDIV 590
C                                                                       PDIV 600
C     START REDUCTION                                                   PDIV 610
C                                                                       PDIV 620
   60 IDIMX=IDIMY-1                                                     PDIV 630
      I=IDIMP                                                           PDIV 640
   70 II=I+IDIMX                                                        PDIV 650
      P(I)=X(II)/Y(IDIMY)                                               PDIV 660
C                                                                       PDIV 670
C     SUBTRACT MULTIPLE OF DIVISOR                                      PDIV 680
C                                                                       PDIV 690
      DO 80 K=1,IDIMX                                                   PDIV 700
      J=K-1+I                                                           PDIV 710
      X(J)=X(J)-P(I)*Y(K)                                               PDIV 720
   80 CONTINUE                                                          PDIV 730
      I=I-1                                                             PDIV 740
      IF(I) 90,90,70                                                    PDIV 750
C                                                                       PDIV 760
C     NORMALIZE REMAINDER POLYNOMIAL                                    PDIV 770
C                                                                       PDIV 780
   90 CALL PNORM(X,IDIMX,TOL)                                           PDIV 790
      GO TO 30                                                          PDIV 800
      END                                                               PDIV 810
```

Subroutine PCLA

```
C                                                                       PCLA  10
C     ...................................................................PCLA  20
C                                                                       PCLA  30
C        SUBROUTINE PCLA                                                PCLA  40
C                                                                       PCLA  50
C        PURPOSE                                                        PCLA  60
C           MOVE POLYNOMIAL X TO Y                                      PCLA  70
C                                                                       PCLA  80
C        USAGE                                                          PCLA  90
C           CALL PCLA(Y,IDIMY,X,IDIMX)                                  PCLA 100
C                                                                       PCLA 110
C        DESCRIPTION OF PARAMETERS                                      PCLA 120
C           Y      - VECTOR OF RESULTANT COEFFICIENTS, ORDERED FROM     PCLA 130
C                    SMALLEST TO LARGEST POWER                          PCLA 140
C           IDIMY - DIMENSION OF Y                                      PCLA 150
C           X      - VECTOR OF COEFFICIENTS FOR POLYNOMIAL, ORDERED     PCLA 160
C                    FROM SMALLEST TO LARGEST POWER                     PCLA 170
C           IDIMX - DIMENSION OF X                                      PCLA 180
C                                                                       PCLA 190
C        REMARKS                                                        PCLA 200
C           NONE                                                        PCLA 210
C                                                                       PCLA 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PCLA 230
C           NONE                                                        PCLA 240
C                                                                       PCLA 250
C        METHOD                                                         PCLA 260
C           IDIMY IS REPLACED BY IDIMX AND VECTOR X IS MOVED TO Y       PCLA 270
C                                                                       PCLA 280
C     ...................................................................PCLA 290
C                                                                       PCLA 300
      SUBROUTINE PCLA (Y,IDIMY,X,IDIMX)                                 PCLA 310
      DIMENSION X(1),Y(1)                                               PCLA 320
C                                                                       PCLA 330
      IDIMY=IDIMX                                                       PCLA 340
      IF(IDIMX) 30,30,10                                                PCLA 350
   10 DO 20 I=1,IDIMX                                                   PCLA 360
   20 Y(I)=X(I)                                                         PCLA 370
   30 RETURN                                                            PCLA 380
      END                                                               PCLA 390
```

Subroutine PADDM

```
C                                                                       PDDM  10
C     ...................................................................PDDM  20
C                                                                       PDDM  30
C        SUBROUTINE PADDM                                               PDDM  40
C                                                                       PDDM  50
C        PURPOSE                                                        PDDM  60
C           ADD COEFFICIENTS OF ONE POLYNOMIAL TO THE PRODUCT OF A      PDDM  70
C           FACTOR BY COEFFICIENTS OF ANOTHER POLYNOMIAL                PDDM  80
C                                                                       PDDM  90
C        USAGE                                                          PDDM 100
C           CALL PADDM(Z,IDIMZ,X,IDIMX,FACT,Y,IDIMY)                    PDDM 110
C                                                                       PDDM 120
C        DESCRIPTION OF PARAMETERS                                      PDDM 130
C           Z      - VECTOR OF RESULTANT COEFFICIENTS, ORDERED FROM     PDDM 140
C                    SMALLEST TO LARGEST POWER                          PDDM 150
C           IDIMZ - DIMENSION OF Z (CALCULATED)                         PDDM 160
C           X      - VECTOR OF COEFFICIENTS FOR FIRST POLYNOMIAL, ORDEREDPDDM 170
C                    FROM SMALLEST TO LARGEST POWER                     PDDM 180
C           IDIMX - DIMENSION OF X (DEGREE IS IDIMX-1)                  PDDM 190
C           FACT  - FACTOR TO BE MULTIPLIED BY VECTOR Y                 PDDM 200
C           Y      - VECTOR OF COEFFICIENTS FOR SECOND POLYNOMIAL,      PDDM 210
C                    ORDERED FROM SMALLEST TO LARGEST POWER             PDDM 220
C           IDIMY - DIMENSION OF Y (DEGREE IS IDIMY-1)                  PDDM 230
C                                                                       PDDM 240
C        REMARKS                                                        PDDM 250
C           VECTOR Z MAY BE IN SAME LOCATION AS EITHER VECTOR X OR      PDDM 260
C           VECTOR Y ONLY IF THE DIMENSION OF THAT VECTOR IS NOT LESS   PDDM 270
C           THAN THE OTHER INPUT VECTOR                                 PDDM 280
C           THE RESULTANT POLYNOMIAL MAY HAVE TRAILING ZERO COEFFICIENTSPDDM 290
C                                                                       PDDM 300
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PDDM 310
C           NONE                                                        PDDM 320
C                                                                       PDDM 330
C        METHOD                                                         PDDM 340
C           DIMENSION OF RESULTANT VECTOR IDIMZ IS CALCULATED AS THE    PDDM 350
C           LARGER OF THE TWO INPUT VECTOR DIMENSIONS. COEFFICIENT IN   PDDM 360
C           VECTOR X IS THEN ADDED TO COEFFICIENT IN VECTOR Y MULTIPLIEDPDDM 370
C           BY FACTOR TO FORM Z.                                        PDDM 380
C                                                                       PDDM 390
C     ...................................................................PDDM 400
C                                                                       PDDM 410
      SUBROUTINE PADDM(Z,IDIMZ,X,IDIMX,FACT,Y,IDIMY)                    PDDM 420
      DIMENSION Z(1),X(1),Y(1)                                          PDDM 430
C                                                                       PDDM 440
C     TEST DIMENSIONS OF SUMMANDS                                       PDDM 450
C                                                                       PDDM 460
      NDIM=IDIMX                                                        PDDM 470
      IF(IDIMX-IDIMY) 10,20,20                                          PDDM 480
   10 NDIM=IDIMY                                                        PDDM 490
   20 IF(NDIM) 90,90,30                                                 PDDM 500
   30 DO 80 I=1,NDIM                                                    PDDM 510
      IF(I-IDIMX) 40,40,60                                              PDDM 520
   40 IF(I-IDIMY) 50,50,70                                              PDDM 530
   50 Z(I)=FACT*Y(I)+X(I)                                               PDDM 540
      GO TO 80                                                          PDDM 550
   60 Z(I)=FACT*Y(I)                                                    PDDM 560
      GO TO 80                                                          PDDM 570
   70 Z(I)=X(I)                                                         PDDM 580
   80 CONTINUE                                                          PDDM 590
   90 IDIMZ=NDIM                                                        PDDM 600
      RETURN                                                            PDDM 610
      END                                                               PDDM 620
```

Subroutine PVAL

```
C                                                                       PVAL  10
C     ..................................................................PVAL  20
C                                                                       PVAL  30
C         SUBROUTINE PVAL                                               PVAL  40
C                                                                       PVAL  50
C         PURPOSE                                                       PVAL  60
C            EVALUATE A POLYNOMIAL FOR A GIVEN VALUE OF THE VARIABLE    PVAL  70
C                                                                       PVAL  80
C         USAGE                                                         PVAL  90
C            CALL PVAL(RES,ARG,X,IDIMX)                                 PVAL 100
C                                                                       PVAL 110
C         DESCRIPTION OF PARAMETERS                                     PVAL 120
C            RES    - RESULTANT VALUE OF POLYNOMIAL                    PVAL 130
C            ARG    - GIVEN VALUE OF THE VARIABLE                      PVAL 140
C            X      - VECTOR OF COEFFICIENTS, ORDERED FROM SMALLEST TO PVAL 150
C                     LARGEST POWER                                     PVAL 160
C            IDIMX  - DIMENSION OF X                                    PVAL 170
C                                                                       PVAL 180
C         REMARKS                                                       PVAL 190
C            NONE                                                       PVAL 200
C                                                                       PVAL 210
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 PVAL 220
C            NONE                                                       PVAL 230
C                                                                       PVAL 240
C         METHOD                                                        PVAL 250
C            EVALUATION IS DONE BY MEANS OF NESTED MULTIPLICATION       PVAL 260
C                                                                       PVAL 270
C     ..................................................................PVAL 280
C                                                                       PVAL 290
      SUBROUTINE PVAL(RES,ARG,X,IDIMX)                                  PVAL 300
      DIMENSION X(1)                                                    PVAL 310
C                                                                       PVAL 320
      RES=0.                                                            PVAL 330
      J=IDIMX                                                           PVAL 340
    1 IF(J)3,3,2                                                        PVAL 350
    2 RES=RES*ARG+X(J)                                                  PVAL 360
      J=J-1                                                             PVAL 370
      GO TO 1                                                           PVAL 380
    3 RETURN                                                            PVAL 390
      END                                                               PVAL 400
```

Subroutine PVSUB

```
C                                                                       PVSU  10
C     ..................................................................PVSU  20
C                                                                       PVSU  30
C         SUBROUTINE PVSUB                                              PVSU  40
C                                                                       PVSU  50
C         PURPOSE                                                       PVSU  60
C            SUBSTITUTE VARIABLE OF A POLYNOMIAL BY ANOTHER POLYNOMIAL  PVSU  70
C                                                                       PVSU  80
C         USAGE                                                         PVSU  90
C            CALL PVSUB(Z,ICIPZ,X,IDIMX,Y,IDIMY,WORK1,WORK2)            PVSU 100
C                                                                       PVSU 110
C         DESCRIPTION OF PARAMETERS                                     PVSU 120
C            Z      - VECTOR OF COEFFICIENTS FOR RESULTANT POLYNOMIAL, / PVSU 130
C                     ORDERED FROM SMALLEST TO LARGEST POWER            PVSU 140
C            ICIPZ  - DIMENSION OF Z                                    PVSU 150
C            X      - VECTOR OF COEFFICIENTS FOR ORIGINAL POLYNOMIAL,   PVSU 160
C                     ORDERED FROM SMALLEST TO LARGEST POWER            PVSU 170
C            IDIMX  - DIMENSION OF X                                    PVSU 180
C            Y      - VECTOR OF COEFFICIENTS FOR POLYNOMIAL WHICH IS    PVSU 190
C                     SUBSTITUTED FOR VARIABLE, ORDERED FROM SMALLEST TO PVSU 200
C                     LARGEST POWER                                     PVSU 210
C            IDIMY  - DIMENSION OF Y                                    PVSU 220
C            WORK1  - WORKING STORAGE ARRAY (SAME DIMENSION AS Z)       PVSU 230
C            WORK2  - WORKING STORAGE ARRAY (SAME DIMENSION AS Z)       PVSU 240
C                                                                       PVSU 250
C         REMARKS                                                       PVSU 260
C            NONE                                                       PVSU 270
C                                                                       PVSU 280
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 PVSU 290
C            FPFY                                                       PVSU 300
C            FACCM                                                      PVSU 310
C            PCLA                                                       PVSU 320
C                                                                       PVSU 330
C         METHOD                                                        PVSU 340
C            VARIABLE OF POLYNOMIAL X IS SUBSTITUTED BY POLYNOMIAL Y    PVSU 350
C            TO FORM POLYNOMIAL Z. DIMENSION OF NEW POLYNOMIAL IS       PVSU 360
C            ((IDIMX-1)*(IDIMY-1)+1. SUBROUTINE REQUIRES THE WORK AREAS PVSU 370
C                                                                       PVSU 380
C     ..................................................................PVSU 390
C                                                                       PVSU 400
      SUBROUTINE PVSUB(Z,ICIPZ,X,IDIMX,Y,IDIMY,WORK1,WORK2)             PVSU 410
      DIMENSION Z(1),X(1),Y(1),WORK1(1),WORK2(1)                        PVSU 420
C                                                                       PVSU 430
C     TEST OF DIMENSIONS                                                PVSU 440
C                                                                       PVSU 450
      IF (IDIMX-1) 1,3,3                                                PVSU 460
    1 ICIPZ=0                                                           PVSU 470
    2 RETURN                                                            PVSU 480
C                                                                       PVSU 490
    3 ICIPZ=1                                                           PVSU 500
      Z(1)=X(1)                                                         PVSU 510
      IF (IDIMY*IDIMX-IDIMY) 2,2,4                                      PVSU 520
    4 IW1=1                                                             PVSU 530
      WORK1(1)=1.                                                       PVSU 540
C                                                                       PVSU 550
      DO 5 I=2,IDIMX                                                    PVSU 560
      CALL FPFY(WORK2,IW2,Y,IDIMY,WORK1,IW1)                            PVSU 570
      CALL PCLA(WORK1,IW1,WORK2,IW2)                                    PVSU 580
      FACT=X(I)                                                         PVSU 590
      CALL FACCM(Z,IDIMZ,Z,ICIPZ,FACT,WORK1,IW1)                        PVSU 600
      ICIPZ=IDIMZ                                                       PVSU 605
    5 CONTINUE                                                          PVSU 610
      GO TO 2                                                           PVSU 620
      END                                                               PVSU 630
```

Subroutine PILD

```
C                                                                       PILD  10
C     ...................................................................PILD  20
C                                                                       PILD  30
C        SUBROUTINE PILD                                                PILD  40
C                                                                       PILD  50
C        PURPOSE                                                        PILD  60
C           EVALUATE POLYNOMIAL AND ITS FIRST DERIVATIVE FOR A GIVEN    PILD  70
C           ARGUMENT                                                    PILD  80
C                                                                       PILD  90
C        USAGE                                                          PILD 100
C           CALL PILD(POLY,DVAL,ARGUM,X,IDIMX)                          PILD 110
C                                                                       PILD 120
C        DESCRIPTION OF PARAMETERS                                      PILD 130
C           POLY  - VALUE OF POLYNOMIAL                                 PILD 140
C           DVAL  - DERIVATIVE                                          PILD 150
C           ARGUM - ARGUMENT                                            PILD 160
C           X     - VECTOR OF COEFFICIENTS FOR POLYNOMIAL, ORDERED      PILD 170
C                   FROM SMALLEST TO LARGEST POWER                      PILD 180
C           IDIMX - DIMENSION OF X                                      PILD 190
C                                                                       PILD 200
C        REMARKS                                                        PILD 210
C           NONE                                                        PILD 220
C                                                                       PILD 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PILD 240
C           PQSD                                                        PILD 250
C                                                                       PILD 260
C        METHOD                                                         PILD 270
C           EVALUATION IS DONE BY MEANS OF SUBROUTINE PQSO (QUADRATIC   PILD 280
C           SYNTHETIC DIVISION)                                         PILD 290
C                                                                       PILD 300
C     ...................................................................PILD 310
C                                                                       PILD 320
      SUBROUTINE PILD (POLY,DVAL,ARGUM,X,IDIMX)                         PILD 330
      DIMENSION X(1)                                                    PILD 340
C                                                                       PILD 350
      P=ARGUM+ARGUM                                                     PILD 360
      Q=-ARGUM*ARGUM                                                    PILD 370
C                                                                       PILD 380
      CALL PQSO (DVAL,POLY,P,Q,X,IDIMX)                                 PILD 390
C                                                                       PILD 400
      POLY=ARGUM*DVAL+POLY                                              PILD 410
C                                                                       PILD 420
      RETURN                                                            PILD 430
      END                                                               PILD 440
```

Subroutine PDER

```
C                                                                       PDER  10
C     ...................................................................PDER  20
C                                                                       PDER  30
C        SUBROUTINE PDER                                                PDER  40
C                                                                       PDER  50
C        PURPOSE                                                        PDER  60
C           FIND DERIVATIVE OF A POLYNOMIAL                             PDER  70
C                                                                       PDER  80
C        USAGE                                                          PDER  90
C           CALL PDER(Y,IDIMY,X,IDIMX)                                  PDER 100
C                                                                       PDER 110
C        DESCRIPTION OF PARAMETERS                                      PDER 120
C           Y     - VECTOR OF COEFFICIENTS FOR DERIVATIVE, ORDERED FROM PDER 130
C                   SMALLEST TO LARGEST POWER                           PDER 140
C           IDIMY - DIMENSION OF Y (EQUAL TO IDIMX-1)                   PDER 150
C           X     - VECTOR OF COEFFICIENTS FOR ORIGINAL POLYNOMIAL,     PDER 160
C                   ORDERED FROM SMALLEST TO LARGEST POWER              PDER 170
C           IDIMX - DIMENSION OF X                                      PDER 180
C                                                                       PDER 190
C        REMARKS                                                        PDER 200
C           NONE                                                        PDER 210
C                                                                       PDER 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PDER 230
C           NONE                                                        PDER 240
C                                                                       PDER 250
C        METHOD                                                         PDER 260
C           DIMENSION OF Y IS SET AT DIMENSION OF X LESS ONE. DERIVATIVEPDER 270
C           IS THEN CALCULATED BY MULTIPLYING COEFFICIENTS BY THEIR      PDER 280
C           RESPECTIVE EXPONENTS.                                       PDER 290
C                                                                       PDER 300
C     ...................................................................PDER 310
C                                                                       PDER 320
      SUBROUTINE PDER(Y,IDIMY,X,IDIMX)                                  PDER 330
      DIMENSION X(1),Y(1)                                               PDER 340
C                                                                       PDER 350
C     TEST OF DIMENSION                                                 PDER 360
      IF (IDIMX-1) 3,3,1                                                PDER 370
    1 IDIMY=IDIMX-1                                                     PDER 380
      EXPT=0.                                                           PDER 390
      DO 2 I=1,IDIMY                                                    PDER 400
      EXPT=EXPT+1.                                                      PDER 410
    2 Y(I)=X(I+1)*EXPT                                                  PDER 420
      GO TO 4                                                           PDER 430
    3 IDIMY=0                                                           PDER 440
    4 RETURN                                                            PDER 450
      END                                                               PDER 460
```

Subroutine PINT

```
C                                                                       PINT  10
C     ...................................................................PINT  20
C                                                                       PINT  30
C        SUBROUTINE PINT                                                PINT  40
C                                                                       PINT  50
C        PURPOSE                                                        PINT  60
C           FIND INTEGRAL OF A POLYNOMIAL WITH CONSTANT OF INTEGRATION  PINT  70
C           EQUAL TO ZERO                                               PINT  80
C                                                                       PINT  90
C        USAGE                                                          PINT 100
C           CALL PINT(Y,IDIMY,X,IDIMX)                                  PINT 110
C                                                                       PINT 120
C        DESCRIPTION OF PARAMETERS                                      PINT 130
C           Y      - VECTOR OF COEFFICIENTS FOR INTEGRAL, ORDERED FROM  PINT 140
C                    SMALLEST TO LARGEST POWER                          PINT 150
C           IDIMY - DIMENSION OF Y (EQUAL TO IDIMX+1)                   PINT 160
C           X      - VECTOR OF COEFFICIENTS FOR ORIGINAL POLYNOMIAL,    PINT 170
C                    ORDERED FROM SMALLEST TO LARGEST POWER             PINT 180
C           IDIMX - DIMENSION OF X                                      PINT 190
C                                                                       PINT 200
C        REMARKS                                                        PINT 210
C           NONE                                                        PINT 220
C                                                                       PINT 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PINT 240
C           NONE                                                        PINT 250
C                                                                       PINT 260
C        METHOD                                                         PINT 270
C           DIMENSION OF Y IS SET AT DIMENSION OF X PLUS ONE, AND THE   PINT 280
C           CONSTANT TERM IS SET TO ZERO. INTEGRAL IS THEN CALCULATED   PINT 290
C           BY DIVIDING COEFFICIENTS BY THEIR RESPECTIVE EXPONENTS.     PINT 300
C                                                                       PINT 310
C     ...................................................................PINT 320
C                                                                       PINT 330
      SUBROUTINE PINT(Y,IDIMY,X,IDIMX)                                  PINT 340
      DIMENSION X(1),Y(1)                                               PINT 350
C                                                                       PINT 360
      IDIMY=IDIMX+1                                                     PINT 370
      Y(1)=0.                                                           PINT 380
      IF(IDIMX)1,1,2                                                    PINT 390
    1 RETURN                                                            PINT 400
    2 EXPT=1.                                                           PINT 410
      DO 3 I=2,IDIMY                                                    PINT 420
      Y(I)=X(I-1)/EXPT                                                  PINT 430
    3 EXPT=EXPT+1.                                                      PINT 440
      GO TO 1                                                           PINT 450
      END                                                               PINT 460
```

Subroutine PQSD

```
C                                                                       PQSD  10
C     ...................................................................PQSD  20
C                                                                       PQSD  30
C        SUBROUTINE PQSD                                                PQSD  40
C                                                                       PQSD  50
C        PURPOSE                                                        PQSD  60
C           PERFORM QUADRATIC SYNTHETIC DIVISION                        PQSD  70
C                                                                       PQSD  80
C        USAGE                                                          PQSD  90
C           CALL PQSD(A,B,P,Q,X,IDIMX)                                  PQSD 100
C                                                                       PQSD 110
C        DESCRIPTION OF PARAMETERS                                      PQSD 120
C           A      - COEFFICIENT OF Z IN REMAINDER (CALCULATED)         PQSD 130
C           B      - CONSTANT TERM IN REMAINDER (CALCULATED)            PQSD 140
C           P      - COEFFICIENT OF Z IN QUADRATIC POLYNOMIAL           PQSD 150
C           Q      - CONSTANT TERM IN QUADRATIC POLYNOMIAL              PQSD 160
C           X      - COEFFICIENT VECTOR FOR GIVEN POLYNOMIAL, ORDERED   PQSD 170
C                    FROM SMALLEST TO LARGEST POWER                     PQSD 180
C           IDIMX - DIMENSION OF X                                      PQSD 190
C                                                                       PQSD 200
C        REMARKS                                                        PQSD 210
C           NONE                                                        PQSD 220
C                                                                       PQSD 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PQSD 240
C           NONE                                                        PQSD 250
C                                                                       PQSD 260
C        METHOD                                                         PQSD 270
C           POLYNOMIAL IS DIVIDED BY THE QUADRATIC Z**2-P*Z-Q GIVING    PQSD 280
C           THE LINEAR REMAINDER A*Z+B                                  PQSD 290
C                                                                       PQSD 300
C     ...................................................................PQSD 310
C                                                                       PQSD 320
      SUBROUTINE PQSD(A,B,P,Q,X,IDIMX)                                  PQSD 330
      DIMENSION X(1)                                                    PQSD 340
C                                                                       PQSD 350
      A=0.                                                              PQSD 360
      B=0.                                                              PQSD 370
      J=IDIMX                                                           PQSD 380
    1 IF(J)3,3,2                                                        PQSD 390
    2 Z=P*A+B                                                           PQSD 400
      B=Q*A+X(J)                                                        PQSD 410
      A=Z                                                               PQSD 420
      J=J-1                                                             PQSD 430
      GO TO 1                                                           PQSD 440
    3 RETURN                                                            PQSD 450
      END                                                               PQSD 460
```

Subroutine PCLD

```
C                                                                       PCLD  10
C     ...................................................................PCLD  20
C                                                                       PCLD  30
C        SUBROUTINE PCLD                                                PCLD  40
C                                                                       PCLD  50
C        PURPOSE                                                        PCLD  60
C           SHIFT OF ORIGIN (COMPLETE LINEAR SYNTHETIC DIVISION)        PCLD  70
C                                                                       PCLD  80
C        USAGE                                                          PCLD  90
C           CALL PCLD(X,IDIMX,U)                                        PCLD 100
C                                                                       PCLD 110
C        DESCRIPTION OF PARAMETERS                                      PCLD 120
C           X      - VECTOR OF COEFFICIENTS, ORDERED FROM SMALLEST TO   PCLD 130
C                    LARGEST POWER. IT IS REPLACED BY VECTOR OF         PCLD 140
C                    TRANSFORMED COEFFICIENTS.                          PCLD 150
C           IDIMX - DIMENSION OF X                                      PCLD 160
C           U      - SHIFT PARAMETER                                    PCLD 170
C                                                                       PCLD 180
C        REMARKS                                                        PCLD 190
C           NONE                                                        PCLD 200
C                                                                       PCLD 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PCLD 220
C           NONE                                                        PCLD 230
C                                                                       PCLD 240
C        METHOD                                                         PCLD 250
C           COEFFICIENT VECTOR X(I) OF POLYNOMIAL P(Z) IS TRANSFORMED   PCLD 260
C           SUCH THAT Q(Z)=P(Z-U) WHERE Q(Z) DENOTES THE POLYNOMIAL     PCLD 270
C           WITH TRANSFORMED COEFFICIENT VECTOR.                        PCLD 280
C                                                                       PCLD 290
C     ...................................................................PCLD 300
C                                                                       PCLD 310
      SUBROUTINE PCLD (X,IDIMX,U)                                       PCLD 320
      DIMENSION X(1)                                                    PCLD 330
C                                                                       PCLD 340
      K=1                                                               PCLD 350
    1 J=IDIMX                                                           PCLD 360
    2 IF (J-K) 4,4,3                                                    PCLD 370
    3 X(J-1)=X(J-1)+U*X(J)                                              PCLD 380
      J=J-1                                                             PCLD 390
      GO TO 2                                                           PCLD 400
    4 K=K+1                                                             PCLD 410
      IF (IDIMX-K) 5,5,1                                                PCLD 420
    5 RETURN                                                            PCLD 430
      END                                                               PCLD 440
```

Subroutine PGCD

```
C                                                                       PGCD  10
C     ...................................................................PGCD  20
C                                                                       PGCD  30
C        SUBROUTINE PGCD                                                PGCD  40
C                                                                       PGCD  50
C        PURPOSE                                                        PGCD  60
C           DETERMINE GREATEST COMMON DIVISOR OF TWO POLYNOMIALS        PGCD  70
C                                                                       PGCD  80
C        USAGE                                                          PGCD  90
C           CALL PGCD(X,IDIMX,Y,IDIMY,WORK,EPS,IER)                     PGCD 100
C                                                                       PGCD 110
C        DESCRIPTION OF PARAMETERS                                      PGCD 120
C           X      -  VECTOR OF COEFFICIENTS FOR FIRST POLYNOMIAL,      PGCD 130
C                     ORDERED FROM SMALLEST TO LARGEST POWER           PGCD 140
C           IDIMX  -  DIMENSION OF X                                    PGCD 150
C           Y      -  VECTOR OF COEFFICIENTS FOR SECOND POLYNOMIAL,     PGCD 160
C                     ORDERED FROM SMALLEST TO LARGEST POWER.          PGCD 170
C                     THIS IS REPLACED BY GREATEST COMMON DIVISOR       PGCD 180
C           IDIMY  -  DIMENSION OF Y                                    PGCD 190
C           WORK   -  WORKING STORAGE ARRAY                             PGCD 200
C           EPS    -  TOLERANCE VALUE BELOW WHICH COEFFICIENT IS        PGCD 210
C                     ELIMINATED DURING NORMALIZATION                   PGCD 220
C           IER    -  RESULTANT ERROR CODE WHERE                        PGCD 230
C                     IER=0  NO ERROR                                   PGCD 240
C                     IER=1  X OR Y IS ZERO POLYNOMIAL                  PGCD 250
C                                                                       PGCD 260
C        REMARKS                                                        PGCD 270
C           IDIMX MUST BE GREATER THAN IDIMY                            PGCD 280
C           IDIMY=1 ON RETURN MEANS X AND Y ARE PRIME, THE GCD IS A     PGCD 290
C           CONSTANT. IDIMX IS DESTROYED DURING COMPUTATION.            PGCD 300
C                                                                       PGCD 310
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PGCD 320
C           PDIV                                                        PGCD 330
C           PNORM                                                       PGCD 340
C                                                                       PGCD 350
C        METHOD                                                         PGCD 360
C           GREATEST COMMON DIVISOR OF TWO POLYNOMIALS X AND Y IS       PGCD 370
C           DETERMINED BY MEANS OF EUCLIDEAN ALGORITHM. COEFFICIENT     PGCD 380
C           VECTORS X AND Y ARE DESTROYED AND GREATEST COMMON           PGCD 390
C           DIVISOR IS GENERATED IN Y.                                  PGCD 400
C                                                                       PGCD 410
C     ...................................................................PGCD 420
C                                                                       PGCD 430
      SUBROUTINE PGCD(X,IDIMX,Y,IDIMY,WORK,EPS,IER)                     PGCD 440
      DIMENSION X(1),Y(1),WORK(1)                                       PGCD 450
C                                                                       PGCD 460
C     DIMENSION REQUIRED FOR VECTOR NAMED  WORK  IS   IDIMX-IDIMY+1     PGCD 470
C                                                                       PGCD 480
    1 CALL PDIV(WORK,NDIM,X,IDIMX,Y,IDIMY,EPS,IER)                      PGCD 490
      IF(IER) 5,2,5                                                     PGCD 500
    2 IF(IDIMX) 5,5,3                                                   PGCD 510
C                                                                       PGCD 520
C     INTERCHANGE X AND Y                                               PGCD 530
C                                                                       PGCD 540
    3 DO 4 J=1,IDIMY                                                    PGCD 550
      WORK(1)=X(J)                                                      PGCD 560
      X(J)=Y(J)                                                         PGCD 570
    4 Y(J)=WORK(1)                                                      PGCD 580
      NDIM=IDIMX                                                        PGCD 590
      IDIMX=IDIMY                                                       PGCD 600
      IDIMY=NDIM                                                        PGCD 610
      GO TO 1                                                           PGCD 620
    5 RETURN                                                            PGCD 630
      END                                                               PGCD 640
```

Subroutine PNORM

```
C                                                                       PNOR  10
C     ...................................................................PNOR  20
C                                                                       PNOR  30
C        SUBROUTINE PNORM                                               PNOR  40
C                                                                       PNOR  50
C        PURPOSE                                                        PNOR  60
C           NORMALIZE COEFFICIENT VECTOR OF A POLYNOMIAL                PNOR  70
C                                                                       PNOR  80
C        USAGE                                                          PNOR  90
C           CALL PNORM(X,IDIMX,EPS)                                     PNOR 100
C                                                                       PNOR 110
C        DESCRIPTION OF PARAMETERS                                      PNOR 120
C           X      - VECTOR OF ORIGINAL COEFFICIENTS, ORDERED FROM      PNOR 130
C                    SMALLEST TO LARGEST POWER. IT REMAINS UNCHANGED    PNOR 140
C           IDIMX  - DIMENSION OF X. IT IS REPLACED BY FINAL DIMENSION  PNOR 150
C           EPS    - TOLERANCE BELOW WHICH COEFFICIENT IS ELIMINATED    PNOR 160
C                                                                       PNOR 170
C        REMARKS                                                        PNOR 180
C           IF ALL COEFFICIENTS ARE LESS THAN EPS, RESULT IS A ZERO     PNOR 190
C           POLYNOMIAL WITH IDIMX=0 BUT VECTOR X REMAINS INTACT         PNOR 200
C                                                                       PNOR 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PNOR 220
C           NONE                                                        PNOR 230
C                                                                       PNOR 240
C        METHOD                                                         PNOR 250
C           DIMENSION OF VECTOR X IS REDUCED BY ONE FOR EACH TRAILING   PNOR 260
C           COEFFICIENT WITH AN ABSOLUTE VALUE LESS THAN OR EQUAL TO EPSPNOR 270
C                                                                       PNOR 280
C     ...................................................................PNOR 290
C                                                                       PNOR 300
      SUBROUTINE PNORM(X,IDIMX,EPS)                                     PNOR 310
      DIMENSION X(1)                                                    PNOR 320
C                                                                       PNOR 330
    1 IF(IDIMX) 4,4,2                                                   PNOR 340
    2 IF(ABS(X(IDIMX))-EPS) 3,3,4                                       PNOR 350
    3 IDIMX=IDIMX-1                                                     PNOR 360
      GO TO 1                                                           PNOR 370
    4 RETURN                                                            PNOR 380
      END                                                               PNOR 390
```

Subroutines PECN and DPECN

These subroutines perform the economization of a polynomial for symmetric range.

A given polynomial P(x) with coefficient vector $P = (p_1, \ldots, p_n)$, representing a function f(x) with a maximum error eps over the range (-bound, bound) -- that is, $\left| f(x) - \sum_{i=1}^{n} p_i x^{i-1} \right| \leqq \text{eps for} \left| x \right| \leqq$ bound -- is reduced to a shorter coefficient vector, if possible, representing f(x) over the same range with a maximal error absolutely less than tol by means of telescoping.

The Chebyshev polynomial $T_{n-1}(t)$ has 2^{n-2} as coefficient of t^{n-1}. As a consequence, t^{n-1} may be replaced by $T_{n-1}(t)/2^{n-2}$ plus a polynomial in t of degree n-2.

This means that the telescoped polynomial:

$$P_1(x) = \sum_{i=1}^{n} p_i x^{i-1} - (p_n \cdot \text{bound}^{n-1} / 2^{n-2}) \; T_{n-1}(x/\text{bound})$$

is of degree n - 2 representing f(x) over the range $|x| \leqq$ bound with a maximal error err absolutely less than $\text{eps}_1 = \text{eps} + |p_n| \cdot \text{bound}^{n-1}/2^{n-2}$, since $|T_{n-1}(t)| \leqq 1$ for $|t| \leqq 1$.

If eps_1 is less than the tolerance tol, the procedure may be repeated with P_1 instead of P, and eps_1 instead of eps.

This iterative scheme results in a polynomial approximation to f(x) which possibly consists of fewer terms and thus may allow the computation of f(x) with less effort than the original approximation P(x).

Naturally, tol should be greater than eps.

For reference see K.A. Brons, Algorithm 38, Telescope 2, CACM vol. 4, 1961, no. 3, pp. 151-152.

```
C                                                                       PECN  10
C     ...................................................................PECN  20
C                                                                       PECN  30
C        SUBROUTINE PECN                                                PECN  40
C                                                                       PECN  50
C        PURPOSE                                                        PECN  60
C           ECONOMIZE A POLYNOMIAL FOR SYMMETRIC RANGE                  PECN  70
C                                                                       PECN  80
C        USAGE                                                          PECN  90
C           CALL PECN (P,N,BOUND,EPS,TOL,WORK)                          PECN 100
C                                                                       PECN 110
C        DESCRIPTION OF PARAMETERS                                      PECN 120
C           P      - COEFFICIENT VECTOR OF GIVEN POLYNOMIAL             PECN 130
C                    ON RETURN P CONTAINS THE ECONOMIZED POLYNOMIAL     PECN 140
C           N      - DIMENSION OF COEFFICIENT VECTOR P                  PECN 150
C                    ON RETURN N CONTAINS DIMENSION OF ECONOMIZED       PECN 160
C                    POLYNOMIAL                                         PECN 170
C           BOUND  - RIGHT HAND BOUNDARY OF RANGE                       PECN 180
C           EPS    - INITIAL ERROR BOUND                                PECN 190
C                    ON RETURN EPS CONTAINS AN ERROR BOUND FOR THE      PECN 200
C                    ECONOMIZED POLYNOMIAL                              PECN 210
C           TOL    - TOLERANCE FOR ERROR                                PECN 220
C                    FINAL VALUE OF EPS MUST BE LESS THAN TOL           PECN 230
C           WORK   - WORKING STORAGE OF DIMENSION N (STARTING VALUE     PECN 240
C                    OF N RATHER THAN FINAL VALUE)                      PECN 250
C                                                                       PECN 260
C        REMARKS                                                        PECN 270
C           THE OPERATION IS BYPASSED IN CASE OF N LESS THAN 1.         PECN 280
C           IN CASE OF AN ARBITRARY INTERVAL (XL,XR) IT IS NECESSARY    PECN 290
C           FIRST TO CALCULATE THE EXPANSION OF THE GIVEN POLYNOMIAL    PECN 300
C           WITH ARGUMENT X IN POWERS OF T = (X-(XR-XL)/2).             PECN 310
C           THIS IS ACCOMPLISHED THROUGH SUBROUTINE PCLD.               PECN 320
C                                                                       PECN 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PECN 340
C           NONE                                                        PECN 350
C                                                                       PECN 360
C        METHOD                                                         PECN 370
C           SUBROUTINE PECN TAKES AN (N-1)ST DEGREE POLYNOMIAL          PECN 380
C           APPROXIMATION TO A FUNCTION F(X) VALID WITHIN A TOLERANCE   PECN 390
C           EPS OVER THE INTERVAL (-BOUND,BOUND) AND REDUCES IT IF      PECN 400
C           POSSIBLE TO A POLYNOMIAL OF LOWER DEGREE VALID WITHIN       PECN 410
C           THE GIVEN TOLERANCE TOL.                                    PECN 420
C           THE INITIAL COEFFICIENT VECTOR P IS REPLACED BY THE FINAL   PECN 430
C           VECTOR. THE INITIAL ERROR BOUND EPS IS REPLACED BY A FINAL  PECN 440
C           ERROR BOUND.                                                PECN 450
C           N IS REPLACED BY THE DIMENSION OF THE REDUCED POLYNOMIAL.   PECN 460
C           THE COEFFICIENT VECTOR OF THE N-TH CHEBYSHEV POLYNOMIAL     PECN 470
C           IS CALCULATED FROM THE RECURSION FORMULA                    PECN 480
C           A(K-1)=-A(K+1)*K*L*L*(K-1)/((N+K-2)*(N-K+2))                PECN 490
C           REFERENCE                                                   PECN 500
C           K. A. BRONS, ALGORITHM 38, TELESCOPE 2, CACM VOL. 4, 1961,  PECN 510
C           NO. 3, PP. 151-152.                                         PECN 520
C                                                                       PECN 530
C     ...................................................................PECN 540
C                                                                       PECN 550
      SUBROUTINE PECN(P,N,BOUND,EPS,TOL,WORK)                           PECN 560
C                                                                       PECN 570
      DIMENSION P(1),WORK(1)                                            PECN 580
      FL=BOUND*BOUND                                                    PECN 590
C                                                                       PECN 600
C     TEST OF DIMENSION                                                 PECN 610
C                                                                       PECN 620
    1 IF(N-1)2,3,6                                                      PECN 630
    2 RETURN                                                            PECN 640
    3 IF(EPS+ABS(P(1))-TOL)4,4,5                                        PECN 650
    4 N=0                                                               PECN 660
      EPS=EPS+ABS(P(1))                                                 PECN 670
    5 RETURN                                                            PECN 680
C                                                                       PECN 690
C     CALCULATE EXPANSION OF CHEBYSHEV POLYNOMIAL                       PECN 700
C                                                                       PECN 710
    6 NEND=N-2                                                          PECN 720
      WORK(N)=-P(N)                                                     PECN 730
      DO 7 J=1,NEND,2                                                   PECN 740
      K=N-J                                                             PECN 750
      FN=(NEND-1+K)*(NEND+3-K)                                          PECN 760
      FK=K*(K-1)                                                        PECN 770
    7 WORK(K-1)=-WORK(K+1)*FK*FL/FN                                     PECN 780
C                                                                       PECN 790
C     TEST FOR FEASIBILITY OF REDUCTION                                 PECN 800
C                                                                       PECN 810
      IF(K-2)8,8,9                                                      PECN 820
    8 FN=ABS(WORK(1))                                                   PECN 830
      GOTO 10                                                           PECN 840
    9 FN=N-1                                                            PECN 850
      FN=ABS(WORK(2)/FN)                                                PECN 860
   10 IF(EPS+FN-TOL)11,11,5                                             PECN 870
C                                                                       PECN 880
C     REDUCE POLYNOMIAL                                                 PECN 890
C                                                                       PECN 900
   11 EPS=EPS+FN                                                        PECN 910
      N=N-1                                                             PECN 920
      DO 12 J=K,N,2                                                     PECN 930
   12 P(J-1)=P(J-1)+WORK(J-1)                                           PECN 940
      GOTO 1                                                            PECN 950
      END                                                               PECN 960
```

```
C                                                                       DPCN  10
C     ...................................................................DPCN  20
C                                                                       DPCN  30
C        SUBROUTINE DPECN                                               DPCN  40
C                                                                       DPCN  50
C        PURPOSE                                                        DPCN  60
C           ECONOMIZE A POLYNOMIAL FOR SYMMETRIC RANGE                  DPCN  70
C                                                                       DPCN  80
C        USAGE                                                          DPCN  90
C           CALL DPECN(P,N,BOUND,EPS,TOL,WORK)                          DPCN 100
C                                                                       DPCN 110
C        DESCRIPTION OF PARAMETERS                                      DPCN 120
C           P      - DOUBLE PRECISION COEFFICIENT VECTOR OF GIVEN       DPCN 130
C                    POLYNOMIAL                                         DPCN 140
C                    ON RETURN P CONTAINS THE ECONOMIZED POLYNOMIAL     DPCN 150
C           N      - DIMENSION OF COEFFICIENT VECTOR P                  DPCN 160
C                    ON RETURN N CONTAINS DIMENSION OF ECONOMIZED       DPCN 170
C                    POLYNOMIAL                                         DPCN 180
C           BOUND  - SINGLE PRECISION RIGHT HAND BOUNDARY OF RANGE      DPCN 190
C           EPS    - SINGLE PRECISION INITIAL ERROR BOUND               DPCN 200
C                    ON RETURN EPS CONTAINS AN ERROR BOUND FOR THE      DPCN 210
C                    ECONOMIZED POLYNOMIAL                              DPCN 220
C           TOL    - SINGLE PRECISION TOLERANCE FOR ERROR               DPCN 230
C                    FINAL VALUE OF EPS MUST BE LESS THAN TOL           DPCN 240
C           WORK   - DOUBLE PRECISION WORKING STORAGE OF DIMENSION N    DPCN 250
C                    (STARTING VALUE OF N RATHER THAN FINAL VALUE)      DPCN 260
C                                                                       DPCN 270
C        REMARKS                                                        DPCN 280
C           THE OPERATION IS BYPASSED IN CASE OF N LESS THAN 1.         DPCN 290
C           IN CASE OF AN ARBITRARY INTERVAL (XL,XR) IT IS NECESSARY    DPCN 300
C           FIRST TO CALCULATE THE EXPANSION OF THE GIVEN POLYNOMIAL    DPCN 310
C           WITH ARGUMENT X IN POWERS OF T = (X-(XR-XL)/2).             DPCN 320
C           THIS IS ACCOMPLISHED THROUGH SUBROUTINE DPCLD.              DPCN 330
C                                                                       DPCN 340
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DPCN 350
C           NONE                                                        DPCN 360
C                                                                       DPCN 370
C        METHOD                                                         DPCN 380
C           SUBROUTINE DPECN TAKES AN (N-1)ST DEGREE POLYNOMIAL         DPCN 390
C           APPROXIMATION TO A FUNCTION F(X) VALID WITHIN A TOLERANCE   DPCN 400
C           EPS OVER THE INTERVAL (-BOUND,BOUND) AND REDUCES IT IF      DPCN 410
C           POSSIBLE TO A POLYNOMIAL OF LOWER DEGREE VALID WITHIN       DPCN 420
C           THE GIVEN TOLERANCE TOL.                                    DPCN 430
C           THE INITIAL COEFFICIENT VECTOR P IS REPLACED BY THE FINAL   DPCN 440
C           VECTOR. THE INITIAL ERROR BOUND EPS IS REPLACED BY A FINAL  DPCN 450
C           ERROR BOUND.                                                DPCN 460
C           N IS REPLACED BY THE DIMENSION OF THE REDUCED POLYNOMIAL.   DPCN 470
C           THE COEFFICIENT VECTOR OF THE N-TH CHEBYSHEV POLYNOMIAL     DPCN 480
C           IS CALCULATED FROM THE RECURSION FORMULA                    DPCN 490
C           A(K-1)=-A(K+1)*K*L*L*(K-1)/((N+K-2)*(N-K+2))                DPCN 500
C           REFERENCE                                                   DPCN 510
C           K. A. BRONS, ALGORITHM 38, TELESCOPE 2, CACM VOL. 4, 1961,  DPCN 520
C           NO. 3, PP. 151-152.                                         DPCN 530
C                                                                       DPCN 540
C     ...................................................................DPCN 550
C                                                                       DPCN 560
      SUBROUTINE DPECN(P,N,BOUND,EPS,TOL,WORK)                          DPCN 570
C                                                                       DPCN 580
      DIMENSION P(1),WORK(1)                                            DPCN 590
      DOUBLE PRECISION P,WORK                                           DPCN 600
C                                                                       DPCN 610
      FL=BOUND*BOUND                                                    DPCN 620
C                                                                       DPCN 630
C        TEST OF DIMENSION                                              DPCN 640
C                                                                       DPCN 650
    1 IF(N-1)2,3,6                                                      DPCN 660
    2 RETURN                                                            DPCN 670
C                                                                       DPCN 680
    3 IF(EPS+ABS(SNGL(P(1)))-TOL)4,4,5                                  DPCN 690
    4 N=0                                                               DPCN 700
      EPS=EPS+ABS(SNGL(P(1)))                                           DPCN 710
    5 RETURN                                                            DPCN 720
C                                                                       DPCN 730
C        CALCULATE EXPANSION OF CHEBYSHEV POLYNOMIAL                    DPCN 740
C                                                                       DPCN 750
    6 NEND=N-2                                                          DPCN 760
      WORK(N)=-P(N)                                                     DPCN 770
      DO 7 J=1,NEND,2                                                   DPCN 780
      K=N-J                                                             DPCN 790
      FN=(NEND-1+K)*(NEND+3-K)                                          DPCN 800
      FK=K*(K-1)                                                        DPCN 810
    7 WORK(K-1)=-WORK(K+1)*DBLE(FK*FL/FN)                               DPCN 820
C                                                                       DPCN 830
C        TEST FOR FEASIBILITY OF REDUCTION                              DPCN 840
C                                                                       DPCN 850
      IF(K-2)8,8,9                                                      DPCN 860
    8 FN=DABS(WORK(1))                                                  DPCN 870
      GOTO 10                                                           DPCN 880
    9 FN=N-1                                                            DPCN 890
      FN=ABS(SNGL(WORK(2))/FN)                                          DPCN 900
   10 IF(EPS+FN-TOL)11,11,5                                             DPCN 910
C                                                                       DPCN 920
C        REDUCE POLYNOMIAL                                              DPCN 930
C                                                                       DPCN 940
   11 EPS=EPS+FN                                                        DPCN 950
      N=N-1                                                             DPCN 960
      DO 12 J=K,N,2                                                     DPCN 970
   12 P(J-1)=P(J-1)+WORK(J-1)                                           DPCN 980
      GOTO 1                                                            DPCN 990
      END                                                               DPCN1000
```

Subroutines PECS and DPECS

These subroutines perform the economization of a polynomial for unsymmetric range.

A given polynomial P(x) with coefficient vector $P = (p_1, \ldots, p_n)$, representing a function f(x) with a maximal error eps over the range (0, bound) -- that is, $\left| f(x) - \sum_{i=1}^{n} p_i x^{i-1} \right| \leqq$ eps for $0 \leqq x \leqq$ bound -- is reduced to a shorter coefficient vector, if possible, representing f(x) over the same range with a maximal error absolutely less than tol by means of telescoping.

The shifted Chebyshev polynomial $T^s_{n-1}(t) = T_{n-1}(2t - 1)$ has 2^{2n-3} as coefficient of t^{n-1}. As a consequence, t^{n-1} may be replaced by $T^s_{n-1}(t)/2^{2n-3}$ plus a polynomial in t of degree n - 2.

This means that the telescoped polynomial

$$P_1(x) = \sum_{i=1}^{n} p_i x^{i-1} - (p_n \cdot (\text{bound})^{n-1} / 2^{2n-3}) T^s_{n-1}(x/\text{bound})$$

is of degree n - 2 representing f(x) over the range $0 \leqq x \leqq$ bound with a maximal error err absolutely less than $\text{eps}_1 = \text{eps} + \left| p_n \right| \cdot \text{bound}^{n-1} / 2^{2n-3}$, since $\left| T^s_{n-1}(t) \right| \leqq 1$ for $0 \leqq t \leqq 1$.

If eps_1 is less than the tolerance tol, the procedure may be repeated with P_1 instead of P, and eps_1 instead of eps.

This iterative scheme results in a polynomial approximation to f(x) which possibly consists of fewer terms and thus may allow the computation of f(x) with less effort than the original approximation P(x).

Naturally, tol should be greater than eps.

For reference see K.A. Brons, Algorithm 37, Telescope 1, CACM vol. 4, 1961, no. 3, p. 151.

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C                                                                       PECS  10
C     ...................................................................PECS  20
C                                                                       PECS  30
C        SUBROUTINE PECS                                                PECS  40
C                                                                       PECS  50
C        PURPOSE                                                        PECS  60
C           ECONOMIZATION OF A POLYNOMIAL FOR UNSYMMETRIC RANGE         PECS  70
C                                                                       PECS  80
C        USAGE                                                          PECS  90
C           CALL PECS (P,N,BOUND,EPS,TOL,WORK)                          PECS 100
C                                                                       PECS 110
C        DESCRIPTION OF PARAMETERS                                      PECS 120
C           P      - COEFFICIENT VECTOR OF GIVEN POLYNOMIAL             PECS 130
C           N      - DIMENSION OF COEFFICIENT VECTOR                    PECS 140
C           BOUND  - RIGHT HAND BOUNDARY OF INTERVAL                    PECS 150
C           EPS    - INITIAL ERROR BOUND                                PECS 160
C           TOL    - TOLERANCE FOR ERROR                                PECS 170
C           WORK   - WORKING STORAGE OF DIMENSION N                     PECS 180
C                                                                       PECS 190
C        REMARKS                                                        PECS 200
C           THE INITIAL COEFFICIENT VECTOR P IS REPLACED BY THE         PECS 210
C           ECONOMIZED VECTOR.                                          PECS 220
C           THE INITIAL ERROR BOUND EPS IS REPLACED BY A FINAL          PECS 230
C           ERROR BOUND.                                                PECS 240
C           N IS REPLACED BY THE DIMENSION OF THE REDUCED POLYNOMIAL.   PECS 250
C           IN CASE OF AN ARBITRARY INTERVAL (XL,XR) IT IS NECESSARY    PECS 260
C           FIRST TO CALCULATE THE EXPANSION OF THE GIVEN POLYNOMIAL    PECS 270
C           WITH ARGUMENT X IN POWERS OF T = (X-XL).                    PECS 280
C           THIS IS ACCOMPLISHED THROUGH SUBROUTINE PCLD.               PECS 290
C           OPERATION IS BYPASSED IN CASE OF N LESS THAN 1.             PECS 300
C                                                                       PECS 310
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PECS 320
C           NONE                                                        PECS 330
C                                                                       PECS 340
C        METHOD                                                         PECS 350
C           SUBROUTINE PECS TAKES AN (N-1)ST DEGREE POLYNOMIAL          PECS 360
C           APPROXIMATION TO A FUNCTION F(X) VALID WITHIN A TOLERANCE   PECS 370
C           EPS OVER THE INTERVAL (0,BOUND) AND REDUCES IT IF POSSIBLE  PECS 380
C           TO A POLYNOMIAL OF LOWER DEGREE VALID WITHIN TOLERANCE      PECS 390
C           TOL.                                                        PECS 400
C           THE COEFFICIENT VECTOR OF THE N-TH SHIFTED CHEBYSHEV        PECS 410
C           POLYNOMIAL IS CALCULATED FROM THE RECURSION FORMULA         PECS 420
C           A(K) = -A(K+1)*K*L*(2*K-1)/(2*(N+K-1)*(N-K+1)).             PECS 430
C           REFERENCE                                                   PECS 440
C           K. A. BRONS, ALGORITHM 37, TELESCOPE 1, CACM VOL. 4, 1961,  PECS 450
C           NO. 3, PP. 151.                                             PECS 460
C                                                                       PECS 470
C     ...................................................................PECS 480
C                                                                       PECS 490
      SUBROUTINE PECS(P,N,BOUND,EPS,TOL,WORK)                           PECS 500
C                                                                       PECS 510
      DIMENSION P(1),WORK(1)                                            PECS 520
      FL=BOUND*0.5                                                      PECS 530
C                                                                       PECS 540
C     TEST OF DIMENSION                                                 PECS 550
C                                                                       PECS 560
    1 IF(N-1)2,3,6                                                      PECS 570
    2 RETURN                                                            PECS 580
    3 IF(EPS+ABS(P(1))-TOL)4,4,5                                        PECS 590
    4 N=0                                                               PECS 600
      EPS=EPS+ABS(P(1))                                                 PECS 610
    5 RETURN                                                            PECS 620
C                                                                       PECS 630
C     CALCULATE EXPANSION OF CHEBYSHEV POLYNOMIAL                       PECS 640
C                                                                       PECS 650
    6 NEND=N-1                                                          PECS 660
      WORK(N)=-P(N)                                                     PECS 670
      DO 7 J=1,NEND                                                     PECS 680
      K=N-J                                                             PECS 690
      FN=(NEND-1+K)*(N-K)                                               PECS 700
      FK=K*(K+K-1)                                                      PECS 710
    7 WORK(K)=-WORK(K+1)*FK*FL/FN                                       PECS 720
C                                                                       PECS 730
C        TEST FOR FEASIBILITY OF REDUCTION                              PECS 740
C                                                                       PECS 750
      FN=ABS(WORK(1))                                                   PECS 760
      IF(EPS+FN-TOL)8,8,5                                               PECS 770
C                                                                       PECS 780
C     REDUCE POLYNOMIAL                                                 PECS 790
C                                                                       PECS 800
    8 EPS=EPS+FN                                                        PECS 810
      N=NEND                                                            PECS 820
      DO 9 J=1,NEND                                                     PECS 830
    9 P(J)=P(J)+WORK(J)                                                 PECS 840
      GOTO 1                                                            PECS 850
      END                                                               PECS 860
```

```
C
C     ..................................................................
C
C        SUBROUTINE DPECS
C
C        PURPOSE
C           ECONOMIZATION OF A POLYNOMIAL FOR UNSYMMETRIC RANGE
C
C        USAGE
C           CALL DPECS(P,N,BOUND,EPS,TOL,WORK)
C
C        DESCRIPTION OF PARAMETERS
C           P      - DOUBLE PRECISION COEFFICIENT VECTOR OF GIVEN
C                    POLYNOMIAL
C           N      - DIMENSION OF COEFFICIENT VECTOR P
C           BOUND  - SINGLE PRECISION RIGHT HAND BOUNDARY OF INTERVAL
C           EPS    - SINGLE PRECISION INITIAL ERROR BOUND
C           TOL    - SINGLE PRECISION TOLERANCE FOR ERROR
C           WORK   - DOUBLE PRECISION WORKING STORAGE OF DIMENSION N
C
C        REMARKS
C           THE INITIAL COEFFICIENT VECTOR P IS REPLACED BY THE
C           ECONOMIZED VECTOR.
C           THE INITIAL ERROR BOUND EPS IS REPLACED BY A FINAL
C           ERROR BOUND.
C           N IS REPLACED BY THE DIMENSION OF THE REDUCED POLYNOMIAL.
C           IN CASE OF AN ARBITRARY INTERVAL (XL,XR) IT IS NECESSARY
C           FIRST TO CALCULATE THE EXPANSION OF THE GIVEN POLYNOMIAL
C           WITH ARGUMENT X IN POWERS OF T = (X-XL).
C           THIS IS ACCOMPLISHED THROUGH SUBROUTINE DPCLD.
C           OPERATION IS BYPASSED IN CASE OF N LESS THAN 1.
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           SUBROUTINE DPECS TAKES AN (N-1)ST DEGREE POLYNOMIAL
C           APPROXIMATION TO A FUNCTION F(X) VALID WITHIN A TOLERANCE
C           EPS OVER THE INTERVAL (0,BOUND) AND REDUCES IT IF POSSIBLE
C           TO A POLYNOMIAL OF LOWER DEGREE VALID WITHIN TOLERANCE
C           TOL.
C           THE COEFFICIENT VECTOR OF THE N-TH SHIFTED CHEBYSHEV
C           POLYNOMIAL IS CALCULATED FROM THE RECURSION FORMULA
C           A(K) = -A(K+1)*K*L*(2*K-1)/(2*(N+K-1)*(N-K+1)).
C           REFERENCE
C           K. A. BRONS, ALGORITHM 37, TELESCOPE 1, CACM VOL. 4, 1961,
C           NO. 3, PP. 151.
C
C     ..................................................................
C
      SUBROUTINE DPECS(P,N,BOUND,EPS,TOL,WORK)
C
      DIMENSION P(1),WORK(1)
      DOUBLE PRECISION P,WORK
C
      FL=BOUND*0.5
C
C        TEST OF DIMENSION
C
    1 IF(N-1)2,3,6
    2 RETURN
C
    3 IF(EPS+ABS(SNGL(P(1)))-TOL)4,4,5
    4 N=0
      EPS=EPS+ABS(SNGL(P(1)))
    5 RETURN
C
C        CALCULATE EXPANSION OF CHEBYSHEV POLYNOMIAL
C
    6 NEND=N-1
      WORK(N)=-P(N)
      DO 7 J=1,NEND
      K=N-J
      FN=(NEND-1+K)*(N-K)
      FK=K*(K+K-1)
    7 WORK(K)=-WORK(K+1)*DBLE(FK)*DBLE(FL)/DBLE(FN)
C
C        TEST FOR FEASIBILITY OF REDUCTION
C
      FN=DABS(WORK(1))
      IF(EPS+FN-TOL)8,8,5
C
C        REDUCE POLYNOMIAL
C
    8 EPS=EPS+FN
      N=NEND
      DO 9 J=1,NEND
    9 P(J)=P(J)+WORK(J)
      GOTO 1
      END
```

DPCS 10 DPCS 20 DPCS 30 DPCS 40 DPCS 50 DPCS 60 DPCS 70 DPCS 80 DPCS 90 DPCS 100 DPCS 110 DPCS 120 DPCS 130 DPCS 140 DPCS 150 DPCS 160 DPCS 170 DPCS 180 DPCS 190 DPCS 200 DPCS 210 DPCS 220 DPCS 230 DPCS 240 DPCS 250 DPCS 260 DPCS 270 DPCS 280 DPCS 290 DPCS 300 DPCS 310 DPCS 320 DPCS 330 DPCS 340 DPCS 350 DPCS 360 DPCS 370 DPCS 380 DPCS 390 DPCS 400 DPCS 410 DPCS 420 DPCS 430 DPCS 440 DPCS 450 DPCS 460 DPCS 470 DPCS 480 DPCS 490 DPCS 500 DPCS 510 DPCS 520 DPCS 530 DPCS 540 DPCS 550 DPCS 560 DPCS 570 DPCS 580 DPCS 590 DPCS 600 DPCS 610 DPCS 620 DPCS 630 DPCS 640 DPCS 650 DPCS 660 DPCS 670 DPCS 680 DPCS 690 DPCS 700 DPCS 710 DPCS 720 DPCS 730 DPCS 740 DPCS 750 DPCS 760 DPCS 770 DPCS 780 DPCS 790 DPCS 800 DPCS 810 DPCS 820 DPCS 830 DPCS 840 DPCS 850 DPCS 860 DPCS 870 DPCS 880 DPCS 890 DPCS 900

Subroutine POLRT

This subroutine computes the real and complex roots of a real polynomial.

Given a polynomial

$$f(z) = \sum_{n=0}^{N} a_n z^n \qquad (1)$$

let

$Z = X + iY$ be a starting value for a root of f(z).

Then:

$$Z^n = (X + iY)^n \qquad (2)$$

Define X_n as real terms of expanded equation (2).

Define Y_n as imaginary terms of expanded equation (2).

Then for:

$n = 0$

$X_o = 1.0$

$Y_o = 0.0$

$n > 0$

$$X_n = X \cdot X_{n-1} - Y \cdot Y_{n-1} \qquad (3)$$

$$Y_n = X \cdot Y_{n-1} + Y \cdot X_{n-1} \qquad (4)$$

Let:

U be the real terms of (1)
V be the imaginary terms of (1)

Then:

$$U = \sum_{n=0}^{N} a_n X_n \qquad (5)$$

$$V = \sum_{n=0}^{N} a_n Y_n \qquad (6)$$

or:

$$U = a_o + \sum_{n=1}^{N} a_n X_n \qquad (7)$$

$$V = \sum_{n=1}^{N} a_n Y_n \qquad (8)$$

$$\frac{\partial U}{\partial X} = \sum_{n=1}^{N} n \cdot X_{n-1} \cdot a_n \qquad (9)$$

$$\frac{\partial U}{\partial Y} = -\sum_{n=1}^{N} n\, Y_{n-1}\, a_n \qquad (10)$$

Note that equations (3), (4), (7), (8), (9), and (10) can be performed iteratively for n = 1 to N by saving X_{n-1} and Y_{n-1}.

Using the Newton-Raphson method for computing ΔX, ΔY, the result is:

$$\Delta X = \left(V\frac{\partial U}{\partial Y} - U\frac{\partial U}{\partial X}\right) \Bigg/ \left[\left(\frac{\partial U}{\partial X}\right)^2 + \left(\frac{\partial U}{\partial Y}\right)^2\right] \qquad (11)$$

$$\Delta Y = -\left(U\frac{\partial U}{\partial Y} + V\frac{\partial U}{\partial X}\right) \Bigg/ \left[\left(\frac{\partial U}{\partial X}\right)^2 + \left(\frac{\partial U}{\partial Y}\right)^2\right] \qquad (12)$$

after applying the Cauchy-Riemann equations.

Thus, for the next iteration:

$$X' = X + \Delta X$$

$$Y' = Y + \Delta Y$$

```
C
C     ..................................................................
C
C        SUBROUTINE POLRT
C
C        PURPOSE
C           COMPUTES THE REAL AND COMPLEX ROOTS OF A REAL POLYNOMIAL
C
C        USAGE
C           CALL POLRT(XCOF,COF,M,ROOTR,ROOTI,IER)
C
C        DESCRIPTION OF PARAMETERS
C           XCOF -VECTOR OF M+1 COEFFICIENTS OF THE POLYNOMIAL
C                 ORDERED FROM SMALLEST TO LARGEST POWER
C           COF  -WORKING VECTOR OF LENGTH M+1
C           M    -ORDER OF POLYNOMIAL
C           ROOTR-RESULTANT VECTOR OF LENGTH M CONTAINING REAL ROOTS
C                 OF THE POLYNOMIAL
C           ROOTI-RESULTANT VECTOR OF LENGTH M CONTAINING THE
C                 CORRESPONDING IMAGINARY ROOTS OF THE POLYNOMIAL
C           IER  -ERROR CODE WHERE
C                 IER=0  NO ERROR
C                 IER=1  M LESS THAN ONE
C                 IER=2  M GREATER THAN 36
C                 IER=3  UNABLE TO DETERMINE ROOT WITH 500 INTERATIONS
C                        ON 5 STARTING VALUES
C                 IER=4  HIGH ORDER COEFFICIENT IS ZERO
C
C        REMARKS
C           LIMITED TO 36TH ORDER POLYNOMIAL OR LESS.
C           FLOATING POINT OVERFLOW MAY OCCUR FOR HIGH ORDER
C           POLYNOMIALS BUT WILL NOT AFFECT THE ACCURACY OF THE RESULTS.
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           NEWTON-RAPHSON ITERATIVE TECHNIQUE.  THE FINAL ITERATIONS
C           ON EACH ROOT ARE PERFORMED USING THE ORIGINAL POLYNOMIAL
C           RATHER THAN THE REDUCED POLYNOMIAL TO AVOID ACCUMULATED
C           ERRORS IN THE REDUCED POLYNOMIAL.
C
C     ..................................................................
C
      SUBROUTINE POLRT(XCOF,COF,M,ROOTR,ROOTI,IER)
      DIMENSION XCOF(1),COF(1),ROOTR(1),ROOTI(1)
      DOUBLE PRECISION XO,YO,X,Y,XPR,YPR,UX,UY,V,YT,XT,U,XT2,YT2,SUMSQ,
     1 DX,DY,TEMP,ALPHA
C
C     ..................................................................
C
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION
C        STATEMENT WHICH FOLLOWS.
C
C     DOUBLE PRECISION XCOF,COF,ROOTR,ROOTI
C
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS
C        ROUTINE.
C
C        THE DOUBLE PRECISION VERSION MAY BE MODIFIED BY CHANGING THE
C        CONSTANT IN STATEMENT 78 TO 1.0D-12 AND IN STATEMENT 122 TO
C        1.0D-10.  THIS WILL PROVIDE HIGHER PRECISION RESULTS AT THE
C        COST OF EXECUTION TIME
C
C        ..................................................................
C
      IFIT=0
      N=M
      IER=0
      IF(XCOF(N+1))10,25,10
   10 IF(N) 15,15,32
C
C        SET ERROR CODE TO 1
C
   15 IER=1
   20 RETURN
C
C        SET ERROR CODE TO 4
C
   25 IER=4
      GO TO 20
C
C        SET ERROR CODE TO 2
C
   30 IER=2
      GO TO 20
   32 IF(N-36) 35,35,30
   35 NX=N
      NXX=N+1
      NZ=1
      KJ1 = N+1
      DO 40 L=1,KJ1
      MT=KJ1-L+1
   40 COF(MT)=XCOF(L)
C
C        SET INITIAL VALUES
C
   45 XO=.00500101
      YO=0.01000101
C
C        ZERO INITIAL VALUE COUNTER
C
      IN=0
   50 X=XO
C
C        INCREMENT INITIAL VALUES AND COUNTER
C
      XO=-10.0*YO
      YO=-10.0*X
C
C        SET X AND Y TO CURRENT VALUE
C
      X=XO
      Y=YO
      IN=IN+1
      GO TO 59
   55 IFIT=1
      XPR=X
      YPR=Y
C
C        EVALUATE POLYNOMIAL AND DERIVATIVES
C
   59 ICT=0
   60 UX=0.0
      UY=0.0
      V =0.0
      YT=0.0
      XT=1.0
      U=COF(N+1)
      IF(U) 65,130,65
   65 DO 70 I=1,N
      L =N-I+1
      TEMP=COF(L)
      XT2=X*XT-Y*YT
      YT2=X*YT+Y*XT
      U=U+TEMP*XT2
      V=V+TEMP*YT2
      FI=I
      UX=UX+FI*XT*TEMP
      UY=UY-FI*YT*TEMP
      XT=XT2
   70 YT=YT2
      SUMSQ=UX*UX+UY*UY
      IF(SUMSQ) 75,110,75
   75 DX=(V*UY-U*UX)/SUMSQ
      X=X+DX
      DY=-(U*UY+V*UX)/SUMSQ
      Y=Y+DY
   78 IF(DABS(DY)+DABS(DX)-1.0D-05) 100,80,80
C
C        STEP ITERATION COUNTER
C
   80 ICT=ICT+1
      IF(ICT-500) 60,85,85
   85 IF(IFIT)100,90,100
   90 IF(IN-5) 50,95,95
C
C        SET ERROR CODE TO 3
C
   95 IER=3
      GO TO 20
  100 DO 105 L=1,NXX
      MT=KJ1-L+1
      TEMP=XCOF(MT)
      XCOF(MT)=COF(L)
  105 COF(L)=TEMP
      ITEMP=N
      N=NX
      NX=ITEMP
      IF(IFIT) 120,55,120
  110 IF(IFIT) 115,50,115
  115 X=XPR
      Y=YPR
  120 IFIT=0
  122 IF(DABS(Y)-1.0D-4*DABS(X)) 135,125,125
  125 ALPHA=X+X
      SUMSQ=X*X+Y*Y
      N=N-2
      GO TO 140
  130 X=0.0
      NX=NX-1
      NXX=NXX-1
  135 Y=0.0
      SUMSQ=0.0
      ALPHA=X
      N=N-1
  140 COF(2)=COF(2)+ALPHA*COF(1)
```

```
      DO 150 L=2,N                                                    PLRT1890
  150 COF(L+1)=COF(L+1)+ALPHA*COF(L)-SUMSQ*COF(L-1)                   PLRT1900
  155 ROOTI(N2)=Y                                                     PLRT1910
      ROOTR(N2)=X                                                     PLRT1920
      N2=N2+1                                                         PLRT1930
      IF(SUMSQ) 160,165,160                                           PLRT1940
  160 Y=-Y                                                            PLRT1950
      SUMSQ=0.0                                                       PLRT1960
      GO TO 155                                                       PLRT1970
  165 IF(N) 20,20,45                                                  PLRT1980
      END                                                             PLRT1990
```

Subroutines PRQD and DPRQD

These subroutines find the roots of a real polynomial by means of the QD-algorithm with displacement. The progressive QD-algorithm is a fast device for calculation of all roots of a polynomial P(x) with real coefficients when there are no approximations to the roots available.

The roots of P(x) = 0 are determined by solving for the poles of Q(x)/P(x) where Q(x) is some polynomial of smaller degree than P(x). In the following, n is used as the symbol for the degree of P(x). Using the derivative P'(x) for Q(x) has the advantage that the poles are simple even in case of multiple roots of P(x).

Start of the QD-algorithm requires the continued S-fraction:

$$\cfrac{c}{x-q_1 - \cfrac{1}{1-e_1 - \cfrac{1}{x-q_2 - \cfrac{1}{1- \ddots - \cfrac{q_n}{1}}}}} \quad \text{of } P'(x)/P(x)$$

This calculation is performed using the Euclidean algorithm. By means of normalization such that the highest coefficient is 1, $Q_0(x)$ is obtained from P(x), and $P_1(x)$ from P'(x). Then e_k and q_k are calculated from the iteration scheme:

$$q_k Q_k(x) = x \cdot P_k(x) - Q_{k-1}(x), \quad k = 1,2,\ldots,n \qquad (1)$$

$$e_k P_{k+1}(x) = Q_k(x) - P_k(x), \quad k = 1,2,\ldots,n-1 \qquad (2)$$

using the fact that all elements $Q_i(x)$ and $P_i(x)$ are normalized by definition.

The following example is an illustration for this iteration scheme:

$$P(x) = 1 + 3x + 3x^2 + x^3 \quad , n = 3$$

$$Q_0(x) = x^3 + 3x^2 + 3x + 1$$

$$P_1(x) = x^2 + 2x + 1 \quad , q_1 Q_1(x) = -x^2 - 2x - 1, \; q_1 = -1$$

$$Q_1(x) = x^2 + 2x + 1 \quad , e_1 P_2(x) = 0 \quad , e_1 = 0$$

where $Q_1(x)$ is a common divisor of $P'(x)/P(x)$ and $q_1 = -1$ is the value of the real root which factors out first.

The above iteration scheme breaks down if some intermediate value of q_1 with $0 < i < n$ is equal or approximately equal to zero. In this case an error code is set to 4, which indicates that no S-fraction exists for $P'(x)/P(x)$.

If Q_0 and P_1 have a common divisor of degree j, this common divisor is obtained as Q_{n-j}, and necessarily $e_{n-j} P_{n-j+1} = 0$.

Due to roundoff errors, all coefficients of $e_{n-j} P_{n-j+1}$ cannot be expected to vanish exactly; therefore, allowance is made for coefficients of small absolute value.

If the highest coefficient of $e_{n-j} P_{n-j+1}$ is small in absolute value but some lower coefficient is not, the error code is set to 4, and the subroutine is abandoned.

The coefficients e_k, q_k obtained by the Euclidean algorithm form the first row of the QD-array indicated by superscript 0.

e_0	q_1	e_1	q_2	e_2	...	q_m	e_m
0	$q_1^{(0)}$	$e_1^{(0)}$	$q_2^{(0)}$	$e_2^{(0)}$	...	$q_m^{(0)}$	$e_m^{(0)}$
0	$q_1^{(1)}$	$e_1^{(1)}$	$q_2^{(1)}$	$e_2^{(1)}$	...	$q_m^{(1)}$	$e_m^{(1)}$
. . . . .							

Normally m is equal to n but it may be smaller if a common factor exists.

The following rows are obtained by means of the relationships:

$$q_i^{(v+1)} = q_i^{(v)} + e_i^{(v)} - e_{i-1}^{(v+1)}, \quad i = 1, \ldots, m \tag{3}$$

$$e_i^{(v+1)} = \frac{e_i^{(v)} \cdot q_{i+1}^{(v)}}{q_i^{(v+1)}}, \quad i = 1, \ldots, m-1 \tag{4}$$

together with $e_0^{(v)} = e_m^{(v)} = 0$.

Let x_i denote the roots of P(x) ordered in decreasing absolute value. If P(x) has only roots of different absolute value, there is convergence of the q_k-column to the value x_k. Complex roots are indicated by oscillation of certain q-values.

If x_k and x_{k+1} are of equal absolute value, then the roots of

$$x^2 - (q_k^{(v+1)} + q_{k+1}^{(v)})\, x + q_k^{(v)} q_{k+1}^{(v)} = 0 \tag{5}$$

converge to x_k and x_{k+1}. The same reasoning applies if the relation $|x_k| = |x_{k+1}|$ holds only approximately.

The QD-algorithm in the form (3), (4) suffers from the fact that convergence is rather slow. By means of displacement of the origin a form is obtained which is asymptotically of quadratic convergence.

The strategy is as follows. Start with displacement $t = 0$.

I. As soon as convergence is indicated to a real root -- that is, $e_{m-1}^{(v)}$ is sufficiently small (internal test value 0.01) -- perform a displacement by the amount $q_m^{(v)}$.

Starting with $q_k^{(v)}$, $e_k^{(v)}$, use instead of (3), (4) the iteration scheme:

$$t = t + q_m^{(v)} \tag{6}$$

$$q_k^{(v+1)} = q_k^{(v)} + e_k^{(v)} - e_{k-1}^{(v+1)} - q_m^{(v)}$$

$$, \quad k = 1, 2, \ldots, m \tag{7}$$

$$e_k^{(v+1)} = q_{k+1}^{(v)} \cdot e_k^{(v)} \Big/ q_k^{(v+1)}$$

$$, \quad k = 1, 2, \ldots, m-1 \tag{8}$$

Values $e_0^{(v+1)}$ and $e_m^{(v)}$ are thereby set equal to zero.

II. If convergence is indicated to a root pair -- that is, $e_{m-2}^{(v)}$ is less than $e_{m-1}^{(v)}$ and sufficiently small (internal test value 0.01) -- calculate the discriminant of the quadratic equation (5):

$$D = p * p - q_m^{(v)} * q_{m-1}^{(v)}$$

with

$$P = 0.5\,(q_{m-1}^{(v)} + e_{m-1}^{(v)} + q_m^{(v)})$$

If D is positive, provide for a real displacement of amount $P - \sqrt{D}$ or $P + \sqrt{D}$, whichever has the smaller absolute value, and proceed according to (7), (8).

If D is negative, three complex displacements are applied in sequence: the first by amount $P + i\sqrt{|D|}$, the second by $-2i\sqrt{|D|}$, and the third by $V + i\sqrt{|D|}$, resulting in a total real displacement of amount P.

Instead of (6), (7), (8) the following iteration scheme is then obtained. Starting with:

$$t = t + P \tag{9}$$

$$q_1^* = q_1^{(v)} + e_1^{(v)} - P \tag{10}$$

$$P_1 = -D/q_1^{*2} \tag{11}$$

$$e_1^* = e_1^{(v)} q_2^{(v)} / \left[q_1^* (1 + p_1)\right] \tag{12}$$

$$q_1^{**} = q_1^* + e_1^* \tag{13}$$

calculate for $k = 2, 3, \ldots, m$:

$$q_k^* = q_k^{(v)} + e_k^{(v)} - e_{k-1}^* - P \tag{14}$$

$$e_{k-1}^{**} = e_{k-1}^* q_k^* / q_{k-1}^{**} \tag{15}$$

$$p_k = p_{k-1} (q_{k-1}^{**} / q_k^*)^2 \tag{16}$$

$$q_{k-1}^{(v+3)} = q_{k-1}^{**} + e_{k-1}^{**} - e_{k-2}^{(v+3)} \tag{17}$$

$$e_k^* = q_{k+1}^{(v)} e_k^{(v)} / \left[q_k^* (1+p_k)\right] \tag{18}$$

$$q_k^{**} = q_k^* + e_k^* - e_{k-1}^{**} \tag{19}$$

$$e_{k-1}^{(v+3)} = (e_{k-1}^{**} q_k^{**} / q_{k-1}^{(v+3)}) (1 + p_k) \tag{20}$$

Finally set:

$$q_m^{(v+3)} = q_m^{**} - e_{m-1}^{(v+3)} \tag{21}$$

Values $e_0^{(v+3)}$, $e_m^{(v)}$ and $q_{m+1}^{(v)}$ are thereby set equal to zero.

III. If none of the values $e_{m-1}^{(v)}$ and $e_{m-2}^{(v)}$ is sufficiently small, the relationship (3), (4) is used with no displacement at all.

Regarding termination of the iterative scheme given by I., II., III. there are two possibilities:

1. If $e_{m-1}^{(v)}$ is negligible (internal test value is 10^{-6} in single precision and 10^{-16} in double precision), a real root is factored out.

2. If $e_{m-2}^{(v)}$ is negligible (with the same internal test values), a pair of roots is factored out.

A maximum of ten times the number of coefficients using I., II. or III. is allowed. At every iteration step for one and the same root or root pair, the internal test value for convergence and the internal test value for acceptance of a displacement are increased by ten percent.

In case of convergence:

1. For a real root --
   real part of root = $t + q_m$
   complex part of root = 0
2. For a real root pair (characterized by $D > 0$) --
   real part of first root = $t + P + \sqrt{D}$
   complex part of first root = 0
   real part of second root = $t + P - \sqrt{D}$
   complex part of second root = 0
3. For a complex root pair (characterized by $D < 0$) --
   real part of first root = $t + P$
   complex part of first root = $\sqrt{-D}$
   real part of second root = $t + P$
   complex part of second root = $-\sqrt{-D}$

As soon as a root or root pair has been factored out, m is reduced by 1 or 2 respectively and the whole procedure I., II., III. is repeated with original values of internal test values, until m = 0 -- that is, all roots have been calculated -- or m = 1, when the last real root is factored immediately. If $P'(x)$, $P(x)$ have a common divisor, the whole process is repeated for this common divisor. Thus, the complete factorization of the original polynomial $P(x)$ is obtained.

Some remarks are in order:

1. The QD-algorithm is a nonlinear relationship and therefore sensitive to roundoff errors. Small intermediate q-values cause loss of accuracy. Therefore, all divisors are checked before division is actually performed. If a divisor is small in

absolute value due to loss of significant digits, the error parameter is set to 3 indicating possible instability of calculation, and further calculation is bypassed.

2. If a maximum of 10 * n iteration steps is insufficient for calculation of all roots, the error parameter is set to 1, indicating poor convergence. Further calculation is bypassed again.

3. If the original polynomial has a degree less than one, the error parameter is set to 2 indicating that no root exists.

4. If, in case of a complex displacement, q^{**}_{m-1} or q^{*}_{m} gets very small due to loss of significant digits, and the calculated $e^{(v+3)}_{m-2}$ is less than the internal test value TOL, a pair of roots is calculated from the quadratic equation:

$$x^2 - x\cdot(q^{**}_{n-1} + q^{*}_{n} - e^{(v+3)}_{n-2}) + (q^{**}_{n-1} - e^{*}_{n-1}) \left[q^{*}_{n} - e^{*}_{n-1}\,p_{n-1} - q^{*}_{n}\,\frac{e^{**}_{n-2}}{q^{(v+3)}_{n-2}}(1+p_{n-1})\right] \qquad (22)$$

which is easily obtained from (5).

5. A final test of accuracy is made after calculation of all roots of the given polynomial. The calculated roots are used for calculation of the corresponding coefficient vector. If this calculated coefficient vector has less than a specified number of correct digits (the maximal relative error must be less than TOL), the error parameter is set to -1 indicating that calculation of all roots was successful only with poor accuracy of results.

```
C                                                                       PRQD  10
C     ...................................................................PRQD  20
C                                                                       PRQD  30
C        SUBROUTINE PRQD                                                PRQD  40
C                                                                       PRQD  50
C        PURPOSE                                                        PRQD  60
C           CALCULATE ALL REAL AND COMPLEX ROOTS OF A GIVEN POLYNOMIAL  PRQD  70
C           WITH REAL COEFFICIENTS.                                     PRQD  80
C                                                                       PRQD  90
C        USAGE                                                          PRQD 100
C           CALL PRQD(C,IC,Q,E,POL,IR,IER)                              PRQD 110
C                                                                       PRQD 120
C        DESCRIPTION OF PARAMETERS                                      PRQD 130
C           C      - COEFFICIENT VECTOR OF GIVEN POLYNOMIAL             PRQD 140
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          PRQD 150
C                    THE GIVEN COEFFICIENT VECTOR GETS DIVIDED BY THE   PRQD 160
C                    LAST NONZERO TERM                                  PRQD 170
C           IC     - DIMENSION OF VECTOR C                              PRQD 180
C           Q      - WORKING STORAGE OF DIMENSION IC                    PRQD 190
C                    ON RETURN Q CONTAINS REAL PARTS OF ROOTS           PRQD 200
C           E      - WORKING STORAGE OF DIMENSION IC                    PRQD 210
C                    ON RETURN E CONTAINS COMPLEX PARTS OF ROOTS        PRQD 220
C           POL    - WORKING STORAGE OF DIMENSION IC                    PRQD 230
C                    ON RETURN POL CONTAINS THE COEFFICIENTS OF THE     PRQD 240
C                    POLYNOMIAL WITH CALCULATED ROOTS                   PRQD 250
C                    THIS RESULTING COEFFICIENT VECTOR HAS DIMENSION IR+1PRQD 260
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          PRQD 270
C           IR     - NUMBER OF CALCULATED ROOTS                         PRQD 280
C                    NORMALLY IR IS EQUAL TO DIMENSION IC MINUS ONE     PRQD 290
C           IER    - RESULTING ERROR PARAMETER. SEE REMARKS             PRQD 300
C                                                                       PRQD 310
C        REMARKS                                                        PRQD 320
C           THE REAL PART OF THE ROOTS IS STORED IN Q(I) UP TO Q(IR)    PRQD 330
C           CORRESPONDING COMPLEX PARTS ARE STORED IN E(I) UP TO E(IR). PRQD 340
C           IER = 0 MEANS NO ERRORS                                     PRQD 350
C           IER = 1 MEANS NO CONVERGENCE WITH FEASIBLE TOLERANCE        PRQD 360
C           IER = 2 MEANS POLYNOMIAL IS DEGENERATE (CONSTANT OR ZERO)   PRQD 370
C           IER = 3 MEANS SUBROUTINE WAS ABANDONED DUE TO ZERO DIVISOR  PRQD 380
C           IER = 4 MEANS THERE EXISTS NO S-FRACTION                    PRQD 390
C           IER =-1 MEANS CALCULATED COEFFICIENT VECTOR REVEALS POOR    PRQD 400
C                   ACCURACY OF THE CALCULATED ROOTS.                   PRQD 410
C                   THE CALCULATED COEFFICIENT VECTOR HAS LESS THAN     PRQD 420
C                   3 CORRECT DIGITS.                                   PRQD 430
C           THE FINAL COMPARISON BETWEEN GIVEN AND CALCULATED           PRQD 440
C           COEFFICIENT VECTOR IS PERFORMED ONLY IF ALL ROOTS HAVE BEEN PRQD 450
C           CALCULATED.                                                 PRQD 460
C           THE MAXIMAL RELATIVE ERROR OF THE COEFFICIENT VECTOR IS     PRQD 470
C           RECORDED IN Q(IR+1).                                        PRQD 480
C                                                                       PRQD 490
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PRQD 500
C           NONE                                                        PRQD 510
C                                                                       PRQD 520
C        METHOD                                                         PRQD 530
C           THE ROOTS OF THE POLYNOMIAL ARE CALCULATED BY MEANS OF      PRQD 540
C           THE QUOTIENT-DIFFERENCE ALGORITHM WITH DISPLACEMENT.        PRQD 550
C           REFERENCE                                                   PRQD 560
C           H.RUTISHAUSER, DER QUOTIENTEN-DIFFERENZEN-ALGORITHMUS,      PRQD 570
C           BIRKHAEUSER, BASEL/STUTTGART, 1957.                         PRQD 580
C                                                                       PRQD 590
C     ...................................................................PRQD 600
C                                                                       PRQD 610
      SUBROUTINE PRQD(C,IC,Q,E,POL,IR,IER)                              PRQD 620
C                                                                       PRQD 630
C     DIMENSIONED DUMMY VARIABLES                                       PRQD 640
      DIMENSION E(1),Q(1),C(1),POL(1)                                   PRQD 650
C                                                                       PRQD 660
C        NORMALIZATION OF GIVEN POLYNOMIAL                              PRQD 670
C           TEST OF DIMENSION                                           PRQD 680
C        IR CONTAINS INDEX OF HIGHEST COEFFICIENT                       PRQD 690
      IER=0                                                             PRQD 700
      IR=IC                                                             PRQD 710
      EPS=1.E-6                                                         PRQD 720
      TOL=1.E-3                                                         PRQD 730
      LIMIT=10*IC                                                       PRQD 740
      KOUNT=0                                                           PRQD 750
    1 IF(C(IR-1))79,79,2                                                PRQD 760
C                                                                       PRQD 770
C        DROP TRAILING ZERO COEFFICIENTS                                PRQD 780
    2 IF(C(IR))4,3,4                                                    PRQD 790
    3 IR=IR-1                                                           PRQD 800
      GOTO 1                                                            PRQD 810
C                                                                       PRQD 820
C           REARRANGEMENT OF GIVEN POLYNOMIAL                           PRQD 830
C        EXTRACTION OF ZERO ROOTS                                       PRQD 840
    4 Q=1./C(IR)                                                        PRQD 850
      IEND=IR-1                                                         PRQD 860
      ISTA=1                                                            PRQD 870
      NSAV=IR+1                                                         PRQD 880
      JBEG=1                                                            PRQD 890
C                                                                       PRQD 900
C        Q(J)=1.                                                        PRQD 910
C        Q(J+I)=C(IR-I)/C(IR)                                           PRQD 920
C        Q(IR)=C(J)/C(IR)                                               PRQD 930
C        WHERE J IS THE INDEX OF THE LOWEST NONZERO COEFFICIENT         PRQD 940
      DO 9 I=1,IR                                                       PRQD 950
      J=NSAV-I                                                          PRQD 960
      IF(C(I))7,5,7                                                     PRQD 970
    5 GOTO(6,8),JBEG                                                    PRQD 980
    6 NSAV=NSAV+1                                                       PRQD 990
      Q(ISTA)=0.                                                        PRQD1000
      E(ISTA)=0.                                                        PRQD1010
      ISTA=ISTA+1                                                       PRQD1020
      GOTO 9                                                            PRQD1030
    7 JBEG=2                                                            PRQD1040
    8 Q(J)=C(I)*Q                                                       PRQD1050
      C(I)=Q(J)                                                         PRQD1060
    9 CONTINUE                                                          PRQD1070
C                                                                       PRQD1080
C           INITIALIZATION                                              PRQD1090
      ESAV=0.                                                           PRQD1100
      Q(ISTA)=0.                                                        PRQD1110
   10 NSAV=IR                                                           PRQD1120
C                                                                       PRQD1130
C        COMPUTATION OF DERIVATIVE                                      PRQD1140
      EXPT=IR-ISTA                                                      PRQD1150
      E(ISTA)=EXPT                                                      PRQD1160
      DO 11 I=ISTA,IEND                                                 PRQD1170
      EXPT=EXPT-1.0                                                     PRQD1180
      POL(I+1)=EPS*ABS(Q(I+1))+EPS                                      PRQD1190
   11 E(I+1)=Q(I+1)*EXPT                                                PRQD1200
C                                                                       PRQD1210
C        TEST OF REMAINING DIMENSION                                    PRQD1220
      IF(ISTA-IEND)12,20,60                                             PRQD1230
   12 JEND=IEND-1                                                       PRQD1240
C                                                                       PRQD1250
C        COMPUTATION OF S-FRACTION                                      PRQD1260
      DO 19 I=ISTA,JEND                                                 PRQD1270
      IF(I-ISTA)13,16,13                                                PRQD1280
   13 IF(ABS(E(I))-POL(I+1))14,14,16                                    PRQD1290
C                                                                       PRQD1300
C        THE GIVEN POLYNOMIAL HAS MULTIPLE ROOTS, THE COEFFICIENTS OF   PRQD1310
C        THE COMMON FACTOR ARE STORED FROM Q(NSAV) UP TO Q(IR)          PRQD1320
   14 NSAV=I                                                            PRQD1330
      DO 15 K=I,JEND                                                    PRQD1340
      IF(ABS(E(K))-POL(K+1))15,15,80                                    PRQD1350
   15 CONTINUE                                                          PRQD1360
      GOTO 21                                                           PRQD1370
C                                                                       PRQD1380
C           EUCLIDEAN ALGORITHM                                         PRQD1390
   16 DO 19 K=I,IEND                                                    PRQD1400
      E(K+1)=E(K+1)/E(I)                                                PRQD1410
      Q(K+1)=E(K+1)-Q(K+1)                                              PRQD1420
      IF(K-I)18,17,18                                                   PRQD1430
C                                                                       PRQD1440
C        TEST FOR SMALL DIVISOR                                         PRQD1450
   17 IF(ABS(Q(I+1))-POL(I+1))80,80,19                                  PRQD1460
   18 Q(K+1)=Q(K+1)/Q(I+1)                                              PRQD1470
      POL(K+1)=POL(K+1)/ABS(Q(I+1))                                     PRQD1480
      E(K)=Q(K+1)-E(K)                                                  PRQD1490
   19 CONTINUE                                                          PRQD1500
   20 Q(IR)=-Q(IR)                                                      PRQD1510
C                                                                       PRQD1520
C           THE DISPLACEMENT EXPT IS SET TO 0 AUTOMATICALLY.            PRQD1530
C           E(ISTA)=0.,Q(ISTA+1),....,E(NSAV-1),Q(NSAV),E(NSAV)=0.,     PRQD1540
C           FORM A DIAGONAL OF THE QD-ARRAY.                            PRQD1550
C        INITIALIZATION OF BOUNDARY VALUES                              PRQD1560
   21 E(ISTA)=0.                                                        PRQD1570
      NRAN=NSAV-1                                                       PRQD1580
   22 E(NRAN+1)=0.                                                      PRQD1590
C                                                                       PRQD1600
C           TEST FOR LINEAR OR CONSTANT FACTOR                          PRQD1610
C        NRAN-ISTA IS DEGREE-1                                          PRQD1620
      IF(NRAN-ISTA)24,23,31                                             PRQD1630
C                                                                       PRQD1640
C        LINEAR FACTOR                                                  PRQD1650
   23 Q(ISTA+1)=Q(ISTA+1)+EXPT                                          PRQD1660
      E(ISTA+1)=0.                                                      PRQD1670
C                                                                       PRQD1680
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C        TEST FOR UNFACTORED COMMON DIVISOR                          PRQD1690
   24 E(ISTA)=ESAV                                                    PRQD1700
      IF(IR-NSAV)60,60,25                                             PRQD1710
C                                                                     PRQD1720
C        INITIALIZE QD-ALGORITHM FOR COMMON DIVISOR                   PRQD1730
   25 ISTA=NSAV                                                       PRQD1740
      ESAV=E(ISTA)                                                    PRQD1750
      GOTO 10                                                         PRQD1760
C                                                                     PRQD1770
C        COMPUTATION OF ROOT PAIR                                     PRQD1780
   26 P=P+EXPT                                                        PRQD1790
C                                                                     PRQD1800
C           TEST FOR REALITY                                          PRQD1810
      IF(D)27,28,28                                                   PRQD1820
C                                                                     PRQD1830
C           COMPLEX ROOT PAIR                                         PRQD1840
   27 Q(NRAN)=P                                                       PRQD1850
      Q(NRAN+1)=P                                                     PRQD1860
      E(NRAN)=T                                                       PRQD1870
      E(NRAN+1)=-T                                                    PRQD1880
      GOTO 29                                                         PRQD1890
C                                                                     PRQD1900
C           REAL ROOT PAIR                                            PRQD1910
   28 Q(NRAN)=P-T                                                     PRQD1920
      Q(NRAN+1)=P+T                                                   PRQD1930
      E(NRAN)=0.                                                      PRQD1940
C                                                                     PRQD1950
C           REDUCTION OF DEGREE BY 2 (DEFLATION)                      PRQD1960
   29 NRAN=NRAN-2                                                     PRQD1970
      GOTO 22                                                         PRQD1980
C                                                                     PRQD1990
C        COMPUTATION OF REAL ROOT                                     PRQD2000
   30 Q(NRAN+1)=EXPT+P                                                PRQD2010
C                                                                     PRQD2020
C           REDUCTION OF DEGREE BY 1 (DEFLATION)                      PRQD2030
      NRAN=NRAN-1                                                     PRQD2040
      GOTO 22                                                         PRQD2050
C                                                                     PRQD2060
C        START QD-ITERATION                                           PRQD2070
   31 JBEG=ISTA+1                                                     PRQD2080
      JEND=NRAN-1                                                     PRQD2090
      TEPS=EPS                                                        PRQD2100
      TDELT=1.E-2                                                     PRQD2110
   32 KOUNT=KOUNT+1                                                   PRQD2120
      P=Q(NRAN+1)                                                     PRQD2130
      R=ABS(E(NRAN))                                                  PRQD2140
C                                                                     PRQD2150
C           TEST FOR CONVERGENCE                                      PRQD2160
      IF(R-TEPS)30,30,33                                              PRQD2170
   33 S=ABS(E(JEND))                                                  PRQD2180
C                                                                     PRQD2190
C        IS THERE A REAL ROOT NEXT                                    PRQD2200
      IF(S-R)38,38,34                                                 PRQD2210
C                                                                     PRQD2220
C        IS DISPLACEMENT SMALL ENOUGH                                 PRQD2230
   34 IF(R-TDELT)36,35,35                                             PRQD2240
   35 P=0.                                                            PRQD2250
   36 D=P                                                             PRQD2260
      DO 37 J=JBEG,NRAN                                               PRQD2270
      Q(J)=Q(J)+E(J)-E(J-1)-D                                         PRQD2280
C                                                                     PRQD2290
C           TEST FOR SMALL DIVISOR                                    PRQD2300
      IF(ABS(Q(J))-POL(J)*1.E-81,81,37                                PRQD2310
   37 E(J)=Q(J+1)*E(J)/Q(J)                                           PRQD2320
      Q(NRAN+1)=-E(NRAN)+Q(NRAN+1)-D                                  PRQD2330
      GOTO 54                                                         PRQD2340
C                                                                     PRQD2350
C        CALCULATE DISPLACEMENT FOR DOUBLE ROOTS                      PRQD2360
C           QUADRATIC EQUATION FOR DOUBLE ROOTS                       PRQD2370
C           X**2-(Q(NRAN)+Q(NRAN+1)+E(NRAN))*X+Q(NRAN)*Q(NRAN+1)=0    PRQD2380
   38 P=0.5*(Q(NRAN)+E(NRAN)+Q(NRAN+1))                               PRQD2390
      D=P*P-Q(NRAN)*Q(NRAN+1)                                         PRQD2400
      T=SQRT(ABS(D))                                                  PRQD2410
C                                                                     PRQD2420
C        TEST FOR CONVERGENCE                                         PRQD2430
      IF(S-TEPS)26,26,39                                              PRQD2440
C                                                                     PRQD2450
C        ARE THERE COMPLEX ROOTS                                      PRQD2460
   39 IF(D)43,40,40                                                   PRQD2470
   40 IF(P)42,41,41                                                   PRQD2480
   41 T=-T                                                            PRQD2490
   42 P=P+T                                                           PRQD2500
      R=S                                                             PRQD2510
      GOTO 34                                                         PRQD2520
C                                                                     PRQD2530
C        MODIFICATION FOR COMPLEX ROOTS                               PRQD2540
C        IS DISPLACEMENT SMALL ENOUGH                                 PRQD2550
   43 IF(S-TDELT)44,35,35                                             PRQD2560
C                                                                     PRQD2570
C        INITIALIZATION                                               PRQD2580
   44 D=Q(JBEG)+E(JBEG)-P                                             PRQD2590
C                                                                     PRQD2600
C           TEST FOR SMALL DIVISOR                                    PRQD2610
      IF(ABS(D)-POL(JBEG)*1.E-81,81,45                                PRQD2620
   45 T=(T/D)**2                                                      PRQD2630
      U=E(JBEG)*Q(JBEG+1)/(D*(1.+T))                                  PRQD2640
      V=D+U                                                           PRQD2650
      KOUNT=KOUNT+2                                                   PRQD2660
C                                                                     PRQD2670
C        THREEFOLD LOOP FOR COMPLEX DISPLACEMENT                      PRQD2680
      DO 53 J=JBEG,NRAN                                               PRQD2690
      D=Q(J+1)+E(J+1)-U-P                                             PRQD2700
C                                                                     PRQD2710
C           TEST FOR SMALL DIVISOR                                    PRQD2720
      IF(ABS(V)-POL(J))46,46,49                                       PRQD2730
   46 IF(J-NRAN)81,47,81                                              PRQD2740
   47 EXPT=EXPT+P                                                     PRQD2750
      IF(ABS(E(JEND))-TOL)48,48,81                                    PRQD2760
   48 P=0.5*(V+D-E(JEND))                                             PRQD2770
      D=P*P-(V-U)*(D-U*T-D*W*(1.+T)/Q(JEND))                          PRQD2780
      T=SQRT(ABS(D))                                                  PRQD2790
      GOTO 26                                                         PRQD2800
C                                                                     PRQD2810
C           TEST FOR SMALL DIVISOR                                    PRQD2820
   49 IF(ABS(D)-POL(J+1))46,46,50                                     PRQD2830
   50 W=U*D/V                                                         PRQD2840
      T=T*(V/D)**2                                                    PRQD2850
      Q(J)=V+W-E(J-1)                                                 PRQD2860
      U=0.                                                            PRQD2870
      IF(J-NRAN)51,52,52                                              PRQD2880
   51 U=Q(J+2)*E(J+1)/(D*(1.+T))                                      PRQD2890
   52 V=D+U-W                                                         PRQD2900
C                                                                     PRQD2910
C        TEST FOR SMALL DIVISOR                                       PRQD2920
      IF(ABS(Q(J))-POL(J))81,81,53                                    PRQD2930
   53 E(J)=W*V*(1.+T)/Q(J)                                            PRQD2940
      Q(NRAN+1)=V-E(NRAN)                                             PRQD2950
   54 EXPT=EXPT+P                                                     PRQD2960
      TEPS=TEPS*1.1                                                   PRQD2970
      TDELT=TDELT*1.1                                                 PRQD2980
      IF(KOUNT-LIMIT)32,55,55                                         PRQD2990
C                                                                     PRQD3000
C        NO CONVERGENCE WITH FEASIBLE TOLERANCE                       PRQD3010
C           ERROR RETURN IN CASE OF UNSATISFACTORY CONVERGENCE        PRQD3020
   55 IER=1                                                           PRQD3030
C                                                                     PRQD3040
C        REARRANGE CALCULATED ROOTS                                   PRQD3050
   56 IEND=NSAV-NRAN-1                                                PRQD3060
      E(ISTA)=ESAV                                                    PRQD3070
      IF(IEND)59,59,57                                                PRQD3080
   57 DO 58 I=1,IEND                                                  PRQD3090
      J=ISTA+I                                                        PRQD3100
      K=NRAN+1+I                                                      PRQD3110
      E(J)=E(K)                                                       PRQD3120
   58 Q(J)=Q(K)                                                       PRQD3130
   59 IR=ISTA+IEND                                                    PRQD3140
C                                                                     PRQD3150
C        NORMAL RETURN                                                PRQD3160
   60 IR=IR-1                                                         PRQD3170
      IF(IR)78,78,61                                                  PRQD3180
C                                                                     PRQD3190
C        REARRANGE CALCULATED ROOTS                                   PRQD3200
   61 DO 62 I=1,IR                                                    PRQD3210
      Q(I)=Q(I+1)                                                     PRQD3220
   62 E(I)=E(I+1)                                                     PRQD3230
C                                                                     PRQD3240
C        CALCULATE COEFFICIENT VECTOR FROM ROOTS                      PRQD3250
      POL(IR+1)=1.                                                    PRQD3260
      IEND=IR-1                                                       PRQD3270
      JBEG=1                                                          PRQD3280
      DO 69 J=1,IR                                                    PRQD3290
      ISTA=IR+1-J                                                     PRQD3300
      D=0.                                                            PRQD3310
      P=Q(ISTA)                                                       PRQD3320
      T=E(ISTA)                                                       PRQD3330
      IF(T)65,63,65                                                   PRQD3340
C                                                                     PRQD3350
C        MULTIPLY WITH LINEAR FACTOR                                  PRQD3360
   63 DO 64 I=ISTA,IR                                                 PRQD3370
      POL(I)=D-P*POL(I+1)                                             PRQD3380
   64 D=POL(I+1)                                                      PRQD3390
      GOTO 69                                                         PRQD3400
   65 GOTO(66,67),JBEG                                                PRQD3410
   66 JBEG=2                                                          PRQD3420
      POL(ISTA)=0.                                                    PRQD3430
      GOTO 69                                                         PRQD3440
C                                                                     PRQD3450
C        MULTIPLY WITH QUADRATIC FACTOR                               PRQD3460
   67 JBEG=1                                                          PRQD3470
      U=P*P+T*T                                                       PRQD3480
      P=P+P                                                           PRQD3490
      DO 68 I=ISTA,IEND                                               PRQD3500
      POL(I)=D-P*POL(I+1)+U*POL(I+2)                                  PRQD3510
   68 D=POL(I+1)                                                      PRQD3520
      POL(IR)=D-P                                                     PRQD3530
   69 CONTINUE                                                        PRQD3540
      IF(IER)78,70,78                                                 PRQD3550
C                                                                     PRQD3560
C        COMPARISON OF COEFFICIENT VECTORS, IE. TEST OF ACCURACY      PRQD3570
   70 P=0.                                                            PRQD3580
      DO 75 I=1,IR                                                    PRQD3590
      IF(C(I))72,71,72                                                PRQD3600
   71 D=ABS(POL(I))                                                   PRQD3610
      GOTO 73                                                         PRQD3620
   72 D=ABS((POL(I)-C(I))/C(I))                                       PRQD3630
   73 IF(P-D)74,75,75                                                 PRQD3640
   74 P=D                                                             PRQD3650
   75 CONTINUE                                                        PRQD3660
      IF(P-TOL)77,76,76                                               PRQD3670
   76 IER=-1                                                          PRQD3680
   77 Q(IR+1)=P                                                       PRQD3690
      E(IR+1)=0.                                                      PRQD3700
   78 RETURN                                                          PRQD3710
C                                                                     PRQD3720
C        ERROR RETURNS                                                PRQD3730
C           ERROR RETURN FOR POLYNOMIALS OF DEGREE LESS THAN 1        PRQD3740
   79 IER=2                                                           PRQD3750
      IR=0                                                            PRQD3760
      RETURN                                                          PRQD3770
C                                                                     PRQD3780
C           ERROR RETURN IF THERE EXISTS NO S-FRACTION                PRQD3790
   80 IER=4                                                           PRQD3800
      IR=ISTA                                                         PRQD3810
      GOTO 60                                                         PRQD3820
C                                                                     PRQD3830
C           ERROR RETURN IN CASE OF INSTABLE QD-ALGORITHM             PRQD3840
   81 IER=3                                                           PRQD3850
      GOTO 56                                                         PRQD3860
      END                                                             PRQD3870
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C                                                                     DPRQ  10
C     ..............................................................DPRQ  20
C                                                                     DPRQ  30
C        SUBROUTINE DPRQD                                           DPRQ  40
C                                                                     DPRQ  50
C        PURPOSE                                                    DPRQ  60
C           CALCULATE ALL REAL AND COMPLEX ROOTS OF A GIVEN POLYNOMIAL DPRQ  70
C           WITH REAL COEFFICIENTS.                                 DPRQ  80
C                                                                     DPRQ  90
C        USAGE                                                      DPRQ 100
C           CALL DPRQD(C,IC,Q,E,POL,IR,IER)                         DPRQ 110
C                                                                   DPRQ 120
C        DESCRIPTION OF PARAMETERS                                  DPRQ 130
C           C      - COEFFICIENT VECTOR OF GIVEN POLYNOMIAL         DPRQ 140
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH      DPRQ 150
C                    THE GIVEN COEFFICIENT VECTOR GETS DIVIDED BY THE DPRQ 160
C                    LAST NONZERO TERM                              DPRQ 170
C                    DOUBLE PRECISION ARRAY                         DPRQ 180
C           IC     - DIMENSION OF VECTOR C                          DPRQ 190
C           Q      - WORKING STORAGE OF DIMENSION IC                DPRQ 200
C                    ON RETURN Q CONTAINS REAL PARTS OF ROOTS       DPRQ 210
C                    DOUBLE PRECISION ARRAY                         DPRQ 220
C           E      - WORKING STORAGE OF DIMENSION IC                DPRQ 230
C                    ON RETURN E CONTAINS COMPLEX PARTS OF ROOTS     DPRQ 240
C                    DOUBLE PRECISION ARRAY                         DPRQ 250
C           POL    - WORKING STORAGE OF DIMENSION IC                DPRQ 260
C                    ON RETURN POL CONTAINS THE COEFFICIENTS OF THE DPRQ 270
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C                    POLYNOMIAL WITH CALCULATED ROOTS                    DPRQ 280
C                    THIS RESULTING COEFFICIENT VECTOR HAS DIMENSION IR+1DPRQ 290
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH           DPRQ 300
C                    DOUBLE PRECISION ARRAY                              DPRQ 310
C             IR     - NUMBER OF CALCULATED ROOTS                        DPRQ 320
C                    NORMALLY IR IS EQUAL TO DIMENSION IC MINUS ONE      DPRQ 330
C     .       IER    - RESULTING ERROR PARAMETER. SEE REMARKS            DPRQ 340
C                                                                        DPRQ 350
C          REMARKS                                                       DPRQ 360
C             THE REAL PART OF THE ROOTS IS STORED IN Q(1) UP TO Q(IR)   DPRQ 370
C             CORRESPONDING COMPLEX PARTS ARE STORED IN E(1) UP TO E(IR). DPRQ 380
C             IER = 0 MEANS NO ERRORS                                    DPRQ 390
C             IER = 1 MEANS NO CONVERGENCE WITH FEASIBLE TOLERANCE       DPRQ 400
C             IER = 2 MEANS POLYNOMIAL IS DEGENERATE (CONSTANT OR ZERO)  DPRQ 410
C             IER = 3 MEANS SUBROUTINE WAS ABANDONED DUE TO ZERO DIVISOR DPRQ 420
C             IER = 4 MEANS THERE EXISTS NO S-FRACTION                   DPRQ 430
C             IER =-1 MEANS CALCULATED COEFFICIENT VECTOR REVEALS POOR   DPRQ 440
C                     ACCURACY OF THE CALCULATED ROOTS.                  DPRQ 450
C                     THE CALCULATED COEFFICIENT VECTOR HAS LESS THAN    DPRQ 460
C                     6 CORRECT DIGITS.                                  DPRQ 470
C             THE FINAL COMPARISON BETWEEN GIVEN AND CALCULATED          DPRQ 480
C             COEFFICIENT VECTOR IS PERFORMED ONLY IF ALL ROOTS HAVE BEEN DPRQ 490
C             CALCULATED.                                                DPRQ 500
C             THE MAXIMAL RELATIVE ERROR OF THE COEFFICIENT VECTOR IS    DPRQ 510
C             RECORDED IN Q(IR+1).                                       DPRQ 520
C                                                                        DPRQ 530
C          SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 DPRQ 540
C             NONE                                                       DPRQ 550
C                                                                        DPRQ 560
C          METHOD                                                        DPRQ 570
C             THE ROOTS OF THE POLYNOMIAL ARE CALCULATED BY MEANS OF     DPRQ 580
C             THE QUOTIENT-DIFFERENCE ALGORITHM WITH DISPLACEMENT.       DPRQ 590
C             REFERENCE                                                  DPRQ 600
C             H.RUTISHAUSER, DER QUOTIENTEN-DIFFERENZEN-ALGORITHMUS,     DPRQ 610
C             BIRKHAEUSER, BASEL/STUTTGART, 1957.                        DPRQ 620
C                                                                        DPRQ 630
C     ------------------------------------------------------------------ DPRQ 640
C                                                                        DPRQ 650
      SUBROUTINE DPRQD(C,IC,Q,E,POL,IR,IER)                              DPRQ 660
C                                                                        DPRQ 670
C      DIMENSIONED DUMMY VARIABLES                                       DPRQ 680
      DIMENSION E(1),Q(1),C(1),POL(1)                                   DPRQ 690
      DOUBLE PRECISION Q,E,O,P,T,EXPT,ESAV,U,V,W,C,POL,EPS              DPRQ 700
C                                                                       DPRQ 710
C        NORMALIZATION OF GIVEN POLYNOMIAL                              DPRQ 720
C           TEST OF DIMENSION                                           DPRQ 730
C        IR CONTAINS INDEX OF HIGHEST COEFFICIENT                       DPRQ 740
      IR=IC                                                             DPRQ 750
      IER=0                                                             DPRQ 760
      EPS=1.D-16                                                        DPRQ 770
      TOL=1.E-6                                                         DPRQ 780
      LIMIT=10*IC                                                       DPRQ 790
      KOUNT=0                                                           DPRQ 800
    1 IF(IR-1)79,79,2                                                   DPRQ 810
C                                                                       DPRQ 820
C        DROP TRAILING ZERO COEFFICIENTS                                DPRQ 830
    2 IF(C(IR))4,3,4                                                    DPRQ 840
    3 IR=IR-1                                                           DPRQ 850
      GOTO 1                                                            DPRQ 860
C                                                                       DPRQ 870
C           REARRANGEMENT OF GIVEN POLYNOMIAL                           DPRQ 880
C        EXTRACTION OF ZERO ROOTS                                       DPRQ 890
    4 O=1.0D0/C(IR)                                                     DPRQ 900
      IEND=IR-1                                                         DPRQ 910
      ISTA=1                                                            DPRQ 920
      NSAV=IR+1                                                         DPRQ 930
      JBEG=1                                                            DPRQ 940
C                                                                       DPRQ 950
C        Q(J)=1.                                                        DPRQ 960
C        Q(J+I)=C(IR-I)/C(IR)                                           DPRQ 970
C        Q(IR)=C(J)/C(IR)                                               DPRQ 980
C        WHERE J IS THE INDEX OF THE LOWEST NONZERO COEFFICIENT         DPRQ 990
      DO 9 I=1,IR                                                       DPRQ1000
      J=NSAV-I                                                          DPRQ1010
      IF(C(I))7,5,7                                                     DPRQ1020
    5 GOTO(6,8),JBEG                                                    DPRQ1030
    6 NSAV=NSAV+1                                                       DPRQ1040
      Q(ISTA)=0.D0                                                      DPRQ1050
      E(ISTA)=0.D0                                                      DPRQ1060
      ISTA=ISTA+1                                                       DPRQ1070
      GOTO 9                                                            DPRQ1080
    7 JBEG=2                                                            DPRQ1090
    8 Q(J)=C(I)*O                                                       DPRQ1100
      C(I)=Q(J)                                                         DPRQ1110
    9 CONTINUE                                                          DPRQ1120
C                                                                       DPRQ1130
C           INITIALIZATION                                              DPRQ1140
      ESAV=0.D0                                                         DPRQ1150
      Q(ISTA)=0.D0                                                      DPRQ1160
   10 NSAV=IR                                                           DPRQ1170
C                                                                       DPRQ1180
C        COMPUTATION OF DERIVATIVE                                      DPRQ1190
      EXPT=IR-ISTA                                                      DPRQ1200
      E(ISTA)=EXPT                                                      DPRQ1210
      DO 11 I=ISTA,IEND                                                 DPRQ1220
      EXPT=EXPT-1.0D0                                                   DPRQ1230
      POL(I+1)=EPS*DABS(Q(I+1))+EPS                                     DPRQ1240
   11 E(I+1)=Q(I+1)*EXPT                                                DPRQ1250
C                                                                       DPRQ1260
C        TEST OF REMAINING DIMENSION                                    DPRQ1270
      IF(ISTA-IEND)12,20,60                                             DPRQ1280
   12 JEND=IEND-1                                                       DPRQ1290
C                                                                       DPRQ1300
C        COMPUTATION OF S-FRACTION                                      DPRQ1310
      DO 19 I=ISTA,JEND                                                 DPRQ1320
      IF(I-ISTA)13,16,13                                                DPRQ1330
   13 IF(DABS(E(I))-POL(I+1))14,14,16                                   DPRQ1340
C                                                                       DPRQ1350
C        THE GIVEN POLYNOMIAL HAS MULTIPLE ROOTS, THE COEFFICIENTS OF   DPRQ1360
C        THE COMMON FACTOR ARE STORED FROM Q(NSAV) UP TO Q(IR)          DPRQ1370
   14 NSAV=I                                                            DPRQ1380
      DO 15 K=I,JEND                                                    DPRQ1390
      IF(DABS(E(K))-POL(K+1))15,15,80                                   DPRQ1400
   15 CONTINUE                                                          DPRQ1410
      GOTO 21                                                           DPRQ1420
C                                                                       DPRQ1430
C           EUCLIDEAN ALGORITHM                                         DPRQ1440
   16 DO 19 K=I,IEND                                                    DPRQ1450
      E(K+1)=E(K+1)/E(I)                                                DPRQ1460
      Q(K+1)=E(K+1)-Q(K+1)                                              DPRQ1470
      IF(K-I)18,17,18                                                   DPRQ1480
C                                                                       DPRQ1490
C        TEST FOR SMALL DIVISOR                                         DPRQ1500
   17 IF(DABS(Q(I+1))-POL(I+1))80,80,19                                 DPRQ1510
   18 Q(K+1)=Q(K+1)/Q(I+1)                                              DPRQ1520
      POL(K+1)=POL(K+1)/DABS(Q(I+1))                                    DPRQ1530
      E(K)=Q(K+1)-E(K)                                                  DPRQ1540
   19 CONTINUE                                                          DPRQ1550
   20 Q(IR)=-Q(IR)                                                      DPRQ1560
C                                                                       DPRQ1570
C           THE DISPLACEMENT EXPT IS SET TO 0 AUTOMATICALLY.            DPRQ1580
C           E(ISTA)=0.,Q(ISTA+1),...,E(NSAV-1),Q(NSAV),E(NSAV)=0.,      DPRQ1590
C           FORM A DIAGONAL OF THE QD-ARRAY.                            DPRQ1600
C        INITIALIZATION OF BOUNDARY VALUES                              DPRQ1610
   21 E(ISTA)=0.D0                                                      DPRQ1620
      NRAN=NSAV-1                                                       DPRQ1630
   22 E(NRAN+1)=0.D0                                                    DPRQ1640
C                                                                       DPRQ1650
C           TEST FOR LINEAR OR CONSTANT FACTOR                          DPRQ1660
C        NRAN-ISTA IS DEGREE-1                                          DPRQ1670
      IF(NRAN-ISTA)24,23,31                                             DPRQ1680
C                                                                       DPRQ1690
C        LINEAR FACTOR                                                  DPRQ1700
   23 Q(ISTA+1)=Q(ISTA+1)+EXPT                                          DPRQ1710
      E(ISTA+1)=0.D0                                                    DPRQ1720
C                                                                       DPRQ1730
C        TEST FOR UNFACTORED COMMON DIVISOR                             DPRQ1740
   24 E(ISTA)=ESAV                                                      DPRQ1750
      IF(IR-NSAV)60,60,25                                               DPRQ1760
C                                                                       DPRQ1770
C        INITIALIZE QD-ALGORITHM FOR COMMON DIVISOR                     DPRQ1780
   25 ISTA=NSAV                                                         DPRQ1790
      ESAV=E(ISTA)                                                      DPRQ1800
      GOTO 10                                                           DPRQ1810
C                                                                       DPRQ1820
C        COMPUTATION OF ROOT PAIR                                       DPRQ1830
   26 P=P+EXPT                                                          DPRQ1840
C                                                                       DPRQ1850
C        TEST FOR REALITY                                               DPRQ1860
      IF(O)27,28,28                                                     DPRQ1870
C                                                                       DPRQ1880
C        COMPLEX ROOT PAIR                                              DPRQ1890
   27 Q(NRAN)=P                                                         DPRQ1900
      Q(NRAN+1)=P                                                       DPRQ1910
      E(NRAN)=T                                                         DPRQ1920
      E(NRAN+1)=-T                                                      DPRQ1930
      GOTO 29                                                           DPRQ1940
C                                                                       DPRQ1950
C        REAL ROOT PAIR                                                 DPRQ1960
   28 Q(NRAN)=P-T                                                       DPRQ1970
      Q(NRAN+1)=P+T                                                     DPRQ1980
      E(NRAN)=0.D0                                                      DPRQ1990
C                                                                       DPRQ2000
C           REDUCTION OF DEGREE BY 2 (DEFLATION)                        DPRQ2010
   29 NRAN=NRAN-2                                                       DPRQ2020
      GOTO 22                                                           DPRQ2030
C                                                                       DPRQ2040
C        COMPUTATION OF REAL ROOT                                       DPRQ2050
   30 Q(NRAN+1)=EXPT+P                                                  DPRQ2060
C                                                                       DPRQ2070
C           REDUCTION OF DEGREE BY 1 (DEFLATION)                        DPRQ2080
      NRAN=NRAN-1                                                       DPRQ2090
      GOTO 22                                                           DPRQ2100
C                                                                       DPRQ2110
C        START QD-ITERATION                                             DPRQ2120
   31 JBEG=ISTA+1                                                       DPRQ2130
      JEND=NRAN-1                                                       DPRQ2140
      TEPS=EPS                                                          DPRQ2150
      TOELT=1.E-2                                                       DPRQ2160
   32 KOUNT=KOUNT+1                                                     DPRQ2170
      P=Q(NRAN+1)                                                       DPRQ2180
      R=ABS(SNGL(E(NRAN)))                                              DPRQ2190
C                                                                       DPRQ2200
C           TEST FOR CONVERGENCE                                        DPRQ2210
      IF(R-TEPS)30,30,33                                                DPRQ2220
   33 S=ABS(SNGL(E(JEND)))                                              DPRQ2230
C                                                                       DPRQ2240
C        IS THERE A REAL ROOT NEXT                                      DPRQ2250
      IF(S-R)38,38,34                                                   DPRQ2260
C                                                                       DPRQ2270
C        IS DISPLACEMENT SMALL ENOUGH                                   DPRQ2280
   34 IF(R-TOELT)36,35,35                                               DPRQ2290
   35 P=0.D0                                                            DPRQ2300
   36 O=P                                                               DPRQ2310
      DO 37 J=JBEG,NRAN                                                 DPRQ2320
      Q(J)=Q(J)+E(J)-E(J-1)-O                                           DPRQ2330
C                                                                       DPRQ2340
C           TEST FOR SMALL DIVISOR                                      DPRQ2350
      IF(DABS(Q(J))-POL(J))81,81,37                                     DPRQ2360
   37 E(J)=Q(J+1)*E(J)/Q(J)                                             DPRQ2370
      Q(NRAN+1)=-E(NRAN)+Q(NRAN+1)-O                                    DPRQ2380
      GOTO 54                                                           DPRQ2390
C                                                                       DPRQ2400
C        CALCULATE DISPLACEMENT FOR DOUBLE ROOTS                        DPRQ2410
C           QUADRATIC EQUATION FOR DOUBLE ROOTS                         DPRQ2420
C           X**2-(Q(NRAN)+Q(NRAN+1)+E(NRAN))*X+Q(NRAN)*Q(NRAN+1)=0      DPRQ2430
   38 P=0.500*(Q(NRAN)+E(NRAN)+Q(NRAN+1))                               DPRQ2440
      O=P*P-Q(NRAN)*Q(NRAN+1)                                           DPRQ2450
      T=DSQRT(DABS(O))                                                  DPRQ2460
C                                                                       DPRQ2470
C        TEST FOR CONVERGENCE                                           DPRQ2480
      IF(S-TEPS)26,26,39                                                DPRQ2490
C                                                                       DPRQ2500
C        ARE THERE COMPLEX ROOTS                                        DPRQ2510
   39 IF(O)43,40,40                                                     DPRQ2520
   40 IF(P)42,41,41                                                     DPRQ2530
   41 T=-T                                                              DPRQ2540
   42 P=P+T                                                             DPRQ2550
      R=S                                                               DPRQ2560
      GOTO 34                                                           DPRQ2570
C                                                                       DPRQ2580
C        MODIFICATION FOR COMPLEX ROOTS                                 DPRQ2590
C        IS DISPLACEMENT SMALL ENOUGH                                   DPRQ2600
   43 IF(S-TOELT)44,35,35                                               DPRQ2610
C                                                                       DPRQ2620
C           INITIALIZATION                                              DPRQ2630
   44 O=Q(JBEG)+E(JBEG)-P                                               DPRQ2640
C                                                                       DPRQ2650
C           TEST FOR SMALL DIVISOR                                      DPRQ2660
      IF(DABS(O)-POL(JBEG))81,81,45                                     DPRQ2670
   45 T=(T/O)**2                                                        DPRQ2680
      U=E(JBEG)*Q(JBEG+1)/(O*(1.000+T))                                 DPRQ2690
      V=O+U                                                             DPRQ2700
C                                                                       DPRQ2710
C        THREEFOLD LOOP FOR COMPLEX DISPLACEMENT                        DPRQ2720
      KOUNT=KOUNT+2                                                     DPRQ2730
      DO 53 J=JBEG,NRAN                                                 DPRQ2740
      O=Q(J+1)+E(J+1)-U-P                                               DPRQ2750
C                                                                       DPRQ2760
C           TEST FOR SMALL DIVISOR                                      DPRQ2770
      IF(DABS(V)-POL(J))46,46,49                                        DPRQ2780
   46 IF(J-NRAN)81,47,81                                                DPRQ2790
   47 EXPT=EXPT+P                                                       DPRQ2800
      IF(ABS(SNGL(E(JEND)))-TOL)48,48,81                                DPRQ2810
   48 P=0.500*(V+O-E(JEND))                                             DPRQ2820
      O=P*P-(V-U)*(O-U*T-O*W*(1.DO+T)/Q(JEND))                          DPRQ2830
      T=DSQRT(DABS(O))                                                  DPRQ2840
      GOTO 26                                                           DPRQ2850
```

```
C
C            TEST FOR SMALL DIVISOR
   49 IF(DABS(D)-POL(J+1))46,46,50
   50 W=U*D/V
      T=T*(V/D)**2
      Q(J)=V+W-E(J-1)
      U=0.D0
      IF(J-NRAN)51,52,52
   51 U=Q(J+2)*E(J+1)/(D*(1.D0+T))
   52 V=D+U-W
C
C            TEST FOR SMALL DIVISOR
      IF(DABS(Q(J))-POL(J))81,81,53
   53 E(J)=W*V*(1.D0+T)/Q(J)
      Q(NRAN+1)=V-E(NRAN)
   54 EXPT=EXPT+P
      TEPS=TEPS*1.1
      TDELT=TDELT*1.1
      IF(KOUNT-LIMIT)32,55,55
C
C        NO CONVERGENCE WITH FEASIBLE TOLERANCE
C           ERROR RETURN IN CASE OF UNSATISFACTORY CONVERGENCE
   55 IER=1
C
C           REARRANGE CALCULATED ROOTS
   56 IEND=NSAV-NRAN-1
      E(ISTA)=ESAV
      IF(IEND)59,59,57
   57 DO 58 I=1,IEND
      J=ISTA+I
      K=NRAN+1+I
      E(J)=E(K)
   58 Q(J)=Q(K)
   59 IR=ISTA+IEND
C
C           NORMAL RETURN
   60 IR=IR-1
      IF(IR)78,78,61
C
C           REARRANGE CALCULATED ROOTS
   61 DO 62 I=1,IR
      Q(I)=Q(I+1)
   62 E(I)=E(I+1)
C
C           CALCULATE COEFFICIENT VECTOR FROM ROOTS
      POL(IR+1)=1.D0
      IEND=IR-1
      JBEG=1
      DO 69 J=1,IR
      ISTA=IR+1-J
      D=0.D0
      P=Q(ISTA)
      T=E(ISTA)
      IF(T)65,63,65
C
C           MULTIPLY WITH LINEAR FACTOR
   63 DO 64 I=ISTA,IR
      POL(I)=D-P*POL(I+1)
   64 D=POL(I+1)
      GOTO 69
   65 GOTO(66,67),JBEG
   66 JBEG=2
      POL(ISTA)=0.D0
      GOTO 69
C
C           MULTIPLY WITH QUADRATIC FACTOR
   67 JBEG=1
      U=P*P+T*T
      P=P+P
      DO 68 I=ISTA,IEND
      POL(I)=D-P*POL(I+1)+U*POL(I+2)
   68 D=POL(I+1)
      POL(IR)=D-P
   69 CONTINUE
      IF(IER)78,70,78
C
C           COMPARISON OF COEFFICIENT VECTORS, IE. TEST OF ACCURACY
   70 P=0.D0
      DO 75 I=1,IR
      IF(C(I))72,71,72
   71 D=DABS(POL(I))
      GOTO 73
   72 D=DABS((POL(I)-C(I))/C(I))
   73 IF(P-D)74,75,75
   74 P=D
   75 CONTINUE
      IF(SNGL(P)-TOL)77,76,76
   76 IER=-1
   77 Q(IR+1)=P
      E(IR+1)=0.D0
   78 RETURN
C
C           ERROR RETURNS
C              ERROR RETURN FOR POLYNOMIALS OF DEGREE LESS THAN 1
   79 IER=2
      IR=0
      RETURN
C
C              ERROR RETURN IF THERE EXISTS NO S-FRACTION
   80 IER=4
      IR=ISTA
      GOTO 60
C
C              ERROR RETURN IN CASE OF INSTABLE QD-ALGORITHM
   81 IER=3
      GOTO 56
      END
```

DPRQ2860 DPRQ2870 DPRQ2880 DPRQ2890 DPRQ2900 DPRQ2910 DPRQ2920 DPRQ2930 DPRQ2940 DPRQ2950 DPRQ2960 DPRQ2970 DPRQ2980 DPRQ2990 DPRQ3000 DPRQ3010 DPRQ3020 DPRQ3030 DPRQ3040 DPRQ3050 DPRQ3060 DPRQ3070 DPRQ3080 DPRQ3090 DPRQ3100 DPRQ3110 DPRQ3120 DPRQ3130 DPRQ3140 DPRQ3150 DPRQ3160 DPRQ3170 DPRQ3180 DPRQ3190 DPRQ3200 DPRQ3210 DPRQ3220 DPRQ3230 DPRQ3240 DPRQ3250 DPRQ3260 DPRQ3270 DPRQ3280 DPRQ3290 DPRQ3300 DPRQ3310 DPRQ3320 DPRQ3330 DPRQ3340 DPRQ3350 DPRQ3360 DPRQ3370 DPRQ3380 DPRQ3390 DPRQ3400 DPRQ3410 DPRQ3420 DPRQ3430 DPRQ3440 DPRQ3450 DPRQ3460 DPRQ3470 DPRQ3480 DPRQ3490 DPRQ3500 DPRQ3510 DPRQ3520 DPRQ3530 DPRQ3540 DPRQ3550 DPRQ3560 DPRQ3570 DPRQ3580 DPRQ3590 DPRQ3600 DPRQ3610 DPRQ3620 DPRQ3630 DPRQ3640 DPRQ3650 DPRQ3660 DPRQ3670 DPRQ3680 DPRQ3690 DPRQ3700 DPRQ3710 DPRQ3720 DPRQ3730 DPRQ3740 DPRQ3750 DPRQ3760 DPRQ3770 DPRQ3780 DPRQ3790 DPRQ3800 DPRQ3810 DPRQ3820 DPRQ3830 DPRQ3840 DPRQ3850 DPRQ3860 DPRQ3870 DPRQ3880 DPRQ3890 DPRQ3900 DPRQ3910 DPRQ3920

Subroutines PRBM and DPRBM

These subroutines compute the real and complex roots of a real polynomial

$$p(x) = c_1 + c_2 x + \ldots + c_{n+1} x^n$$

using Bairstow's iterative method of quadratic factorization.

1. Mathematical background

Every real polynomial of degree greater than one can be factored in the form $p(x) = q(x)r(x)$ where $q(x) = x^2 + q_2 x + q_1$ is quadratic. If q(x) is reducible, that is, if q(x) is a product of two real linear factors, p(x) has a pair of real roots; and if q(x) is irreducible, p(x) has a complex conjugate pair of roots. If r(x) has degree exceeding one, it too may be factored as above, and so on. The quadratic factors of p(x) are determined by subroutines PQFB and DPQFB. See those routines for a detailed description of Bairstow's method.

2. Programming considerations

The subroutines need only the coefficient vector $C = (c_1, \ldots, c_{IC})$ and the number of coefficients IC = n+1 as input. They give as output an error parameter IER, the number of computed roots IR, the real and complex parts of the computed roots in vectors RR and RC, and -- if all the roots have been computed -- the coefficients of the polynomial with the computed roots stored in the vector POL.

If p(x) is a constant, that is, if $c_2 = c_3 = \ldots = 0$, we set IR = 0, IER = 2, and return to the call program.

Otherwise, let $IR = \max \left\{ j \mid c_j \neq 0 \right\}$. Then we may write:

$$p(x) = c_{IR}\, \bar{p}(x)\, \bar{\bar{p}}(x)$$

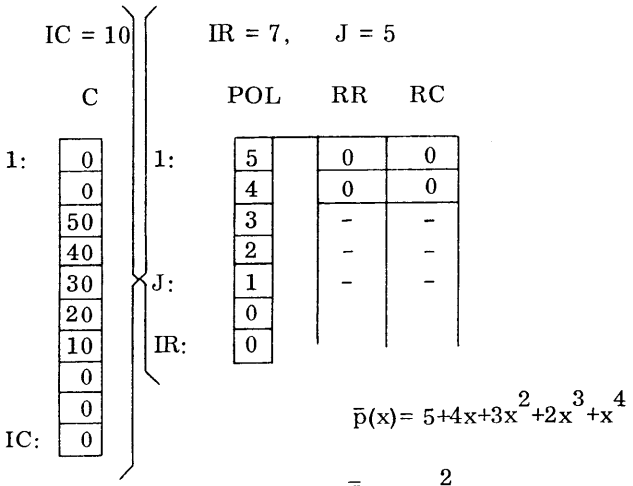
$$\bar{p}(x) = p_1 + p_2 x + \ldots + p_J x^{J-1}$$

$$\bar{\bar{p}}(x) = x^K$$

where $K \geq 0$, $J = IR - K$, and $p_j = c_{K+j}/c_{IR}$, $j = 1, 2, \ldots, J$, and $p_1 \neq 0$. The coefficients of $\bar{p}$ are stored in POL(1) up to POL(J) and POL(J+1) up to POL(IR) are initialized to zero. If an exponential overflow occurs during the calculation of the p_i we again set IR = 0, IER = 2 and return control to the calling program.

The following example illustrates the procedure so far:

$$p(x) = 0+0\cdot x+50\cdot x^2 + 40\cdot x^3 + 30\cdot x^4 + 20\cdot x^5 + 10\cdot x^6 + 0\cdot x^7 + 0\cdot x^8 + 0\cdot x^9$$



$$\bar{p}(x) = 5+4x+3x^2+2x^3+x^4$$

$$\bar{\bar{p}}(x) = x^2$$

3. The Bairstow iteration

Upon entering the main part of the routine we assume

$$p(x) = c_{IR}\,\bar{p}(x)\,\bar{\bar{p}}(x)$$

where

$$\bar{p}(x) = p_1 + p_2x + \ldots + p_jx^{j-1} \qquad (p_j = 1)$$

is the polynomial with the unknown roots, and

$$\bar{\bar{p}}(x) = p_{j+1} + p_{j+2}x + \ldots + p_{IR}x^{IR-j-1} + x^{IR-j}$$

is the polynomial generated from the computed roots. The coefficients $p_1, p_2, \ldots, p_{IR}$ are stored in POL(1), POL (2), . . ., POL(IR). Now there are three possibilities:

(1) j = 1. All the roots have been computed. IR is decreased by 1 in order to record the number of computed roots and control is passed on to the last phase of the subroutine (the appendix).

(2) j = 2. The last root is $x = -p_1$. This is recorded by setting $RR(IR - 1) = -p_1$ and $RC(IR - 1) = 0$. The polynomial $\bar{p}(x)$ is multiplied by the linear factor $x + p_1$, occupying after multiplication the locations POL(2) up to POL(IR). IR is decreased by 1, thus recording the number of computed roots, and control is passed on to the appendix.

(3) $j \geq 3$. In this case the polynomial $\bar{p}(x)$ is factored by means of subroutine PQFB or DPQFB, where the quadratic factor $q_1 + q_2x + x^2$ of the previous step is used as the initial guess (in the first factorization x^2 is used). If factorization is not successful, it is restarted with the initial guesses $-q_1+q_2x+x^2$, $-q_1-q_2x+x^2$ and $q_1-q_2x+x^2$. If none of these trials leads to a successful factorization, q_1 and q_2 are increased by 1 (at most nine times). If after a maximum of 40 trials factorization is still unsuccessful, IR is decreased by J, thus recording the number of computed roots, and the rest of the subroutine is bypassed giving the error message IER = 3.

If any one of these trials is successful, $\bar{p}(x)$ is divided by the determined quadratic factor, occupying after division the locations POL(1) up to POL (J-2). Then the polynomial $\bar{\bar{p}}(x)$ is multiplied by the same quadratic factor and occupies after multiplication the locations POL(J-1) up to POL(IR). At least the quadratic equation is solved, and the real and complex parts of the two roots are stored in the corresponding locations of RR and RC. After decreasing j by 2, the main part of the subroutine is reentered.

Assuming that all the roots of the polynomial have been computed, the coefficients of the polynomial $\bar{\bar{p}}(x)$ are shifted into the locations POL(1) up to POL(IR), and POL(IR+1) is set to 1 (IR is the number of computed roots).

Furthermore, the absolutely greatest error of the coefficients of the resulting polynomial is generated using the formula

$$a = \max_i |\,\delta_i\,|$$

where $\delta_i = \begin{cases} (p_i - c_i)/c_i & \text{if } c_i \neq 0 \\ p_i & \text{if } c_i = 0 \end{cases}$ $\quad i = 1, \ldots, IR$

The number a is stored in RR(IR+1) giving the user some indication of the accuracy reached by the subroutines. The warning IER = -1 is given if $a > \epsilon$ ($\epsilon = 10^{-3}$ in single precision and $\epsilon = 10^{-6}$ in double precision). The warning IER = -1 is overridden by the warning IER = 1, which is given if any quadratic factorization fails to converge. (See PQFB.)

For reference see J. H. Wilkinson, "The Evaluation of the Zeros of Ill-Conditioned Polynomials (Parts 1 and 2)", Numerische Mathematik, vol. 1 (1959), pp 150-180.

```
C                                                                       PRBM  10
C     ..................................................................PRBM  20
C                                                                       PRBM  30
C        SUBROUTINE PRBM                                                PRBM  40
C                                                                       PRBM  50
C        PURPOSE                                                        PRBM  60
C           TO CALCULATE ALL REAL AND COMPLEX ROOTS OF A GIVEN          PRBM  70
C           POLYNOMIAL WITH REAL COEFFICIENTS.                          PRBM  80
C                                                                       PRBM  90
C        USAGE                                                          PRBM 100
C           CALL PRBM (C,IC,RR,RC,POL,IR,IER)                           PRBM 110
C                                                                       PRBM 120
C        DESCRIPTION OF PARAMETERS                                      PRBM 130
C           C      - INPUT VECTOR CONTAINING THE COEFFICIENTS OF THE    PRBM 140
C                    GIVEN POLYNOMIAL. COEFFICIENTS ARE ORDERED FROM    PRBM 150
C                    LOW TO HIGH. ON RETURN COEFFICIENTS ARE DIVIDED    PRBM 160
C                    BY THE LAST NONZERO TERM.                          PRBM 170
C           IC     - DIMENSION OF VECTORS C, RR, RC, AND POL.           PRBM 180
C           RR     - RESULTANT VECTOR OF REAL PARTS OF THE ROOTS.       PRBM 190
C           RC     - RESULTANT VECTOR OF COMPLEX PARTS OF THE ROOTS.    PRBM 200
C           POL    - RESULTANT VECTOR OF COEFFICIENTS OF THE POLYNOMIAL PRBM 210
C                    WITH CALCULATED ROOTS. COEFFICIENTS ARE ORDERED    PRBM 220
C                    FROM LOW TO HIGH (SEE REMARK 4).                   PRBM 230
C           IR     - OUTPUT VALUE SPECIFYING THE NUMBER OF CALCULATED   PRBM 240
C                    ROOTS. NORMALLY IR IS EQUAL TO IC-1.               PRBM 250
C           IER    - RESULTANT ERROR PARAMETER CODED AS FOLLOWS         PRBM 260
C                      IER=0  - NO ERROR,                               PRBM 270
C                      IER=1  - SUBROUTINE PQFB RECORDS POOR CONVERGENCE PRBM 280
C                               AT SOME QUADRATIC FACTORIZATION WITHIN   PRBM 290
C                               50 ITERATION STEPS,                      PRBM 300
C                      IER=2  - POLYNOMIAL IS DEGENERATE, I.E. ZERO OR  PRBM 310
C                               CONSTANT,                                PRBM 320
C                               OR OVERFLOW IN NORMALIZATION OF GIVEN    PRBM 330
C                               POLYNOMIAL,                              PRBM 340
C                      IER=3  - THE SUBROUTINE IS BYPASSED DUE TO       PRBM 350
C                               SUCCESSIVE ZERO DIVISORS OR OVERFLOWS    PRBM 360
C                               IN QUADRATIC FACTORIZATION OR DUE TO     PRBM 370
C                               COMPLETELY UNSATISFACTORY ACCURACY,      PRBM 380
C                      IER=-1 - CALCULATED COEFFICIENT VECTOR HAS LESS   PRBM 390
C                               THAN THREE CORRECT SIGNIFICANT DIGITS.   PRBM 400
C                               THIS REVEALS POOR ACCURACY OF CALCULATED PRBM 410
C                               ROOTS.                                   PRBM 420
C                                                                        PRBM 430
C        REMARKS                                                         PRBM 440
C           (1) REAL PARTS OF THE ROOTS ARE STORED IN RR(1) UP TO RR(IR) PRBM 450
C               AND CORRESPONDING COMPLEX PARTS IN RC(1) UP TO RC(IR).   PRBM 460
C           (2) ERROR MESSAGE IER=1 INDICATES POOR CONVERGENCE WITHIN    PRBM 470
C               50 ITERATION STEPS AT SOME QUADRATIC FACTORIZATION       PRBM 480
C               PERFORMED BY SUBROUTINE PQFB.                            PRBM 490
C           (3) NO ACTION BESIDES ERROR MESSAGE IER=2 IN CASE OF A ZERO  PRBM 500
C               OR CONSTANT POLYNOMIAL. THE SAME ERROR MESSAGE IS GIVEN  PRBM 510
C               IN CASE OF AN OVERFLOW IN NORMALIZATION OF GIVEN         PRBM 520
C               POLYNOMIAL.                                              PRBM 530
C           (4) ERROR MESSAGE IER=3 INDICATES SUCCESSIVE ZERO DIVISORS   PRBM 540
C               OR OVERFLOWS OR COMPLETELY UNSATISFACTORY ACCURACY AT    PRBM 550
C               ANY QUADRATIC FACTORIZATION PERFORMED BY                 PRBM 560
C               SUBROUTINE PQFB. IN THIS CASE CALCULATION IS BYPASSED.   PRBM 570
C               IR RECORDS THE NUMBER OF CALCULATED ROOTS.               PRBM 580
C               POL(1),...,POL(J-IR) ARE THE COEFFICIENTS OF THE         PRBM 590
C               REMAINING POLYNOMIAL, WHERE J IS THE ACTUAL NUMBER OF    PRBM 600
C               COEFFICIENTS IN VECTOR C (NORMALLY J=IC).                PRBM 610
C           (5) IF CALCULATED COEFFICIENT VECTOR HAS LESS THAN THREE     PRBM 620
C               CORRECT SIGNIFICANT DIGITS THOUGH ALL QUADRATIC          PRBM 630
C               FACTORIZATIONS SHOWED SATISFACTORY ACCURACY, THE ERROR   PRBM 640
C               MESSAGE IER=-1 IS GIVEN.                                 PRBM 650
C           (6) THE FINAL COMPARISON BETWEEN GIVEN AND CALCULATED        PRBM 660
C               COEFFICIENT VECTOR IS PERFORMED ONLY IF ALL ROOTS HAVE   PRBM 670
C               BEEN CALCULATED. IN THIS CASE THE NUMBER OF ROOTS IR IS  PRBM 680
C               EQUAL TO THE ACTUAL DEGREE OF THE POLYNOMIAL (NORMALLY   PRBM 690
C               IR=IC-1). THE MAXIMAL RELATIVE ERROR OF THE COEFFICIENT  PRBM 700
C               VECTOR IS RECORDED IN RR(IR+1).                          PRBM 710
C                                                                        PRBM 720
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   PRBM 730
C           SUBROUTINE PQFB      QUADRATIC FACTORIZATION OF A POLYNOMIAL PRBM 740
C                                BY BAIRSTOW ITERATION.                  PRBM 750
C                                                                        PRBM 760
C        METHOD                                                          PRBM 770
C           THE ROOTS OF THE POLYNOMIAL ARE CALCULATED BY MEANS OF       PRBM 780
C           SUCCESSIVE QUADRATIC FACTORIZATION PERFORMED BY BAIRSTOW     PRBM 790
C           ITERATION. X**2 IS USED AS INITIAL GUESS FOR THE FIRST       PRBM 800
C           QUADRATIC FACTOR, AND FURTHER EACH CALCULATED QUADRATIC      PRBM 810
C           FACTOR IS USED AS INITIAL GUESS FOR THE NEXT ONE. AFTER      PRBM 820
C           COMPUTATION OF ALL ROOTS THE COEFFICIENT VECTOR IS           PRBM 830
C           CALCULATED AND COMPARED WITH THE GIVEN ONE.                  PRBM 840
C           FOR REFERENCE, SEE J. H. WILKINSON, THE EVALUATION OF THE    PRBM 850
C           ZEROS OF ILL-CONDITIONED POLYNOMIALS (PART ONE AND TWO),     PRBM 860
C           NUMERISCHE MATHEMATIK, VOL.1 (1959), PP.150-180.             PRBM 870
C                                                                        PRBM 880
C     ..................................................................PRBM 890
C                                                                        PRBM 900
      SUBROUTINE PRBM(C,IC,RR,RC,POL,IR,IER)                             PRBM 910
C                                                                        PRBM 920
C                                                                        PRBM 930
      DIMENSION C(1),RR(1),RC(1),POL(1),Q(4)                             PRBM 940
C                                                                        PRBM 950
C        TEST ON LEADING ZERO COEFFICIENTS                               PRBM 960
      EPS=1.E-3                                                          PRBM 970
      LIM=50                                                             PRBM 980
      IR=IC+1                                                            PRBM 990
    1 IR=IR-1                                                            PRBM1000
      IF(IR-1)42,42,2                                                    PRBM1010
    2 IF(C(IR))3,1,3                                                     PRBM1020
C                                                                        PRBM1030
C        WORK UP ZERO ROOTS AND NORMALIZE REMAINING POLYNOMIAL           PRBM1040
    3 IER=0                                                              PRBM1050
      J=IR                                                               PRBM1060
      L=0                                                                PRBM1070
      A=C(IR)                                                            PRBM1080
      DO 8 I=1,IR                                                        PRBM1090
      IF(L)4,4,7                                                         PRBM1100
    4 IF(C(I))6,5,6                                                      PRBM1110
    5 RR(I)=0.                                                           PRBM1120
      RC(I)=0.                                                           PRBM1130
      POL(J)=0.                                                          PRBM1140
      J=J-1                                                              PRBM1150
      GO TO 8                                                            PRBM1160
    6 L=1                                                                PRBM1170
      IST=I                                                              PRBM1180
      J=0                                                                PRBM1190
    7 J=J+1                                                              PRBM1200
      C(I)=C(I)/A                                                        PRBM1210
      POL(J)=C(I)                                                        PRBM1220
      CALL OVERFL(N)                                                     PRBM1230
      IF(N-2)42,8,8                                                      PRBM1240
    8 CONTINUE                                                           PRBM1250
C                                                                        PRBM1260
C        START BAIRSTOW ITERATION                                        PRBM1270
      Q1=0.                                                              PRBM1280
      Q2=0.                                                              PRBM1290
    9 IF(J-2)33,10,14                                                    PRBM1300
C                                                                        PRBM1310
C        DEGREE OF RESTPOLYNOMIAL IS EQUAL TO ONE                        PRBM1320
   10 A=POL(1)                                                           PRBM1330
      RR(IST)=-A                                                         PRBM1340
      RC(IST)=0.                                                         PRBM1350
      IR=IR-1                                                            PRBM1360
      Q2=0.                                                              PRBM1370
      IF(IR-1)13,13,11                                                   PRBM1380
   11 DO 12 I=2,IR                                                       PRBM1390
      Q1=Q2                                                              PRBM1400
      Q2=POL(I+1)                                                        PRBM1410
   12 POL(I)=A*Q2+Q1                                                     PRBM1420
   13 POL(IR+1)=A*Q2                                                     PRBM1430
      GO TO 34                                                           PRBM1440
C        THIS IS BRANCH TO COMPARISON OF COEFFICIENT VECTORS C AND POL   PRBM1450
C                                                                        PRBM1460
C        DEGREE OF RESTPOLYNOMIAL IS GREATER THAN ONE                    PRBM1470
   14 DO 22 L=1,10                                                       PRBM1480
      N=1                                                                PRBM1490
   15 Q(1)=Q1                                                            PRBM1500
      Q(2)=Q2                                                            PRBM1510
      CALL PQFB(POL,J,Q,EPS,LIM,I)                                       PRBM1520
      IF(I)16,24,23                                                      PRBM1530
   16 IF(Q1)18,17,18                                                     PRBM1540
   17 IF(Q2)18,21,18                                                     PRBM1550
   18 GO TO (19,20,19,21),N                                              PRBM1560
   19 Q1=-Q1                                                             PRBM1570
      N=N+1                                                              PRBM1580
      GO TO 15                                                           PRBM1590
   20 Q2=-Q2                                                             PRBM1600
      N=N+1                                                              PRBM1610
      GO TO 15                                                           PRBM1620
   21 Q1=1.+Q1                                                           PRBM1630
   22 Q2=1.-Q2                                                           PRBM1640
C                                                                        PRBM1650
C        ERROR EXIT DUE TO UNSATISFACTORY RESULTS OF FACTORIZATION       PRBM1660
      IER=3                                                              PRBM1670
      IR=IR-J                                                            PRBM1680
      RETURN                                                             PRBM1690
C                                                                        PRBM1700
C        WORK UP RESULTS OF QUADRATIC FACTORIZATION                      PRBM1710
   23 IER=1                                                              PRBM1720
   24 Q1=Q(1)                                                            PRBM1730
      Q2=Q(2)                                                            PRBM1740
C                                                                        PRBM1750
C        PERFORM DIVISION OF FACTORIZED POLYNOMIAL BY QUADRATIC FACTOR   PRBM1760
      B=0.                                                               PRBM1770
      A=0.                                                               PRBM1780
      I=J                                                                PRBM1790
   25 H=-Q1*B-Q2*A+POL(I)                                                PRBM1800
      POL(I)=B                                                           PRBM1810
      B=A                                                                PRBM1820
      A=H                                                                PRBM1830
      I=I-1                                                              PRBM1840
      IF(I-2)26,25,25                                                    PRBM1850
   26 POL(2)=B                                                           PRBM1860
      POL(1)=A                                                           PRBM1870
C                                                                        PRBM1880
C        MULTIPLY POLYNOMIAL WITH CALCULATED ROOTS BY QUADRATIC FACTOR   PRBM1890
      L=IR-1                                                             PRBM1900
      IF(J-L)27,27,29                                                    PRBM1910
   27 DO 28 I=J,L                                                        PRBM1920
   28 POL(I-1)=POL(I-1)+POL(I)*Q2+POL(I+1)*Q1                            PRBM1930
   29 POL(L)=POL(L)+POL(L+1)*Q2+Q1                                       PRBM1940
      POL(IR)=POL(IR)+Q2                                                 PRBM1950
C                                                                        PRBM1960
C        CALCULATE ROOT-PAIR FROM QUADRATIC FACTOR X*X+Q2*X+Q1           PRBM1970
      H=-.5*Q2                                                           PRBM1980
      A=H*H-Q1                                                           PRBM1990
      B=SQRT(ABS(A))                                                     PRBM2000
      IF(A)30,30,31                                                      PRBM2010
   30 RR(IST)=H                                                          PRBM2020
      RC(IST)=B                                                          PRBM2030
      IST=IST+1                                                          PRBM2040
      RR(IST)=H                                                          PRBM2050
      RC(IST)=-B                                                         PRBM2060
      GO TO 32                                                           PRBM2070
   31 B=H+SIGN(B,H)                                                      PRBM2080
      RR(IST)=Q1/B                                                       PRBM2090
      RC(IST)=0.                                                         PRBM2100
      IST=IST+1                                                          PRBM2110
      RR(IST)=B                                                          PRBM2120
      RC(IST)=0.                                                         PRBM2130
   32 IST=IST+1                                                          PRBM2140
      J=J-2                                                              PRBM2150
      GO TO 9                                                            PRBM2160
C                                                                        PRBM2170
C        SHIFT BACK ELEMENTS OF POL BY 1 AND COMPARE VECTORS POL AND C   PRBM2180
   33 IR=IR-1                                                            PRBM2190
   34 A=0.                                                               PRBM2200
      DO 38 I=1,IR                                                       PRBM2210
      Q1=C(I)                                                            PRBM2220
      Q2=POL(I+1)                                                        PRBM2230
      POL(I)=Q2                                                          PRBM2240
      IF(Q1)35,36,35                                                     PRBM2250
   35 Q2=(Q1-Q2)/Q1                                                      PRBM2260
   36 Q2=ABS(Q2)                                                         PRBM2270
      IF(Q2-A)38,38,37                                                   PRBM2280
   37 A=Q2                                                               PRBM2290
   38 CONTINUE                                                           PRBM2300
      I=IR+1                                                             PRBM2310
      POL(I)=1.                                                          PRBM2320
      RR(I)=A                                                            PRBM2330
      RC(I)=0.                                                           PRBM2340
      IF(IER)39,39,41                                                    PRBM2350
   39 IF(A-EPS)41,41,40                                                  PRBM2360
C                                                                        PRBM2370
C        WARNING DUE TO POOR ACCURACY OF CALCULATED COEFFICIENT VECTOR   PRBM2380
   40 IER=-1                                                             PRBM2390
   41 RETURN                                                             PRBM2400
C                                                                        PRBM2410
C        ERROR EXIT DUE TO DEGENERATE POLYNOMIAL OR OVERFLOW IN          PRBM2420
C        NORMALIZATION                                                   PRBM2430
   42 IER=2                                                              PRBM2440
      IR=0                                                               PRBM2450
      RETURN                                                             PRBM2460
      END                                                                PRBM2470
```

```
C                                                                       DPRB  10
C     ..................................................................DPRB  20
C                                                                       DPRB  30
C        SUBROUTINE DPRBM                                               DPRB  40
C                                                                       DPRB  50
C        PURPOSE                                                        DPRB  60
C           TO CALCULATE ALL REAL AND COMPLEX ROOTS OF A GIVEN          DPRB  70
C           POLYNOMIAL WITH REAL COEFFICIENTS.                          DPRB  80
C                                                                       DPRB  90
C        USAGE                                                          DPRB 100
C           CALL DPRBM (C,IC,RR,RC,POL,IR,IER)                          DPRB 110
C                                                                       DPRB 120
C        DESCRIPTION OF PARAMETERS                                      DPRB 130
C           C   - DOUBLE PRECISION INPUT VECTOR CONTAINING THE          DPRB 140
C                 COEFFICIENTS OF THE GIVEN POLYNOMIAL. COEFFICIENTS    DPRB 150
C                 ARE ORDERED FROM LOW TO HIGH. ON RETURN COEFFI-       DPRB 160
C                 CIENTS ARE DIVIDED BY THE LAST NONZERO TERM.          DPRB 170
C           IC  - DIMENSION OF VECTORS C, RR, RC, AND POL.              DPRB 180
C           RR  - RESULTANT DOUBLE PRECISION VECTOR OF REAL PARTS       DPRB 190
C                 OF THE ROOTS.                                         DPRB 200
C           RC  - RESULTANT DOUBLE PRECISION VECTOR OF COMPLEX PARTS    DPRB 210
C                 OF THE ROOTS.                                         DPRB 220
C           POL - RESULTANT DOUBLE PRECISION VECTOR OF COEFFICIENTS     DPRB 230
C                 OF THE POLYNOMIAL WITH CALCULATED ROOTS.              DPRB 240
C                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH (SEE        DPRB 250
C                 REMARK 4).                                            DPRB 260
C           IR  - OUTPUT VALUE SPECIFYING THE NUMBER OF CALCULATED      DPRB 270
C                 ROOTS. NORMALLY IR IS EQUAL TO IC-1.                  DPRB 280
C           IER - RESULTANT ERROR PARAMETER CODED AS FOLLOWS            DPRB 290
C                 IER=0  - NO ERROR,                                    DPRB 300
C                 IER=1  - SUBROUTINE DPQFB RECORDS POOR CONVERGENCE    DPRB 310
C                          AT SOME QUADRATIC FACTORIZATION WITHIN       DPRB 320
C                          100 ITERATION STEPS,                         DPRB 330
C                 IER=2  - POLYNOMIAL IS DEGENERATE, I.E. ZERO OR       DPRB 340
C                          CONSTANT,                                    DPRB 350
C                          OR OVERFLOW IN NORMALIZATION OF GIVEN        DPRB 360
C                          POLYNOMIAL,                                  DPRB 370
C                 IER=3  - THE SUBROUTINE IS BYPASSED DUE TO            DPRB 380
C                          SUCCESSIVE ZERO DIVISORS OR OVERFLOWS        DPRB 390
C                          IN QUADRATIC FACTORIZATION OR DUE TO         DPRB 400
C                          COMPLETELY UNSATISFACTORY ACCURACY,          DPRB 410
C                 IER=-1 - CALCULATED COEFFICIENT VECTOR HAS LESS       DPRB 420
C                          THAN SIX CORRECT SIGNIFICANT DIGITS.         DPRB 430
C                          THIS REVEALS POOR ACCURACY OF CALCULATED     DPRB 440
C                          ROOTS.                                       DPRB 450
C                                                                       DPRB 460
C        REMARKS                                                        DPRB 470
C           (1) REAL PARTS OF THE ROOTS ARE STORED IN RR(1) UP TO RR(IR)DPRB 480
C               AND CORRESPONDING COMPLEX PARTS IN RC(1) UP TO RC(IR).  DPRB 490
C           (2) ERROR MESSAGE IER=1 INDICATES POOR CONVERGENCE WITHIN   DPRB 500
C               100 ITERATION STEPS AT SOME QUADRATIC FACTORIZATION     DPRB 510
C               PERFORMED BY SUBROUTINE DPQFB.                          DPRB 520
C           (3) NO ACTION BESIDES ERROR MESSAGE IER=2 IN CASE OF A ZERO DPRB 530
C               OR CONSTANT POLYNOMIAL. THE SAME ERROR MESSAGE IS GIVEN DPRB 540
C               IN CASE OF AN OVERFLOW IN NORMALIZATION OF GIVEN        DPRB 550
C               POLYNOMIAL.                                             DPRB 560
C           (4) ERROR MESSAGE IER=3 INDICATES SUCCESSIVE ZERO DIVISORS  DPRB 570
C               OR OVERFLOWS OR COMPLETELY UNSATISFACTORY ACCURACY AT   DPRB 580
C               ANY QUADRATIC FACTORIZATION PERFORMED BY                DPRB 590
C               SUBROUTINE DPQFB. IN THIS CASE CALCULATION IS BYPASSED. DPRB 600
C               IR RECORDS THE NUMBER OF CALCULATED ROOTS.              DPRB 610
C               POL(1),...,POL(J-IR) ARE THE COEFFICIENTS OF THE        DPRB 620
C               REMAINING POLYNOMIAL, WHERE J IS THE ACTUAL NUMBER OF   DPRB 630
C               COEFFICIENTS IN VECTOR C (NORMALLY J=IC).               DPRB 640
C           (5) IF CALCULATED COEFFICIENT VECTOR HAS LESS THAN SIX      DPRB 650
C               CORRECT SIGNIFICANT DIGITS THOUGH ALL QUADRATIC         DPRB 660
C               FACTORIZATIONS SHOWED SATISFACTORY ACCURACY, THE ERROR  DPRB 670
C               MESSAGE IER=-1 IS GIVEN.                                DPRB 680
C           (6) THE FINAL COMPARISON BETWEEN GIVEN AND CALCULATED       DPRB 690
C               COEFFICIENT VECTOR IS PERFORMED ONLY IF ALL ROOTS HAVE  DPRB 700
C               BEEN CALCULATED. IN THIS CASE THE NUMBER OF ROOTS IR IS DPRB 710
C               EQUAL TO THE ACTUAL DEGREE OF THE POLYNOMIAL (NORMALLY  DPRB 720
C               IR=IC-1). THE MAXIMAL RELATIVE ERROR OF THE COEFFICIENT DPRB 730
C               VECTOR IS RECORDED IN RR(IR+1).                         DPRB 740
C                                                                       DPRB 750
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DPRB 760
C           SUBROUTINE DPQFB    QUADRATIC FACTORIZATION OF A POLYNOMIAL DPRB 770
C                               BY BAIRSTOW ITERATION.                  DPRB 780
C                                                                       DPRB 790
C        METHOD                                                         DPRB 800
C           THE ROOTS OF THE POLYNOMIAL ARE CALCULATED BY MEANS OF      DPRB 810
C           SUCCESSIVE QUADRATIC FACTORIZATION PERFORMED BY BAIRSTOW    DPRB 820
C           ITERATION. X**2 IS USED AS INITIAL GUESS FOR THE FIRST      DPRB 830
C           QUADRATIC FACTOR, AND FURTHER EACH CALCULATED QUADRATIC     DPRB 840
C           FACTOR IS USED AS INITIAL GUESS FOR THE NEXT ONE. AFTER     DPRB 850
C           COMPUTATION OF ALL ROOTS THE COEFFICIENT VECTOR IS          DPRB 860
C           CALCULATED AND COMPARED WITH THE GIVEN ONE.                 DPRB 870
C           FOR REFERENCE, SEE J. H. WILKINSON, THE EVALUATION OF THE   DPRB 880
C           ZEROS OF ILL-CONDITIONED POLYNOMIALS (PART ONE AND TWO),    DPRB 890
C           NUMERISCHE MATHEMATIK, VOL.1 (1959), PP.150-180.            DPRB 900
C                                                                       DPRB 910
C     ..................................................................DPRB 920
C                                                                       DPRB 930
      SUBROUTINE DPRBM(C,IC,RR,RC,POL,IR,IER)                           DPRB 940
C                                                                       DPRB 950
C                                                                       DPRB 960
      DIMENSION C(1),RR(1),RC(1),POL(1),Q(4)                            DPRB 970
      DOUBLE PRECISION C,RR,RC,POL,Q,EPS,A,B,H,Q1,Q2                    DPRB 980
C                                                                       DPRB 990
C        TEST ON LEADING ZERO COEFFICIENTS                              DPRB1000
      EPS=1.D-6                                                         DPRB1010
      LIM=100                                                           DPRB1020
      IR=IC+1                                                           DPRB1030
    1 IR=IR-1                                                           DPRB1040
      IF(IR-1)42,42,2                                                   DPRB1050
    2 IF(C(IR))3,1,3                                                    DPRB1060
C                                                                       DPRB1070
C        WORK UP ZERO ROOTS AND NORMALIZE REMAINING POLYNOMIAL          DPRB1080
    3 IER=0                                                             DPRB1090
      J=IR                                                              DPRB1100
      L=0                                                               DPRB1110
      A=C(IR)                                                           DPRB1120
      DO 8 I=1,IR                                                       DPRB1130
      IF(L)4,4,7                                                        DPRB1140
    4 IF(C(I))6,5,6                                                     DPRB1150
    5 RR(I)=0.D0                                                        DPRB1160
      RC(I)=0.D0                                                        DPRB1170
      POL(J)=0.D0                                                       DPRB1180
      J=J-1                                                             DPRB1190
      GO TO 8                                                           DPRB1200
    6 L=1                                                               DPRB1210
      IST=I                                                             DPRB1220
      J=0                                                               DPRB1230
    7 J=J+1                                                             DPRB1240
      C(I)=C(I)/A                                                       DPRB1250
      POL(J)=C(I)                                                       DPRB1260
      CALL OVERFL(N)                                                    DPRB1270
      IF(N-2)42,8,8                                                     DPRB1280
    8 CONTINUE                                                          DPRB1290
C                                                                       DPRB1300
C        START BAIRSTOW ITERATION                                       DPRB1310
      Q1=0.D0                                                           DPRB1320
      Q2=0.D0                                                           DPRB1330
    9 IF(J-2)33,10,14                                                   DPRB1340
C                                                                       DPRB1350
C        DEGREE OF RESTPOLYNOMIAL IS EQUAL TO ONE                       DPRB1360
   10 A=POL(1)                                                          DPRB1370
      RR(IST)=-A                                                        DPRB1380
      RC(IST)=0.D0                                                      DPRB1390
      IR=IR-1                                                           DPRB1400
      Q2=0.D0                                                           DPRB1410
      IF(IR-1)13,13,11                                                  DPRB1420
   11 DO 12 I=2,IR                                                      DPRB1430
      Q1=Q2                                                             DPRB1440
      Q2=POL(I+1)                                                       DPRB1450
   12 POL(I)=A*Q2+Q1                                                    DPRB1460
   13 POL(IR+1)=A*Q2                                                    DPRB1470
      GO TO 34                                                          DPRB1480
C        THIS IS BRANCH TO COMPARISON OF COEFFICIENT VECTORS C AND POL  DPRB1490
C                                                                       DPRB1500
C        DEGREE OF RESTPOLYNOMIAL IS GREATER THAN ONE                   DPRB1510
   14 DO 22 L=1,10                                                      DPRB1520
      N=1                                                               DPRB1530
   15 Q(1)=Q1                                                           DPRB1540
      Q(2)=Q2                                                           DPRB1550
      CALL DPQFB(POL,J,Q,LIM,I)                                         DPRB1560
      IF(I)16,24,23                                                     DPRB1570
   16 IF(Q1)18,17,18                                                    DPRB1580
   17 IF(Q2)18,21,18                                                    DPRB1590
   18 GO TO (19,20,19,21),N                                             DPRB1600
   19 Q1=-Q1                                                            DPRB1610
      N=N+1                                                             DPRB1620
      GO TO 15                                                          DPRB1630
   20 Q2=-Q2                                                            DPRB1640
      N=N+1                                                             DPRB1650
      GO TO 15                                                          DPRB1660
   21 Q1=1.D0+Q1                                                        DPRB1670
   22 Q2=1.D0-Q2                                                        DPRB1680
C                                                                       DPRB1690
C        ERROR EXIT DUE TO UNSATISFACTORY RESULTS OF FACTORIZATION      DPRB1700
      IER=3                                                             DPRB1710
      IR=IR-J                                                           DPRB1720
      RETURN                                                            DPRB1730
C                                                                       DPRB1740
C        WORK UP RESULTS OF QUADRATIC FACTORIZATION                     DPRB1750
   23 IER=1                                                             DPRB1760
   24 Q1=Q(1)                                                           DPRB1770
      Q2=Q(2)                                                           DPRB1780
C                                                                       DPRB1790
C        PERFORM DIVISION OF FACTORIZED POLYNOMIAL BY QUADRATIC FACTOR  DPRB1800
      B=0.D0                                                            DPRB1810
      A=0.D0                                                            DPRB1820
      I=J                                                               DPRB1830
   25 H=-Q1*B-Q2*A+POL(I)                                               DPRB1840
      POL(I)=B                                                          DPRB1850
      B=A                                                               DPRB1860
      A=H                                                               DPRB1870
      I=I-1                                                             DPRB1880
      IF(I-2)26,26,25                                                   DPRB1890
   26 POL(2)=B                                                          DPRB1900
      POL(1)=A                                                          DPRB1910
C                                                                       DPRB1920
C        MULTIPLY POLYNOMIAL WITH CALCULATED ROOTS BY QUADRATIC FACTOR  DPRB1930
      L=IR-1                                                            DPRB1940
      IF(J-L)27,27,29                                                   DPRB1950
   27 DO 28 I=J,L                                                       DPRB1960
   28 POL(I-1)=POL(I-1)+POL(I)*Q2+POL(I+1)*Q1                           DPRB1970
   29 POL(L)=POL(L)+POL(L+1)*Q2+Q1                                      DPRB1980
      POL(IR)=POL(IR)+Q2                                                DPRB1990
C                                                                       DPRB2000
C        CALCULATE ROOT-PAIR FROM QUADRATIC FACTOR X**X+Q2*X+Q1         DPRB2010
      H=-.5D0*Q2                                                        DPRB2020
      A=H*H-Q1                                                          DPRB2030
      B=DSQRT(DABS(A))                                                  DPRB2040
      IF(A)30,30,31                                                     DPRB2050
   30 RR(IST)=H                                                         DPRB2060
      RC(IST)=B                                                         DPRB2070
      IST=IST+1                                                         DPRB2080
      RR(IST)=H                                                         DPRB2090
      RC(IST)=-B                                                        DPRB2100
      GO TO 32                                                          DPRB2110
   31 B=H+DSIGN(B,H)                                                    DPRB2120
      RR(IST)=Q1/B                                                      DPRB2130
      RC(IST)=0.D0                                                      DPRB2140
      IST=IST+1                                                         DPRB2150
      RR(IST)=B                                                         DPRB2160
      RC(IST)=0.D0                                                      DPRB2170
   32 IST=IST+1                                                         DPRB2180
      J=J-2                                                             DPRB2190
      GO TO 9                                                           DPRB2200
C                                                                       DPRB2210
C        SHIFT BACK ELEMENTS OF POL BY 1 AND COMPARE VECTORS POL AND C  DPRB2220
   33 IR=IR-1                                                           DPRB2230
   34 A=0.D0                                                            DPRB2240
      DO 38 I=1,IR                                                      DPRB2250
      Q1=C(I)                                                           DPRB2260
      Q2=POL(I+1)                                                       DPRB2270
      POL(I)=Q2                                                         DPRB2280
      IF(Q1)35,36,35                                                    DPRB2290
   35 Q2=(Q1-Q2)/Q1                                                     DPRB2300
   36 Q2=DABS(Q2)                                                       DPRB2310
      IF(Q2-A)38,38,37                                                  DPRB2320
   37 A=Q2                                                              DPRB2330
   38 CONTINUE                                                          DPRB2340
      I=IR+1                                                            DPRB2350
      POL(I)=1.D0                                                       DPRB2360
      RR(I)=A                                                           DPRB2370
      RC(I)=0.D0                                                        DPRB2380
      IF(IER)39,39,41                                                   DPRB2390
   39 IF(A-EPS)41,41,40                                                 DPRB2400
C                                                                       DPRB2410
C        WARNING DUE TO POOR ACCURACY OF CALCULATED COEFFICIENT VECTOR  DPRB2420
   40 IER=-1                                                            DPRB2430
   41 RETURN                                                            DPRB2440
C                                                                       DPRB2450
C        ERROR EXIT DUE TO DEGENERATE POLYNOMIAL OR OVERFLOW IN         DPRB2460
C        NORMALIZATION                                                  DPRB2470
   42 IER=2                                                             DPRB2480
      IR=0                                                              DPRB2490
      RETURN                                                            DPRB2500
      END                                                               DPRB2510
```

Subroutines PQFB and DPQFB

These subroutines use Bairstow's iterative method to find an approximation to a quadratic factor of a given polynomial $p(x) = c_1+c_2x+\ldots+c_{n+1}x^n$ (deg $p(x) = n \geq 2$, c_i real).

1. Mathematical background

Let $Q(x) = x^2 + Q_2x+Q_1$ be any quadratic polynomial with real coefficients. Then $p(x) = R(x)Q(x) + B(Q_1, Q_2)x + C(Q_1, Q_2)$, where $C(Q_1, Q_2) = a_1$, $B(Q_1, Q_2) = a_2$, $R(x) = a_3+a_4x+\ldots+a_{n+1}x^{n-2}$, and

$$a_i = \begin{cases} 0 & \text{if } i > n+1 \\ c_i - Q_2 a_{i+1} - Q_1 a_{i+2} & \text{if } i=n+1,\ldots,2 \\ c_1 - Q_1 a_3 & \text{if } i=1 \end{cases}$$

Of course, if $q(x)=x^2 + q_2x+q_1$ is a factor of $p(x)$, then:

$$\left.\begin{aligned} C(q_1, q_2) &= 0 \\ \text{and} \\ B(q_1, q_2) &= 0 \end{aligned}\right\}$$

Suppose that $Q(x)$ is an approximation to $q(x)$; then Q_1 and Q_2 are approximations to q_1 and q_2 respectively, and if ΔQ_1 and ΔQ_2 are such that:

$$\left.\begin{aligned} q_1 &= Q_1 + \Delta Q_1 \\ \text{and} \\ q_2 &= Q_2 + \Delta Q_2 \end{aligned}\right\}$$

Then:

$$\left.\begin{aligned} C(Q_1 + \Delta Q_1, Q_2 + \Delta Q_2) &= 0 \\ \text{and} \\ B(Q_1 + \Delta Q_1, Q_2 + \Delta Q_2) &= 0 \end{aligned}\right\} \qquad (1)$$

Instead of solving (1) for ΔQ_1 and ΔQ_2, we solve:

$$\left.\begin{aligned} C(Q_1, Q_2) + \frac{\partial}{\partial Q_1} C(Q_1, Q_2)\,\Delta Q_1 \\ + \frac{\partial}{\partial Q_2} C(Q_1, Q_2)\,\Delta Q_2 = 0 \\ \text{and} \\ B(Q_1, Q_2) + \frac{\partial}{\partial Q_1} B(Q_1, Q_2)\,\Delta Q_1 \\ + \frac{\partial}{\partial Q_2} B(Q_1, Q_2)\,\Delta Q_2 = 0 \end{aligned}\right\} \qquad (2)$$

for ΔQ_1 and ΔQ_2. Equation (2) is the linearization of (1). To solve (2) we must find $\frac{\partial}{\partial Q_i} B(Q_1, Q_2)$ and $\frac{\partial}{\partial Q_i} C(Q_1, Q_2)$, $i = 1, 2$. To do this we define

$$r_i = \begin{cases} a_i & \text{if } i>1 \\ a_1 - Q_2 B & \text{if } i=1 \end{cases}$$

and then

$$s_i = \begin{cases} 0 & \text{if } i>n+1 \\ r_i - Q_2 s_{i+1} - Q_1 s_{i+2} & \text{if } i = n+1, n, n-1,\ldots,1 \end{cases}$$

Now:

$$\left.\begin{aligned} \frac{\partial r_i}{\partial Q_2} &= -r_{i+1} - Q_2 \frac{\partial r_{i+1}}{\partial Q_e} - Q_1 \frac{\partial r_{i+2}}{\partial Q_2} \\ \text{and} \\ \frac{\partial r_i}{\partial Q_1} &= -r_{i+2} - Q_2 \frac{\partial r_{i+1}}{\partial Q_1} - Q_1 \frac{\partial r_{i+2}}{\partial Q_1} \end{aligned}\right\}$$

By an easy induction on i it follows that:

$$\frac{\partial r_i}{\partial Q_2} = -S_{i+1} \quad \text{and} \quad \frac{\partial r_i}{\partial Q_1} = -S_{i+2}, \qquad i=1,\ldots,n+1$$

In particular:

$$\left.\begin{aligned} \frac{\partial B}{\partial Q_1} &= \frac{\partial a_2}{\partial Q_1} = \frac{\partial r_2}{\partial Q_1} = -S_4 \\ \frac{\partial B}{\partial Q_2} &= \frac{\partial a_2}{\partial Q_2} = \frac{\partial r_2}{\partial Q_2} = -S_3 \\ \frac{\partial C}{\partial Q_1} &= \frac{\partial a_1}{\partial Q_1} = \frac{\partial r_1}{\partial Q_1} + Q_2 \frac{\partial r_2}{\partial Q_1} = \\ & -S_3 - Q_2 S_4 \\ \frac{\partial C}{\partial Q_2} &= \frac{\partial a_1}{\partial Q_2} = \frac{\partial r_1}{\partial Q_2} + Q_2 \frac{\partial r_2}{\partial Q_2} + r_2 = \\ & -S_2 - Q_2 S_3 + r_4 \end{aligned}\right\}$$

and if we let:

$$\left.\begin{aligned} C_1 &= s_4 \\ B_1 &= s_3 \\ A_1 &= s_2 - r_2 \\ A &= r_1 \end{aligned}\right\}$$

then we can rewrite (2) as:

$$\left.\begin{aligned} (B_1 + Q_2 C_1)\,\Delta Q_1 + (A_1 + Q_2 B_1)\,\Delta Q_2 &= A + Q_2 B \\ C_1\,\Delta Q_1 + \qquad B_1\,\Delta Q_2 &= B \end{aligned}\right\}$$

which simplifies to:

$$\left.\begin{aligned} B_1\,\Delta Q_1 + A_1\,\Delta Q_2 &= A \\ C_1\,\Delta Q_1 + B_1\,\Delta Q_2 &= B \end{aligned}\right\} \qquad (3)$$

Solving (3) we find that:

$$\left.\begin{aligned} \Delta Q_1 &= \frac{A_1 B - B_1 A}{A_1 C_1 - B_1^2} \\ \Delta Q_2 &= \frac{C_1 A - B_1 B}{A_1 C_1 - B_1^2} \end{aligned}\right\}$$

We can now replace Q_i by $Q_i + \Delta Q_i$, $i = 1, 2$, and repeat the above procedure.

2. Programming considerations

The input consists of a vector C of polynomial coefficients (C(1) is the constant term), the dimension IC of C, a vector Q of dimension 4 with Q(1) and Q(2) containing initial guesses for the coefficients of a quadratic factor, and an upper bound LIM for the number of iterations to be performed.

First $J \le IC$ is determined such that $C(J) \neq 0$, $C(K) = 0$ for $K > J$. If $J \le 1$, there is no computation and the error parameter IER is set to -1. If $J > 1$, the polynomial is normalized by dividing all the coefficients of C by C(J), the coefficient of the leading term. If overflow occurs during the normalization, computation is terminated and IER is set to -1. If no overflow occurs, the degree (J-1) of the polynomial p(x) is tested; if p is of degree 1, there is no further computation and IER is set to -2; if p is of degree 2, Q(1) and Q(2) are set to C(1) and C(2) respectively, Q(3) and Q(4) are set to zero, IER is set to zero, and computation is terminated; if p is of degree greater than 2, the main part of the subroutine--the Bairstow iterative procedure--is entered.

Every approximation $Q(x) = x^2 + Q_2 x + Q_1$ to a quadratic factor of p has associated with it a constant CC, called the norm of the modified linear remainder and hereafter referred to as the norm. It is given by $CC = CA \cdot |A| + CB \cdot |B|$ where:

$$CA = \begin{cases} 1 & \text{if } |C(1)| \le |C(2)| \\ \left|\dfrac{C(2)}{C(1)}\right| & \text{if } |C(1)| > |C(2)| \end{cases}$$

and

$$CB = \begin{cases} \left|\dfrac{C(1)}{C(2)}\right| & \text{if } |C(1)| < |C(2)| \\ 1 & \text{if } |C(1)| \ge |C(2)| \end{cases}$$

Since there is no guarantee that the Bairstow method will converge, several accuracy tests are performed at the end of each iteration. Depending on the outcome of these tests, which in part involve CC, either the computation is terminated or another iteration is performed.

Letting:

$$EPS = \begin{cases} 10^{-6} & \text{in single precision} \\ 10^{-14} & \text{in double precision} \end{cases}$$

and:

$$EPS1 = \begin{cases} 10^{-3} & \text{in single precision} \\ 10^{-16} & \text{in double precision} \end{cases}$$

the tests are described below.

a. If $|A| \le EPS^* |C(1)|$ and $|B| \le EPS^* |C(2)|$, or if $|\Delta Q_1| \le EPS^* |Q_1|$ and $|\Delta Q_2| \le EPS^* |Q_2|$, computation is terminated after setting IER = 0, $Q(1) = Q_1$, $Q(2) = Q_2$, Q(3) = A, and Q(4) = B.

b. If $|\Delta Q_1| \le EPS1^* |Q_1|$ and $|\Delta Q_2| \le EPS1^* |Q_2|$, and if $|\Delta Q_1/Q_1|$ or $|\Delta Q_2/Q_2|$ is not smaller than its value for the previous iteration (this is generally due to roundoff errors), computation is terminated after setting IER = 0, $Q(1) = QQ_1$, $Q(2) = QQ_2$, Q(3) = AA, and Q(4) = BB where QQ_1, QQ_2, AA, and BB are the values of Q_1, Q_2, A, and B belonging to

a previous iteration--the iteration with the smallest norm.

c. If no convergence occurs within LIM iterations and if the last norm is not greater than CD/10, where CD is the norm associated with the quadratic factor x^2, results are generated as in b. with the exception that IER is set to 1. If the last norm is greater than CD/10:

(1) If the initial guess for the quadratic factor was x^2, the results are generated as in b. with the exception that IER is set to -3.

(2) If the initial guess for the quadratic factor was not x^2, the subroutine restarts with x^2 as the initial guess.

d. If exponential overflow or division by 0 occurs during any iteration, results are generated as in b. with the exception that IER is set to -3.

For reference see:

(1) J. H. Wilkinson, "The Evaluation of the Zeros of Ill-Conditioned Polynomials (Part I and II)," Numerische Mathematik, vol. 1 (1959), pp. 150-180.

(2) F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 472-476.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C                                                                       PQFB  10
C ..................................................................  PQFB  20
C                                                                       PQFB  30
C    SUBROUTINE PQFB                                                    PQFB  40
C                                                                       PQFB  50
C    PURPOSE                                                            PQFB  60
C       TO FIND AN APPROXIMATION Q(X)=Q1+Q2*X+X**2 TO A QUADRATIC       PQFB  70
C       FACTOR OF A GIVEN POLYNOMIAL P(X) WITH REAL COEFFICIENTS.       PQFB  80
C                                                                       PQFB  90
C    USAGE                                                              PQFB 100
C       CALL PQFB(C,IC,Q,LIM,IER)                                       PQFB 110
C                                                                       PQFB 120
C    DESCRIPTION OF PARAMETERS                                          PQFB 130
C       C   - INPUT VECTOR CONTAINING THE COEFFICIENTS OF P(X) -        PQFB 140
C             C(1) IS THE CONSTANT TERM (DIMENSION IC)                  PQFB 150
C       IC  - DIMENSION OF C                                            PQFB 160
C       Q   - VECTOR OF DIMENSION 4 - ON INPUT Q(1) AND Q(2) MUST       PQFB 170
C             CONTAIN INITIAL GUESSES FOR Q1 AND Q2 - ON RETURN Q(1)    PQFB 180
C             AND Q(2) CONTAIN THE REFINED COEFFICIENTS Q1 AND Q2 OF    PQFB 190
C             Q(X), WHILE Q(3) AND Q(4) CONTAIN THE COEFFICIENTS A      PQFB 200
C             AND B OF A+B*X, WHICH IS THE REMAINDER OF THE QUOTIENT    PQFB 210
C             OF P(X) BY Q(X)                                           PQFB 220
C       LIM - INPUT VALUE SPECIFYING THE MAXIMUM NUMBER OF              PQFB 230
C             ITERATIONS TO BE PERFORMED                                PQFB 240
C       IER - RESULTING ERROR PARAMETER (SEE REMARKS)                   PQFB 250
C             IER= 0 - NO ERROR                                         PQFB 260
C             IER= 1 - NO CONVERGENCE WITHIN LIM ITERATIONS             PQFB 270
C             IER=-1 - THE POLYNOMIAL P(X) IS CONSTANT OR UNDEFINED     PQFB 280
C                      - OR OVERFLOW OCCURRED IN NORMALIZING P(X)       PQFB 290
C             IER=-2 - THE POLYNOMIAL P(X) IS OF DEGREE 1               PQFB 300
C             IER=-3 - NO FURTHER REFINEMENT OF THE APPROXIMATION TO    PQFB 310
C                      A QUADRATIC FACTOR IS FEASIBLE, DUE TO EITHER    PQFB 320
C                      DIVISION BY 0, OVERFLOW OR AN INITIAL GUESS      PQFB 330
C                      THAT IS NOT SUFFICIENTLY CLOSE TO A FACTOR OF    PQFB 340
C                      P(X)                                             PQFB 350
C                                                                       PQFB 360
C    REMARKS                                                            PQFB 370
C       (1)  IF IER=-1 THERE IS NO COMPUTATION OTHER THAN THE           PQFB 380
C            POSSIBLE NORMALIZATION OF C.                               PQFB 390
C       (2)  IF IER=-2 THERE IS NO COMPUTATION OTHER THAN THE           PQFB 400
C            NORMALIZATION OF C.                                        PQFB 410
C       (3)  IF IER =-3  IT IS SUGGESTED THAT A NEW INITIAL GUESS BE    PQFB 420
C            MADE FOR A QUADRATIC FACTOR.  Q, HOWEVER, WILL CONTAIN     PQFB 430
C            THE VALUES ASSOCIATED WITH THE ITERATION THAT YIELDED      PQFB 440
C            THE SMALLEST NORM OF THE MODIFIED LINEAR REMAINDER.        PQFB 450
C       (4)  IF IER=1, THEN, ALTHOUGH THE NUMBER OF ITERATIONS LIM      PQFB 460
C            WAS TOO SMALL TO INDICATE CONVERGENCE, NO OTHER PROB-      PQFB 470
C            LEMS HAVE BEEN DETECTED, AND Q WILL CONTAIN THE VALUES     PQFB 480
C            ASSOCIATED WITH THE ITERATION THAT YIELDED THE SMALLEST    PQFB 490
C            NORM OF THE MODIFIED LINEAR REMAINDER.                     PQFB 500
C       (5)  FOR COMPLETE DETAIL SEE THE DOCUMENTATION FOR              PQFB 510
C            SUBROUTINES PQFB AND DPQFB.                                PQFB 520
C                                                                       PQFB 530
C    SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                      PQFB 540
C       NONE                                                            PQFB 550
C                                                                       PQFB 560
C    METHOD                                                             PQFB 570
C       COMPUTATION IS BASED ON BAIRSTOW'S ITERATIVE METHOD.  (SEE      PQFB 580
C       WILKINSON, J.H., THE EVALUATION OF THE ZEROS OF ILL-CON-        PQFB 590
C       DITIONED POLYNOMIALS (PART ONE AND TWO), NUMERISCHE MATHE-      PQFB 600
C       MATIK, VOL.1 (1959), PP. 150-180, OR HILDEBRAND, F.B.,          PQFB 610
C       INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/     PQFB 620
C       TORONTO/LONDON, 1956, PP. 472-476.)                             PQFB 630
C                                                                       PQFB 640
C ..................................................................  PQFB 650
C                                                                       PQFB 660
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      SUBROUTINE PQFB(C,IC,Q,LIM,IER)                                   PQFB 670
C                                                                       PQFB 680
C                                                                       PQFB 690
      DIMENSION C(1),Q(1)                                               PQFB 700
C                                                                       PQFB 710
C     .    TEST ON LEADING ZERO COEFFICIENTS                            PQFB 720
      IER=0                                                             PQFB 730
      J=IC+1                                                            PQFB 740
    1 J=J-1                                                             PQFB 750
      IF(J-1)40,40,2                                                    PQFB 760
    2 IF(C(J))3,1,3                                                     PQFB 770
C                                                                       PQFB 780
C        NORMALIZATION OF REMAINING COEFFICIENTS                        PQFB 790
    3 A=C(J)                                                            PQFB 800
      IF(A-1.)4,6,4                                                     PQFB 810
    4 DO 5 I=1,J                                                        PQFB 820
      C(I)=C(I)/A                                                       PQFB 830
      CALL OVERFL(N)                                                    PQFB 840
      IF(N-2)40,5,5                                                     PQFB 850
    5 CONTINUE                                                          PQFB 860
C                                                                       PQFB 870
C        TEST ON NECESSITY OF BAIRSTOW ITERATION                        PQFB 880
    6 IF(J-3)41,38,7                                                    PQFB 890
C                                                                       PQFB 900
C        PREPARE BAIRSTOW ITERATION                                     PQFB 910
    7 EPS=1.E-6                                                         PQFB 920
      EPS1=1.E-3                                                        PQFB 930
      L=0                                                               PQFB 940
      LL=0                                                              PQFB 950
      Q1=Q(1)                                                           PQFB 960
      Q2=Q(2)                                                           PQFB 970
      QQ1=0.                                                            PQFB 980
      QQ2=0.                                                            PQFB 990
      AA=C(1)                                                           PQFB1000
      BB=C(2)                                                           PQFB1010
      CB=ABS(AA)                                                        PQFB1020
      CA=ABS(BB)                                                        PQFB1030
      IF(CB-CA)8,9,10                                                   PQFB1040
    8 CC=CB+CB                                                          PQFB1050
      CB=CB/CA                                                          PQFB1060
      CA=1.                                                             PQFB1070
      GO TO 11                                                          PQFB1080
    9 CC=CA+CA                                                          PQFB1090
      CA=1.                                                             PQFB1100
      CB=1.                                                             PQFB1110
      GO TO 11                                                          PQFB1120
   10 CC=CA+CA                                                          PQFB1130
      CA=CA/CB                                                          PQFB1140
      CB=1.                                                             PQFB1150
   11 CD=CC*.1                                                          PQFB1160
C                                                                       PQFB1170
C        START BAIRSTOW ITERATION                                       PQFB1180
C        PREPARE NESTED MULTIPLICATION                                  PQFB1190
   12 A=0.                                                              PQFB1200
      B=A                                                               PQFB1210
      A1=A                                                              PQFB1220
      B1=A                                                              PQFB1230
      I=J                                                               PQFB1240
      QQQ1=Q1                                                           PQFB1250
      QQQ2=Q2                                                           PQFB1260
      DQ1=HH                                                            PQFB1270
      DQ2=H                                                             PQFB1280
C                                                                       PQFB1290
C        START NESTED MULTIPLICATION                                    PQFB1300
   13 H=-Q1*B-Q2*A+C(I)                                                 PQFB1310
      CALL OVERFL(N)                                                    PQFB1320
      IF(N-2)42,14,14                                                   PQFB1330
   14 B=A                                                               PQFB1340
      A=H                                                               PQFB1350
      I=I-1                                                             PQFB1360
      IF(I-1)18,15,16                                                   PQFB1370
   15 H=0.                                                              PQFB1380
   16 H=-Q1*B1-Q2*A1+H                                                  PQFB1390
      CALL OVERFL(N)                                                    PQFB1400
      IF(N-2)42,17,17                                                   PQFB1410
   17 C1=B1                                                             PQFB1420
      B1=A1                                                             PQFB1430
      A1=H                                                              PQFB1440
      GO TO 13                                                          PQFB1450
C        END OF NESTED MULTIPLICATION                                   PQFB1460
C                                                                       PQFB1470
C        TEST ON SATISFACTORY ACCURACY                                  PQFB1480
   18 H=CA*ABS(A)+CB*ABS(B)                                             PQFB1490
      IF(LL)19,19,39                                                    PQFB1500
   19 L=L+1                                                             PQFB1510
      IF(ABS(A)-EPS*ABS(C(1)))20,20,21                                  PQFB1520
   20 IF(ABS(B)-EPS*ABS(C(2)))39,39,21                                  PQFB1530
C                                                                       PQFB1540
C        TEST ON LINEAR REMAINDER OF MINIMUM NORM                       PQFB1550
   21 IF(H-CC)22,22,23                                                  PQFB1560
   22 AA=A                                                              PQFB1570
      BB=B                                                              PQFB1580
      CC=H                                                              PQFB1590
      CQ1=Q1                                                            PQFB1600
      CQ2=Q2                                                            PQFB1610
C                                                                       PQFB1620
C        TEST ON LAST ITERATION STEP                                    PQFB1630
   23 IF(L-LIM)28,28,24                                                 PQFB1640
C                                                                       PQFB1650
C        TEST ON RESTART OF BAIRSTOW ITERATION WITH ZERO INITIAL GUESS  PQFB1660
   24 IF(H-CD)43,43,25                                                  PQFB1670
   25 IF(Q(1))27,26,27                                                  PQFB1680
   26 IF(Q(2))27,42,27                                                  PQFB1690
   27 Q(1)=0.                                                           PQFB1700
      Q(2)=0.                                                           PQFB1710
      GO TO 7                                                           PQFB1720
C                                                                       PQFB1730
C        PERFORM ITERATION STEP                                         PQFB1740
   28 HH=AMAX1(ABS(A1),ABS(B1),ABS(C1))                                 PQFB1750
      IF(HH)42,42,29                                                    PQFB1760
   29 A1=A1/HH                                                          PQFB1770
      B1=B1/HH                                                          PQFB1780
      C1=C1/HH                                                          PQFB1790
      H=A1*C1-B1*B1                                                     PQFB1800
      IF(H)30,42,30                                                     PQFB1810
   30 A=A/HH                                                            PQFB1820
      B=B/HH                                                            PQFB1830
      HH=(B*A1-A*B1)/H                                                  PQFB1840
      H=(A*C1-B*B1)/H                                                   PQFB1850
      Q1=Q1+HH                                                          PQFB1860
      Q2=Q2+H                                                           PQFB1870
C        END OF ITERATION STEP                                          PQFB1880
C                                                                       PQFB1890
C        TEST ON SATISFACTORY RELATIVE ERROR OF ITERATED VALUES         PQFB1900
      IF(ABS(HH)-EPS*ABS(Q1))31,31,33                                   PQFB1910
   31 IF(ABS(H)-EPS*ABS(Q2))32,32,33                                    PQFB1920
   32 LL=1                                                              PQFB1930
      GO TO 12                                                          PQFB1940
C                                                                       PQFB1950
C        TEST ON DECREASING RELATIVE ERRORS                             PQFB1960
   33 IF(L-1)12,17,34                                                   PQFB1970
   34 IF(ABS(HH)-EPS1*ABS(Q1))35,35,12                                  PQFB1980
   35 IF(ABS(H)-EPS1*ABS(Q2))36,36,12                                   PQFB1990
   36 IF(ABS(QQQ1*HH)-ABS(Q1*DQ1))37,44,44                              PQFB2000
   37 IF(ABS(QQQ2*H)-ABS(Q2*DC2))12,44,44                               PQFB2010
C        END OF BAIRSTOW ITERATION                                      PQFB2020
C                                                                       PQFB2030
C        EXIT IN CASE OF QUADRATIC POLYNOMIAL                           PQFB2040
   38 Q(1)=C(1)                                                         PQFB2050
      Q(2)=C(2)                                                         PQFB2060
      Q(3)=0.                                                           PQFB2070
      Q(4)=0.                                                           PQFB2080
      RETURN                                                            PQFB2090
C                                                                       PQFB2100
C        EXIT IN CASE OF SUFFICIENT ACCURACY                            PQFB2110
   39 Q(1)=Q1                                                           PQFB2120
      Q(2)=Q2                                                           PQFB2130
      Q(3)=A                                                            PQFB2140
      Q(4)=B                                                            PQFB2150
      RETURN                                                            PQFB2160
C                                                                       PQFB2170
C        ERROR EXIT IN CASE OF ZERO OR CONSTANT POLYNOMIAL              PQFB2180
   40 IER=-1                                                            PQFB2190
      RETURN                                                            PQFB2200
C                                                                       PQFB2210
C        ERROR EXIT IN CASE OF LINEAR POLYNOMIAL                        PQFB2220
   41 IER=-2                                                            PQFB2230
      RETURN                                                            PQFB2240
C                                                                       PQFB2250
C        ERROR EXIT IN CASE OF NONREFINED QUADRATIC FACTOR              PQFB2260
   42 IER=-3                                                            PQFB2270
      GO TO 44                                                          PQFB2280
C                                                                       PQFB2290
C        ERROR EXIT IN CASE OF UNSATISFACTORY ACCURACY                  PQFB2300
   43 IER=1                                                             PQFB2310
   44 Q(1)=QQ1                                                          PQFB2320
      Q(2)=QQ2                                                          PQFB2330
      Q(3)=AA                                                           PQFB2340
      Q(4)=BB                                                           PQFB2350
      RETURN                                                            PQFB2360
      END                                                               PQFB2370
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C                                                                       DPQF  10
C     ..................................................................DPQF  20
C                                                                       DPQF  30
C        SUBROUTINE DPQFB                                               DPQF  40
C                                                                       DPQF  50
C        PURPOSE                                                        DPQF  60
C           TO FIND AN APPROXIMATION Q(X)=Q1+Q2*X+X**2 TO A QUADRATIC   DPQF  70
C           FACTOR OF A GIVEN POLYNOMIAL P(X) WITH REAL COEFFICIENTS.   DPQF  80
C                                                                       DPQF  90
C        USAGE                                                          DPQF 100
C           CALL DPQFB(C,IC,Q,LIM,IER)                                  DPQF 110
C                                                                       DPQF 120
C        DESCRIPTION OF PARAMETERS                                      DPQF 130
C           C   - DOUBLE PRECISION INPUT VECTOR CONTAINING THE          DPQF 140
C                 COEFFICIENTS OF P(X) - C(1) IS THE CONSTANT TERM       DPQF 150
C                 (DIMENSION IC)                                        DPQF 160
C           IC  - DIMENSION OF C                                        DPQF 170
C           Q   - DOUBLE PRECISION VECTOR OF DIMENSION 4 - ON INPUT Q(1)DPQF 180
C                 AND Q(2) CONTAIN INITIAL GUESSES FOR Q1 AND Q2 - ON   DPQF 190
C                 RETURN Q(1) AND Q(2) CONTAIN THE REFINED COEFFICIENTS DPQF 200
C                 Q1 AND Q2 OF Q(X), WHILE Q(3) AND Q(4) CONTAIN THE    DPQF 210
C                 COEFFICIENTS A AND B OF A+B*X, WHICH IS THE REMAINDER DPQF 220
C                 OF THE QUOTIENT OF P(X) BY Q(X)                       DPQF 230
C           LIM - INPUT VALUE SPECIFYING THE MAXIMUM NUMBER OF          DPQF 240
C                 ITERATIONS TO BE PERFORMED                            DPQF 250
C           IER - RESULTING ERROR PARAMETER (SEE REMARKS)               DPQF 260
C                 IER= 0 - NO ERROR                                     DPQF 270
C                 IER= 1 - NO CONVERGENCE WITHIN LIM ITERATIONS         DPQF 280
C                 IER=-1 - THE POLYNOMIAL P(X) IS CONSTANT OR UNDEFINED DPQF 290
C                        - OR OVERFLOW OCCURRED IN NORMALIZING P(X)     DPQF 300
C                 IER=-2 - THE POLYNOMIAL P(X) IS OF DEGREE 1           DPQF 310
C                 IER=-3 - NO FURTHER REFINEMENT OF THE APPROXIMATION TODPQF 320
C                          A QUADRATIC FACTOR IS FEASIBLE, DUE TO EITHERDPQF 330
C                          DIVISION BY 0, OVERFLOW OR AN INITIAL GUESS  DPQF 340
C                          THAT IS NOT SUFFICIENTLY CLOSE TO A FACTOR OFDPQF 350
C                          P(X)                                         DPQF 360
C                                                                       DPQF 370
C        REMARKS                                                        DPQF 380
C           (1)  IF IER=-1 THERE IS NO COMPUTATION OTHER THAN THE       DPQF 390
C                POSSIBLE NORMALIZATION OF C.                           DPQF 400
C           (2)  IF IER=-2 THERE IS NO COMPUTATION OTHER THAN THE       DPQF 410
C                NORMALIZATION OF C.                                    DPQF 420
C           (3)  IF IER =-3  IT IS SUGGESTED THAT A NEW INITIAL GUESS BEDPQF 430
C                MADE FOR A QUADRATIC FACTOR, Q. HOWEVER, WILL CONTAIN DPQF 440
C                THE VALUES ASSOCIATED WITH THE ITERATION THAT YIELDED  DPQF 450
C                THE SMALLEST NORM OF THE MODIFIED LINEAR REMAINDER.    DPQF 460
C           (4)  IF IER=1, THEN, ALTHOUGH THE NUMBER OF ITERATIONS LIM  DPQF 470
C                WAS TOO SMALL TO INDICATE CONVERGENCE, NO OTHER PROB-  DPQF 480
C                LEMS HAVE BEEN DETECTED, AND Q WILL CONTAIN THE VALUES DPQF 490
C                ASSOCIATED WITH THE ITERATION THAT YIELDED THE SMALLESTDPQF 500
C                NORM OF THE MODIFIED LINEAR REMAINDER.                 DPQF 510
C           (5)  FOR COMPLETE DETAIL SEE THE DOCUMENTATION FOR          DPQF 520
C                SUBROUTINES PQFB AND DPQFB.                            DPQF 530
C                                                                       DPQF 540
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DPQF 550
C           NONE                                                        DPQF 560
C                                                                       DPQF 570
C        METHOD                                                         DPQF 580
C           COMPUTATION IS BASED ON BAIRSTOW'S ITERATIVE METHOD.  (SEE  DPQF 590
C           WILKINSON, J.H., THE EVALUATION OF THE ZEROS OF ILL-CON-    DPQF 600
C           DITIONED POLYNOMIALS (PART ONE AND TWO), NUMERISCHE MATHE-  DPQF 610
C           MATIK, VOL.1 (1959), PP. 150-180, OR HILDEBRAND, F.B.,      DPQF 620
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/ DPQF 630
C           TORONTO/LONDON, 1956, PP. 472-476.)                         DPQF 640
C                                                                       DPQF 650
C     ..................................................................DPQF 660
C                                                                       DPQF 670
      SUBROUTINE DPQFB(C,IC,Q,LIM,IER)                                  DPQF 680
C                                                                       DPQF 690
C                                                                       DPQF 700
      DIMENSION C(1),Q(1)                                               DPQF 710
      DOUBLE PRECISION A,B,AA,BB,CA,CB,CC,CD,A1,B1,C1,H,HH,Q1,Q2,QQ1,   DPQF 720
     1                 QQ2,QQQ1,QQQ2,DQ1,DQ2,EPS,EPS1,C,Q               DPQF 730
C                                                                       DPQF 740
C        TEST ON LEADING ZERO COEFFICIENTS                              DPQF 750
      IER=0                                                             DPQF 760
      J=IC+1                                                            DPQF 770
    1 J=J-1                                                             DPQF 780
```

```
      IF(J-1)40,40,2                                                    DPQF 790
    2 IF(C(J))3,1,3                                                     DPQF 800
C                                                                       DPQF 810
C        NORMALIZATION OF REMAINING COEFFICIENTS                        DPQF 820
    3 A=C(J)                                                            DPQF 830
      IF(A-1.D0)4,6,4                                                   DPQF 840
    4 DO 5 I=1,J                                                        DPQF 850
      C(I)=C(I)/A                                                       DPQF 860
      CALL OVERFL(N)                                                    DPQF 870
      IF(N-2)40,5,5                                                     DPQF 880
    5 CONTINUE                                                          DPQF 890
C                                                                       DPQF 900
C        TEST ON NECESSITY OF BAIRSTOW ITERATION                        DPQF 910
    6 IF(J-3)41,38,7                                                    DPQF 920
C                                                                       DPQF 930
C        PREPARE BAIRSTOW ITERATION                                     DPQF 940
    7 EPS=1.D-14                                                        DPQF 950
      EPS1=1.D-6                                                        DPQF 960
      L=0                                                               DPQF 970
      LL=0                                                              DPQF 980
      Q1=Q(1)                                                           DPQF 990
      Q2=Q(2)                                                           DPQF1000
      QQ1=0.D0                                                          DPQF1010
      QQ2=0.D0                                                          DPQF1020
      AA=C(1)                                                           DPQF1030
      BB=C(2)                                                           DPQF1040
      CB=DABS(AA)                                                       DPQF1050
      CA=DABS(BB)                                                       DPQF1060
      IF(CB-CA)8,9,10                                                   DPQF1070
    8 CC=CB+CB                                                          DPQF1080
      CB=CB/CA                                                          DPQF1090
      CA=1.D0                                                           DPQF1100
      GO TO 11                                                          DPQF1110
    9 CC=CA+CA                                                          DPQF1120
      CA=1.D0                                                           DPQF1130
      CB=1.D0                                                           DPQF1140
      GO TO 11                                                          DPQF1150
   10 CC=CA+CA                                                          DPQF1160
      CA=CA/CB                                                          DPQF1170
      CB=1.D0                                                           DPQF1180
   11 CD=CC*.1D0                                                        DPQF1190
C                                                                       DPQF1200
C        START BAIRSTOW ITERATION                                       DPQF1210
C        PREPARE NESTED MULTIPLICATION                                  DPQF1220
   12 A=0.D0                                                            DPQF1230
      B=A                                                               DPQF1240
      A1=A                                                              DPQF1250
      B1=A                                                              DPQF1260
      I=J                                                               DPQF1270
      QQQ1=Q1                                                           DPQF1280
      QQQ2=Q2                                                           DPQF1290
      DQ1=HH                                                            DPQF1300
      DQ2=H                                                             DPQF1310
C                                                                       DPQF1320
C        START NESTED MULTIPLICATION                                    DPQF1330
   13 H=-Q1*B-Q2*A+C(I)                                                 DPQF1340
      CALL OVERFL(N)                                                    DPQF1350
      IF(N-2)42,14,14                                                   DPQF1360
   14 B=A                                                               DPQF1370
      A=H                                                               DPQF1380
      I=I-1                                                             DPQF1390
      IF(I-1)18,15,16                                                   DPQF1400
   15 H=0.D0                                                            DPQF1410
   16 H=-Q1*B1-Q2*A1+H                                                  DPQF1420
      CALL OVERFL(N)                                                    DPQF1430
      IF(N-2)42,17,17                                                   DPQF1440
   17 C1=B1                                                             DPQF1450
      B1=A1                                                             DPQF1460
      A1=H                                                              DPQF1470
      GO TO 13                                                          DPQF1480
C        END OF NESTED MULTIPLICATION                                   DPQF1490
C                                                                       DPQF1500
C        TEST ON SATISFACTORY ACCURACY                                  DPQF1510
   18 H=CA*DABS(A)+CB*DABS(B)                                           DPQF1520
      IF(LL)19,19,39                                                    DPQF1530
   19 L=L+1                                                             DPQF1540
      IF(DABS(A)-EPS*DABS(C(1)))20,20,21                                DPQF1550
   20 IF(DABS(B)-EPS*DABS(C(2)))39,39,21                                DPQF1560
C                                                                       DPQF1570
C        TEST ON LINEAR REMAINDER OF MINIMUM NORM                       DPQF1580
   21 IF(H-CC)22,22,23                                                  DPQF1590
   22 AA=A                                                              DPQF1600
      BB=B                                                              DPQF1610
      CC=H                                                              DPQF1620
      QQ1=Q1                                                            DPQF1630
      QQ2=Q2                                                            DPQF1640
C                                                                       DPQF1650
C        TEST ON LAST ITERATION STEP                                    DPQF1660
   23 IF(L-LIM)28,28,24                                                 DPQF1670
C                                                                       DPQF1680
C        TEST ON RESTART OF BAIRSTOW ITERATION WITH ZERO INITIAL GUESS  DPQF1690
   24 IF(H-CD)43,43,25                                                  DPQF1700
   25 IF(Q(1))27,26,27                                                  DPQF1710
   26 IF(Q(2))27,42,27                                                  DPQF1720
   27 Q(1)=0.D0                                                         DPQF1730
      Q(2)=0.D0                                                         DPQF1740
      GO TO 7                                                           DPQF1750
C                                                                       DPQF1760
C        PERFORM ITERATION STEP                                         DPQF1770
   28 HH=DMAX1(DABS(A1),DABS(B1),DABS(C1))                              DPQF1780
      IF(HH)42,42,29                                                    DPQF1790
   29 A1=A1/HH                                                          DPQF1800
      B1=B1/HH                                                          DPQF1810
      C1=C1/HH                                                          DPQF1820
      H=A1*C1-B1*B1                                                     DPQF1830
      IF(H)30,42,30                                                     DPQF1840
   30 A=A/HH                                                            DPQF1850
      B=B/HH                                                            DPQF1860
      HH=(B*A1-A*B1)/H                                                  DPQF1870
      H=(A*C1-B*B1)/H                                                   DPQF1880
      Q1=Q1+HH                                                          DPQF1890
      Q2=Q2+H                                                           DPQF1900
C        END OF ITERATION STEP                                          DPQF1910
C                                                                       DPQF1920
C        TEST ON SATISFACTORY RELATIVE ERROR OF ITERATED VALUES         DPQF1930
      IF(DABS(HH)-EPS*DABS(Q1))31,31,33                                 DPQF1940
   31 IF(DABS(H)-EPS*DABS(Q2))32,32,33                                  DPQF1950
   32 LL=1                                                              DPQF1960
      GO TO 12                                                          DPQF1970
C                                                                       DPQF1980
C        TEST ON DECREASING RELATIVE ERRORS                             DPQF1990
   33 IF(L-1)12,12,34                                                   DPQF2000
   34 IF(DABS(HH)-EPS1*DABS(Q1))35,35,12                                DPQF2010
   35 IF(DABS(H)-EPS1*DABS(Q2))36,36,12                                 DPQF2020
   36 IF(DABS(QQQ1*HH)-DABS(Q1*DQ1))37,44,44                            DPQF2030
   37 IF(DABS(QQQ2*H)-DABS(Q2*DQ2))12,44,44                             DPQF2040
C        END OF BAIRSTOW ITERATION                                      DPQF2050
C                                                                       DPQF2060
C        EXIT IN CASE OF QUADRATIC POLYNOMIAL                           DPQF2070
   38 Q(1)=C(1)                                                         DPQF2080
      Q(2)=C(2)                                                         DPQF2090
      Q(3)=0.D0                                                         DPQF2100
      Q(4)=0.D0                                                         DPQF2110
      RETURN                                                            DPQF2120
C                                                                       DPQF2130
C        EXIT IN CASE OF SUFFICIENT ACCURACY                            DPQF2140
   39 Q(1)=Q1                                                           DPQF2150
      Q(2)=Q2                                                           DPQF2160
      Q(3)=A                                                            DPQF2170
      Q(4)=B                                                            DPQF2180
      RETURN                                                            DPQF2190
C                                                                       DPQF2200
C        ERROR EXIT IN CASE OF ZERO OR CONSTANT POLYNOMIAL              DPQF2210
   40 IER=-1                                                            DPQF2220
      RETURN                                                            DPQF2230
C                                                                       DPQF2240
C        ERROR EXIT IN CASE OF LINEAR POLYNOMIAL                        DPQF2250
   41 IER=-2                                                            DPQF2260
      RETURN                                                            DPQF2270
C                                                                       DPQF2280
C        ERROR EXIT IN CASE OF NONREFINED QUADRATIC FACTOR              DPQF2290
   42 IER=-3                                                            DPQF2300
      GO TO 44                                                          DPQF2310
C                                                                       DPQF2320
C        ERROR EXIT IN CASE OF UNSATISFACTORY ACCURACY                  DPQF2330
   43 IER=1                                                             DPQF2340
   44 Q(1)=QQ1                                                          DPQF2350
      Q(2)=QQ2                                                          DPQF2360
      Q(3)=AA                                                           DPQF2370
      Q(4)=BB                                                           DPQF2380
      RETURN                                                            DPQF2390
      END                                                               DPQF2400
```

Subroutines CNP and DCNP

These subroutines compute the values of the Chebyshev polynomials for a given argument x and orders zero up to N. The Chebyshev polynomial $T_n(x)$ satisfies the recurrence equation

$$T_{n+1}(x) = 2x \cdot T_n(x) - T_{n-1}(x)$$

with starting values $T_0(x) = 1$, $T_1(x) = x$. From this equation it follows immediately that roundoff errors grow at worst linearly under the tacit assumption that the argument has an absolute value less than one.

If e_{n+r} is the error in $T_{n+r}(x)$ due to a single roundoff error e in $T_n(x)$:

$$e_{n+r+1} = 2x \cdot e_{n+r} - e_{n+r-1}$$

with initial conditions $e_n = e$, $e_{n-1} = 0$.

The solution of this difference equation has its maximum for $|x| = 1$:

$$e_{n-1} = 0,\ e_n = e,\ \left|e_{n+1}\right| = 2e, \ldots, \left|e_{n+r}\right| = (r+1)e$$

The order is assumed to be zero for negative values of N.

```
C                                                                       CNP   10
C     ..................................................................CNP   20
C                                                                       CNP   30
C        SUBROUTINE CNP                                                 CNP   40
C                                                                       CNP   50
C        PURPOSE                                                        CNP   60
C           COMPUTE THE VALUES OF THE CHEBYSHEV POLYNOMIALS T(N,X)      CNP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  CNP   80
C                                                                       CNP   90
C        USAGE                                                          CNP  100
C           CALL CNP(Y,X,N)                                             CNP  110
C                                                                       CNP  120
C        DESCRIPTION OF PARAMETERS                                      CNP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESCNP  140
C                    OF CHEBYSHEV POLYNOMIALS OF ORDER 0 UP TO N        CNP  150
C                    FOR GIVEN ARGUMENT X.                              CNP  160
C           Y      - RESULT VALUE                                      CNP  170
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          CNP  180
C           X      - ARGUMENT OF CHEBYSHEV POLYNOMIAL                  CNP  190
C           N      - ORDER OF CHEBYSHEV POLYNOMIAL                     CNP  200
C                                                                       CNP  210
C        REMARKS                                                        CNP  220
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     CNP  230
C                                                                       CNP  240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CNP  250
C           NONE                                                        CNP  260
C                                                                       CNP  270
C        METHOD                                                         CNP  280
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          CNP  290
C           CHEBYSHEV POLYNOMIALS T(N,X)                                CNP  300
C           T(N+1,X)=2*X*T(N,X)-T(N-1,X),                               CNP  310
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              CNP  320
C           THE SECOND IS THE ARGUMENT.                                 CNP  330
C           STARTING VALUES ARE T(0,X)=1, T(1,X)=X.                     CNP  340
C                                                                       CNP  350
C     ..................................................................CNP  360
C                                                                       CNP  370
      SUBROUTINE CNP(Y,X,N)                                             CNP  380
C                                                                       CNP  390
      DIMENSION Y(1)                                                    CNP  400
      Y(1)=1.                                                           CNP  410
      IF(N)1,1,2                                                        CNP  420
    1 RETURN                                                            CNP  430
C                                                                       CNP  440
    2 Y(2)=X                                                            CNP  450
      IF(N-1)1,1,3                                                      CNP  460
C                                                                       CNP  470
C        INITIALIZATION                                                 CNP  480
    3 F=X+X                                                             CNP  490
C                                                                       CNP  500
      DO 4 I=2,N                                                        CNP  510
    4 Y(I+1)=F*Y(I)-Y(I-1)                                              CNP  520
      RETURN                                                            CNP  530
      END                                                               CNP  540
```

```
C                                                                       DNP   10
C     ..................................................................DNP   20
C                                                                       DNP   30
C        SUBROUTINE DCNP                                                DNP   40
C                                                                       DNP   50
C        PURPOSE                                                        DNP   60
C           COMPUTE THE VALUES OF THE CHEBYSHEV POLYNOMIALS T(N,X)      DNP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  DNP   80
C                                                                       DNP   90
C        USAGE                                                          DNP  100
C           CALL DCNP,Y,X,N)                                            DNP  110
C                                                                       DNP  120
C        DESCRIPTION OF PARAMETERS                                      DNP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESDNP  140
C                    OF CHEBYSHEV POLYNOMIALS OF ORDER 0 UP TO N        DNP  150
C                    FOR GIVEN ARGUMENT X.                              DNP  160
C                    DOUBLE PRECISION VECTOR.                           DNP  170
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          DNP  180
C           Y      - RESULT VALUE                                      DNP  190
C                    DOUBLE PRECISION VARIABLE.                         DNP  200
C           X      - ARGUMENT OF CHEBYSHEV POLYNOMIAL                  DNP  210
C           N      - ORDER OF CHEBYSHEV POLYNOMIAL                     DNP  220
C                                                                       DNP  230
C        REMARKS                                                        DNP  240
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     DNP  250
C                                                                       DNP  260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DNP  270
C           NONE                                                        DNP  280
C                                                                       DNP  290
C        METHOD                                                         DNP  300
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          DNP  310
C           CHEBYSHEV POLYNOMIALS T(N,X)                                DNP  320
C           T(N+1,X)=2*X*T(N,X)-T(N-1,X),                               DNP  330
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              DNP  340
C           THE SECOND IS THE ARGUMENT.                                 DNP  350
C           STARTING VALUES ARE T(0,X)=1, T(1,X)=X.                     DNP  360
C                                                                       DNP  370
C     ..................................................................DNP  380
C                                                                       DNP  390
      SUBROUTINE DCNP(Y,X,N)                                            DNP  400
C                                                                       DNP  410
      DIMENSION Y(1)                                                    DNP  420
      DOUBLE PRECISION Y,X,F                                            DNP  430
C                                                                       DNP  440
      Y(1)=1.D0                                                         DNP  450
      IF(N)1,1,2                                                        DNP  460
    1 RETURN                                                            DNP  470
C                                                                       DNP  480
    2 Y(2)=X                                                            DNP  490
      IF(N-1)1,1,3                                                      DNP  500
C                                                                       DNP  510
C        INITIALIZATION                                                 DNP  520
    3 F=X+X                                                             DNP  530
C                                                                       DNP  540
      DO 4 I=2,N                                                        DNP  550
    4 Y(I+1)=F*Y(I)-Y(I-1)                                              DNP  560
      RETURN                                                            DNP  570
      END                                                               DNP  580
```

Subroutines CNPS and DCNPS

These subroutines compute the value of a series expansion in Chebyshev polynomials. The Chebyshev polynomial $T_n(x)$ satisfies the recurrence equation

$$T_{n+1}(x) = 2x \cdot T_n(x) - T_{n-1}(x)$$

with starting values $T_0(x) = 1$, $T_1(x) = x$.

An n-term expansion in Chebyshev polynomials with coefficient vector $C = (c_1, \ldots, c_n)$ is evaluated by means of a backward iteration scheme:

$$\text{Arg} = 2x,\ H_1 = 0,\ H_0 = 0$$

$$\left.\begin{aligned} H_2 &= H_1 \\ H_1 &= H_0 \\ H_0 &= \text{Arg} \cdot H_1 - H_2 + c_{n-i+1} \\ Y &= (c_1 - H_2 + H_0)/2. \end{aligned}\right\} \text{ for } i = 1, \ldots, n$$

This gives result $Y(x) = \sum_{i=1}^{n} c_i T_{i-1}(x)$.

Calculation is bypassed in case of a nonpositive value of the dimension n.

```
C                                                                       CNPS  10
C     ...................................................................CNPS  20
C                                                                       CNPS  30
C        SUBROUTINE CNPS                                                CNPS  40
C                                                                       CNPS  50
C        PURPOSE                                                        CNPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN CHEBYSHEV      CNPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. CNPS  80
C                                                                       CNPS  90
C        USAGE                                                          CNPS 100
C           CALL CNPS(Y,X,C,N)                                          CNPS 110
C                                                                       CNPS 120
C        DESCRIPTION OF PARAMETERS                                      CNPS 130
C           Y      - RESULT VALUE                                       CNPS 140
C           X      - ARGUMENT VALUE                                     CNPS 150
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              CNPS 160
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          CNPS 170
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  CNPS 180
C                                                                       CNPS 190
C        REMARKS                                                        CNPS 200
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 CNPS 210
C                                                                       CNPS 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CNPS 230
C           NONE                                                        CNPS 240
C                                                                       CNPS 250
C        METHOD                                                         CNPS 260
C           DEFINITION                                                  CNPS 270
C           Y=SUM(C(I)*T(I-1,X), SUMMED OVER I FROM 1 TO N).            CNPS 280
C           EVALUATION IS DONE BY MEANS OF BACKWARD RECURSION           CNPS 290
C           USING THE RECURRENCE EQUATION FOR CHEBYSHEV POLYNOMIALS     CNPS 300
C           T(N+1,X)=2*X*T(N,X)-T(N-1,X).                               CNPS 310
C                                                                       CNPS 320
C     ...................................................................CNPS 330
C                                                                       CNPS 340
      SUBROUTINE CNPS(Y,X,C,N)                                          CNPS 350
C                                                                       CNPS 360
      DIMENSION C(1)                                                    CNPS 370
C                                                                       CNPS 380
C        TEST OF DIMENSION                                              CNPS 390
      IF(N)1,1,2                                                        CNPS 400
    1 RETURN                                                            CNPS 410
C                                                                       CNPS 420
    2 IF(N-2)3,4,4                                                      CNPS 430
    3 Y=C(1)                                                            CNPS 440
      RETURN                                                            CNPS 450
C                                                                       CNPS 460
C        INITIALIZATION                                                 CNPS 470
    4 ARG=X+X                                                           CNPS 480
      H1=0.                                                             CNPS 490
      H0=0.                                                             CNPS 500
C                                                                       CNPS 510
      DO 5 I=1,N                                                        CNPS 520
      K=N-I                                                             CNPS 530
      H2=H1                                                             CNPS 540
      H1=H0                                                             CNPS 550
    5 H0=ARG*H1-H2+C(K+1)                                               CNPS 560
      Y=0.5*(C(1)-H2+H0)                                                CNPS 570
      RETURN                                                            CNPS 580
      END                                                               CNPS 590
```

```
C                                                                       DNPS  10
C     ...................................................................DNPS  20
C                                                                       DNPS  30
C        SUBROUTINE DCNPS                                               DNPS  40
C                                                                       DNPS  50
C        PURPOSE                                                        DNPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN CHEBYSHEV      DNPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. DNPS  80
C                                                                       DNPS  90
C        USAGE                                                          DNPS 100
C           CALL DCNPS(Y,X,C,N)                                         DNPS 110
C                                                                       DNPS 120
C        DESCRIPTION OF PARAMETERS                                      DNPS 130
C           Y      - RESULT VALUE                                       DNPS 140
C                    DOUBLE PRECISION VARIABLE                          DNPS 150
C           X      - ARGUMENT VALUE                                     DNPS 160
C                    DOUBLE PRECISION VARIABLE                          DNPS 170
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              DNPS 180
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DNPS 190
C                    DOUBLE PRECISION VECTOR                            DNPS 200
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  DNPS 210
C                                                                       DNPS 220
C        REMARKS                                                        DNPS 230
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 DNPS 240
C                                                                       DNPS 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DNPS 260
C           NONE                                                        DNPS 270
C                                                                       DNPS 280
C        METHOD                                                         DNPS 290
C           DEFINITION                                                  DNPS 300
C           Y=SUM(C(I)*T(I-1,X), SUMMED OVER I FROM 1 TO N).            DNPS 310
C           EVALUATION IS DONE BY MEANS OF BACKWARD RECURSION           DNPS 320
C           USING THE RECURRENCE EQUATION FOR CHEBYSHEV POLYNOMIALS     DNPS 330
C           T(N+1,X)=2*X*T(N,X)-T(N-1,X).                               DNPS 340
C                                                                       DNPS 350
C     ...................................................................DNPS 360
      SUBROUTINE DCNPS(Y,X,C,N)                                         DNPS 370
C                                                                       DNPS 380
      DIMENSION C(1)                                                    DNPS 390
      DOUBLE PRECISION C,Y,X,H0,H1,H2,ARG                               DNPS 400
C                                                                       DNPS 410
C        TEST OF DIMENSION                                              DNPS 420
      IF(N)1,1,2                                                        DNPS 430
    1 RETURN                                                            DNPS 440
C                                                                       DNPS 450
    2 IF(N-2)3,4,4                                                      DNPS 460
    3 Y=C(1)                                                            DNPS 470
      RETURN                                                            DNPS 480
C                                                                       DNPS 490
C        INITIALIZATION                                                 DNPS 500
    4 ARG=X+X                                                           DNPS 510
      H1=0.D0                                                           DNPS 520
      H0=0.D0                                                           DNPS 530
C                                                                       DNPS 540
      DO 5 I=1,N                                                        DNPS 550
      K=N-I                                                             DNPS 560
      H2=H1                                                             DNPS 570
      H1=H0                                                             DNPS 580
    5 H0=ARG*H1-H2+C(K+1)                                               DNPS 590
      Y=0.5D0*(C(1)-H2+H0)                                              DNPS 600
      RETURN                                                            DNPS 610
      END                                                               DNPS 620
                                                                        DNPS 630
```

Subroutines TCNP and DTCNP

These subroutines transform a given series expansion in Chebyshev polynomials to a polynomial. The independent variable x of the given expansion is thereby substituted by the independent variable z of the resulting polynomial using the linear transformation $x = A * z + B$ or $z = (x - B)/A$.

This means:
$$\sum_{i=1}^{N} C_i * T_{i-1}(A * z + B)$$

$$= \sum_{i=1}^{N} POL_i * z^{i-1}$$

Calculation is bypassed in case of a nonpositive value of the dimension N.

The range (-1, +1) in x is transformed to the range (z_l, z_r) in z with $z_l = -(1+B)/A$ and $z_r = (1-B)/A$, or vice versa, $A = 2/(z_r - z_l)$ and $B = -(z_r + z_l)/(z_r - z_l)$.

The Chebyshev polynomial $T_n(x)$ satisfies the recurrence equation

$$T_{n+1}(x) = 2x \cdot T_n(x) - T_{n-1}(x)$$

with starting values $T_0(x) = 1$, $T_1(x) = x$. The transformation is performed by means of a forward iteration scheme:

1. The coefficient vector of the Chebyshev polynomial $T_i(x)$ is calculated from the coefficient vectors of $T_{i-1}(x)$, $T_{i-2}(x)$ using the recurrence equation, for i = 3, ..., N.

2. The resulting polynomial coefficient vector is obtained by summation of c_i times coefficient vector of $T_{i-1}(x)$ over i, for i = 1, ..., N.

```
C                                                                       TCNP  10
C     ...................................................................TCNP  20
C                                                                       TCNP  30
C        SUBROUTINE TCNP                                                TCNP  40
C                                                                       TCNP  50
C        PURPOSE                                                        TCNP  60
C           A SERIES EXPANSION IN CHEBYSHEV POLYNOMIALS WITH INDEPENDENTTCNP  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  TCNP  80
C           VARIABLE Z, WHERE X=A*Z+B.                                  TCNP  90
C                                                                       TCNP 100
C        USAGE                                                          TCNP 110
C           CALL TCNP(A,B,POL,N,C,WORK)                                 TCNP 120
C                                                                       TCNP 130
C        DESCRIPTION OF PARAMETERS                                      TCNP 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONTCNP 150
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION       TCNP 160
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) TCNP 170
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          TCNP 180
C           N      - DIMENSION OF COEFFICIENT VECTORS POL AND C         TCNP 190
C           C      - GIVEN COEFFICIENT VECTOR OF EXPANSION              TCNP 200
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          TCNP 210
C                    POL AND C MAY BE IDENTICALLY LOCATED               TCNP 220
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   TCNP 230
C                                                                       TCNP 240
C        REMARKS                                                        TCNP 250
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    TCNP 260
C           WITH COEFFICIENT VECTOR POL.                                TCNP 270
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                TCNP 280
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSTCNP 290
C           THE RANGE (-1,+1) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE     TCNP 300
C           ZL=-(1+B)/A AND ZR=(1-B)/A.                                 TCNP 310
C           FOR GIVEN ZL, ZR WE HAVE A=2/(ZR-ZL) AND B=-(ZR+ZL)/(ZR-ZL) TCNP 320
C                                                                       TCNP 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TCNP 340
C           NONE                                                        TCNP 350
C                                                                       TCNP 360
C        METHOD                                                         TCNP 370
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      TCNP 380
C           FOR CHEBYSHEV POLYNOMIALS T(N,X)                            TCNP 390
C           T(N+1,X)=2*X*T(N,X)-T(N-1,X),                               TCNP 400
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              TCNP 410
C           THE SECOND IS THE ARGUMENT.                                 TCNP 420
C           STARTING VALUES ARE T(0,X)=1, T(1,X)=X.                     TCNP 430
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        TCNP 440
C           X = A*Z+B TOGETHER WITH                                     TCNP 450
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             TCNP 460
C           =SUM(C(I)*T(I-1,X), SUMMED OVER I FROM 1 TO N).             TCNP 470
C                                                                       TCNP 480
C     ...................................................................TCNP 490
C                                                                       TCNP 500
      SUBROUTINE TCNP(A,B,POL,N,C,WORK)                                 TCNP 510
C                                                                       TCNP 520
      DIMENSION POL(1),C(1),WORK(1)                                     TCNP 530
C                                                                       TCNP 540
C        TEST OF DIMENSION                                              TCNP 550
      IF(N-1)2,1,3                                                      TCNP 560
C                                                                       TCNP 570
C        DIMENSION LESS THAN 2                                          TCNP 580
    1 POL(1)=C(1)                                                       TCNP 590
    2 RETURN                                                            TCNP 600
C                                                                       TCNP 610
    3 POL(1)=C(1)+C(2)*B                                                TCNP 620
      POL(2)=C(2)*A                                                     TCNP 630
      IF(N-2)2,2,4                                                      TCNP 640
C                                                                       TCNP 650
C        INITIALIZATION                                                 TCNP 660
    4 WORK(1)=1.                                                        TCNP 670
      WORK(2)=B                                                         TCNP 680
      WORK(3)=0.                                                        TCNP 690
      WORK(4)=A                                                         TCNP 700
      XO=A*A                                                            TCNP 710
      XO=B+B                                                            TCNP 720
C                                                                       TCNP 730
C        CALCULATE COEFFICIENT VECTOR OF NEXT CHEBYSHEV POLYNOMIAL      TCNP 740
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              TCNP 750
      DO 6 J=3,N                                                        TCNP 760
      P=0.                                                              TCNP 770
C                                                                       TCNP 780
      DO 5 K=2,J                                                        TCNP 790
      H=P-WORK(2*K-3)+XO*WORK(2*K-2)                                    TCNP 800
      P=WORK(2*K-2)                                                     TCNP 810
      WORK(2*K-2)=H                                                     TCNP 820
      WORK(2*K-3)=P                                                     TCNP 830
      POL(K-1)=POL(K-1)+H*C(J)                                          TCNP 840
    5 P=XO*P                                                            TCNP 850
      WORK(2*J-1)=0.                                                    TCNP 860
      WORK(2*J)=P                                                       TCNP 870
    6 POL(J)=C(J)*P                                                     TCNP 880
      RETURN                                                            TCNP 890
      END                                                               TCNP 900
```

```
C                                                                       DTCN  10
C     ...................................................................DTCN  20
C                                                                       DTCN  30
C        SUBROUTINE DTCNP                                               DTCN  40
C                                                                       DTCN  50
C        PURPOSE                                                        DTCN  60
C           A SERIES EXPANSION IN CHEBYSHEV POLYNOMIALS WITH INDEPENDENTDTCN  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  DTCN  80
C           VARIABLE Z, WHERE X=A*Z+B.                                  DTCN  90
C                                                                       DTCN 100
C        USAGE                                                          DTCN 110
C           CALL DTCNP(A,B,POL,N,C,WORK)                                DTCN 120
C                                                                       DTCN 130
C        DESCRIPTION OF PARAMETERS                                      DTCN 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONDTCN 150
C                    DOUBLE PRECISION VARIABLE                          DTCN 160
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION       DTCN 170
C                    DOUBLE PRECISION VARIABLE                          DTCN 180
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) DTCN 190
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTCN 200
C                    DOUBLE PRECISION VECTOR                            DTCN 210
C           N      - DIMENSION OF COEFFICIENT VECTORS POL AND C         DTCN 220
C           C      - GIVEN COEFFICIENT VECTOR OF EXPANSION              DTCN 230
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTCN 240
C                    POL AND C MAY BE IDENTICALLY LOCATED               DTCN 250
C                    DOUBLE PRECISION VECTOR                            DTCN 260
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   DTCN 270
C                    DOUBLE PRECISION ARRAY                             DTCN 280
C                                                                       DTCN 290
C        REMARKS                                                        DTCN 300
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    DTCN 310
C           WITH COEFFICIENT VECTOR POL.                                DTCN 320
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                DTCN 330
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSDTCN 340
C           THE RANGE (-1,+1) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE     DTCN 350
C           ZL=-(1+B)/A AND ZR=(1-B)/A.                                 DTCN 360
C           FOR GIVEN ZL, ZR WE HAVE A=2/(ZR-ZL) AND B=-(ZR+ZL)/(ZR-ZL) DTCN 370
C                                                                       DTCN 380
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTCN 390
C           NONE                                                        DTCN 400
C                                                                       DTCN 410
C        METHOD                                                         DTCN 420
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      DTCN 430
C           FOR CHEBYSHEV POLYNOMIALS T(N,X)                            DTCN 440
C           T(N+1,X)=2*X*T(N,X)-T(N-1,X),                               DTCN 450
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              DTCN 460
C           THE SECOND IS THE ARGUMENT.                                 DTCN 470
C           STARTING VALUES ARE T(0,X)=1, T(1,X)=X.                     DTCN 480
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        DTCN 490
C           X = A*Z+B TOGETHER WITH                                     DTCN 500
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             DTCN 510
C           =SUM(C(I)*T(I-1,X), SUMMED OVER I FROM 1 TO N).             DTCN 520
C                                                                       DTCN 530
C     ...................................................................DTCN 540
C                                                                       DTCN 550
      SUBROUTINE DTCNP(A,B,POL,N,C,WORK)                                DTCN 560
C                                                                       DTCN 570
      DIMENSION POL(1),C(1),WORK(1)                                     DTCN 580
      DOUBLE PRECISION A,B,POL,C,WORK,H,P,XO,X0                         DTCN 590
C                                                                       DTCN 600
C        TEST OF DIMENSION                                              DTCN 610
      IF(N-1)2,1,3                                                      DTCN 620
C                                                                       DTCN 630
C        DIMENSION LESS THAN 2                                          DTCN 640
    1 POL(1)=C(1)                                                       DTCN 650
    2 RETURN                                                            DTCN 660
C                                                                       DTCN 670
    3 POL(1)=C(1)+C(2)*B                                                DTCN 680
      POL(2)=C(2)*A                                                     DTCN 690
      IF(N-2)2,2,4                                                      DTCN 700
C                                                                       DTCN 710
C        INITIALIZATION                                                 DTCN 720
    4 WORK(1)=1.D0                                                      DTCN 730
      WORK(2)=B                                                         DTCN 740
      WORK(3)=0.D0                                                      DTCN 750
      WORK(4)=A                                                         DTCN 760
      XO=A+A                                                            DTCN 770
      XO=B+B                                                            DTCN 780
C                                                                       DTCN 790
```

```
C        CALCULATE COEFFICIENT VECTOR OF NEXT CHEBYSHEV POLYNOMIAL      DTCN 800
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              DTCN 810
      DO 6 J=3,N                                                        DTCN 820
      P=0.00                                                            DTCN 830
C                                                                       DTCN 840
      DO 5 K=2,J                                                        DTCN 850
      H=P-WORK(2*K-3)+XO*WORK(2*K-2)                                    DTCN 860
      P=WORK(2*K-2)                                                     DTCN 870
      WORK(2*K-2)=H                                                     DTCN 880
      WORK(2*K-3)=P                                                     DTCN 890
      POL(K-1)=POL(K-1)+H*C(J)                                          DTCN 900
    5 P=XO*P                                                            DTCN 910
      WORK(2*J-1)=0.00                                                  DTCN 920
      WORK(2*J)=P                                                       DTCN 930
    6 POL(J)=C(J)*P                                                     DTCN 940
      RETURN                                                            DTCN 950
      END                                                               DTCN 960
```

Subroutines CSP and DCSP

These subroutines compute the values of the shifted Chebyshev polynomials for a given argument x and orders zero up to N. The shifted Chebyshev polynomial satisfies the recurrence equation.

$$T^S_{n+1}(x) = 2\ (2\ x-1)\ T^S_n(x) - T^S_{n-1}(x)$$

with starting values $T^S_0(x) = 1$, $T^S_1(x) = 2 \cdot x - 1$. From this equation, it follows immediately that roundoff errors grow at worst linearly under the tacit assumption that the argument values are between zero and one.

If e_{n+r} is the error in $T^S_{n+r}(x)$ due to a single rounding error e in $T^S_n(x)$:

$$e_{n+r+1} = 2\ (2\ x-1)\ e_{n+r} - e_{n+r-1}$$

with initial conditions $e_n = e$, $e_{n-1} = 0$.

The solution of this difference equation has its maximum for x = 1 or x = 0.

$$e_{n-1} = 0,\ e_n = e,\ \left|e_{n+1}\right| = 2e,\ \ldots,\ \left|e_{n+r}\right|$$

$$= (1 + r)\ e.$$

The order is assumed to be zero for negative values of N.

```
C                                                                       CSP   10
C     ..................................................................CSP   20
C                                                                       CSP   30
C        SUBROUTINE CSP                                                 CSP   40
C                                                                       CSP   50
C        PURPOSE                                                        CSP   60
C           COMPUTE THE VALUES OF THE SHIFTED CHEBYSHEV POLYNOMIALS     CSP   70
C           TS(N,X) FOR ARGUMENT X AND ORDERS 0 UP TO N.                CSP   80
C                                                                       CSP   90
C        USAGE                                                          CSP  100
C           CALL CSP(Y,X,N)                                             CSP  110
C                                                                       CSP  120
C        DESCRIPTION OF PARAMETERS                                      CSP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESCSP  140
C                    OF SHIFTED CHEBYSHEV POLYNOMIALS OF ORDER 0 UP TO N CSP  150
C                    FOR GIVEN ARGUMENT X.                              CSP  160
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          CSP  170
C           X      - ARGUMENT OF SHIFTED CHEBYSHEV POLYNOMIAL          CSP  180
C           N      - ORDER OF SHIFTED CHEBYSHEV POLYNOMIAL             CSP  190
C                                                                       CSP  200
C        REMARKS                                                        CSP  210
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     CSP  220
C                                                                       CSP  230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CSP  240
C           NONE                                                        CSP  250
C                                                                       CSP  260
C        METHOD                                                         CSP  270
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          CSP  280
C           SHIFTED CHEBYSHEV POLYNOMIALS TS(N,X)                       CSP  290
C           TS(N+1,X)=(4*X-2)*TS(N,X)-TS(N-1,X),                        CSP  300
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              CSP  310
C           THE SECOND IS THE ARGUMENT.                                 CSP  320
C           STARTING VALUES ARE TS(0,X)=1, TS(1,X)=2*X-1.               CSP  330
C                                                                       CSP  340
C     ..................................................................CSP  350
C                                                                       CSP  360
      SUBROUTINE CSP(Y,X,N)                                             CSP  370
C                                                                       CSP  380
      DIMENSION Y(1)                                                    CSP  390
C                                                                       CSP  400
C        TEST OF ORDER                                                  CSP  410
      Y(1)=1.                                                           CSP  420
      IF(N)1,1,2                                                        CSP  430
    1 RETURN                                                            CSP  440
C                                                                       CSP  450
    2 Y(2)=X+X-1.                                                       CSP  460
      IF(N-1)1,1,3                                                      CSP  470
C                                                                       CSP  480
C        INITIALIZATION                                                 CSP  490
    3 F=Y(2)+Y(2)                                                       CSP  500
C                                                                       CSP  510
      DO 4 I=2,N                                                        CSP  520
    4 Y(I+1)=F*Y(I)-Y(I-1)                                              CSP  530
      RETURN                                                            CSP  540
      END                                                               CSP  550
```

```
C                                                                       DSP  10
C     ...................................................................DSP  20
C                                                                       DSP  30
C        SUBROUTINE DCSP                                                DSP  40
C                                                                       DSP  50
C        PURPOSE                                                        DSP  60
C           COMPUTE THE VALUES OF THE SHIFTED CHEBYSHEV POLYNOMIALS     DSP  70
C           TS(N,X) FOR ARGUMENT X AND ORDERS 0 UP TO N.                DSP  80
C                                                                       DSP  90
C        USAGE                                                          DSP 100
C           CALL DCSP(Y,X,N)                                            DSP 110
C                                                                       DSP 120
C        DESCRIPTION OF PARAMETERS                                      DSP 130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESDSP 140
C                    OF SHIFTED CHEBYSHEV POLYNOMIALS OF ORDER 0 UP TO N DSP 150
C                    FOR GIVEN ARGUMENT X.                              DSP 160
C                    DOUBLE PRECISION VECTOR.                           DSP 170
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          DSP 180
C           X      - ARGUMENT OF SHIFTED CHEBYSHEV POLYNOMIAL           DSP 190
C                    DOUBLE PRECISION VARIABLE.                         DSP 200
C           N      - ORDER OF SHIFTED CHEBYSHEV POLYNOMIAL              DSP 210
C                                                                       DSP 220
C        REMARKS                                                        DSP 230
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     DSP 240
C                                                                       DSP 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DSP 260
C           NONE                                                        DSP 270
C                                                                       DSP 280
C        METHOD                                                         DSP 290
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          DSP 300
C           SHIFTED CHEBYSHEV POLYNOMIALS TS(N,X)                       DSP 310
C           TS(N+1,X)=(4*X-2)*TS(N,X)-TS(N-1,X),                        DSP 320
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              DSP 330
C           THE SECOND IS THE ARGUMENT.                                 DSP 340
C           STARTING VALUES ARE TS(0,X)=1, TS(1,X)=2*X-1.               DSP 350
C                                                                       DSP 360
C     ...................................................................DSP 370
C                                                                       DSP 380
      SUBROUTINE DCSP(Y,X,N)                                            DSP 390
C                                                                       DSP 400
      DIMENSION Y(1)                                                    DSP 410
      DOUBLE PRECISION Y,X,F                                            DSP 420
C                                                                       DSP 430
C        TEST OF ORDER                                                  DSP 440
      Y(1)=1.D0                                                         DSP 450
      IF(N)1,1,2                                                        DSP 460
    1 RETURN                                                            DSP 470
C                                                                       DSP 480
    2 Y(2)=X+X-1.D0                                                     DSP 490
      IF(N-1)1,1,3                                                      DSP 500
C                                                                       DSP 510
C        INITIALIZATION                                                 DSP 520
    3 F=Y(2)+Y(2)                                                       DSP 530
C                                                                       DSP 540
      DO 4 I=2,N                                                        DSP 550
    4 Y(I+1)=F*Y(I)-Y(I-1)                                              DSP 560
      RETURN                                                            DSP 570
      END                                                               DSP 580
```

Subroutines CSPS and DCSPS

These subroutines compute the value of a series expansion in shifted Chebyshev polynomials. The shifted Chebyshev polynomial $T^S_n(x)$ satisfies the recurrence equation

$$T^S_{n+1}(x) = 2\,(2x-1)\,T^S_n(x) - T^S_{n-1}(x)$$

with starting values $T^S_0(x) = 1$, $T^S_1(x) = 2x - 1$.

An n-term expansion in shifted Chebyshev polynomials with coefficient vector $C = (c_1, \ldots, c_n)$ is evaluated by means of a backward iteration scheme:

$$\text{Arg} = 4x - 2,\quad H_1 = 0,\quad H_0 = 0$$

$$\left.\begin{aligned} H_2 &= H_1 \\ H_1 &= H_0 \\ H_0 &= \text{Arg} \cdot H_1 - H_2 + c_{n-i+1} \\ Y &= (c_1 - H_2 + H_0)/2. \end{aligned}\right\} \text{ for } i = 1, \ldots, n$$

This gives the result $Y(x) = \sum_{i=1}^{n} c_i\, T^S_{i-1}(x)$.

Calculation is bypassed in case of a nonpositive value of the dimension n.

```
C                                                                       CSPS  10
C     ...................................................................CSPS  20
C                                                                       CSPS  30
C        SUBROUTINE CSPS                                                CSPS  40
C                                                                       CSPS  50
C        PURPOSE                                                        CSPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN SHIFTED        CSPS  70
C           CHEBYSHEV POLYNOMIALS WITH COEFFICIENT VECTOR C             CSPS  80
C           FOR ARGUMENT VALUE X.                                       CSPS  90
C                                                                       CSPS 100
C        USAGE                                                          CSPS 110
C           CALL CSPS(Y,X,C,N)                                          CSPS 120
C                                                                       CSPS 130
C        DESCRIPTION OF PARAMETERS                                      CSPS 140
C           Y      - RESULT VALUE                                       CSPS 150
C           X      - ARGUMENT VALUE                                     CSPS 160
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              CSPS 170
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          CSPS 180
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  CSPS 190
C                                                                       CSPS 200
C        REMARKS                                                        CSPS 210
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 CSPS 220
C                                                                       CSPS 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CSPS 240
C           NONE                                                        CSPS 250
C                                                                       CSPS 260
C        METHOD                                                         CSPS 270
C           DEFINITION                                                  CSPS 280
C           Y=SUM(C(I)*TS(I-1,X), SUMMED OVER I FROM 1 TO N).           CSPS 290
C           EVALUATION IS DONE BY MEANS OF BACKWARD RECURSION           CSPS 300
C           USING THE RECURRENCE EQUATION FOR SHIFTED                   CSPS 310
C           CHEBYSHEV POLYNOMIALS                                       CSPS 320
C           TS(N+1,X)=(4*X-2)*TS(N,X)-TS(N-1,X).                        CSPS 330
C                                                                       CSPS 340
C     ...................................................................CSPS 350
C                                                                       CSPS 360
      SUBROUTINE CSPS(Y,X,C,N)                                          CSPS 370
C                                                                       CSPS 380
      DIMENSION C(1)                                                    CSPS 390
C                                                                       CSPS 400
C        TEST OF DIMENSION                                              CSPS 410
      IF(N)1,1,2                                                        CSPS 420
    1 RETURN                                                            CSPS 430
C                                                                       CSPS 440
    2 IF(N-2)3,4,4                                                      CSPS 450
    3 Y=C(1)                                                            CSPS 460
      RETURN                                                            CSPS 470
C                                                                       CSPS 480
C        INITIALIZATION                                                 CSPS 490
    4 ARG=X+X-1.                                                        CSPS 500
      ARG=ARG+ARG                                                       CSPS 510
      H1=0.                                                             CSPS 520
      H0=0.                                                             CSPS 530
C                                                                       CSPS 540
      DO 5 I=1,N                                                        CSPS 550
      K=N-I                                                             CSPS 560
      H2=H1                                                             CSPS 570
      H1=H0                                                             CSPS 580
    5 H0=ARG*H1-H2+C(K+1)                                               CSPS 590
      Y=0.5*(C(1)-H2+H0)                                                CSPS 600
      RETURN                                                            CSPS 610
      END                                                               CSPS 620
```

```
C                                                                       DSPS  10
C  ...................................................................DSPS  20
C                                                                       DSPS  30
C     SUBROUTINE DCSPS                                                  DSPS  40
C                                                                       DSPS  50
C     PURPOSE                                                           DSPS  60
C        COMPUTES THE VALUE OF AN N-TERM EXPANSION IN SHIFTED           DSPS  70
C        CHEBYSHEV POLYNOMIALS WITH COEFFICIENT VECTOR C                DSPS  80
C        FOR ARGUMENT VALUE X.                                          DSPS  90
C                                                                       DSPS 100
C     USAGE                                                             DSPS 110
C        CALL DCSPS(Y,X,C,N)                                            DSPS 120
C                                                                       DSPS 130
C     DESCRIPTION OF PARAMETERS                                         DSPS 140
C        Y      - RESULT VALUE                                         DSPS 150
C                 DOUBLE PRECISION VARIABLE                            DSPS 160
C        X      - ARGUMENT VALUE                                       DSPS 170
C                 DOUBLE PRECISION VARIABLE                            DSPS 180
C        C      - COEFFICIENT VECTOR OF GIVEN EXPANSION                DSPS 190
C                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH            DSPS 200
C                 DOUBLE PRECISION VECTOR                              DSPS 210
C        N      - DIMENSION OF COEFFICIENT VECTOR C                    DSPS 220
C                                                                       DSPS 230
C     REMARKS                                                           DSPS 240
C        OPERATION IS BYPASSED IN CASE N LESS THAN 1                    DSPS 250
C                                                                       DSPS 260
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DSPS 270
C        NONE                                                           DSPS 280
C                                                                       DSPS 290
C     METHOD                                                            DSPS 300
C        DEFINITION                                                     DSPS 310
C        Y=SUM(C(I)*TS(I-1,X), SUMMED OVER I FROM 1 TO N).              DSPS 320
C        EVALUATION IS DONE BY MEANS OF BACKWARD RECURSION              DSPS 330
C        USING THE RECURRENCE EQUATION FOR SHIFTED                      DSPS 340
C        CHEBYSHEV POLYNOMIALS                                          DSPS 350
C        TS(N+1,X)=(4*X-2)*TS(N,X)-TS(N-1,X).                           DSPS 360
C                                                                       DSPS 370
C  ...................................................................DSPS 380
C                                                                       DSPS 390
      SUBROUTINE DCSPS(Y,X,C,N)                                         DSPS 400
C                                                                       DSPS 410
      DIMENSION C(1)                                                    DSPS 420
      DOUBLE PRECISION C,Y,X,H0,H1,H2,ARG                               DSPS 430
C                                                                       DSPS 440
C        TEST OF DIMENSION                                              DSPS 450
      IF(N)1,1,2                                                        DSPS 460
    1 RETURN                                                            DSPS 470
C                                                                       DSPS 480
    2 IF(N-2)3,4,4                                                      DSPS 490
    3 Y=C(1)                                                            DSPS 500
      RETURN                                                            DSPS 510
C                                                                       DSPS 520
C        INITIALIZATION                                                 DSPS 530
    4 ARG=X+X-1.D0                                                      DSPS 540
      ARG=ARG+ARG                                                       DSPS 550
      H1=0.D0                                                           DSPS 560
      H0=0.D0                                                           DSPS 570
      DO 5 I=1,N                                                        DSPS 580
      K=N-I                                                             DSPS 590
      H2=H1                                                             DSPS 600
      H1=H0                                                             DSPS 610
    5 H0=ARG*H1-H2+C(K+1)                                               DSPS 620
      Y=0.5D0*(C(1)-H2+H0)                                              DSPS 630
      RETURN                                                            DSPS 640
      END                                                               DSPS 650
```

Subroutines TCSP and DTCSP

These subroutines transform a given series expansion in shifted Chebyshev polynomials to a polynomial. The independent variable x of the given expansion is thereby substituted by the independent variable z of the resulting polynomial using the linear transformation x = A * z + B or z = (x - B)/A.

This means:
$$\sum_{i=1}^{N} C_i * T^S_{i-1}(A * z + B)$$
$$= \sum_{i=1}^{N} POL_i * z^{i-1}$$

Calculation is bypassed in case of a nonpositive value of the dimension N.

The range (0, +1) in x is transformed to the range (z_l, z_r) in z with $z_l = -B/A$ and $z_r = (1-B)/A$ or vice versa, $A = 1/(z_r - z_l)$ and $B = -z_l/(z_r - z_l)$.

The shifted Chebyshev polynomial $T^S_n(x)$ satisfies the recurrence equation

$$T^S_{n+1}(x) = 4 \times T^S_n(x) - 2\, T^S_n(x) - T^S_{n-1}(x)$$

with starting values $T^S_0(x) = 1$, $T^S_1(x) = 2 x - 1$. The transformation is performed by means of a forward iteration scheme:

1. The coefficient vector of the shifted Chebyshev polynomial $T^S_i(x)$ is calculated from the coefficient vectors of $T^S_{i-1}(x)$, $T^S_{i-2}(x)$ using the recurrence equation, for i = 3, ..., N.

2. The resulting polynomial coefficient vector is obtained by summation of c_i times $T^S_{i-1}(x)$ over i, for i = 1, ..., N.

```
C                                                                       TCSP  10
C  ...................................................................TCSP  20
C                                                                       TCSP  30
C     SUBROUTINE TCSP                                                   TCSP  40
C                                                                       TCSP  50
C     PURPOSE                                                           TCSP  60
C        A SERIES EXPANSION IN SHIFTED CHEBYSHEV POLYNOMIALS WITH       TCSP  70
C        INDEPENDENT VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH     TCSP  80
C        INDEPENDENT VARIABLE Z, WHERE X=A*Z+B.                         TCSP  90
C                                                                       TCSP 100
C     USAGE                                                             TCSP 110
C        CALL TCSP(A,B,POL,N,C,WORK)                                    TCSP 120
C                                                                       TCSP 130
C     DESCRIPTION OF PARAMETERS                                         TCSP 140
C        A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATION  TCSP 150
C        B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION          TCSP 160
C        POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE)    TCSP 170
C                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH             TCSP 180
C        N      - DIMENSION OF COEFFICIENT VECTORS POL AND C            TCSP 190
C        C      - GIVEN COEFFICIENT VECTOR OF EXPANSION                 TCSP 200
C                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH             TCSP 210
C                 POL AND C MAY BE IDENTICALLY LOCATED                  TCSP 220
C        WORK   - WORKING STORAGE OF DIMENSION 2*N                      TCSP 230
C                                                                       TCSP 240
C     REMARKS                                                           TCSP 250
C        COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING       TCSP 260
C        WITH COEFFICIENT VECTOR POL.                                   TCSP 270
C        OPERATION IS BYPASSED IN CASE N LESS THAN 1.                   TCSP 280
C        THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMS   TCSP 290
C        THE RANGE (0,1) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE          TCSP 300
C        ZL=-B/A AND ZR=(1-B)/A.                                        TCSP 310
C        FOR GIVEN ZL, ZR WE HAVE A=1/(ZR-ZL) AND B=-ZL/(ZR-ZL).        TCSP 320
C                                                                       TCSP 330
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     TCSP 340
C        NONE                                                           TCSP 350
C                                                                       TCSP 360
C     METHOD                                                            TCSP 370
C        THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION FOR     TCSP 380
C        SHIFTED CHEBYSHEV POLYNOMIALS TS(N,X)                          TCSP 390
C        TS(N+1,X)=(4*X-2)*TS(N,X)-TS(N-1,X),                           TCSP 400
C        WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,                 TCSP 410
C        THE SECOND IS THE ARGUMENT.                                    TCSP 420
```

```
C           STARTING VALUES ARE TS(0,X)=1, TS(1,X)=2*X-1.                   TCSP 430
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF            TCSP 440
C           X=A*Z+B TOGETHER WITH                                           TCSP 450
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)                 TCSP 460
C           =SUM(C(I)*TS(I-1,X), SUMMED OVER I FROM 1 TO N).                TCSP 470
C                                                                           TCSP 480
C   ..........................................................              TCSP 490
C                                                                           TCSP 500
      SUBROUTINE TCSP(A,B,POL,N,C,WORK)                                     TCSP 510
C                                                                           TCSP 520
      DIMENSION POL(1),C(1),WORK(1)                                         TCSP 530
C                                                                           TCSP 540
C        TEST OF DIMENSION                                                  TCSP 550
      IF(N-1)2,1,3                                                          TCSP 560
C                                                                           TCSP 570
C        DIMENSION LESS THAN 2                                              TCSP 580
    1 POL(1)=C(1)                                                           TCSP 590
    2 RETURN                                                                TCSP 600
C                                                                           TCSP 610
    3 XD=A+A                                                                TCSP 620
      X0=B+B-1.                                                             TCSP 630
      POL(1)=C(1)+C(2)*X0                                                   TCSP 640
      POL(2)=C(2)*XD                                                        TCSP 650
      IF(N-2)2,2,4                                                          TCSP 660
C                                                                           TCSP 670
C        INITIALIZATION                                                     TCSP 680
    4 WORK(1)=1.                                                            TCSP 690
      WORK(2)=X0                                                            TCSP 700
      WORK(3)=0.                                                            TCSP 710
      WORK(4)=XD                                                            TCSP 720
      XD=XD+XD                                                              TCSP 730
      X0=X0+X0                                                              TCSP 740
C                                                                           TCSP 750
C        CALCULATE COEFFICIENT VECTOR OF NEXT SHIFTED CHEBYSHEV             TCSP 760
C        POLYNOMIAL AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL       TCSP 770
      DO 6 J=3,N                                                            TCSP 780
      P=0.                                                                  TCSP 790
C                                                                           TCSP 800
      DO 5 K=2,J                                                            TCSP 810
      H=P-WORK(2*K-3)+X0*WORK(2*K-2)                                        TCSP 820
      P=WORK(2*K-2)                                                         TCSP 830
      WORK(2*K-2)=H                                                         TCSP 840
      WORK(2*K-3)=P                                                         TCSP 850
      POL(K-1)=POL(K-1)+H*C(J)                                              TCSP 860
    5 P=XD*P                                                                TCSP 870
      WORK(2*J-1)=0.                                                        TCSP 880
      WORK(2*J)=P                                                           TCSP 890
    6 POL(J)=C(J)*P                                                         TCSP 900
      RETURN                                                                TCSP 910
      END                                                                   TCSP 920
```

```
C                                                                           DTCS  10
C   ..........................................................              DTCS  20
C                                                                           DTCS  30
      SUBROUTINE DTCSP                                                      DTCS  40
C                                                                           DTCS  50
C     PURPOSE                                                               DTCS  60
C        A SERIES EXPANSION IN SHIFTED CHEBYSHEV POLYNOMIALS WITH           DTCS  70
C        INDEPENDENT VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH         DTCS  80
C        INDEPENDENT VARIABLE Z, WHERE X=A*Z+B.                             DTCS  90
C                                                                           DTCS 100
C     USAGE                                                                 DTCS 110
C        CALL DTCSP(A,B,POL,N,C,WORK)                                       DTCS 120
C                                                                           DTCS 130
C     DESCRIPTION OF PARAMETERS                                             DTCS 140
C        A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATION      DTCS 150
C                 DOUBLE PRECISION VARIABLE                                 DTCS 160
C        B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION              DTCS 170
C                 DOUBLE PRECISION VARIABLE                                 DTCS 180
C        POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE)        DTCS 190
C                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH                 DTCS 200
C                 DOUBLE PRECISION VECTOR                                   DTCS 210
C        N      - DIMENSION OF COEFFICIENT VECTORS POL AND C                DTCS 220
C        C      - GIVEN COEFFICIENT VECTOR OF EXPANSION                     DTCS 230
C                 POL AND C MAY BE IDENTICALLY LOCATED                      DTCS 240
C                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH                 DTCS 250
C                 DOUBLE PRECISION VECTOR                                   DTCS 260
C        WORK   - WORKING STORAGE OF DIMENSION 2*N                          DTCS 270
C                 DOUBLE PRECISION ARRAY                                    DTCS 280
C                                                                           DTCS 290
C     REMARKS                                                               DTCS 300
C        COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING           DTCS 310
C        WITH COEFFICIENT VECTOR POL.                                       DTCS 320
C        OPERATION IS BYPASSED IN CASE N LESS THAN 1.                       DTCS 330
C        THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)*(X-B) TRANSFORMS      DTCS 340
C        THE RANGE (0,1) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE              DTCS 350
C        ZL=-B/A AND ZR=(1-B)/A.                                            DTCS 360
C        FOR GIVEN ZL, ZR WE HAVE A=1/(ZR-ZL) AND B=-ZL/(ZR-ZL).            DTCS 370
C                                                                           DTCS 380
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                         DTCS 390
C        NONE                                                               DTCS 400
C                                                                           DTCS 410
C     METHOD                                                                DTCS 420
C        THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION FOR          DTCS 430
C        SHIFTED CHEBYSHEV POLYNOMIALS TS(N,X)                              DTCS 440
C        TS(N+1,X)=(4*X-2)*TS(N,X)-TS(N-1,X),                               DTCS 450
C        WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,                     DTCS 460
C        THE SECOND IS THE ARGUMENT.                                        DTCS 470
C        STARTING VALUES ARE TS(0,X)=1, TS(1,X)=2*X-1.                      DTCS 480
C        THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF               DTCS 490
C        X=A*Z+B TOGETHER WITH                                              DTCS 500
C        SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)                    DTCS 510
C        =SUM(C(I)*TS(I-1,X), SUMMED OVER I FROM 1 TO N).                   DTCS 520
C                                                                           DTCS 530
C   ..........................................................              DTCS 540
C                                                                           DTCS 550
      SUBROUTINE DTCSP(A,B,POL,N,C,WORK)                                    DTCS 560
C                                                                           DTCS 570
      DIMENSION POL(1),C(1),WORK(1)                                         DTCS 580
      DOUBLE PRECISION A,B,POL,C,WORK,H,P,XD,X0                             DTCS 590
C                                                                           DTCS 600
C        TEST OF DIMENSION                                                  DTCS 610
      IF(N-1)2,1,3                                                          DTCS 620
C                                                                           DTCS 630
C        DIMENSION LESS THAN 2                                              DTCS 640
    1 POL(1)=C(1)                                                           DTCS 650
    2 RETURN                                                                DTCS 660
C                                                                           DTCS 670
    3 XD=A+A                                                                DTCS 680
      X0=B+B-1.D0                                                           DTCS 690
      POL(1)=C(1)+C(2)*X0                                                   DTCS 700
      POL(2)=C(2)*XD                                                        DTCS 710
      IF(N-2)2,2,4                                                          DTCS 720
C                                                                           DTCS 730
C        INITIALIZATION                                                     DTCS 740
    4 WORK(1)=1.D0                                                          DTCS 750
      WORK(2)=X0                                                            DTCS 760
      WORK(3)=0.D0                                                          DTCS 770
      WORK(4)=XD                                                            DTCS 780
      XD=XD+XD                                                              DTCS 790
      X0=X0+X0                                                              DTCS 800
C                                                                           DTCS 810
C        CALCULATE COEFFICIENT VECTOR OF NEXT SHIFTED CHEBYSHEV             DTCS 820
C        POLYNOMIAL AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL       DTCS 830
      DO 6 J=3,N                                                            DTCS 840
      P=0.D0                                                                DTCS 850
C                                                                           DTCS 860
      DO 5 K=2,J                                                            DTCS 870
      H=P-WORK(2*K-3)+X0*WORK(2*K-2)                                        DTCS 880
      P=WORK(2*K-2)                                                         DTCS 890
      WORK(2*K-2)=H                                                         DTCS 900
      WORK(2*K-3)=P                                                         DTCS 910
      POL(K-1)=POL(K-1)+H*C(J)                                              DTCS 920
    5 P=XD*P                                                                DTCS 930
      WORK(2*J-1)=0.D0                                                      DTCS 940
      WORK(2*J)=P                                                           DTCS 950
    6 POL(J)=C(J)*P                                                         DTCS 960
      RETURN                                                                DTCS 970
      END                                                                   DTCS 980
```

Subroutines HEP and DHEP

These subroutines compute the values of the Hermite polynomials for a given argument x and orders zero up to N. The Hermite polynomial $H_n(x)$ satisfies the recurrence equation

$$H_{n+1}(x) = 2\,(x \cdot H_n(x) - n \cdot H_{n-1}(x))$$

with starting values $H_0(x) = 1$, $H_1(x) = 2\,x$.

The order is assumed to be zero for negative values of N.

```
C                                                                       HEP   10
C     ..................................................................HEP   20
C                                                                       HEP   30
C        SUBROUTINE HEP                                                 HEP   40
C                                                                       HEP   50
C        PURPOSE                                                        HEP   60
C           COMPUTE THE VALUES OF THE HERMITE POLYNOMIALS H(N,X)        HEP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  HEP   80
C                                                                       HEP   90
C        USAGE                                                          HEP  100
C           CALL HEP(Y,X,N)                                             HEP  110
C                                                                       HEP  120
C        DESCRIPTION OF PARAMETERS                                      HEP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESHEP  140
C                    OF HERMITE POLYNOMIALS OF ORDER 0 UP TO N          HEP  150
C                    FOR GIVEN ARGUMENT X.                              HEP  160
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          HEP  170
C           X      - ARGUMENT OF HERMITE POLYNOMIAL                    HEP  180
C           N      - ORDER OF HERMITE POLYNOMIAL                       HEP  190
C                                                                       HEP  200
C        REMARKS                                                        HEP  210
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     HEP  220
C                                                                       HEP  230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  HEP  240
C           NONE                                                        HEP  250
C                                                                       HEP  260
C        METHOD                                                         HEP  270
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          HEP  280
C           HERMITE POLYNOMIALS H(N,X)                                  HEP  290
C           H(N+1,X)=2*(X*H(N,X)-N*H(N-1,X))                            HEP  300
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              HEP  310
C           THE SECOND IS THE ARGUMENT.                                 HEP  320
C           STARTING VALUES ARE H(0,X)=1, H(1,X)=2*X.                   HEP  330
C                                                                       HEP  340
C     ..................................................................HEP  350
C                                                                       HEP  360
      SUBROUTINE HEP(Y,X,N)                                             HEP  370
C                                                                       HEP  380
      DIMENSION Y(1)                                                    HEP  390
C                                                                       HEP  400
C        TEST OF ORDER                                                  HEP  410
      Y(1)=1.                                                           HEP  420
      IF(N)1,1,2                                                        HEP  430
    1 RETURN                                                            HEP  440
C                                                                       HEP  450
    2 Y(2)=X+X                                                          HEP  460
      IF(N-1)1,1,3                                                      HEP  470
C                                                                       HEP  480
    3 DO 4 I=2,N                                                        HEP  490
      F=X*Y(I)-FLOAT(I-1)*Y(I-1)                                        HEP  500
    4 Y(I+1)=F+F                                                        HEP  510
      RETURN                                                            HEP  520
      END                                                               HEP  530
```

```
C                                                                       DHP   10
C     ..................................................................DHP   20
C                                                                       DHP   30
C        SUBROUTINE DHEP                                                DHP   40
C                                                                       DHP   50
C        PURPOSE                                                        DHP   60
C           COMPUTE THE VALUES OF THE HERMITE POLYNOMIALS H(N,X)        DHP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  DHP   80
C                                                                       DHP   90
C        USAGE                                                          DHP  100
C           CALL DHEP(Y,X,N)                                            DHP  110
C                                                                       DHP  120
C        DESCRIPTION OF PARAMETERS                                      DHP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESDHP  140
C                    OF HERMITE POLYNOMIALS OF ORDER 0 UP TO N          DHP  150
C                    FOR GIVEN ARGUMENT X.                              DHP  160
C                    DOUBLE PRECISION VECTOR.                           DHP  170
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          DHP  180
C           X      - ARGUMENT OF HERMITE POLYNOMIAL                    DHP  190
C                    DOUBLE PRECISION VARIABLE.                         DHP  200
C           N      - ORDER OF HERMITE POLYNOMIAL                       DHP  210
C                                                                       DHP  220
C        REMARKS                                                        DHP  230
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     DHP  240
C                                                                       DHP  250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DHP  260
C           NONE                                                        DHP  270
C                                                                       DHP  280
C        METHOD                                                         DHP  290
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          DHP  300
C           HERMITE POLYNOMIALS H(N,X)                                  DHP  310
C           H(N+1,X)=2*(X*H(N,X)-N*H(N-1,X))                            DHP  320
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              DHP  330
C           THE SECOND IS THE ARGUMENT.                                 DHP  340
C           STARTING VALUES ARE H(0,X)=1, H(1,X)=2*X.                   DHP  350
C                                                                       DHP  360
C     ..................................................................DHP  370
C                                                                       DHP  380
      SUBROUTINE DHEP(Y,X,N)                                            DHP  390
C                                                                       DHP  400
      DIMENSION Y(1)                                                    DHP  410
      DOUBLE PRECISION Y,X,F                                            DHP  420
C                                                                       DHP  430
C        TEST OF ORDER                                                  DHP  440
      Y(1)=1.D0                                                         DHP  450
      IF(N)1,1,2                                                        DHP  460
    1 RETURN                                                            DHP  470
C                                                                       DHP  480
    2 Y(2)=X+X                                                          DHP  490
      IF(N-1)1,1,3                                                      DHP  500
C                                                                       DHP  510
    3 DO 4 I=2,N                                                        DHP  520
      F=X*Y(I)-DFLOAT(I-1)*Y(I-1)                                       DHP  530
    4 Y(I+1)=F+F                                                        DHP  540
      RETURN                                                            DHP  550
      END                                                               DHP  560
```

Subroutines HEPS and DHEPS

These subroutines compute the value of a series expansion in Hermite polynomials. The Hermite polynomial $H_n(x)$ satisfies the recurrence equation

$$H_{n+1}(x) = 2\,(x \cdot H_n(x) - n \cdot H_{n-1}(x))$$

with starting values $H_0(x) = 1$, $H_1(x) = 2x$.

An n-term expansion in Hermite polynomials with coefficient vector $C = (c_1, \ldots, c_n)$ is evaluated by means of a forward iteration scheme:

$$\left.\begin{aligned} Y &= c_1,\ H_0 = 1,\ H_1 = 2 \cdot x \\ H_2 &= x \cdot H_1 - (i-1)\,H_0 \\ H_0 &= H_1 \\ H_1 &= H_2 + H_2 \\ Y &= Y + c_i \cdot H_0 \end{aligned}\right\} \quad \text{for } i = 2, \ldots, n$$

This gives the result $Y(x) = \sum_{i=1}^{n} c_i \cdot H_{i-1}(x)$.

Calculation is bypassed in case of a nonpositive value of the dimension n.

```
C                                                                       HEPS  10
C     .................................................................HEPS  20
C                                                                       HEPS  30
C        SUBROUTINE HEPS                                                HEPS  40
C                                                                       HEPS  50
C        PURPOSE                                                        HEPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN HERMITE        HEPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. HEPS  80
C                                                                       HEPS  90
C        USAGE                                                          HEPS 100
C           CALL HEPS(Y,X,C,N)                                          HEPS 110
C                                                                       HEPS 120
C        DESCRIPTION OF PARAMETERS                                      HEPS 130
C           Y      - RESULT VALUE                                       HEPS 140
C           X      - ARGUMENT VALUE                                     HEPS 150
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              HEPS 160
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          HEPS 170
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  HEPS 180
C                                                                       HEPS 190
C        REMARKS                                                        HEPS 200
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 HEPS 210
C                                                                       HEPS 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  HEPS 230
C           NONE                                                        HEPS 240
C                                                                       HEPS 250
C        METHOD                                                         HEPS 260
C           DEFINITION                                                  HEPS 270
C           Y=SUM(C(I)*H(I-1,X), SUMMED OVER I FROM 1 TO N).            HEPS 280
C           EVALUATION IS DONE BY MEANS OF UPWARD RECURSION             HEPS 290
C           USING THE RECURRENCE EQUATION FOR HERMITE POLYNOMIALS       HEPS 300
C           H(N+1,X)=2*(X*H(N,X)-N*H(N-1,X)).                           HEPS 310
C                                                                       HEPS 320
C     .................................................................HEPS 330
C                                                                       HEPS 340
      SUBROUTINE HEPS(Y,X,C,N)                                          HEPS 350
C                                                                       HEPS 360
      DIMENSION C(1)                                                    HEPS 370
C                                                                       HEPS 380
C        TEST OF DIMENSION                                              HEPS 390
      IF(N)1,1,2                                                        HEPS 400
    1 RETURN                                                            HEPS 410
C                                                                       HEPS 420
    2 Y=C(1)                                                            HEPS 430
      IF(N-2)1,3,3                                                      HEPS 440
C                                                                       HEPS 450
C        INITIALIZATION                                                 HEPS 460
    3 H0=1.                                                             HEPS 470
      H1=X+X                                                            HEPS 480
C                                                                       HEPS 490
      DO 4 I=2,N                                                        HEPS 500
      H2=X*H1-FLOAT(I-1)*H0                                             HEPS 510
      H0=H1                                                             HEPS 520
      H1=H2+H2                                                          HEPS 530
    4 Y=Y+C(I)*H0                                                       HEPS 540
      RETURN                                                            HEPS 550
      END                                                               HEPS 560
```

```
C                                                                       DHPS  10
C     .................................................................DHPS  20
C                                                                       DHPS  30
C        SUBROUTINE DHEPS                                               DHPS  40
C                                                                       DHPS  50
C        PURPOSE                                                        DHPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN HERMITE        DHPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. DHPS  80
C                                                                       DHPS  90
C        USAGE                                                          DHPS 100
C           CALL DHEPS(Y,X,C,N)                                         DHPS 110
C                                                                       DHPS 120
C        DESCRIPTION OF PARAMETERS                                      DHPS 130
C           Y      - RESULT VALUE                                       DHPS 140
C                    DOUBLE PRECISION VARIABLE                          DHPS 150
C           X      - ARGUMENT VALUE                                     DHPS 160
C                    DOUBLE PRECISION VARIABLE                          DHPS 170
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              DHPS 180
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DHPS 190
C                    DOUBLE PRECISION VECTOR                            DHPS 200
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  DHPS 210
C                                                                       DHPS 220
C        REMARKS                                                        DHPS 230
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 DHPS 240
C                                                                       DHPS 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DHPS 260
C           NONE                                                        DHPS 270
C                                                                       DHPS 280
C        METHOD                                                         DHPS 290
C           DEFINITION                                                  DHPS 300
C           Y=SUM(C(I)*H(I-1,X), SUMMED OVER I FROM 1 TO N).            DHPS 310
C           EVALUATION IS DONE BY MEANS OF UPWARD RECURSION             DHPS 320
C           USING THE RECURRENCE EQUATION FOR HERMITE POLYNOMIALS       DHPS 330
C           H(N+1,X)=2*(X*H(N,X)-N*H(N-1,X)).                           DHPS 340
C                                                                       DHPS 350
C     .................................................................DHPS 360
C                                                                       DHPS 370
      SUBROUTINE DHEPS(Y,X,C,N)                                         DHPS 380
C                                                                       DHPS 390
      DIMENSION C(1)                                                    DHPS 400
      DOUBLE PRECISION C,Y,X,H0,H1,H2                                   DHPS 410
C                                                                       DHPS 420
C        TEST OF DIMENSION                                              DHPS 430
      IF(N)1,1,2                                                        DHPS 440
    1 RETURN                                                            DHPS 450
C                                                                       DHPS 460
    2 Y=C(1)                                                            DHPS 470
      IF(N-2)1,3,3                                                      DHPS 480
C                                                                       DHPS 490
C        INITIALIZATION                                                 DHPS 500
    3 H0=1.D0                                                           DHPS 510
      H1=X+X                                                            DHPS 520
C                                                                       DHPS 530
      DO 4 I=2,N                                                        DHPS 540
      H2=X*H1-DFLOAT(I-1)*H0                                            DHPS 550
      H0=H1                                                             DHPS 560
      H1=H2+H2                                                          DHPS 570
    4 Y=Y+C(I)*H0                                                       DHPS 580
      RETURN                                                            DHPS 590
      END                                                               DHPS 600
```

Subroutines THEP and DTHEP

These subroutines transform a given series expansion in Hermite polynomials to a polynomial. The independent variable x of the given expansion is thereby substituted by the independent variable z of the resulting polynomial using the linear transformation x = A * z + B or z = (x-B)/A.

This means:
$$\sum_{i=1}^{N} C_i * H_{i-1}(A * z + B)$$
$$= \sum_{i=1}^{N} POL_i * z^{i-1}$$

Calculation is bypassed in case of a nonpositive value of the dimension N.

The range (-c, + c) in x is transformed to the range (z_l, z_r) in z with $z_l = -(c + B)/A$ and $z_r = (c-B)/A$, or vice versa, $A = 2c/(z_r - z_l)$ and $B = -c(z_r + z_l)/(z_r - z_l)$.

The Hermite polynomial $H_n(x)$ satisfies the recurrence equation

$$H_{n+1}(x) = 2(x \cdot H_n(x) - n \cdot H_{n-1}(x))$$

with starting values $H_0(x) = 1$, $H_1(x) = 2x$.

The transformation is performed by means of a forward iteration scheme:

1. The coefficient vector of the Hermite polynomial $H_i(x)$ is calculated from the coefficient vectors of $H_{i-1}(x)$, $H_{i-2}(x)$ using the recurrence equation, for i = 3, . . ., N.

2. The resulting polynomial coefficient vector is obtained by summation of c_i times coefficient vector of $H_{i-1}(x)$ over i, for i = 1, . . ., N.

```
C                                                                       THEP  10
C     ..................................................................THEP  20
C                                                                       THEP  30
C        SUBROUTINE THEP                                                THEP  40
C                                                                       THEP  50
C        PURPOSE                                                        THEP  60
C           A SERIES EXPANSION IN HERMITE POLYNOMIALS WITH INDEPENDENT  THEP  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  THEP  80
C           VARIABLE Z, WHERE X=A*Z+B                                   THEP  90
C                                                                       THEP 100
C        USAGE                                                          THEP 110
C           CALL THEP(A,B,POL,N,C,WORK)                                 THEP 120
C                                                                       THEP 130
C        DESCRIPTION OF PARAMETERS                                      THEP 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONTHEP 150
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION       THEP 160
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) THEP 170
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          THEP 180
C           N      - DIMENSION OF COEFFICIENT VECTOR POL AND C          THEP 190
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              THEP 200
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          THEP 210
C                    POL AND C MAY BE IDENTICALLY LOCATED               THEP 220
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   THEP 230
C                                                                       THEP 240
C        REMARKS                                                        THEP 250
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    THEP 260
C           WITH COEFFICIENT VECTOR POL.                                THEP 270
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                THEP 280
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSTHEP 290
C           THE RANGE (-C,C) IN X TO THE RANGE (ZL,ZR) IN Z WHERE       THEP 300
C           ZL=-(C+B)/A AND ZR=(C-B)/A.                                 THEP 310
C           FOR GIVEN ZL, ZR AND C WE HAVE A=2C/(ZR-ZL) AND             THEP 320
C           B=-C(ZR+ZL)/(ZR-ZL)                                         THEP 330
C                                                                       THEP 340
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  THEP 350
C           NONE                                                        THEP 360
C                                                                       THEP 370
C        METHOD                                                         THEP 380
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      THEP 390
C           FOR HERMITE POLYNOMIALS H(N,X)                              THEP 400
C           H(N+1,X)=2*(X*H(N,X)-N*H(N-1,X)),                           THEP 410
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX               THEP 420
C           THE SECOND IS THE ARGUMENT.                                 THEP 430
C           STARTING VALUES ARE H(0,X)=1,H(1,X)=2*X.                    THEP 440
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        THEP 450
C           X=A*Z+B TOGETHER WITH                                       THEP 460
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             THEP 470
C           =SUM(C(I)*H(I-1,X), SUMMED OVER I FROM 1 TO N).             THEP 480
C                                                                       THEP 490
C     ..................................................................THEP 500
C                                                                       THEP 510
      SUBROUTINE THEP(A,B,POL,N,C,WORK)                                 THEP 520
C                                                                       THEP 530
      DIMENSION POL(1),C(1),WORK(1)                                     THEP 540
C                                                                       THEP 550
C        TEST OF DIMENSION                                              THEP 560
      IF(N-1)2,1,3                                                      THEP 570
C                                                                       THEP 580
C        DIMENSION LESS THAN 2                                          THEP 590
    1 POL(1)=C(1)                                                       THEP 600
    2 RETURN                                                            THEP 610
C                                                                       THEP 620
    3 XO=A+A                                                            THEP 630
      XO=B+B                                                            THEP 640
      POL(1)=C(1)+C(2)*XO                                               THEP 650
      POL(2)=C(2)*XD                                                    THEP 660
      IF(N-2)2,2,4                                                      THEP 670
C                                                                       THEP 680
C        INITIALIZATION                                                 THEP 690
    4 WORK(1)=1.                                                        THEP 700
      WORK(2)=XO                                                        THEP 710
      WORK(3)=0.                                                        THEP 720
      WORK(4)=XD                                                        THEP 730
      FI=2.                                                             THEP 740
C                                                                       THEP 750
C        CALCULATE COEFFICIENT VECTOR OF NEXT HERMITE POLYNOMIAL        THEP 760
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              THEP 770
      DO 6 J=3,N                                                        THEP 780
      P=0.                                                              THEP 790
C                                                                       THEP 800
      DO 5 K=2,J                                                        THEP 810
      H=P*XD+WORK(2*K-2)*XO-FI*WORK(2*K-3)                              THEP 820
      P=WORK(2*K-2)                                                     THEP 830
      WORK(2*K-2)=H                                                     THEP 840
      WORK(2*K-3)=P                                                     THEP 850
    5 POL(K-1)=POL(K-1)+H*C(J)                                          THEP 860
      WORK(2*J-1)=0.                                                    THEP 870
      WORK(2*J)=P*XD                                                    THEP 880
      FI=FI+2.                                                          THEP 890
    6 POL(J)=C(J)*WORK(2*J)                                             THEP 900
      RETURN                                                            THEP 910
      END                                                               THEP 920
```

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C                                                                       DTHE  10
C     ...................................................................DTHE  20
C                                                                       DTHE  30
C        SUBROUTINE DTHEP                                               DTHE  40
C                                                                       DTHE  50
C        PURPOSE                                                        DTHE  60
C           A SERIES EXPANSION IN HERMITE POLYNOMIALS WITH INDEPENDENT  DTHE  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  DTHE  80
C           VARIABLE Z, WHERE X=A*Z+B                                   DTHE  90
C                                                                       DTHE 100
C        USAGE                                                          DTHE 110
C           CALL DTHEP(A,B,POL,N,C,WORK)                                DTHE 120
C                                                                       DTHE 130
C        DESCRIPTION OF PARAMETERS                                      DTHE 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONDTHE 150
C                    DOUBLE PRECISION VARIABLE                          DTHE 160
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION      DTHE 170
C                    DOUBLE PRECISION VARIABLE                          DTHE 180
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) DTHE 190
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTHE 200
C                    DOUBLE PRECISION VECTOR                            DTHE 210
C           N      - DIMENSION OF COEFFICIENT VECTOR POL AND C         DTHE 220
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION             DTHE 230
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTHE 240
C                    POL AND C MAY BE IDENTICALLY LOCATED               DTHE 250
C                    DOUBLE PRECISION VECTOR                            DTHE 260
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   DTHE 270
C                    DOUBLE PRECISION ARRAY                             DTHE 280
C                                                                       DTHE 290
C        REMARKS                                                        DTHE 300
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    DTHE 310
C           WITH COEFFICIENT VECTOR POL.                                DTHE 320
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                DTHE 330
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSDTHE 340
C           THE RANGE (-C,C) IN X TO THE RANGE (ZL,ZR) IN Z WHERE       DTHE 350
C           ZL=-(C+B)/A AND ZR=(C-B)/A.                                 DTHE 360
C           FOR GIVEN ZL, ZR AND C WE HAVE A=2C/(ZR-ZL) AND             DTHE 370
C           B=-C(ZR+ZL)/(ZR-ZL)                                         DTHE 380
C                                                                       DTHE 390
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTHE 400
C           NONE                                                        DTHE 410
C                                                                       DTHE 420
C        METHOD                                                         DTHE 430
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      DTHE 440
C           FOR HERMITE POLYNOMIALS H(N,X)                              DTHE 450
C           H(N+1,X)=2*(X*H(N,X)-(N)*H(N-1,X)),                         DTHE 460
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX               DTHE 470
C           THE SECOND IS THE ARGUMENT.                                 DTHE 480
C           STARTING VALUES ARE H(0,X)=1,H(1,X)=2*X.                    DTHE 490
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        DTHE 500
C           X=A*Z+B TOGETHER WITH                                       DTHE 510
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             DTHE 520
C           =SUM(C(I)*H(I-1,X), SUMMED OVER I FROM 1 TO N).             DTHE 530
C                                                                       DTHE 540
C     ...................................................................DTHE 550
C                                                                       DTHE 560
      SUBROUTINE DTHEP(A,B,POL,N,C,WORK)                                DTHE 570
C                                                                       DTHE 580
      DIMENSION POL(1),C(1),WORK(1)                                     DTHE 590
      DOUBLE PRECISION A,B,POL,C,WORK,H,P,FI,XO,XO                      DTHE 600
C                                                                       DTHE 610
C        TEST OF DIMENSION                                              DTHE 620
      IF(N-1)2,1,3                                                      DTHE 630
C                                                                       DTHE 640
C        DIMENSION LESS THAN 2                                          DTHE 650
    1 POL(1)=C(1)                                                       DTHE 660
    2 RETURN                                                            DTHE 670
C                                                                       DTHE 680
    3 XO=A+A                                                            DTHE 690
      XO=B+B                                                            DTHE 700
      POL(1)=C(1)+C(2)*XO                                               DTHE 710
      POL(2)=C(2)*XO                                                    DTHE 720
      IF(N-2)2,2,4                                                      DTHE 730
C                                                                       DTHE 740
C        INITIALIZATION                                                 DTHE 750
    4 WORK(1)=1.DO                                                      DTHE 760
      WORK(2)=XO                                                        DTHE 770
      WORK(3)=0.DO                                                      DTHE 780
      WORK(4)=XO                                                        DTHE 790
      FI=2.DO                                                           DTHE 800
C                                                                       DTHE 810
C        CALCULATE COEFFICIENT VECTOR OF NEXT HERMITE POLYNOMIAL        DTHE 820
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              DTHE 830
      DO 6 J=3,N                                                        DTHE 840
      P=0.DO                                                            DTHE 850
C                                                                       DTHE 860
      DO 5 K=2,J                                                        DTHE 870
      H=P*XO+WORK(2*K-2)*XO-FI*WORK(2*K-3)                              DTHE 880
      P=WORK(2*K-2)                                                     DTHE 890
      WORK(2*K-2)=H                                                     DTHE 900
      WORK(2*K-3)=P                                                     DTHE 910
    5 POL(K-1)=POL(K-1)+H*C(J)                                          DTHE 920
      WORK(2*J-1)=0.DO                                                  DTHE 930
      WORK(2*J)=P*XO                                                    DTHE 940
      FI=FI+2.DO                                                        DTHE 950
    6 POL(J)=C(J)*WORK(2*J)                                             DTHE 960
      RETURN                                                            DTHE 970
      END                                                               DTHE 980
```

Subroutines LAP and DLAP

These subroutines compute the values of the normalized Laguerre polynomials for a given argument x and orders zero up to N. The polynomial $L_n(x)/n!$, termed $L_n(x)$ below, satisfies the recurrence equation

$$L_{n+1}(x) = \left[(2n + 1 - x)\, L_n(x) - n\, L_{n-1}(x)\right]/(n+1)$$

with starting values $L_0(x) = 1$, $L_1(x) = 1 - x$.

For reasons of economy and numerical stability the recurrence equation is used in the form

$$L_{n+1}(x) = L_n(x) - L_{n-1}(x) + L_n(x)$$

$$-\left[(1+x)\, L_n(x) - L_{n-1}(x)\right]/(n+1).$$

For large values of n the last term is negligible, giving the approximation

$$L_{n+1}(x) = 2\, L_n(x) - L_{n-1}(x).$$

This form shows that roundoff errors grow at worst linearly as long as x is small compared to n.

If e_{n+r} is the error in $L_{n+r}(x)$ due to a single rounding error e in $L_n(x)$, the approximation is:

$$e_{n+r+1} = 2 \cdot e_{n+r} - e_{n+r-1}$$

with initial conditions $e_n = e$, $e_{n-1} = 0$. This implies:

$$e_{n+1} = 2e,\ e_{n+2} = 3 \cdot e,\ \ldots,\ e_{n+r} = (r+1)e$$

The order is assumed to be zero for negative values of N.

```
C                                                                       LAP  10
C     ...................................................................LAP  20
C                                                                       LAP  30
C        SUBROUTINE LAP                                                 LAP  40
C                                                                       LAP  50
C        PURPOSE                                                        LAP  60
C           COMPUTE THE VALUES OF THE LAGUERRE POLYNOMIALS L(N,X)       LAP  70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  LAP  80
C                                                                       LAP  90
C        USAGE                                                          LAP 100
C           CALL LAP(Y,X,N)                                             LAP 110
C                                                                       LAP 120
C        DESCRIPTION OF PARAMETERS                                      LAP 130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESLAP 140
C                    OF LAGUERRE POLYNOMIALS OF ORDER 0 UP TO N         LAP 150
C                    FOR GIVEN ARGUMENT X.                              LAP 160
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          LAP 170
C           X      - ARGUMENT OF LAGUERRE POLYNOMIAL                   LAP 180
C           N      - ORDER OF LAGUERRE POLYNOMIAL                      LAP 190
C                                                                       LAP 200
C        REMARKS                                                        LAP 210
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     LAP 220
C                                                                       LAP 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  LAP 240
C           NONE                                                        LAP 250
C                                                                       LAP 260
C        METHOD                                                         LAP 270
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          LAP 280
C           LAGUERRE POLYNOMIALS L(N,X)                                 LAP 290
C           L(N+1,X)=2*L(N,X)-L(N-1,X)-((1+X)*L(N,X)-L(N-1,X))/(N+1),   LAP 300
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              LAP 310
C           THE SECOND IS THE ARGUMENT.                                 LAP 320
C           STARTING VALUES ARE L(0,X)=1, L(1,X)=1.-X.                  LAP 330
C                                                                       LAP 340
C     ...................................................................LAP 350
C                                                                       LAP 360
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      SUBROUTINE LAP(Y,X,N)                                          LAP  370
C                                                                    LAP  380
      DIMENSION Y(1)                                                 LAP  390
C                                                                    LAP  400
C        TEST OF ORDER                                               LAP  410
      Y(1)=1.                                                        LAP  420
      IF(N)1,1,2                                                     LAP  430
    1 RETURN                                                         LAP  440
C                                                                    LAP  450
    2 Y(2)=1.-X                                                      LAP  460
      IF(N-1)1,1,3                                                   LAP  470
C                                                                    LAP  480
C        INITIALIZATION                                              LAP  490
    3 T=1.+X                                                         LAP  500
C                                                                    LAP  510
      DO 4 I=2,N                                                     LAP  520
    4 Y(I+1)=Y(I)-Y(I-1)+Y(I)-(T*Y(I)-Y(I-1))/FLOAT(I)               LAP  530
      RETURN                                                         LAP  540
      END                                                            LAP  550
```

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C                                                                    DAP   10
C     ..............................................................DAP   20
C                                                                    DAP   30
C        SUBROUTINE DLAP                                             DAP   40
C                                                                    DAP   50
C        PURPOSE                                                     DAP   60
C           COMPUTE THE VALUES OF THE LAGUERRE POLYNOMIALS L(N,X)    DAP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.               DAP   80
C                                                                    DAP   90
C        USAGE                                                       DAP  100
C           CALL DLAP(Y,X,N)                                         DAP  110
C                                                                    DAP  120
C        DESCRIPTION OF PARAMETERS                                   DAP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESDAP  140
C                    OF LAGUERRE POLYNOMIALS OF ORDER 0 UP TO N      DAP  150
C                    FOR GIVEN ARGUMENT X.                           DAP  160
C                    DOUBLE PRECISION VECTOR.                        DAP  170
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER       DAP  180
C           X      - ARGUMENT OF LAGUERRE POLYNOMIAL                 DAP  190
C                    DOUBLE PRECISION VARIABLE.                      DAP  200
C           N      - ORDER OF LAGUERRE POLYNOMIAL                    DAP  210
C                                                                    DAP  220
C        REMARKS                                                     DAP  230
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                  DAP  240
C                                                                    DAP  250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED               DAP  260
C           NONE                                                     DAP  270
C                                                                    DAP  280
C        METHOD                                                      DAP  290
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR       DAP  300
C           LAGUERRE POLYNOMIALS L(N,X)                              DAP  310
C           L(N+1,X)=2*L(N,X)-L(N-1,X)-((1+X)*L(N,X)-L(N-1,X))/(N+1), DAP 320
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,           DAP  330
C           THE SECOND IS THE ARGUMENT.                              DAP  340
C           STARTING VALUES ARE L(0,X)=1, L(1,X)=1.-X.               DAP  350
C                                                                    DAP  360
C     ..............................................................DAP  370
C                                                                    DAP  380
      SUBROUTINE DLAP(Y,X,N)                                         DAP  390
C                                                                    DAP  400
      DIMENSION Y(1)                                                 DAP  410
      DOUBLE PRECISION Y,X,T                                         DAP  420
C                                                                    DAP  430
C        TEST OF ORDER                                               DAP  440
      Y(1)=1.D0                                                      DAP  450
      IF(N)1,1,2                                                     DAP  460
    1 RETURN                                                         DAP  470
C                                                                    DAP  480
    2 Y(2)=1.D0-X                                                    DAP  490
      IF(N-1)1,1,3                                                   DAP  500
C                                                                    DAP  510
C        INITIALIZATION                                              DAP  520
    3 T=1.D0+X                                                       DAP  530
C                                                                    DAP  540
      DO 4 I=2,N                                                     DAP  550
    4 Y(I+1)=Y(I)-Y(I-1)+Y(I)-(T*Y(I)-Y(I-1))/DFLOAT(I)              DAP  560
      RETURN                                                         DAP  570
      END                                                            DAP  580
```

Subroutines LAPS and DLAPS

These subroutines compute the value of a series expansion in normalized Laguerre polynomials. The polynomial $L_n(x)/n!$, termed $L_n(x)$ below, satisfies the recurrence equation

$$L_{n+1}(x) = 2 \cdot L_n(x) - L_{n-1}(x) - \left[(1 + x) \cdot L_n(x) - L_{n-1}(x)\right] /(n+1)$$

with starting values $L_0(x) = 1$, $L_1(x) = 1 - x$.

An n-term expansion in Laguerre polynomials with coefficient vector $C = (c_1, \ldots, c_n)$ is evaluated by means of a forward iteration scheme:

$$Y = c_1,\ H_0 = 1,\ H_1 = 1 - x,\ T = 1 - x$$

$$\left.\begin{aligned} H_2 &= H_1 - H_0 + H_1 - (T \cdot H_1 - H_0)/i \\ H_0 &= H_1 \\ H_1 &= H_2 \\ Y &= Y + c_i \cdot H_0 \end{aligned}\right\} \text{ for } i = 2, \ldots, n$$

This gives the result $Y(x) = \sum_{i=1}^{n} c_i \cdot L_{i-1}(x)$.

Calculation is bypassed in case of a nonpositive value of the dimension n.

```
C                                                                    LAPS   10
C     ..............................................................LAPS   20
C                                                                    LAPS   30
C        SUBROUTINE LAPS                                             LAPS   40
C                                                                    LAPS   50
C        PURPOSE                                                     LAPS   60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN LAGUERRE    LAPS   70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. LAPS 80
C                                                                    LAPS   90
C        USAGE                                                       LAPS  100
C           CALL LAPS(Y,X,C,N)                                       LAPS  110
C                                                                    LAPS  120
C        DESCRIPTION OF PARAMETERS                                   LAPS  130
C           Y      - RESULT VALUE                                    LAPS  140
C           X      - ARGUMENT VALUE                                  LAPS  150
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION           LAPS  160
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH       LAPS  170
C           N      - DIMENSION OF COEFFICIENT VECTOR C               LAPS  180
C                                                                    LAPS  190
C        REMARKS                                                     LAPS  200
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1              LAPS  210
C                                                                    LAPS  220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED               LAPS  230
C           NONE                                                     LAPS  240
C                                                                    LAPS  250
C        METHOD                                                      LAPS  260
C           DEFINITION                                               LAPS  270
C           Y=SUM(C(I)*L(I-1,X), SUMMED OVER I FROM 1 TO N).         LAPS  280
C           EVALUATION IS DONE BY MEANS OF UPWARD RECURSION          LAPS  290
C           USING THE RECURRENCE EQUATION FOR LAGUERRE POLYNOMIALS   LAPS  300
C           L(N+1,X)=2*L(N,X)-L(N-1,X)-((1+X)*L(N,X)-L(N-1,X))/(N+1). LAPS 310
C                                                                    LAPS  320
C     ..............................................................LAPS  330
C                                                                    LAPS  340
      SUBROUTINE LAPS(Y,X,C,N)                                       LAPS  350
C                                                                    LAPS  360
      DIMENSION C(1)                                                 LAPS  370
C                                                                    LAPS  380
C        TEST OF DIMENSION                                           LAPS  390
      IF(N)1,1,2                                                     LAPS  400
    1 RETURN                                                         LAPS  410
C                                                                    LAPS  420
    2 Y=C(1)                                                         LAPS  430
      IF(N-2)1,3,3                                                   LAPS  440
C                                                                    LAPS  450
C        INITIALIZATION                                              LAPS  460
    3 H0=1.                                                          LAPS  470
      H1=1.-X                                                        LAPS  480
      T=1.+X                                                         LAPS  490
C                                                                    LAPS  500
      DO 4 I=2,N                                                     LAPS  510
      H2=H1-H0+H1-(T*H1-H0)/FLOAT(I)                                 LAPS  520
      H0=H1                                                          LAPS  530
      H1=H2                                                          LAPS  540
    4 Y=Y+C(I)*H0                                                    LAPS  550
      RETURN                                                         LAPS  560
      END                                                            LAPS  570
```

```
C                                                                       DAPS  10
C     ...................................................................DAPS  20
C                                                                       DAPS  30
C        SUBROUTINE DLAPS                                               DAPS  40
C                                                                       DAPS  50
C        PURPOSE                                                        DAPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN LAGUERRE       DAPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. DAPS  80
C                                                                       DAPS  90
C        USAGE                                                          DAPS 100
C           CALL DLAPS(Y,X,C,N)                                         DAPS 110
C                                                                       DAPS 120
C        DESCRIPTION OF PARAMETERS                                      DAPS 130
C           Y      - RESULT VALUE                                       DAPS 140
C                    DOUBLE PRECISION VARIABLE                          DAPS 150
C           X      - ARGUMENT VALUE                                     DAPS 160
C                    DOUBLE PRECISION VARIABLE                          DAPS 170
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              DAPS 180
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DAPS 190
C                    DOUBLE PRECISION VECTOR                            DAPS 200
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  DAPS 210
C                                                                       DAPS 220
C        REMARKS                                                        DAPS 230
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 DAPS 240
C                                                                       DAPS 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DAPS 260
C           NONE                                                        DAPS 270
C                                                                       DAPS 280
C        METHOD                                                         DAPS 290
C           DEFINITION                                                  DAPS 300
C           Y=SUM(C(I)*L(I-1,X), SUMMED OVER I FROM 1 TO N).            DAPS 310
C           EVALUATION IS DONE BY MEANS OF UPWARD RECURSION             DAPS 320
C           USING THE RECURRENCE EQUATION FOR LAGUERRE POLYNOMIALS      DAPS 330
C           L(N+1,X)=2*L(N,X)-L(N-1,X)-((1+X)*L(N,X)-L(N-1,X))/(N+1).   DAPS 340
C                                                                       DAPS 350
C     ...................................................................DAPS 360
C                                                                       DAPS 370
      SUBROUTINE DLAPS(Y,X,C,N)                                         DAPS 380
C                                                                       DAPS 390
      DIMENSION C(1)                                                    DAPS 400
      DOUBLE PRECISION C,Y,X,H0,H1,H2,T                                 DAPS 410
C                                                                       DAPS 420
C        TEST OF DIMENSION                                              DAPS 430
      IF(N)1,1,2                                                        DAPS 440
    1 RETURN                                                            DAPS 450
C                                                                       DAPS 460
    2 Y=C(1)                                                            DAPS 470
      IF(N-2)1,3,3                                                      DAPS 480
C                                                                       DAPS 490
C        INITIALIZATION                                                 DAPS 500
    3 H0=1.D0                                                           DAPS 510
      H1=1.D0-X                                                         DAPS 520
      T=1.D0+X                                                          DAPS 530
      DO 4 I=2,N                                                        DAPS 540
      H2=H1-H0+H1-(T*H1-H0)/DFLOAT(I)                                   DAPS 550
      H0=H1                                                             DAPS 560
      H1=H2                                                             DAPS 570
    4 Y=Y+C(I)*H0                                                       DAPS 580
      RETURN                                                            DAPS 590
      END                                                               DAPS 600
```

Subroutines TLAP and DTLAP

These subroutines transform a given series expansion in Laguerre polynomials to a polynomial. The independent variable x of the given expansion is thereby substituted by the independent variable z of the resulting polynomial using the linear transformation $x = A * z + B$ or $z = (x-B)/A$.

This means: $$\sum_{i=1}^{N} C_i * L_{i-1}(A * z + B)$$

$$= \sum_{i=1}^{N} POL_i * z^{i-1}$$

Calculation is bypassed in case of a nonpositive value of the dimension N.

The range (0, c) in x is transformed to the range (z_l, z_r) in z with $z_l = -B/A$ and $z_r = (c - B)/A$, or vice versa, $A = c/(z_r - z_l)$ and $B = -c * z_l/(z_r - z_l)$.

The Laguerre polynomial $L_n(x)$ satisfies the recurrence equation

$$L_{n+1}(x) = x/(n+1) \cdot L_n(x) + \left[2 - 1/(n+1)\right] L_n(x) - \left[1 - 1/(n+1)\right] L_{n-1}(x)$$

with starting values $L_0(x) = 1$, $L_1(x) = 1 - x$.

The transformation is performed by means of a forward iteration scheme:

1. The coefficient vector of the Laguerre polynomial $L_i(x)$ is calculated from the coefficient vectors of $L_{i-1}(x)$, $L_{i-2}(x)$ using the recurrence equation, for i = 3, ..., N.
2. The resulting polynomial coefficient vector is obtained by summation of c_i times $L_{i-1}(x)$ over i, for i = 1, ..., N.

```
C                                                                       TLAP  10
C     ...................................................................TLAP  20
C                                                                       TLAP  30
C        SUBROUTINE TLAP                                                TLAP  40
C                                                                       TLAP  50
C        PURPOSE                                                        TLAP  60
C           A SERIES EXPANSION IN LAGUERRE POLYNOMIALS WITH INDEPENDENT TLAP  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  TLAP  80
C           VARIABLE Z, WHERE X=A*Z+B                                   TLAP  90
C                                                                       TLAP 100
C        USAGE                                                          TLAP 110
C           CALL TLAP(A,B,POL,N,C,WORK)                                 TLAP 120
C                                                                       TLAP 130
C        DESCRIPTION OF PARAMETERS                                      TLAP 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONTLAP 150
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION       TLAP 160
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) TLAP 170
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          TLAP 180
C           N      - DIMENSION OF COEFFICIENT VECTORS POL AND C         TLAP 190
C           C      - GIVEN COEFFICIENT VECTOR OF EXPANSION              TLAP 200
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          TLAP 210
C                    POL AND C MAY BE IDENTICALLY LOCATED               TLAP 220
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   TLAP 230
C                                                                       TLAP 240
C        REMARKS                                                        TLAP 250
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    TLAP 260
C           WITH COEFFICIENT VECTOR POL.                                TLAP 270
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                TLAP 280
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSTLAP 290
C           THE RANGE (0,C) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE       TLAP 300
C           ZL=-B/A AND ZR=(C-B)/A.                                     TLAP 310
C           FOR GIVEN ZL, ZR AND C WE HAVE A=C/(ZR-ZL) AND              TLAP 320
C           B=-C*ZL/(ZR-ZL)                                             TLAP 330
C                                                                       TLAP 340
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TLAP 350
C           NONE                                                        TLAP 360
C                                                                       TLAP 370
C        METHOD                                                         TLAP 380
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      TLAP 390
C           FOR LAGUERRE POLYNOMIALS L(N,X)                             TLAP 400
C           L(N+1,X)=2*L(N,X)-L(N-1,X)-((1+X)*L(N,X)-L(N-1,X))/(N+1),   TLAP 410
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              TLAP 420
C           THE SECOND IS THE ARGUMENT.                                 TLAP 430
C           STARTING VALUES ARE L(0,X)=1, L(1,X)=1-X.                   TLAP 440
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        TLAP 450
C           X=A*Z+B TOGETHER WITH                                       TLAP 460
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             TLAP 470
C           =SUM(C(I)*L(I-1,X), SUMMED OVER I FROM 1 TO N).             TLAP 480
C                                                                       TLAP 490
C     ...................................................................TLAP 500
C                                                                       TLAP 510
      SUBROUTINE TLAP(A,B,POL,N,C,WORK)                                 TLAP 520
C                                                                       TLAP 530
      DIMENSION POL(1),C(1),WORK(1)                                     TLAP 540
C                                                                       TLAP 550
C        TEST OF DIMENSION                                              TLAP 560
      IF(N-1)2,1,3                                                      TLAP 570
C                                                                       TLAP 580
C        DIMENSION LESS THAN 2                                          TLAP 590
    1 POL(1)=C(1)                                                       TLAP 600
    2 RETURN                                                            TLAP 610
C                                                                       TLAP 620
    3 POL(1)=C(1)+C(2)-B*C(2)                                           TLAP 630
      POL(2)=-C(2)*A                                                    TLAP 640
      IF(N-2)2,2,4                                                      TLAP 650
C                                                                       TLAP 660
C        INITIALIZATION                                                 TLAP 670
    4 WORK(1)=1.                                                        TLAP 680
      WORK(2)=1.D0-B                                                    TLAP 690
      WORK(3)=0.                                                        TLAP 700
      WORK(4)=-A                                                        TLAP 710
      FI=1.                                                             TLAP 720
C                                                                       TLAP 730
C        CALCULATE COEFFICIENT VECTOR OF NEXT LAGUERRE POLYNOMIAL       TLAP 740
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              TLAP 750
      DO 6 J=3,N                                                        TLAP 760
      FI=FI+1.                                                          TLAP 770
      Q=1./FI                                                           TLAP 780
      Q1=Q-1.                                                           TLAP 790
      Q2=1.-Q1-B*Q                                                      TLAP 800
      Q=Q*A                                                             TLAP 810
      P=0.                                                              TLAP 820
C                                                                       TLAP 830
      DO 5 K=2,J                                                        TLAP 840
      H=-P*Q+WORK(2*K-2)*Q2+WORK(2*K-3)*Q1                              TLAP 850
      P=WORK(2*K-2)                                                     TLAP 860
      WORK(2*K-2)=H                                                     TLAP 870
      WORK(2*K-3)=P                                                     TLAP 880
    5 POL(K-1)=POL(K-1)+H*C(J)                                          TLAP 890
      WORK(2*J-1)=0.                                                    TLAP 900
      WORK(2*J)=-Q*P                                                    TLAP 910
    6 POL(J)=C(J)*WORK(2*J)                                             TLAP 920
      RETURN                                                            TLAP 930
      END                                                               TLAP 940
```

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C                                                                       DTLA  10
C     ...................................................................DTLA  20
C                                                                       DTLA  30
C        SUBROUTINE DTLAP                                               DTLA  40
C                                                                       DTLA  50
C        PURPOSE                                                        DTLA  60
C           A SERIES EXPANSION IN LAGUERRE POLYNOMIALS WITH INDEPENDENT DTLA  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  DTLA  80
C           VARIABLE Z, WHERE X=A*Z+B                                   DTLA  90
C                                                                       DTLA 100
C        USAGE                                                          DTLA 110
C           CALL DTLAP(A,B,POL,N,C,WORK)                                DTLA 120
C                                                                       DTLA 130
C        DESCRIPTION OF PARAMETERS                                      DTLA 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONDTLA 150
C                    DOUBLE PRECISION VARIABLE                          DTLA 160
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION       DTLA 170
C                    DOUBLE PRECISION VARIABLE                          DTLA 180
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) DTLA 190
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTLA 200
C                    DOUBLE PRECISION VECTOR                            DTLA 210
C           N      - DIMENSION OF COEFFICIENT VECTORS POL AND C         DTLA 220
C           C      - GIVEN COEFFICIENT VECTOR OF EXPANSION              DTLA 230
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTLA 240
C                    POL AND C MAY BE IDENTICALLY LOCATED               DTLA 250
C                    DOUBLE PRECISION VECTOR                            DTLA 260
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   DTLA 270
C                    DOUBLE PRECISION ARRAY                             DTLA 280
C                                                                       DTLA 290
C        REMARKS                                                        DTLA 300
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    DTLA 310
C           WITH COEFFICIENT VECTOR POL.                                DTLA 320
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                DTLA 330
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSDTLA 340
C           THE RANGE (0,C) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE       DTLA 350
C           ZL=-B/A AND ZR=(C-B)/A.                                     DTLA 360
C           FOR GIVEN ZL, ZR AND C WE HAVE A=C/(ZR-ZL) AND              DTLA 370
C           B=-C*ZL/(ZR-ZL)                                             DTLA 380
C                                                                       DTLA 390
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTLA 400
C           NONE                                                        DTLA 410
C                                                                       DTLA 420
C        METHOD                                                         DTLA 430
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      DTLA 440
C           FOR LAGUERRE POLYNOMIALS L(N,X)                             DTLA 450
C           L(N+1,X)=2*L(N,X)-L(N-1,X)-((1+X)*L(N,X)-L(N-1,X))/(N+1),   DTLA 460
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              DTLA 470
C           THE SECOND IS THE ARGUMENT.                                 DTLA 480
C           STARTING VALUES ARE L(0,X)=1, L(1,X)=1-X.                   DTLA 490
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        DTLA 500
C           X=A*Z+B TOGETHER WITH                                       DTLA 510
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             DTLA 520
C           =SUM(C(I)*L(I-1,X), SUMMED OVER I FROM 1 TO N).             DTLA 530
C                                                                       DTLA 540
C     ...................................................................DTLA 550
C                                                                       DTLA 560
      SUBROUTINE DTLAP(A,B,POL,N,C,WORK)                                DTLA 570
C                                                                       DTLA 580
      DIMENSION POL(1),C(1),WORK(1)                                     DTLA 590
      DOUBLE PRECISION A,B,POL,C,WORK,H,P,Q,Q1,Q2,FI                    DTLA 600
C                                                                       DTLA 610
C        TEST OF DIMENSION                                              DTLA 620
      IF(N-1)2,1,3                                                      DTLA 630
C                                                                       DTLA 640
C        DIMENSION LESS THAN 2                                          DTLA 650
    1 POL(1)=C(1)                                                       DTLA 660
    2 RETURN                                                            DTLA 670
C                                                                       DTLA 680
    3 POL(1)=C(1)+C(2)-B*C(2)                                           DTLA 690
      POL(2)=-C(2)*A                                                    DTLA 700
      IF(N-2)2,2,4                                                      DTLA 710
C                                                                       DTLA 720
C        INITIALIZATION                                                 DTLA 730
    4 WORK(1)=1.D0                                                      DTLA 740
      WORK(2)=1.D0-B                                                    DTLA 750
      WORK(3)=0.D0                                                      DTLA 760
      WORK(4)=-A                                                        DTLA 770
      FI=1.D0                                                           DTLA 780
C                                                                       DTLA 790
C        CALCULATE COEFFICIENT VECTOR OF NEXT LAGUERRE POLYNOMIAL       DTLA 800
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              DTLA 810
      DO 6 J=3,N                                                        DTLA 820
      FI=FI+1.D0                                                        DTLA 830
      Q=1.D0/FI                                                         DTLA 840
      Q1=Q-1.D0                                                         DTLA 850
      Q2=1.D0-Q1-B*Q                                                    DTLA 860
      Q=Q*A                                                             DTLA 870
      P=0.D0                                                            DTLA 880
C                                                                       DTLA 890
      DO 5 K=2,J                                                        DTLA 900
      H=-P*Q+WORK(2*K-2)*Q2+WORK(2*K-3)*Q1                              DTLA 910
      P=WORK(2*K-2)                                                     DTLA 920
      WORK(2*K-2)=H                                                     DTLA 930
      WORK(2*K-3)=P                                                     DTLA 940
    5 POL(K-1)=POL(K-1)+H*C(J)                                          DTLA 950
      WORK(2*J-1)=0.D0                                                  DTLA 960
      WORK(2*J)=-Q*P                                                    DTLA 970
    6 POL(J)=C(J)*WORK(2*J)                                             DTLA 980
      RETURN                                                            DTLA 990
      END                                                               DTLA1000
```

Subroutines LEP and DLEP

These subroutines compute the values of the Legendre polynomials for a given argument x and orders zero up to N. The Legendre polynomial $P_n(x)$ satisfies the recurrence equation

$$P_{n+1}(x) = ((2n+1) \cdot x \cdot P_n(x) - n \cdot P_{n-1}(x))/(n+1)$$

with starting values $P_0(x) = 1$, $P_1(x) = x$.

For reasons of economy and numerical stability the recurrence equation is used in the form:

$$P_{n+1}(x) = x \cdot P_n(x) - P_{n-1}(x) + x \cdot P_n(x) - (x \cdot P_n(x) - P_{n-1}(x))/(n+1)$$

For large values of n the last term is negligible, giving the approximation:

$$P_{n+1}(x) = 2 \cdot x \cdot P_n(x) - P_{n-1}(x)$$

This form shows that roundoff errors grow at worst linearly, assuming that the argument x is absolutely less than one.

If e_{n+r} is the error in $P_{n+r}(x)$ due to a single rounding error e in $P_n(x)$, the approximation is

$$e_{n+r+1} = 2x \cdot e_{n+r} - e_{n+r-1}$$

with initial conditions $e_n = e$, $e_{n-1} = 0$. The solution of this difference equation has its maximum for $|x| = 1$:

$$e_{n-1} = 0,\ e_n = e,\ |e_{n+1}| = 2e,\ \ldots,\ |e_{n+r}| = (r+1)e$$

The order is assumed to be zero for negative values of N.

```
C                                                                       LEP   10
C     ..................................................................LEP   20
C                                                                       LEP   30
C        SUBROUTINE LEP                                                 LEP   40
C                                                                       LEP   50
C        PURPOSE                                                        LEP   60
C           COMPUTE THE VALUES OF THE LEGENDRE POLYNOMIALS P(N,X)       LEP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  LEP   80
C                                                                       LEP   90
C        USAGE                                                          LEP  100
C           CALL LEP(Y,X,N)                                             LEP  110
C                                                                       LEP  120
C        DESCRIPTION OF PARAMETERS                                      LEP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESLEP  140
C                    OF LEGENDRE POLYNOMIALS OF ORDER 0 UP TO N         LEP  150
C                    FOR GIVEN ARGUMENT X.                              LEP  160
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          LEP  170
C           X      - ARGUMENT OF LEGENDRE POLYNOMIAL                    LEP  180
C           N      - ORDER OF LEGENDRE POLYNOMIAL                       LEP  190
C                                                                       LEP  200
C        REMARKS                                                        LEP  210
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     LEP  220
C                                                                       LEP  230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  LEP  240
C           NONE                                                        LEP  250
C                                                                       LEP  260
C        METHOD                                                         LEP  270
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          LEP  280
C           LEGENDRE POLYNOMIALS P(N,X)                                 LEP  290
C           P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1),     LEP  300
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              LEP  310
C           THE SECOND IS THE ARGUMENT.                                 LEP  320
C           STARTING VALUES ARE P(0,X)=1, P(1,X)=X.                     LEP  330
C                                                                       LEP  340
C     ..................................................................LEP  350
C                                                                       LEP  360
      SUBROUTINE LEP(Y,X,N)                                             LEP  370
C                                                                       LEP  380
      DIMENSION Y(1)                                                    LEP  390
C                                                                       LEP  400
C        TEST OF ORDER                                                  LEP  410
      Y(1)=1.                                                           LEP  420
      IF(N)1,1,2                                                        LEP  430
    1 RETURN                                                            LEP  440
C                                                                       LEP  450
    2 Y(2)=X                                                            LEP  460
      IF(N-1)1,1,3                                                      LEP  470
C                                                                       LEP  480
    3 DO 4 I=2,N                                                        LEP  490
      G=X*Y(I)                                                          LEP  500
    4 Y(I+1)=G-Y(I-1)+G-(G-Y(I-1))/FLOAT(I)                             LEP  510
      RETURN                                                            LEP  520
      END                                                               LEP  530
```

```
C                                                                       DEP   10
C     ..................................................................DEP   20
C                                                                       DEP   30
C        SUBROUTINE DLEP                                                DEP   40
C                                                                       DEP   50
C        PURPOSE                                                        DEP   60
C           COMPUTE THE VALUES OF THE LEGENDRE POLYNOMIALS P(N,X)       DEP   70
C           FOR ARGUMENT VALUE X AND ORDERS 0 UP TO N.                  DEP   80
C                                                                       DEP   90
C        USAGE                                                          DEP  100
C           CALL DLEP(Y,X,N)                                            DEP  110
C                                                                       DEP  120
C        DESCRIPTION OF PARAMETERS                                      DEP  130
C           Y      - RESULT VECTOR OF DIMENSION N+1 CONTAINING THE VALUESDEP  140
C                    OF LEGENDRE POLYNOMIALS OF ORDER 0 UP TO N         DEP  150
C                    FOR GIVEN ARGUMENT X.                              DEP  160
C                    DOUBLE PRECISION VECTOR.                           DEP  170
C                    VALUES ARE ORDERED FROM LOW TO HIGH ORDER          DEP  180
C           X      - ARGUMENT OF LEGENDRE POLYNOMIAL                    DEP  190
C                    DOUBLE PRECISION VARIABLE.                         DEP  200
C           N      - ORDER OF LEGENDRE POLYNOMIAL                       DEP  210
C                                                                       DEP  220
C        REMARKS                                                        DEP  230
C           N LESS THAN 0 IS TREATED AS IF N WERE 0                     DEP  240
C                                                                       DEP  250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DEP  260
C           NONE                                                        DEP  270
C                                                                       DEP  280
C        METHOD                                                         DEP  290
C           EVALUATION IS BASED ON THE RECURRENCE EQUATION FOR          DEP  300
C           LEGENDRE POLYNOMIALS P(N,X)                                 DEP  310
C           P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1),     DEP  320
C           WHERE THE FIRST TERM IN BRACKETS IS THE ORDER,              DEP  330
C           THE SECOND IS THE ARGUMENT.                                 DEP  340
C           STARTING VALUES ARE P(0,X)=1, P(1,X)=X.                     DEP  350
C                                                                       DEP  360
C     ..................................................................DEP  370
C                                                                       DEP  380
      SUBROUTINE DLEP(Y,X,N)                                            DEP  390
C                                                                       DEP  400
      DIMENSION Y(1)                                                    DEP  410
      DOUBLE PRECISION Y,X,G                                            DEP  420
C                                                                       DEP  430
C        TEST OF ORDER                                                  DEP  440
      Y(1)=1.D0                                                         DEP  450
      IF(N)1,1,2                                                        DEP  460
    1 RETURN                                                            DEP  470
C                                                                       DEP  480
    2 Y(2)=X                                                            DEP  490
      IF(N-1)1,1,3                                                      DEP  500
C                                                                       DEP  510
    3 DO 4 I=2,N                                                        DEP  520
      G=X*Y(I)                                                          DEP  530
    4 Y(I+1)=G-Y(I-1)+G-(G-Y(I-1))/DFLOAT(I)                            DEP  540
      RETURN                                                            DEP  550
      END                                                               DEP  560
```

Subroutines LEPS and DLEPS

These subroutines compute the value of a series expansion in Legendre polynomials. The Legendre polynomial $P_n(x)$ satisfies the recurrence equation

$$P_{n+1}(x) = 2x \cdot P_n(x) - P_{n-1}(x) - (x \cdot P_n(x) - P_{n-1}(x))/(n+1)$$

with starting values $P_0(x) = 1$, $P_1(x) = x$.

An n-term expansion in Legendre polynomials with coefficient vector $C = (c_1, \ldots, c_n)$ is evaluated by means of a forward iteration scheme:

$$Y = c_1,\ H_0 = 1,\ H_1 = x$$

$$\left.\begin{aligned} H_2 &= x \cdot H_1 \\ H_2 &= H_2 - H_0 + H_2 - (H_2 - H_0)/i \\ H_0 &= H_1 \\ H_1 &= H_2 \end{aligned}\right\} \quad \text{for } i = 2, \ldots, n$$

$$Y = Y + c_i \cdot H_0$$

This gives the result $Y(x) = \sum_{i=1}^{n} c_i \cdot P_{i-1}(x)$.

Calculation is bypassed in case of a nonpositive value of the dimension N.

```
C                                                                       LEPS  10
C     ..................................................................LEPS  20
C                                                                       LEPS  30
C        SUBROUTINE LEPS                                                LEPS  40
C                                                                       LEPS  50
C        PURPOSE                                                        LEPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN LEGENDRE       LEPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. LEPS  80
C                                                                       LEPS  90
C        USAGE                                                          LEPS 100
C           CALL LEPS(Y,X,C,N)                                          LEPS 110
C                                                                       LEPS 120
C        DESCRIPTION OF PARAMETERS                                      LEPS 130
C           Y      - RESULT VALUE                                       LEPS 140
C           X      - ARGUMENT VALUE                                     LEPS 150
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              LEPS 160
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          LEPS 170
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  LEPS 180
C                                                                       LEPS 190
C        REMARKS                                                        LEPS 200
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 LEPS 210
C                                                                       LEPS 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  LEPS 230
C           NONE                                                        LEPS 240
C                                                                       LEPS 250
C        METHOD                                                         LEPS 260
C           DEFINITION                                                  LEPS 270
C           Y=SUM(C(I)*P(I-1,X), SUMMED OVER I FROM 1 TO N).            LEPS 280
C           EVALUATION IS DONE BY MEANS OF UPWARD RECURSION             LEPS 290
C           USING THE RECURRENCE EQUATION FOR LEGENDRE POLYNOMIALS      LEPS 300
C           P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1).     LEPS 310
C                                                                       LEPS 320
C     ..................................................................LEPS 330
C                                                                       LEPS 340
      SUBROUTINE LEPS(Y,X,C,N)                                          LEPS 350
C                                                                       LEPS 360
      DIMENSION C(1)                                                    LEPS 370
C                                                                       LEPS 380
C        TEST OF DIMENSION                                              LEPS 390
      IF(N)1,1,2                                                        LEPS 400
    1 RETURN                                                            LEPS 410
C                                                                       LEPS 420
    2 Y=C(1)                                                            LEPS 430
      IF(N-2)1,3,3                                                      LEPS 440
C                                                                       LEPS 450
C        INITIALIZATION                                                 LEPS 460
    3 H0=1.                                                             LEPS 470
      H1=X                                                              LEPS 480
C                                                                       LEPS 490
      DO 4 I=2,N                                                        LEPS 500
      H2=X*H1                                                           LEPS 510
      H2=H2-H0+H2-(H2-H0)/FLOAT(I)                                      LEPS 520
      H0=H1                                                             LEPS 530
      H1=H2                                                             LEPS 540
    4 Y=Y+C(I)*H0                                                       LEPS 550
      RETURN                                                            LEPS 560
      END                                                               LEPS 570
```

```
C                                                                       DEPS  10
C     ..................................................................DEPS  20
C                                                                       DEPS  30
C        SUBROUTINE DLEPS                                               DEPS  40
C                                                                       DEPS  50
C        PURPOSE                                                        DEPS  60
C           COMPUTES THE VALUE OF AN N-TERM EXPANSION IN LEGENDRE       DEPS  70
C           POLYNOMIALS WITH COEFFICIENT VECTOR C FOR ARGUMENT VALUE X. DEPS  80
C                                                                       DEPS  90
C        USAGE                                                          DEPS 100
C           CALL DLEPS(Y,X,C,N)                                         DEPS 110
C                                                                       DEPS 120
C        DESCRIPTION OF PARAMETERS                                      DEPS 130
C           Y      - RESULT VALUE                                       DEPS 140
C                    DOUBLE PRECISION VARIABLE                          DEPS 150
C           X      - ARGUMENT VALUE                                     DEPS 160
C                    DOUBLE PRECISION VARIABLE                          DEPS 170
C           C      - COEFFICIENT VECTOR OF GIVEN EXPANSION              DEPS 180
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DEPS 190
C                    DOUBLE PRECISION VECTOR                            DEPS 200
C           N      - DIMENSION OF COEFFICIENT VECTOR C                  DEPS 210
C                                                                       DEPS 220
C        REMARKS                                                        DEPS 230
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1                 DEPS 240
C                                                                       DEPS 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DEPS 260
C           NONE                                                        DEPS 270
C                                                                       DEPS 280
C        METHOD                                                         DEPS 290
C           DEFINITION                                                  DEPS 300
C           Y=SUM(C(I)*P(I-1,X), SUMMED OVER I FROM 1 TO N).            DEPS 310
C           EVALUATION IS DONE BY MEANS OF UPWARD RECURSION             DEPS 320
C           USING THE RECURRENCE EQUATION FOR LEGENDRE POLYNOMIALS      DEPS 330
C           P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1).     DEPS 340
C                                                                       DEPS 350
C     ..................................................................DEPS 360
C                                                                       DEPS 370
      SUBROUTINE DLEPS(Y,X,C,N)                                         DEPS 380
C                                                                       DEPS 390
      DIMENSION C(1)                                                    DEPS 400
      DOUBLE PRECISION C,Y,X,H0,H1,H2                                   DEPS 410
C                                                                       DEPS 420
C        TEST OF DIMENSION                                              DEPS 430
      IF(N)1,1,2                                                        DEPS 440
    1 RETURN                                                            DEPS 450
C                                                                       DEPS 460
    2 Y=C(1)                                                            DEPS 470
      IF(N-2)1,3,3                                                      DEPS 480
C                                                                       DEPS 490
C        INITIALIZATION                                                 DEPS 500
    3 H0=1.D0                                                           DEPS 510
      H1=X                                                              DEPS 520
C                                                                       DEPS 530
      DO 4 I=2,N                                                        DEPS 540
      H2=X*H1                                                           DEPS 550
      H2=H2-H0+H2-(H2-H0)/DFLOAT(I)                                     DEPS 560
      H0=H1                                                             DEPS 570
      H1=H2                                                             DEPS 580
    4 Y=Y+C(I)*H0                                                       DEPS 590
      RETURN                                                            DEPS 600
      END                                                               DEPS 610
```

Subroutines TLEP and DTLEP

These subroutines transform a given series expansion in Legendre polynomials to a polynomial. The independent variable x of the given expansion is thereby substituted by the independent variable z of the resulting polynomial using the linear transformation $x = A * z + B$ or $z = (x - B)/A$.

This means:

$$\sum_{i=1}^{N} C_i * P_{i-1}(A * z + B)$$

$$= \sum_{i=1}^{N} POL_i * z^{i-1}$$

Calculation is bypassed in case of a nonpositive value of the dimension N.

The range (-1, +1) in x is transformed to the range (z_1, z_r) in z with $z_1 = -(1 + B)/A$ and $z_r = (1 - B)/A$, or vice versa, $A = 2/(z_r - z_1)$ and $B = -(z_r + z_1)/(z_r - z_1)$.

The Legendre polynomial $P_n(x)$ satisfies the recurrence equation

$$P_{n+1}(x) = x\left[2-1/(n+1)\right] P_n(x) - \left[1-1/(n+1)\right] P_{n-1}(x)$$

with starting values $P_0(x) = 1$, $P_1(x) = x$.

The transformation is performed by means of a forward iteration scheme:

1. The coefficient vector of the Legendre polynomial $P_i(x)$ is calculated from the coefficient vectors of $P_{i-1}(x)$, $P_{i-2}(x)$ using the recurrence equation, for i = 3, ..., N.

2. The resulting polynomial coefficient vector is obtained by summation of c_i times coefficient vector of $P_{i-1}(x)$ over i, for i = 1, ..., N.

```
C                                                                       TLEP  10
C     ...................................................................TLEP  20
C                                                                       TLEP  30
C        SUBROUTINE TLEP                                                TLEP  40
C                                                                       TLEP  50
C        PURPOSE                                                        TLEP  60
C           A SERIES EXPANSION IN LEGENDRE POLYNOMIALS WITH INDEPENDENT TLEP  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  TLEP  80
C           VARIABLE Z, WHERE X=A*Z+B                                   TLEP  90
C                                                                       TLEP 100
C        USAGE                                                          TLEP 110
C           CALL TLEP(A,B,POL,N,C,WORK)                                 TLEP 120
C                                                                       TLEP 130
C        DESCRIPTION OF PARAMETERS                                      TLEP 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONTLEP 150
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION       TLEP 160
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) TLEP 170
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          TLEP 180
C           N      - DIMENSION OF COEFFICIENT VECTORS POL AND C         TLEP 190
C           C      - GIVEN COEFFICIENT VECTOR OF EXPANSION              TLEP 200
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          TLEP 210
C                    POL AND C MAY BE IDENTICALLY LOCATED               TLEP 220
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                   TLEP 230
C                                                                       TLEP 240
C        REMARKS                                                        TLEP 250
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    TLEP 260
C           WITH COEFFICIENT VECTOR POL.                                TLEP 270
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                TLEP 280
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSTLEP 290
C           THE RANGE (-1,+1) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE     TLEP 300
C           ZL=-(1+B)/A AND ZR=(1-B)/A.                                 TLEP 310
C           FOR GIVEN ZL, ZR WE HAVE A=2/(ZR-ZL) AND B=-(ZR+ZL)/(ZR-ZL) TLEP 320
C                                                                       TLEP 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TLEP 340
C           NONE                                                        TLEP 350
C                                                                       TLEP 360
C        METHOD                                                         TLEP 370
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      TLEP 380
C           FOR LEGENDRE POLYNOMIALS P(N,X)                             TLEP 390
C           P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1),     TLEP 400
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              TLEP 410
C           THE SECOND IS THE ARGUMENT.                                 TLEP 420
C           STARTING VALUES ARE P(0,X)=1, P(1,X)=X.                     TLEP 430
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        TLEP 440
C           X=A*Z+B TOGETHER WITH                                       TLEP 450
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             TLEP 460
C           =SUM(C(I)*P(I-1,X), SUMMED OVER I FROM 1 TO N).             TLEP 470
C                                                                       TLEP 480
C     ...................................................................TLEP 490
C                                                                       TLEP 500
      SUBROUTINE TLEP(A,B,POL,N,C,WORK)                                 TLEP 510
C                                                                       TLEP 520
      DIMENSION POL(1),C(1),WORK(1)                                     TLEP 530
C                                                                       TLEP 540
C        TEST OF DIMENSION                                              TLEP 550
      IF(N-1)2,1,3                                                      TLEP 560
C                                                                       TLEP 570
C        DIMENSION LESS THAN 2                                          TLEP 580
    1 POL(1)=C(1)                                                       TLEP 590
    2 RETURN                                                            TLEP 600
C                                                                       TLEP 610
    3 POL(1)=C(1)+B*C(2)                                                TLEP 620
      POL(2)=A*C(2)                                                     TLEP 630
      IF(N-2)2,2,4                                                      TLEP 640
C                                                                       TLEP 650
C        INITIALIZATION                                                 TLEP 660
    4 WORK(1)=1.                                                        TLEP 670
      WORK(2)=B                                                         TLEP 680
      WORK(3)=0.                                                        TLEP 690
      WORK(4)=A                                                         TLEP 700
      FI=1.                                                             TLEP 710
C                                                                       TLEP 720
C        CALCULATE COEFFICIENT VECTOR OF NEXT LEGENDRE POLYNOMIAL       TLEP 730
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              TLEP 740
      DO 6 J=3,N                                                        TLEP 750
      FI=FI+1.                                                          TLEP 760
      Q=1./FI-1.                                                        TLEP 770
      Q1=1.-Q                                                           TLEP 780
      P=0.                                                              TLEP 790
C                                                                       TLEP 800
      DO 5 K=2,J                                                        TLEP 810
      H=(A*P+B*WORK(2*K-2))*Q1+Q*WORK(2*K-3)                            TLEP 820
      P=WORK(2*K-2)                                                     TLEP 830
      WORK(2*K-2)=H                                                     TLEP 840
      WORK(2*K-3)=P                                                     TLEP 850
    5 POL(K-1)=POL(K-1)+H*C(J)                                          TLEP 860
      WORK(2*J-1)=0.                                                    TLEP 870
      WORK(2*J)=A*P*Q1                                                  TLEP 880
    6 POL(J)=C(J)*WORK(2*J)                                             TLEP 890
      RETURN                                                            TLEP 900
      END                                                               TLEP 910
```

```
C                                                                       DTLE  10
C     ...................................................................DTLE  20
C                                                                       DTLE  30
C        SUBROUTINE DTLEP                                               DTLE  40
C                                                                       DTLE  50
C        PURPOSE                                                        DTLE  60
C           A SERIES EXPANSION IN LEGENDRE POLYNOMIALS WITH INDEPENDENT DTLE  70
C           VARIABLE X IS TRANSFORMED TO A POLYNOMIAL WITH INDEPENDENT  DTLE  80
C           VARIABLE Z, WHERE X=A*Z+B                                   DTLE  90
C                                                                       DTLE 100
C        USAGE                                                          DTLE 110
C           CALL DTLEP(A,B,POL,N,C,WORK)                                DTLE 120
C                                                                       DTLE 130
C        DESCRIPTION OF PARAMETERS                                      DTLE 140
C           A      - FACTOR OF LINEAR TERM IN GIVEN LINEAR TRANSFORMATIONDTLE 150
C                    DOUBLE PRECISION VARIABLE                          DTLE 160
C           B      - CONSTANT TERM IN GIVEN LINEAR TRANSFORMATION      DTLE 170
C                    DOUBLE PRECISION VARIABLE                          DTLE 180
C           POL    - COEFFICIENT VECTOR OF POLYNOMIAL (RESULTANT VALUE) DTLE 190
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTLE 200
C                    DOUBLE PRECISION VECTOR                            DTLE 210
C           N      - DIMENSION OF COEFFICIENT VECTORS POL AND C        DTLE 220
C           C      - GIVEN COEFFICIENT VECTOR OF EXPANSION             DTLE 230
C                    COEFFICIENTS ARE ORDERED FROM LOW TO HIGH          DTLE 240
C                    POL AND C MAY BE IDENTICALLY LOCATED               DTLE 250
C                    DOUBLE PRECISION VECTOR                            DTLE 260
C           WORK   - WORKING STORAGE OF DIMENSION 2*N                  DTLE 270
C                    DOUBLE PRECISION ARRAY                             DTLE 280
C                                                                       DTLE 290
C        REMARKS                                                        DTLE 300
C           COEFFICIENT VECTOR C REMAINS UNCHANGED IF NOT COINCIDING    DTLE 310
C           WITH COEFFICIENT VECTOR POL.                                DTLE 320
C           OPERATION IS BYPASSED IN CASE N LESS THAN 1.                DTLE 330
C           THE LINEAR TRANSFORMATION X=A*Z+B OR Z=(1/A)(X-B) TRANSFORMSDTLE 340
C           THE RANGE (-1,+1) IN X TO THE RANGE (ZL,ZR) IN Z, WHERE     DTLE 350
C           ZL=-(1+B)/A AND ZR=(1-B)/A.                                 DTLE 360
C           FOR GIVEN ZL, ZR WE HAVE A=2/(ZR-ZL) AND B=-(ZR+ZL)/(ZR-ZL) DTLE 370
C                                                                       DTLE 380
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTLE 390
C           NONE                                                        DTLE 400
C                                                                       DTLE 410
C        METHOD                                                         DTLE 420
C           THE TRANSFORMATION IS BASED ON THE RECURRENCE EQUATION      DTLE 430
C           FOR LEGENDRE POLYNOMIALS P(N,X)                             DTLE 440
C           P(N+1,X)=2*X*P(N,X)-P(N-1,X)-(X*P(N,X)-P(N-1,X))/(N+1),     DTLE 450
C           WHERE THE FIRST TERM IN BRACKETS IS THE INDEX,              DTLE 460
C           THE SECOND IS THE ARGUMENT.                                 DTLE 470
C           STARTING VALUES ARE P(0,X)=1, P(1,X)=X.                     DTLE 480
C           THE TRANSFORMATION IS IMPLICITLY DEFINED BY MEANS OF        DTLE 490
C           X=A*Z+B TOGETHER WITH                                       DTLE 500
C           SUM(POL(I)*Z**(I-1), SUMMED OVER I FROM 1 TO N)             DTLE 510
C           =SUM(C(I)*P(I-1,X), SUMMED OVER I FROM 1 TO N).             DTLE 520
C                                                                       DTLE 530
C     ...................................................................DTLE 540
C                                                                       DTLE 550
      SUBROUTINE DTLEP(A,B,POL,N,C,WORK)                                DTLE 560
C                                                                       DTLE 570
      DIMENSION POL(1),C(1),WORK(1)                                     DTLE 580
      DOUBLE PRECISION A,B,POL,C,WORK,H,P,Q,Q1,FI                       DTLE 590
C                                                                       DTLE 600
C        TEST OF DIMENSION                                              DTLE 610
      IF(N-1)2,1,3                                                      DTLE 620
C                                                                       DTLE 630
C        DIMENSION LESS THAN 2                                          DTLE 640
    1 POL(1)=C(1)                                                       DTLE 650
    2 RETURN                                                            DTLE 660
C                                                                       DTLE 670
    3 POL(1)=C(1)+B*C(2)                                                DTLE 680
      POL(2)=A*C(2)                                                     DTLE 690
      IF(N-2)2,2,4                                                      DTLE 700
C                                                                       DTLE 710
C        INITIALIZATION                                                 DTLE 720
    4 WORK(1)=1.D0                                                      DTLE 730
      WORK(2)=B                                                         DTLE 740
      WORK(3)=0.D0                                                      DTLE 750
      WORK(4)=A                                                         DTLE 760
      FI=1.D0                                                           DTLE 770
C                                                                       DTLE 780
C        CALCULATE COEFFICIENT VECTOR OF NEXT LEGENDRE POLYNOMIAL       DTLE 790
C        AND ADD MULTIPLE OF THIS VECTOR TO POLYNOMIAL POL              DTLE 800
      DO 6 J=3,N                                                        DTLE 810
      FI=FI+1.D0                                                        DTLE 820
      Q=1.D0/FI-1.D0                                                    DTLE 830
      Q1=1.D0-Q                                                         DTLE 840
      P=0.D0                                                            DTLE 850
C                                                                       DTLE 860
      DO 5 K=2,J                                                        DTLE 870
      H=(A*P+B*WORK(2*K-2))*Q1+Q*WORK(2*K-3)                            DTLE 880
      P=WORK(2*K-2)                                                     DTLE 890
      WORK(2*K-2)=H                                                     DTLE 900
      WORK(2*K-3)=P                                                     DTLE 910
    5 POL(K-1)=POL(K-1)+H*C(J)                                          DTLE 920
      WORK(2*J-1)=0.D0                                                  DTLE 930
      WORK(2*J)=A*P*Q1                                                  DTLE 940
    6 POL(J)=C(J)*WORK(2*J)                                             DTLE 950
      RETURN                                                            DTLE 960
      END                                                               DTLE 970
```

Roots of Nonlinear Equations

Subroutines RTWI and DRTWI

These subroutines refine the initial guess x_0 of a root of the general nonlinear equation $x = f(x)$. Wegstein's iteration scheme is used in order to get accelerated convergence in case of a function f (x), which has at least continuous first derivative in the range in which iteration moves.

Following Figure 14, set $x_1 = y_0 = f(x_0)$ and $y_1 = f(x_1)$.

Refinement of x_1 is done by determination of the intersection of the linear function $y = x$ and the secant through the points (x_0, y_0) and (x_1, y_1), thus getting:

$$x_2 = x_1 + \frac{\dfrac{x_1 - x_0}{x_0 - y_0}}{\dfrac{x_1 - y_1}{x_1 - y_1}} - 1$$

and $y_2 = f(x_2)$

The next step is done by starting at (x_2, y_2) and setting:

$$x_3 = x_2 + \frac{\dfrac{x_2 - x_1}{x_1 - y_1}}{\dfrac{x_2 - y_2}{x_2 - y_2}} - 1$$

$$y_3 = f(x_3)$$

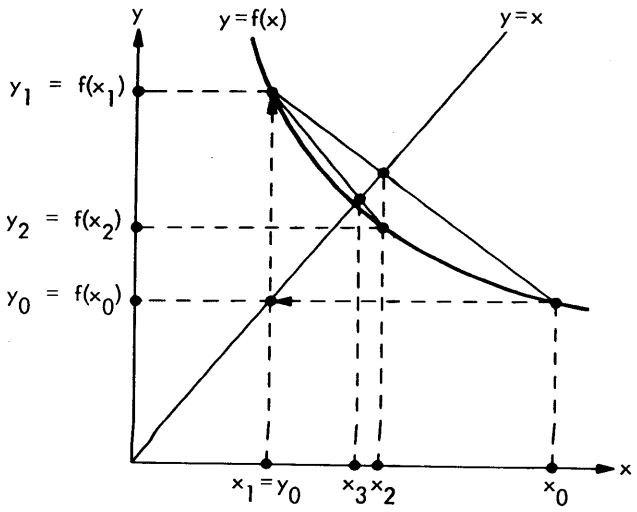

Figure 14. Wegstein's iterative method

It is easily seen that this determines the intersection between y = x and the secant through the points (x_1, y_1) and (x_2, y_2). Therefore Wegstein's iteration scheme is often called the secant modification of the normal iteration scheme $x_{i+1} = f(x_i)$.

Repeating these steps, the result is the iteration scheme:

$$\left.\begin{aligned} x_{i+1} &= x_i + \frac{x_i - x_{i-1}}{\dfrac{x_{i-1} - y_{i-1}}{x_i - y_i} - 1} \\ y_{i+1} &= f(x_{i+1}) \end{aligned}\right\} (i = 1, 2, \ldots) \quad (1)$$

Each step requires one evaluation of f(x).

This iterative procedure is terminated if the following two conditions are satisfied:

$$\delta_1 \leqq \varepsilon \quad \text{and} \quad \delta_2 \leqq 10 \cdot \varepsilon$$

with

$$\delta_1 = \begin{cases} \left| \dfrac{x_{i+1} - x_i}{x_{i+1}} \right| & \text{in case of } |x_{i+1}| > 1 \\ |x_{i+1} - x_i| & \text{in case of } |x_{i+1}| \leqq 1, \end{cases} \quad (2)$$

$$\delta_2 = \begin{cases} \left| \dfrac{x_{i+1} - y_{i+1}}{x_{i+1}} \right| & \text{in case of } |x_{i+1}| > 1 \\ |x_{i+1} - y_{i+1}| & \text{in case of } |x_{i+1}| \leqq 1 \end{cases}$$

and tolerance ε given by input.

The procedure described above may not converge within a specified number of iteration steps. Reasons for this behavior, which is indicated by an error message may be:

1. Too few iteration steps are specified.
2. The initial guess x_0 is too far away from any root.
3. The tolerance ε is too small with respect to roundoff errors.
4. The root to be determined is of multiplicity greater than one.

Furthermore, the procedure fails if at any iteration step the denominator of equation (1) becomes zero. This is also indicated by an error message. This failure may have two reasons:

1. The secant has the slope 1, either exactly or due to roundoff errors. In both cases it is probable that there is at least one point ξ in the range in which iteration moves with $f'(\xi) = 1$.

2. $x_i = x_{i-1}$ and $x_i \neq y_i = f(x_i)$. This case is possible due to roundoff errors or to a very steep slope of the secant.

For reference see G. N. Lance, Numerical Methods for High Speed Computers, Iliffe, London, 1960, pp. 134 - 138.

```
C                                                                       RTWI  10
C     ...................................................................RTWI  20
C                                                                       RTWI  30
C        SUBROUTINE RTWI                                                RTWI  40
C                                                                       RTWI  50
C        PURPOSE                                                        RTWI  60
C           TO SOLVE GENERAL NONLINEAR EQUATIONS OF THE FORM X=FCT(X)   RTWI  70
C           BY MEANS OF WEGSTEIN-S ITERATION METHOD.                    RTWI  80
C                                                                       RTWI  90
C        USAGE                                                          RTWI 100
C           CALL RTWI (X,VAL,FCT,XST,EPS,IEND,IER)                      RTWI 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               RTWI 120
C                                                                       RTWI 130
C        DESCRIPTION OF PARAMETERS                                      RTWI 140
C           X      - RESULTANT ROOT OF EQUATION X=FCT(X).               RTWI 150
C           VAL    - RESULTANT VALUE OF X-FCT(X) AT ROOT X.             RTWI 160
C           FCT    - NAME OF THE EXTERNAL FUNCTION SUBPROGRAM USED.     RTWI 170
C           XST    - INPUT VALUE WHICH SPECIFIES THE INITIAL GUESS OF   RTWI 180
C                    THE ROOT X.                                        RTWI 190
C           EPS    - INPUT VALUE WHICH SPECIFIES THE UPPER BOUND OF THE RTWI 200
C                    ERROR OF RESULT X.                                 RTWI 210
C           IEND   - MAXIMUM NUMBER OF ITERATION STEPS SPECIFIED.       RTWI 220
C           IER    - RESULTANT ERROR PARAMETER CODED AS FOLLOWS         RTWI 230
C                    IER=0 - NO ERROR,                                  RTWI 240
C                    IER=1 - NO CONVERGENCE AFTER IEND ITERATION STEPS, RTWI 250
C                    IER=2 - AT ANY ITERATION STEP THE DENOMINATOR OF   RTWI 260
C                            ITERATION FORMULA WAS EQUAL TO ZERO.       RTWI 270
C                                                                       RTWI 280
C        REMARKS                                                        RTWI 290
C           THE PROCEDURE IS BYPASSED AND GIVES THE ERROR MESSAGE IER=2 RTWI 300
C           IF AT ANY ITERATION STEP THE DENOMINATOR OF ITERATION       RTWI 310
C           FORMULA WAS EQUAL TO ZERO. THAT MEANS THAT THERE IS AT      RTWI 320
C           LEAST ONE POINT IN THE RANGE IN WHICH ITERATION MOVES WITH  RTWI 330
C           DERIVATIVE OF FCT(X) EQUAL TO 1.                            RTWI 340
C                                                                       RTWI 350
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RTWI 360
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   RTWI 370
C           BY THE USER.                                                RTWI 380
C                                                                       RTWI 390
C        METHOD                                                         RTWI 400
C           SOLUTION OF EQUATION X=FCT(X) IS DONE BY MEANS OF           RTWI 410
C           WEGSTEIN-S ITERATION METHOD, WHICH STARTS AT THE INITIAL    RTWI 420
C           GUESS XST OF A ROOT X. ONE ITERATION STEP REQUIRES ONE      RTWI 430
C           EVALUATION OF FCT(X). FOR TEST ON SATISFACTORY ACCURACY SEE RTWI 440
C           FORMULAE (2) OF MATHEMATICAL DESCRIPTION.                   RTWI 450
C           FOR REFERENCE, SEE                                          RTWI 460
C           (1) G. N. LANCE, NUMERICAL METHODS FOR HIGH SPEED COMPUTERS,RTWI 470
C               ILIFFE, LONDON, 1960, PP.134-138,                       RTWI 480
C           (2) J. WEGSTEIN, ALGORITHM 2, CACM, VOL.3, ISS.2 (1960),    RTWI 490
C               PP.74,                                                  RTWI 500
C           (3) H.C. THACHER, ALGORITHM 15, CACM, VOL.3, ISS.8 (1960),  RTWI 510
C               PP.475,                                                 RTWI 520
C           (4) J.G. HERRIOT, ALGORITHM 26, CACM, VOL.3, ISS.11 (1960), RTWI 530
C               PP.603.                                                 RTWI 540
C                                                                       RTWI 550
C     ...................................................................RTWI 560
C                                                                       RTWI 570
      SUBROUTINE RTWI(X,VAL,FCT,XST,EPS,IEND,IER)                       RTWI 580
C                                                                       RTWI 590
C                                                                       RTWI 600
C     PREPARE ITERATION                                                 RTWI 610
      IER=0                                                             RTWI 620
      TOL=XST                                                           RTWI 630
      X=FCT(TOL)                                                        RTWI 640
      A=X-XST                                                           RTWI 650
      B=-A                                                              RTWI 660
      TOL=X                                                             RTWI 670
      VAL=X-FCT(TOL)                                                    RTWI 680
C                                                                       RTWI 690
C                                                                       RTWI 700
C     START ITERATION LOOP                                              RTWI 710
      DO 6 I=1,IEND                                                     RTWI 720
      IF(VAL)1,7,1                                                      RTWI 730
C                                                                       RTWI 740
C     EQUATION IS NOT SATISFIED BY X                                    RTWI 750
    1 B=B/VAL-1.                                                        RTWI 760
      IF(B)2,8,2                                                        RTWI 770
C                                                                       RTWI 780
C     ITERATION IS POSSIBLE                                             RTWI 790
    2 A=A/B                                                             RTWI 800
      X=X+A                                                             RTWI 810
      B=VAL                                                             RTWI 820
      TOL=X                                                             RTWI 830
      VAL=X-FCT(TOL)                                                    RTWI 840
C                                                                       RTWI 850
C     TEST ON SATISFACTORY ACCURACY                                     RTWI 860
      TOL=EPS                                                           RTWI 870
      D=ABS(X)                                                          RTWI 880
      IF(D-1.)4,4,3                                                     RTWI 890
    3 TOL=TOL*D                                                         RTWI 900
    4 IF(ABS(A)-TOL)5,5,6                                               RTWI 910
    5 IF(ABS(VAL)-10.*TOL)7,7,6                                         RTWI 920
    6 CONTINUE                                                          RTWI 930
C     END OF ITERATION LOOP                                             RTWI 940
C                                                                       RTWI 950
C                                                                       RTWI 960
C     NO CONVERGENCE AFTER IEND ITERATION STEPS. ERROR RETURN.          RTWI 970
      IER=1                                                             RTWI 980
    7 RETURN                                                            RTWI 990
C                                                                       RTWI1000
C     ERROR RETURN IN CASE OF ZERO DIVISOR                              RTWI1010
    8 IER=2                                                             RTWI1020
      RETURN                                                            RTWI1030
      END                                                               RTWI1040
```

```
C                                                                       DRTW  10
C     ...................................................................DRTW  20
C                                                                       DRTW  30
C        SUBROUTINE DRTWI                                               DRTW  40
C                                                                       DRTW  50
C        PURPOSE                                                        DRTW  60
C           TO SOLVE GENERAL NONLINEAR EQUATIONS OF THE FORM X=FCT(X)   DRTW  70
C           BY MEANS OF WEGSTEIN-S ITERATION METHOD.                    DRTW  80
C                                                                       DRTW  90
C        USAGE                                                          DRTW 100
C           CALL DRTWI (X,VAL,FCT,XST,EPS,IEND,IER)                     DRTW 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               DRTW 120
C                                                                       DRTW 130
C        DESCRIPTION OF PARAMETERS                                      DRTW 140
C           X      - DOUBLE PRECISION RESULTANT ROOT OF EQUATION        DRTW 150
C                    X=FCT(X).                                          DRTW 160
C           VAL    - DOUBLE PRECISION RESULTANT VALUE OF X-FCT(X)       DRTW 170
C                    AT ROOT X.                                         DRTW 180
C           FCT    - NAME OF THE EXTERNAL DOUBLE PRECISION FUNCTION     DRTW 190
C                    SUBPROGRAM USED.                                   DRTW 200
C           XST    - DOUBLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTW 210
C                    INITIAL GUESS OF THE ROOT X.                       DRTW 220
C           EPS    - SINGLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTW 230
C                    UPPER BOUND OF THE ERROR OF RESULT X.              DRTW 240
C           IEND   - MAXIMUM NUMBER OF ITERATION STEPS SPECIFIED.       DRTW 250
C           IER    - RESULTANT ERROR PARAMETER CODED AS FOLLOWS         DRTW 260
C                    IER=0 - NO ERROR,                                  DRTW 270
C                    IER=1 - NO CONVERGENCE AFTER IEND ITERATION STEPS, DRTW 280
C                    IER=2 - AT ANY ITERATION STEP THE DENOMINATOR OF   DRTW 290
C                            ITERATION FORMULA WAS EQUAL TO ZERO.       DRTW 300
C                                                                       DRTW 310
C        REMARKS                                                        DRTW 320
C           THE PROCEDURE IS BYPASSED AND GIVES THE ERROR MESSAGE IER=2 DRTW 330
C           IF AT ANY ITERATION STEP THE DENOMINATOR OF ITERATION       DRTW 340
C           FORMULA WAS EQUAL TO ZERO. THAT MEANS THAT THERE IS AT      DRTW 350
C           LEAST ONE POINT IN THE RANGE IN WHICH ITERATION MOVES WITH  DRTW 360
C           DERIVATIVE OF FCT(X) EQUAL TO 1.                            DRTW 370
C                                                                       DRTW 380
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DRTW 390
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DRTW 400
C           MUST BE FURNISHED BY THE USER.                              DRTW 410
C                                                                       DRTW 420
C        METHOD                                                         DRTW 430
C           SOLUTION OF EQUATION X=FCT(X) IS DONE BY MEANS OF           DRTW 440
C           WEGSTEIN-S ITERATION METHOD, WHICH STARTS AT THE INITIAL    DRTW 450
C           GUESS XST OF A ROOT X. ONE ITERATION STEP REQUIRES ONE      DRTW 460
C           EVALUATION OF FCT(X). FOR TEST ON SATISFACTORY ACCURACY SEE DRTW 470
C           FORMULAE (2) OF MATHEMATICAL DESCRIPTION.                   DRTW 480
C           FOR REFERENCE, SEE                                          DRTW 490
C           (1) G. N. LANCE, NUMERICAL METHODS FOR HIGH SPEED COMPUTERS,DRTW 500
C               ILIFFE, LONDON, 1960, PP.134-138,                       DRTW 510
C           (2) J. WEGSTEIN, ALGORITHM 2, CACM, VOL.3, ISS.2 (1960),    DRTW 520
C               PP.74,                                                  DRTW 530
C           (3) H.C. THACHER, ALGORITHM 15, CACM, VOL.3, ISS.8 (1960),  DRTW 540
C               PP.475,                                                 DRTW 550
C           (4) J.G. HERRIOT, ALGORITHM 26, CACM, VOL.3, ISS.11 (1960), DRTW 560
C               PP.603.                                                 DRTW 570
C                                                                       DRTW 580
C     ...................................................................DRTW 590
C                                                                       DRTW 600
      SUBROUTINE DRTWI(X,VAL,FCT,XST,EPS,IEND,IER)                      DRTW 610
C                                                                       DRTW 620
C                                                                       DRTW 630
      DOUBLE PRECISION X,VAL,FCT,XST,A,B,D,TOL                          DRTW 640
C                                                                       DRTW 650
C     PREPARE ITERATION                                                 DRTW 660
      IER=0                                                             DRTW 670
      TOL=XST                                                           DRTW 680
      X=FCT(TOL)                                                        DRTW 690
      A=X-XST                                                           DRTW 700
      B=-A                                                              DRTW 710
      TOL=X                                                             DRTW 720
      VAL=X-FCT(TOL)                                                    DRTW 730
C                                                                       DRTW 740
C                                                                       DRTW 750
C     START ITERATION LOOP                                              DRTW 760
      DO 6 I=1,IEND                                                     DRTW 770
      IF(VAL)1,7,1                                                      DRTW 780
C                                                                       DRTW 790
C     EQUATION IS NOT SATISFIED BY X                                    DRTW 800
    1 B=B/VAL-1.D0                                                      DRTW 810
      IF(B)2,8,2                                                        DRTW 820
C                                                                       DRTW 830
C     ITERATION IS POSSIBLE                                             DRTW 840
    2 A=A/B                                                             DRTW 850
      X=X+A                                                             DRTW 860
      B=VAL                                                             DRTW 870
      TOL=X                                                             DRTW 880
      VAL=X-FCT(TOL)                                                    DRTW 890
C                                                                       DRTW 900
C     TEST ON SATISFACTORY ACCURACY                                     DRTW 910
      TOL=EPS                                                           DRTW 920
      D=DABS(X)                                                         DRTW 930
      IF(D-1.D0)4,4,3                                                   DRTW 940
    3 TOL=TOL*D                                                         DRTW 950
    4 IF(DABS(A)-TOL)5,5,6                                              DRTW 960
    5 IF(DABS(VAL)-1.D1*TOL)7,7,6                                       DRTW 970
    6 CONTINUE                                                          DRTW 980
C     END OF ITERATION LOOP                                             DRTW 990
C                                                                       DRTW1000
C                                                                       DRTW1010
C     NO CONVERGENCE AFTER IEND ITERATION STEPS. ERROR RETURN.          DRTW1020
      IER=1                                                             DRTW1030
    7 RETURN                                                            DRTW1040
C                                                                       DRTW1050
C     ERROR RETURN IN CASE OF ZERO DIVISOR                              DRTW1060
    8 IER=2                                                             DRTW1070
      RETURN                                                            DRTW1080
      END                                                               DRTW1090
```

Subroutines RTMI and DRTMI

These subroutines determine a root of the general nonlinear equation $f(x) = 0$ in the range of x from x_{li} up to x_{ri} (x_{li}, x_{ri} given by input) by means of Mueller's iteration scheme of successive bisection and inverse parabolic interpolation. The procedure assumes $f(x_{li}) \cdot f(x_{ri}) \leqq 0$.

Starting with $x_l = x_{li}$ and $x_r = x_{ri}$ and following Fig. 15, one iteration step is described.

First, the middle of the interval $x_l \ldots x_r$ is computed:

$$x_m = \frac{1}{2}(x_l + x_r).$$

In case $f(x_m) \cdot f(x_r) < 0$, x_l and x_r are interchanged to ensure that $f(x_m) \cdot f(x_r) > 0$.

In case

$$2 f(x_m)\,[f(x_m)-f(x_l)] - f(x_r)\,[f(x_r) - f(x_l)] \geqq 0 \quad (1)$$

x_r is replaced by x_m and the bisection step is repeated. If, after a specified number of successive bisections, inequality (1) is still satisfied, the procedure is bypassed and an error message is given.

In Fig. 15, the second bisection step leads to a configuration which does not satisfy inequality (1). Thus by inverse parabolic interpolation:

$$\Delta x = f(x_l)\,\frac{x_m - x_l}{f(x_m)-f(x_l)}$$

$$\left\{1 + f(x_m)\,\frac{f(x_r) - 2 f(x_m) + f(x_l)}{[f(x_r)-f(x_m)]\,[f(x_r)-f(x_l)]}\right\} \quad (2)$$

$$\text{and } x = x_l - \Delta x$$

and x is sure to be situated between x_l and x_m.

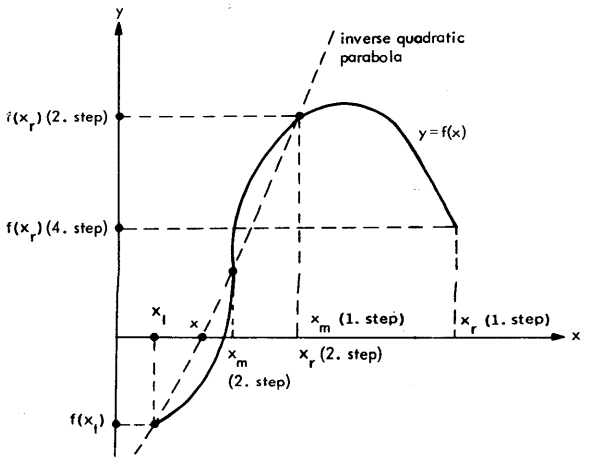

Figure 15. Mueller's iterative method

Now, for the next iteration step, x becomes x_1 and x_m becomes x_r if $f(x) \cdot f(x_1) > 0$, or x becomes x_r if $f(x) \cdot f(x_1) < 0$.

Convergence is either quadratic or linear if the multiplicity of the root to be determined is equal to one or greater than one respectively, and if f(x) can be differentiated continuously at least twice in the range $x_{1i} \cdots x_{ri}$. Each iteration step requires two evaluations of f(x).

This iterative procedure is terminated if either the two conditions (checked in bisection loop)

$$\left.\begin{aligned} |x_r - x_1| &\leq \varepsilon \cdot \max(1, |x_r|) \\ |f(x_r) - f(x_1)| &\leq 100 \cdot \varepsilon \end{aligned}\right\} \quad \text{and} \qquad (3)$$

or the two conditions (checked after inverse parabolic interpolation)

$$\left.\begin{aligned} |\Delta x| &\leq \varepsilon \cdot \max(1, |x|) \\ |f(x)| &\leq 100 \cdot \varepsilon \end{aligned}\right\} \quad \text{and} \qquad (4)$$

are satisfied, where tolerance ε is given by input.

The procedure described above may not converge within a specified number of iteration steps followed by the same number of successive bisections. Reasons for this behaviour, which is indicated by an error message, may be:

1. Too few iteration steps are specified.
2. The initial interval $x_{1i} \cdots x_{ri}$ is too long.
3. The tolerance ε is too small with respect to roundoff errors.

Furthermore, the procedure is bypassed, also giving an error message, if the basic assumption $f(x_{1i}) \cdot f(x_{ri}) \leq 0$ is not satisfied.

For reference see G. K. Kristiansen, "Zero of Arbitrary Function", BIT, vol. 3 (1963), pp. 205-206.

```
C                                                                       RTMI  10
C  ...................................................................RTMI  20
C                                                                       RTMI  30
C     SUBROUTINE RTMI                                                   RTMI  40
C                                                                       RTMI  50
C     PURPOSE                                                           RTMI  60
C        TO SOLVE GENERAL NONLINEAR EQUATIONS OF THE FORM FCT(X)=0      RTMI  70
C        BY MEANS OF MUELLER-S ITERATION METHOD.                        RTMI  80
C                                                                       RTMI  90
C     USAGE                                                             RTMI 100
C        CALL RTMI (X,F,FCT,XLI,XRI,EPS,IEND,IER)                       RTMI 110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.                  RTMI 120
C                                                                       RTMI 130
C     DESCRIPTION OF PARAMETERS                                         RTMI 140
C        X    - RESULTANT ROOT OF EQUATION FCT(X)=0.                    RTMI 150
C        F    - RESULTANT FUNCTION VALUE AT ROOT X.                     RTMI 160
C        FCT  - NAME OF THE EXTERNAL FUNCTION SUBPROGRAM USED.          RTMI 170
C        XLI  - INPUT VALUE WHICH SPECIFIES THE INITIAL LEFT BOUND      RTMI 180
C               OF THE ROOT X.                                          RTMI 190
C        XRI  - INPUT VALUE WHICH SPECIFIES THE INITIAL RIGHT BOUND     RTMI 200
C               OF THE ROOT X.                                          RTMI 210
C        EPS  - INPUT VALUE WHICH SPECIFIES THE UPPER BOUND OF THE      RTMI 220
C               ERROR OF RESULT X.                                      RTMI 230
C        IEND - MAXIMUM NUMBER OF ITERATION STEPS SPECIFIED.            RTMI 240
C        IER  - RESULTANT ERROR PARAMETER CODED AS FOLLOWS              RTMI 250
C               IER=0 - NO ERROR,                                       RTMI 260
C               IER=1 - NO CONVERGENCE AFTER IEND ITERATION STEPS       RTMI 270
C                       FOLLOWED BY IEND SUCCESSIVE STEPS OF            RTMI 280
C                       BISECTION,                                      RTMI 290
C               IER=2 - BASIC ASSUMPTION FCT(XLI)*FCT(XRI) LESS         RTMI 300
C                       THAN OR EQUAL TO ZERO IS NOT SATISFIED.         RTMI 310
C     REMARKS                                                           RTMI 320
C        THE PROCEDURE ASSUMES THAT FUNCTION VALUES AT INITIAL          RTMI 330
C        BOUNDS XLI AND XRI HAVE NOT THE SAME SIGN. IF THIS BASIC       RTMI 340
C        ASSUMPTION IS NOT SATISFIED BY INPUT VALUES XLI AND XRI, THERTRMI 350
C           PROCEDURE IS BYPASSED AND GIVES THE ERROR MESSAGE IER=2.    RTMI 370
C                                                                       RTMI 380
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RTMI 390
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   RTMI 400
C           BY THE USER.                                                RTMI 410
C                                                                       RTMI 420
C        METHOD                                                         RTMI 430
C           SOLUTION OF EQUATION FCT(X)=0 IS DONE BY MEANS OF MUELLER-S RTMI 440
C           ITERATION METHOD OF SUCCESSIVE BISECTIONS AND INVERSE       RTMI 450
C           PARABOLIC INTERPOLATION, WHICH STARTS AT THE INITIAL BOUNDS RTMI 460
C           XLI AND XRI. CONVERGENCE IS QUADRATIC IF THE DERIVATIVE OF  RTMI 470
C           FCT(X) AT ROOT X IS NOT EQUAL TO ZERO. ONE ITERATION STEP   RTMI 480
C           REQUIRES TWO EVALUATIONS OF FCT(X). FOR TEST ON SATISFACTORYRTMI 490
C           ACCURACY SEE FORMULAE (3,4) OF MATHEMATICAL DESCRIPTION.    RTMI 500
C           FOR REFERENCE, SEE G. K. KRISTIANSEN, ZERO OF ARBITRARY     RTMI 510
C           FUNCTION, BIT, VOL. 3 (1963), PP.205-206.                   RTMI 520
C                                                                       RTMI 530
C  ...................................................................RTMI 540
C                                                                       RTMI 550
      SUBROUTINE RTMI(X,F,FCT,XLI,XRI,EPS,IEND,IER)                     RTMI 560
C                                                                       RTMI 570
C                                                                       RTMI 580
C     PREPARE ITERATION                                                 RTMI 590
      IER=0                                                             RTMI 600
      XL=XLI                                                            RTMI 610
      XR=XRI                                                            RTMI 620
      X=XL                                                              RTMI 630
      TOL=X                                                             RTMI 640
      F=FCT(TOL)                                                        RTMI 650
      IF(F)1,16,1                                                       RTMI 660
    1 FL=F                                                              RTMI 670
      X=XR                                                              RTMI 680
      TOL=X                                                             RTMI 690
      F=FCT(TOL)                                                        RTMI 700
      IF(F)2,16,2                                                       RTMI 710
    2 FR=F                                                              RTMI 720
      IF(SIGN(1.,FL)+SIGN(1.,FR))25,3,25                                RTMI 730
C                                                                       RTMI 740
C     BASIC ASSUMPTION FL*FR LESS THAN 0 IS SATISFIED.                  RTMI 750
C     GENERATE TOLERANCE FOR FUNCTION VALUES.                           RTMI 760
    3 I=0                                                               RTMI 770
      TOLF=100.*EPS                                                     RTMI 780
C                                                                       RTMI 790
C                                                                       RTMI 800
C     START ITERATION LOOP                                              RTMI 810
    4 I=I+1                                                             RTMI 820
C                                                                       RTMI 830
C     START BISECTION LOOP                                              RTMI 840
      DO 13 K=1,IEND                                                    RTMI 850
      X=.5*(XL+XR)                                                      RTMI 860
      TOL=X                                                             RTMI 870
      F=FCT(TOL)                                                        RTMI 880
      IF(F)5,16,5                                                       RTMI 890
    5 IF(SIGN(1.,F)+SIGN(1.,FR))7,6,7                                   RTMI 900
C                                                                       RTMI 910
C     INTERCHANGE XL AND XR IN ORDER TO GET THE SAME SIGN IN F AND FR   RTMI 920
    6 TOL=XL                                                            RTMI 930
      XL=XR                                                             RTMI 940
      XR=TOL                                                            RTMI 950
      TOL=FL                                                            RTMI 960
      FL=FR                                                             RTMI 970
      FR=TOL                                                            RTMI 980
    7 TOL=F-FL                                                          RTMI 990
      A=F*TOL                                                           RTMI1000
      A=A+A                                                             RTMI1010
      IF(A-FR*(FR-FL))8,9,9                                             RTMI1020
    8 IF(I-IEND)17,17,9                                                 RTMI1030
    9 XR=X                                                              RTMI1040
      FR=F                                                              RTMI1050
C                                                                       RTMI1060
C     TEST ON SATISFACTORY ACCURACY IN BISECTION LOOP                   RTMI1070
      TOL=EPS                                                           RTMI1080
      A=ABS(XR)                                                         RTMI1090
      IF(A-1.)11,11,10                                                  RTMI1100
   10 TOL=TOL*A                                                         RTMI1110
   11 IF(ABS(XR-XL)-TOL)12,12,13                                        RTMI1120
   12 IF(ABS(FR-FL)-TOLF)14,14,13                                       RTMI1130
   13 CONTINUE                                                          RTMI1140
C     END OF BISECTION LOOP                                             RTMI1150
C                                                                       RTMI1160
C     NO CONVERGENCE AFTER IEND ITERATION STEPS FOLLOWED BY IEND        RTMI1170
C     SUCCESSIVE STEPS OF BISECTION OR STEADILY INCREASING FUNCTION     RTMI1180
C     VALUES AT RIGHT BOUNDS. ERROR RETURN.                             RTMI1190
      IER=1                                                             RTMI1200
   14 IF(ABS(FR)-ABS(FL))16,16,15                                       RTMI1210
   15 X=XL                                                              RTMI1220
      F=FL                                                              RTMI1230
   16 RETURN                                                            RTMI1240
C                                                                       RTMI1250
C     COMPUTATION OF ITERATED X-VALUE BY INVERSE PARABOLIC INTERPOLATIONRTMI1260
   17 A=FR-F                                                            RTMI1270
      DX=(X-XL)*FL*(1.+F*(A-TOL)/(A*(FR-FL)))/TOL                       RTMI1280
      XM=X                                                              RTMI1290
      FM=F                                                              RTMI1300
      X=XL-DX                                                           RTMI1310
      TOL=X                                                             RTMI1320
      F=FCT(TOL)                                                        RTMI1330
      IF(F)18,16,18                                                     RTMI1340
C                                                                       RTMI1350
C     TEST ON SATISFACTORY ACCURACY IN ITERATION LOOP                   RTMI1360
   18 TOL=EPS                                                           RTMI1370
      A=ABS(X)                                                          RTMI1380
      IF(A-1.)20,20,19                                                  RTMI1390
   19 TOL=TOL*A                                                         RTMI1400
   20 IF(ABS(DX)-TOL)21,21,22                                           RTMI1410
   21 IF(ABS(F)-TOLF)16,16,22                                           RTMI1420
C                                                                       RTMI1430
C     PREPARATION OF NEXT BISECTION LOOP                                RTMI1440
   22 IF(SIGN(1.,F)+SIGN(1.,FL))24,23,24                                RTMI1450
   23 XR=X                                                              RTMI1460
      FR=F                                                              RTMI1470
      GO TO 4                                                           RTMI1480
   24 XL=X                                                              RTMI1490
      FL=F                                                              RTMI1500
      XR=XM                                                             RTMI1510
      FR=FM                                                             RTMI1520
      GO TO 4                                                           RTMI1530
C     END OF ITERATION LOOP                                             RTMI1540
C                                                                       RTMI1550
C                                                                       RTMI1560
C     ERROR RETURN IN CASE OF WRONG INPUT DATA                          RTMI1570
   25 IER=2                                                             RTMI1580
      RETURN                                                            RTMI1590
      END                                                               RTMI1600
```

```
C                                                                       DRTM  10
C     ******************************************************************DRTM  20
C                                                                       DRTM  30
C        SUBROUTINE DRTMI                                               DRTM  40
C                                                                       DRTM  50
C        PURPOSE                                                        DRTM  60
C           TO SOLVE GENERAL NONLINEAR EQUATIONS OF THE FORM FCT(X)=0   DRTM  70
C           BY MEANS OF MUELLER-S ITERATION METHOD.                     DRTM  80
C                                                                       DRTM  90
C        USAGE                                                          DRTM 100
C           CALL DRTMI (X,F,FCT,XLI,XRI,EPS,IEND,IER)                   DRTM 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               DRTM 120
C                                                                       DRTM 130
C        DESCRIPTION OF PARAMETERS                                      DRTM 140
C           X      - DOUBLE PRECISION RESULTANT ROOT OF EQUATION        DRTM 150
C                    FCT(X)=0.                                          DRTM 160
C           F      - DOUBLE PRECISION RESULTANT FUNCTION VALUE          DRTM 170
C                    AT ROOT X.                                         DRTM 180
C           FCT    - NAME OF THE EXTERNAL DOUBLE PRECISION FUNCTION     DRTM 190
C                    SUBPROGRAM USED.                                   DRTM 200
C           XLI    - DOUBLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTM 210
C                    INITIAL LEFT BOUND OF THE ROOT X.                  DRTM 220
C           XRI    - DOUBLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTM 230
C                    INITIAL RIGHT BOUND OF THE ROOT X.                 DRTM 240
C           EPS    - SINGLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTM 250
C                    UPPER BOUND OF THE ERROR OF RESULT X.              DRTM 260
C           IEND   - MAXIMUM NUMBER OF ITERATION STEPS SPECIFIED.       DRTM 270
C           IER    - RESULTANT ERROR PARAMETER CODED AS FOLLOWS         DRTM 280
C                      IER=0 - NO ERROR,                                DRTM 290
C                      IER=1 - NO CONVERGENCE AFTER IEND ITERATION STEPS DRTM 300
C                              FOLLOWED BY IEND SUCCESSIVE STEPS OF     DRTM 310
C                              BISECTION,                               DRTM 320
C                      IER=2 - BASIC ASSUMPTION FCT(XLI)*FCT(XRI) LESS  DRTM 330
C                              THAN OR EQUAL TO ZERO IS NOT SATISFIED.  DRTM 340
C                                                                       DRTM 350
C        REMARKS                                                        DRTM 360
C           THE PROCEDURE ASSUMES THAT FUNCTION VALUES AT INITIAL       DRTM 370
C           BOUNDS XLI AND XRI HAVE NOT THE SAME SIGN. IF THIS BASIC    DRTM 380
C           ASSUMPTION IS NOT SATISFIED BY INPUT VALUES XLI AND XRI, THEDRTM 390
C           PROCEDURE IS BYPASSED AND GIVES THE ERROR MESSAGE IER=2.    DRTM 400
C                                                                       DRTM 410
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DRTM 420
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DRTM 430
C           MUST BE FURNISHED BY THE USER.                              DRTM 440
C                                                                       DRTM 450
C        METHOD                                                         DRTM 460
C           SOLUTION OF EQUATION FCT(X)=0 IS DONE BY MEANS OF MUELLER-S DRTM 470
C           ITERATION METHOD OF SUCCESSIVE BISECTIONS AND INVERSE       DRTM 480
C           PARABOLIC INTERPOLATION, WHICH STARTS AT THE INITIAL BOUNDS DRTM 490
C           XLI AND XRI. CONVERGENCE IS QUADRATIC IF THE DERIVATIVE OF  DRTM 500
C           FCT(X) AT ROOT X IS NOT EQUAL TO ZERO. ONE ITERATION STEP   DRTM 510
C           REQUIRES TWO EVALUATIONS OF FCT(X). FOR TEST ON SATISFACTORYDRTM 520
C           ACCURACY SEE FORMULAE (3,4) OF MATHEMATICAL DESCRIPTION.    DRTM 530
C           FOR REFERENCE, SEE G. K. KRISTIANSEN, ZERO OF ARBITRARY     DRTM 540
C           FUNCTION, BIT, VOL. 3 (1963), PP.205-206.                   DRTM 550
C                                                                       DRTM 560
C     ******************************************************************DRTM 570
C                                                                       DRTM 580
      SUBROUTINE DRTMI(X,F,FCT,XLI,XRI,EPS,IEND,IER)                    DRTM 590
C                                                                       DRTM 600
C                                                                       DRTM 610
      DOUBLE PRECISION X,F,FCT,XLI,XRI,XL,XR,FL,FR,TOL,TOLF,A,DX,XM,FM  DRTM 620
C                                                                       DRTM 630
C     PREPARE ITERATION                                                 DRTM 640
      IER=0                                                             DRTM 650
      XL=XLI                                                            DRTM 660
      XR=XRI                                                            DRTM 670
      X=XL                                                              DRTM 680
      TOL=X                                                             DRTM 690
      F=FCT(TOL)                                                        DRTM 700
      IF(F)1,16,1                                                       DRTM 710
    1 FL=F                                                              DRTM 720
      X=XR                                                              DRTM 730
      TOL=X                                                             DRTM 740
      F=FCT(TOL)                                                        DRTM 750
      IF(F)2,16,2                                                       DRTM 760
    2 FR=F                                                              DRTM 770
      IF(DSIGN(1.D0,FL)+DSIGN(1.D0,FR))25,3,25                          DRTM 780
C                                                                       DRTM 790
C     BASIC ASSUMPTION FL*FR LESS THAN 0 IS SATISFIED.                  DRTM 800
C     GENERATE TOLERANCE FOR FUNCTION VALUES.                           DRTM 810
    3 I=0                                                               DRTM 820
      TOLF=100.*EPS                                                     DRTM 830
C                                                                       DRTM 840
C                                                                       DRTM 850
C     START ITERATION LOOP                                              DRTM 860
    4 I=I+1                                                             DRTM 870
C                                                                       DRTM 880
C     START BISECTION LOOP                                              DRTM 890
      DO 13 K=1,IEND                                                    DRTM 900
      X=.5D0*(XL+XR)                                                    DRTM 910
      TOL=X                                                             DRTM 920
      F=FCT(TOL)                                                        DRTM 930
      IF(F)5,16,5                                                       DRTM 940
    5 IF(DSIGN(1.D0,F)+DSIGN(1.D0,FR))7,6,7                             DRTM 950
C                                                                       DRTM 960
C     INTERCHANGE XL AND XR IN ORDER TO GET THE SAME SIGN IN F AND FR   DRTM 970
    6 TOL=XL                                                            DRTM 980
      XL=XR                                                             DRTM 990
      XR=TOL                                                            DRTM1000
      TOL=FL                                                            DRTM1010
      FL=FR                                                             DRTM1020
      FR=TOL                                                            DRTM1030
    7 TOL=F-FL                                                          DRTM1040
      A=F*TOL                                                           DRTM1050
      A=A+A                                                             DRTM1060
      IF(A-FR*(FR-FL))8,9,9                                             DRTM1070
    8 IF(I-IEND)17,17,9                                                 DRTM1080
    9 XR=X                                                              DRTM1090
      FR=F                                                              DRTM1100
C                                                                       DRTM1110
C     TEST ON SATISFACTORY ACCURACY IN BISECTION LOOP                   DRTM1120
      TOL=EPS                                                           DRTM1130
      A=DABS(XR)                                                        DRTM1140
      IF(A-1.D0)11,11,10                                                DRTM1150
   10 TOL=TOL*A                                                         DRTM1160
   11 IF(DABS(XR-XL)-TOL)12,12,13                                       DRTM1170
   12 IF(DABS(FR-FL)-TOLF)14,14,13                                      DRTM1180
   13 CONTINUE                                                          DRTM1190
C     END OF BISECTION LOOP                                             DRTM1200
C                                                                       DRTM1210
C     NO CONVERGENCE AFTER IEND ITERATION STEPS FOLLOWED BY IEND        DRTM1220
C     SUCCESSIVE STEPS OF BISECTION OR STEADILY INCREASING FUNCTION     DRTM1230
C     VALUES AT RIGHT BOUNDS. ERROR RETURN.                             DRTM1240
      IER=1                                                             DRTM1250
   14 IF(DABS(FR)-DABS(FL))16,16,15                                     DRTM1260
   15 X=XL                                                              DRTM1270
      F=FL                                                              DRTM1280
   16 RETURN                                                            DRTM1290
C                                                                       DRTM1300
C     COMPUTATION OF ITERATED X-VALUE BY INVERSE PARABOLIC INTERPOLATIONDRTM1310
   17 A=FR-F                                                            DRTM1320
      DX=(X-XL)*FL*(1.D0+F*(A-TOL)/(A*(FR-FL)))/TOL                     DRTM1330
      XM=X                                                              DRTM1340
      FM=F                                                              DRTM1350
      X=XL-DX                                                           DRTM1360
      TOL=X                                                             DRTM1370
      F=FCT(TOL)                                                        DRTM1380
      IF(F)18,16,18                                                     DRTM1390
C                                                                       DRTM1400
C     TEST ON SATISFACTORY ACCURACY IN ITERATION LOOP                   DRTM1410
   18 TOL=EPS                                                           DRTM1420
      A=DABS(X)                                                         DRTM1430
      IF(A-1.D0)20,20,19                                                DRTM1440
   19 TOL=TOL*A                                                         DRTM1450
   20 IF(DABS(DX)-TOL)21,21,22                                          DRTM1460
   21 IF(DABS(F)-TOLF)16,16,22                                          DRTM1470
C                                                                       DRTM1480
C     PREPARATION OF NEXT BISECTION LOOP                                DRTM1490
   22 IF(DSIGN(1.D0,F)+DSIGN(1.D0,FL))24,23,24                          DRTM1500
   23 XR=X                                                              DRTM1510
      FR=F                                                              DRTM1520
      GO TO 4                                                           DRTM1530
   24 XL=X                                                              DRTM1540
      FL=F                                                              DRTM1550
      XR=XM                                                             DRTM1560
      FR=FM                                                             DRTM1570
      GO TO 4                                                           DRTM1580
C     END OF ITERATION LOOP                                             DRTM1590
C                                                                       DRTM1600
C                                                                       DRTM1610
C     ERROR RETURN IN CASE OF WRONG INPUT DATA                          DRTM1620
   25 IER=2                                                             DRTM1630
      RETURN                                                            DRTM1640
      END                                                               DRTM1650
```

Subroutines RTNI and DRTNI

These subroutines refine the initial guess x_0 of a root of the general nonlinear equation $f(x) = 0$. Newton's iteration scheme is used in the following form:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \qquad (i = 0, 1, 2, \ldots) \qquad (1)$$

Convergence is quadratic or linear if the multiplicity of the root to be determined is equal to one or greater than one respectively, and if f(x) can be differentiated continuously at least twice in the range in which iteration moves. Each iteration step requires one evaluation of f(x) and one evaluation of $f'(x)$.

This iterative procedure is terminated if the following two conditions are satisfied:

$$\delta \leqq \varepsilon \text{ and } |f(x_{i+1})| \leqq 100 \cdot \varepsilon$$

with

$$\delta = \left\{ \begin{array}{ll} \left| \dfrac{x_{i+1} - x_i}{x_{i+1}} \right| & \text{in case of } |x_{i+1}| > 1 \\ |x_{i+1} - x_i| & \text{in case of } |x_{i+1}| \leqq 1 \end{array} \right\} \qquad (2)$$

and tolerance ε given by input.

The procedure described above may not converge within a specified number of iteration steps. Reasons for this behaviour, which is indicated by an error message, may be:

1. Too few iteration steps are specified.
2. The initial guess x_0 is too far away from any root.
3. The tolerance ε is too small with respect to roundoff errors.
4. The root to be determined is of multiplicity greater than one.

Furthermore, the procedure fails and is bypassed if at any iteration step the derivative $f(x_i)$ becomes zero. This is also indicated by an error message.

For reference see:

(1) F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York/Toronto/London, 1956, pp. 447 - 450.

(2) R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker, Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 12 - 17.


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C                                                                       RTNI  10
C     ..................................................................RTNI  20
C                                                                       RTNI  30
C        SUBROUTINE RTNI                                                RTNI  40
C                                                                       RTNI  50
C        PURPOSE                                                        RTNI  60
C           TO SOLVE GENERAL NONLINEAR EQUATIONS OF THE FORM F(X)=0     RTNI  70
C           BY MEANS OF NEWTON-S ITERATION METHOD.                      RTNI  80
C                                                                       RTNI  90
C        USAGE                                                          RTNI 100
C           CALL RTNI (X,F,DERF,FCT,XST,EPS,IEND,IER)                   RTNI 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               RTNI 120
C                                                                       RTNI 130
C        DESCRIPTION OF PARAMETERS                                      RTNI 140
C           X      - RESULTANT ROOT OF EQUATION F(X)=0.                 RTNI 150
C           F      - RESULTANT FUNCTION VALUE AT ROOT X.                RTNI 160
C           DERF   - RESULTANT VALUE OF DERIVATIVE AT ROOT X.           RTNI 170
C           FCT    - NAME OF THE EXTERNAL SUBROUTINE USED. IT COMPUTES  RTNI 180
C                    TO GIVEN ARGUMENT X FUNCTION VALUE F AND DERIVATIVERTNI 190
C                    DERF. ITS PARAMETER LIST MUST BE X,F,DERF.         RTNI 200
C           XST    - INPUT VALUE WHICH SPECIFIES THE INITIAL GUESS OF   RTNI 210
C                    THE ROOT X.                                        RTNI 220
C           EPS    - INPUT VALUE WHICH SPECIFIES THE UPPER BOUND OF THE RTNI 230
C                    ERROR OF RESULT X.                                 RTNI 240
C           IEND   - MAXIMUM NUMBER OF ITERATION STEPS SPECIFIED.       RTNI 250
C           IER    - RESULTANT ERROR PARAMETER CODED AS FOLLOWS         RTNI 260
C                    IER=0 - NO ERROR,                                  RTNI 270
C                    IER=1 - NO CONVERGENCE AFTER IEND ITERATION STEPS, RTNI 280
C                    IER=2 - AT ANY ITERATION STEP DERIVATIVE DERF WAS  RTNI 290
C                            EQUAL TO ZERO.                             RTNI 300
C                                                                       RTNI 310
C        REMARKS                                                        RTNI 320
C           THE PROCEDURE IS BYPASSED AND GIVES THE ERROR MESSAGE IER=2 RTNI 330
C           IF AT ANY ITERATION STEP DERIVATIVE OF F(X) IS EQUAL TO 0.  RTNI 340
C           POSSIBLY THE PROCEDURE WOULD BE SUCCESSFUL IF IT IS STARTED RTNI 350
C           ONCE MORE WITH ANOTHER INITIAL GUESS XST.                   RTNI 360
C                                                                       RTNI 370
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RTNI 380
C           THE EXTERNAL SUBROUTINE FCT(X,F,DERF) MUST BE FURNISHED     RTNI 390
C           BY THE USER.                                                RTNI 400
C                                                                       RTNI 410
C        METHOD                                                         RTNI 420
C           SOLUTION OF EQUATION F(X)=0 IS DONE BY MEANS OF NEWTON-S    RTNI 430
C           ITERATION METHOD, WHICH STARTS AT THE INITIAL GUESS XST OF  RTNI 440
C           A ROOT X. CONVERGENCE IS QUADRATIC IF THE DERIVATIVE OF     RTNI 450
C           F(X) AT ROOT X IS NOT EQUAL TO ZERO. ONE ITERATION STEP     RTNI 460
C           REQUIRES ONE EVALUATION OF F(X) AND ONE EVALUATION OF THE   RTNI 470
C           DERIVATIVE OF F(X). FOR TEST ON SATISFACTORY ACCURACY SEE   RTNI 480
C           FORMULAE (2) OF MATHEMATICAL DESCRIPTION.                   RTNI 490
C           FOR REFERENCE, SEE R. ZURMUEHL, PRAKTISCHE MATHEMATIK FUER  RTNI 500
C           INGENIEURE UND PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/       RTNI 510
C           HEIDELBERG, 1963, PP.12-17.                                 RTNI 520
C                                                                       RTNI 530
C     ..................................................................RTNI 540
      SUBROUTINE RTNI(X,F,DERF,FCT,XST,EPS,IEND,IER)                    RTNI 550
C                                                                       RTNI 560
C                                                                       RTNI 570
C     PREPARE ITERATION                                                 RTNI 580
      IER=0                                                             RTNI 590
      X=XST                                                             RTNI 600
      TOL=X                                                             RTNI 610
      CALL FCT(TOL,F,DERF)                                              RTNI 620
      TOLF=100.*EPS                                                     RTNI 630
C                                                                       RTNI 640
C                                                                       RTNI 650
C     START ITERATION LOOP                                              RTNI 660
      DO 6 I=1,IEND                                                     RTNI 670
      IF(F)1,7,1                                                        RTNI 680
C                                                                       RTNI 690
C     EQUATION IS NOT SATISFIED BY X                                    RTNI 700
    1 IF(DERF)2,8,2                                                     RTNI 710
C                                                                       RTNI 720
C     ITERATION IS POSSIBLE                                             RTNI 730
    2 DX=F/DERF                                                         RTNI 740
      X=X-DX                                                            RTNI 750
      TOL=X                                                             RTNI 760
      CALL FCT(TOL,F,DERF)                                              RTNI 770
C                                                                       RTNI 780
C     TEST ON SATISFACTORY ACCURACY                                     RTNI 790
      TOL=EPS                                                           RTNI 800
      A=ABS(X)                                                          RTNI 810
      IF(A-1.)4,4,3                                                     RTNI 820
    3 TOL=TOL*A                                                         RTNI 830
    4 IF(ABS(DX)-TOL)5,5,6                                              RTNI 840
    5 IF(ABS(F)-TOLF)7,7,6                                              RTNI 850
    6 CONTINUE                                                          RTNI 860
C     END OF ITERATION LOOP                                             RTNI 870
C                                                                       RTNI 880
C                                                                       RTNI 890
C     NO CONVERGENCE AFTER IEND ITERATION STEPS. ERROR RETURN.          RTNI 900
      IER=1                                                             RTNI 910
    7 RETURN                                                            RTNI 920
C                                                                       RTNI 930
C     ERROR RETURN IN CASE OF ZERO DIVISOR                              RTNI 940
    8 IER=2                                                             RTNI 950
      RETURN                                                            RTNI 960
      END                                                               RTNI 970
                                                                        RTNI 980
```

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C                                                                       DRTN  10
C     ...................................................................DRTN  20
C                                                                       DRTN  30
C        SUBROUTINE DRTNI                                               DRTN  40
C                                                                       DRTN  50
C        PURPOSE                                                        DRTN  60
C           TO SOLVE GENERAL NONLINEAR EQUATIONS OF THE FORM F(X)=0     DRTN  70
C           BY MEANS OF NEWTON-S ITERATION METHOD.                      DRTN  80
C                                                                       DRTN  90
C        USAGE                                                          DRTN 100
C           CALL DRTNI (X,F,DERF,FCT,XST,EPS,IEND,IER)                  DRTN 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               DRTN 120
C                                                                       DRTN 130
C        DESCRIPTION OF PARAMETERS                                      DRTN 140
C           X      - DOUBLE PRECISION RESULTANT ROOT OF EQUATION F(X)=0.DRTN 150
C           F      - DOUBLE PRECISION RESULTANT FUNCTION VALUE AT       DRTN 160
C                    ROOT X.                                            DRTN 170
C           DERF   - DOUBLE PRECISION RESULTANT VALUE OF DERIVATIVE     DRTN 180
C                    AT ROOT X.                                         DRTN 190
C           FCT    - NAME OF THE EXTERNAL SUBROUTINE USED. IT COMPUTES  DRTN 200
C                    TO GIVEN ARGUMENT X FUNCTION VALUE F AND DERIVATIVEDRTN 210
C                    DERF. ITS PARAMETER LIST MUST BE X,F,DERF, WHERE   DRTN 220
C                    ALL PARAMETERS ARE DOUBLE PRECISION.               DRTN 230
C           XST    - DOUBLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTN 240
C                    INITIAL GUESS OF THE ROOT X.                       DRTN 250
C           EPS    - SINGLE PRECISION INPUT VALUE WHICH SPECIFIES THE   DRTN 260
C                    UPPER BOUND OF THE ERROR OF RESULT X.              DRTN 270
C           IEND   - MAXIMUM NUMBER OF ITERATION STEPS SPECIFIED.       DRTN 280
C           IER    - RESULTANT ERROR PARAMETER CODED AS FOLLOWS         DRTN 290
C                    IER=0 - NO ERROR,                                  DRTN 300
C                    IER=1 - NO CONVERGENCE AFTER IEND ITERATION STEPS, DRTN 310
C                    IER=2 - AT ANY ITERATION STEP DERIVATIVE DERF WAS  DRTN 320
C                            EQUAL TO ZERO.                             DRTN 330
C                                                                       DRTN 340
C        REMARKS                                                        DRTN 350
C           THE PROCEDURE IS BYPASSED AND GIVES THE ERROR MESSAGE IER=2 DRTN 360
C           IF AT ANY ITERATION STEP DERIVATIVE OF F(X) IS EQUAL TO 0.  DRTN 370
C           POSSIBLY THE PROCEDURE WOULD BE SUCCESSFUL IF IT IS STARTED DRTN 380
C           ONCE MORE WITH ANOTHER INITIAL GUESS XST.                   DRTN 390
C                                                                       DRTN 400
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DRTN 410
C           THE EXTERNAL SUBROUTINE FCT(X,F,DERF) MUST BE FURNISHED     DRTN 420
C           BY THE USER.                                                DRTN 430
C                                                                       DRTN 440
C        METHOD                                                         DRTN 450
C           SOLUTION OF EQUATION F(X)=0 IS DONE BY MEANS OF NEWTON-S    DRTN 460
C           ITERATION METHOD, WHICH STARTS AT THE INITIAL GUESS XST OF  DRTN 470
C           A ROOT X. CONVERGENCE IS QUADRATIC IF THE DERIVATIVE OF     DRTN 480
C           F(X) AT ROOT X IS NOT EQUAL TO ZERO. ONE ITERATION STEP     DRTN 490
C           REQUIRES ONE EVALUATION OF F(X) AND ONE EVALUATION OF THE   DRTN 500
C           DERIVATIVE OF F(X). FOR TEST ON SATISFACTORY ACCURACY SEE   DRTN 510
C           FORMULAE (2) OF MATHEMATICAL DESCRIPTION.                   DRTN 520
C           FOR REFERENCE, SEE R. ZURMUEHL, PRAKTISCHE MATHEMATIK FUER  DRTN 530
C           INGENIEURE UND PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/       DRTN 540
C           HEIDELBERG, 1963, PP.12-17.                                 DRTN 550
C                                                                       DRTN 560
C     ...................................................................DRTN 570
C                                                                       DRTN 580
      SUBROUTINE DRTNI(X,F,DERF,FCT,XST,EPS,IEND,IER)                   DRTN 590
C                                                                       DRTN 600
C                                                                       DRTN 610
      DOUBLE PRECISION X,F,DERF,XST,TOL,TOLF,DX,A                       DRTN 620
C                                                                       DRTN 630
C     PREPARE ITERATION                                                 DRTN 640
      IER=0                                                             DRTN 650
      X=XST                                                             DRTN 660
      TOL=X                                                             DRTN 670
      CALL FCT(TOL,F,DERF)                                              DRTN 680
      TOLF=100.*EPS                                                     DRTN 690
C                                                                       DRTN 700
C                                                                       DRTN 710
C     START ITERATION LOOP                                              DRTN 720
      DO 6 I=1,IEND                                                     DRTN 730
      IF(F)1,7,1                                                        DRTN 740
C                                                                       DRTN 750
C     EQUATION IS NOT SATISFIED BY X                                    DRTN 760
    1 IF(DERF)2,8,2                                                     DRTN 770
C                                                                       DRTN 780
C     ITERATION IS POSSIBLE                                             DRTN 790
    2 DX=F/DERF                                                         DRTN 800
      X=X-DX                                                            DRTN 810
      TOL=X                                                             DRTN 820
      CALL FCT(TOL,F,DERF)                                              DRTN 830
C                                                                       DRTN 840
C     TEST ON SATISFACTORY ACCURACY                                     DRTN 850
      TOL=EPS                                                           DRTN 860
      A=DABS(X)                                                         DRTN 870
      IF(A-1.D0)4,4,3                                                   DRTN 880
    3 TOL=TOL*A                                                         DRTN 890
    4 IF(DABS(DX)-TOL)5,5,6                                             DRTN 900
    5 IF(DABS(F)-TOLF)7,7,6                                             DRTN 910
    6 CONTINUE                                                          DRTN 920
C     END OF ITERATION LOOP                                             DRTN 930
C                                                                       DRTN 940
C                                                                       DRTN 950
C     NO CONVERGENCE AFTER IEND ITERATION STEPS. ERROR RETURN.          DRTN 960
      IER=1                                                             DRTN 970
    7 RETURN                                                            DRTN 980
C                                                                       DRTN 990
C     ERROR RETURN IN CASE OF ZERO DIVISOR                              DRTN1000
    8 IER=2                                                             DRTN1010
      RETURN                                                            DRTN1020
      END                                                               DRTN1030
```

Extremum of Functions

Subroutines FMFP and DFMFP

These subroutines perform the calculation of an unconstrained minimum of a function of several variables using a method proposed by Davidon. The underlying method is described in the article by R. Fletcher and M.J.D. Powell, "A Rapidly Convergent Descent Method for Minimization", Computer Journal, vol. 6, iss. 2, 1963, pp. 163 - 168.

It is assumed that the function f of the n variables $x_1, \ldots, x_n$ (abbreviated as argument vector x) may be computed together with its gradient vector g(x) for any point x. The generalized Taylor expansion for functions of several variables is

$$f(x+u) = f(x) + g(x) \cdot u + \frac{1}{2} u^T G(x) u + \text{higher terms}$$

where g is the gradient vector and G the matrix of second order partial derivatives. Vectors are assumed to be column vectors; u^T means transpose of vector u. It is assumed that in the neighborhood of the required minimum x_{min} the function is approximated closely by the first three terms of its Taylor expansion, giving

$$f(x) = f(x_{min}) + \frac{1}{2} (x - x_{min})^T G(x_{min}) (x - x_{min})$$

since $g(x_{min}) = 0$. Then the gradient is seen to be approximately $g(x) = G(x_{min}) (x - x_{min})$.

Assume now that the symmetric matrix G is positive definite. Then the following equation holds true:

$$x - x_{min} = G^{-1} (x_{min}) \cdot g(x)$$

which would allow x_{min} to be calculated in one step if $G^{-1} (x_{min})$ were available.

To approach $G^{-1} (x_{min})$, a method of successive linear searches in G-conjugate directions is used. Starting with the identity matrix $G^{(0)} = I$, a sequence of symmetric matrices $G^{(i)}$ is generated which tends to G^{-1}. At the $(i+1)^{st}$ iteration step a linear search is made in direction $h^{(i)} = -G^{(i)} g^{(i)}$, where $g^{(i)}$ is an abbreviation for $g(x^{(i)})$. By means of the linear search the minimum of $y(t) = f(x^{(i)} + t \cdot h^{(i)})$ is determined, giving argument $x^{(i+1)} = x^{(i)} + t_i \cdot h^{(i)}$.

The argument of the minimum $x^{(i+1)}$ on the line through $x^{(i)}$ in direction $h^{(i)}$ is determined by the relation that scalar product $(g^{(i+1)}, h^{(i)}) = 0$.

Now:
$$x^{(n)} = x^{(j)} + \sum_{i=j}^{n-1} t_i h^{(i)}$$

and:
$$g^{(n)} = g^{(j)} + \sum_{i=j}^{n-1} t_i G h^{(i)}$$

Therefore:

scalar product
$$(g^{(n)}, h^{(j)}) = \sum_{i=j+1}^{n-1} t_i (G h^{(i)}, h^{(j)})$$

Suppose now that the vectors $h^{(0)}, h^{(1)}, \ldots, h^{(n-1)}$ are G-conjugate, satisfying $(G h^{(i)}, h^{(j)}) = 0$ for $i \neq j$. Then $(g^{(n)}, h^{(j)}) = 0$, and since $h^{(0)}, h^{(1)}, \ldots, h^{(n-1)}$ form a basis, $g^{(n)} = 0$ and $x^{(n)} = x_{min}$. This shows that the minimum is located at the n^{th} iteration for a quadratic function when using successive linear searches for G-conjugate directions.

For the generation of G-conjugate directions, start with $h^{(0)} = -g^{(0)}$ and calculate successive directions $h^{(i)}$ by means of $h^{(i)} = -G^{(i)}g^{(i)}$, where $G^{(i)}$ is modified to $G^{(i+1)}$ so that $h^{(i)}$ is an eigenvector of the matrix $G^{(i+1)}$ G with eigenvalue 1. This ensures that $G^{(i)}$ approaches G^{-1} as $x^{(i)}$ approaches x_{min}. An easy calculation shows:

$$G^{(i+1)} = G^{(i)} + \frac{dx \cdot dx^T}{dx^T \cdot dg} - \frac{G^{(i)} dg \cdot dg^T G^{(i)}}{dg^T G^{(i)} dg}$$

with $dg = g^{(i+1)} - g^{(i)}$

$dx = x^{(i+1)} - x^{(i)}$

where all vectors are regarded as column vectors, and superscript T means transpose of column vector--that is, row vector.

The strategy adopted for termination of the successive linear searches is as follows:

1. If the function value has not decreased in the last iteration step, the search for the minimum is terminated provided the gradient is already sufficiently small; otherwise, the next step is in the direction of steepest descent.

2. If the argument vector and the direction vector change by very small amounts, and at least n iterations are performed, the minimization is terminated again.

3. If the number of iterations exceeds an upper bound furnished by the user, further calculation is bypassed, and an error code is set to 1 indicating poor convergence.

4. If one of the successive linear searches indicates that no constrained minimum exists, further calculation is bypassed again, and the error code is set to 2 indicating that it is likely that no minimum exists.

The i^{th} term $G^{(i)}$ is reset to the identity matrix if there is indication that the current $G^{(i)}$ is not positive definite, or if the formula for $G^{(i+1)}$ breaks down due to zero divisors.

The linear search technique used in subroutines FMFP and DFMFP is as follows. For a given argument vector x and vector h, defining a direction through x, a local minimum of the function $y(t) = f(x+th)$ must be found. This means that a value t_m must be determined for which

$$y'(t_m) = \text{scalar product } (g(x+t_m h), h) = 0$$

From $y'(0) = (g(x), h) < 0$ it is evident that a minimum $y(t_m) < y(0)$ should be found for positive values of t.

The calculation of the minimum is in three stages. The first estimates the magnitude of t_m, the second determines an interval containing t_m, and the third interpolates the value of t_m.

An estimate of the step-size may be obtained, assuming that the true value of the constrained minimum is equal to the estimated value EST of the unconstrained minimum and that y (t) is closely represented by a quadratic polynomial passing through (x, y(0)) with derivative y'(0):
step = 2 (EST - y(0))/y'(0).

This equation tends to overestimate the step-size, since the unconstrained minimum will normally not lie on the line through x with direction h. Therefore, step is taken as step-size s only if it is positive and less than one. Otherwise, s = 1 is taken as step-size.

At the second stage y(t) and y'(t) are examined at the points $t = s, 2s, 4s, \ldots, s_1, s_2$, where successive values are obtained by doubling the step-size.

This search is terminated at $t = s_2$ if:

$$y'(s_2) = 0, \text{ or } y'(s_2) > 0, \text{ or } y(s_2) \geq y(s_1)$$

$$\text{or if } s_2 \cdot \left(\sum_{i=1}^{n} |h_i| \right) > 10^{10}.$$

The last case (search argument runs out of range) is interpreted as an indication that no local minimum exists on the given line. In this case, the error indicator is set to (2) and further calculation is bypassed.

In case $y'(s_2) = 0$, t_m is set to s_2 and $x_m = x = s_2 h$ is used as the argument of a constrained minimum on the line through x with direction h.

In the second and third case ($y'(s_2) > 0$ and/or $y(s_2) \geq y(s_1)$) a minimum lies necessarily between s_1 and s_2. Its argument value gets approximated using cubic interpolation.

The extrema of the cubic interpolation passing through (s_1, $y_1 = y(s_1)$, $y'_1 = y'(s_1)$) and (s_2, $y_2 = y(s_2)$, $y'_2 = y'(s_2)$) are given by solving a quadratic equation. The solution s_3 can be expressed as $s_3 = s_1 + (1-\alpha)(s_2 - s_1) = s_2 - \alpha(s_2 - s_1)$ with

$$\alpha = \frac{y'_2 - z + w}{y'_2 - y'_1 + 2W} = \frac{y'_2 + z - w}{y'_2 + y'_1 + 2z},$$

$$0 < \alpha < 1, \text{ and } z = y'_1 + y'_2 - 3\frac{y_2 - y_2}{s_2 - s_1},$$

$$w = \pm (z^2 - y'_1 y'_2)^{1/2}.$$

The conditions on the problem guarantee a real value of w. The sign of w is so chosen that s_3 is in the interval (s_1, s_2). If this condition is satisfied for the two possible values of s_3, the value closer to s_1 is retained.

As written above, two equivalent formulas can provide α. The choice is based on numerical stability considerations.

If $y(s_3) \leq y(s_1)$ and $y(s_3) \leq y(s_2)$, then t_m is set equal to s_3 and $x_m = x + t_m \cdot h$ is used as argument of the desired minimum along the given line. Otherwise, the interval (s_1, s_2) is reduced by replacing s_1 by s_3 if $y(s_3) \leq y(s_1)$ and $y'(s_3) < 0$ and by replacing s_2 by s_3 in all other cases. The interpolation process is repeated for this new reduced interval.

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C                                                                       FMFP  10
C     ..................................................................FMFP  20
C                                                                       FMFP  30
C        SUBROUTINE FMFP                                                FMFP  40
C                                                                       FMFP  50
C        PURPOSE                                                        FMFP  60
C           TO FIND A LOCAL MINIMUM OF A FUNCTION OF SEVERAL VARIABLES  FMFP  70
C           BY THE METHOD OF FLETCHER AND POWELL                        FMFP  80
C                                                                       FMFP  90
C        USAGE                                                          FMFP 100
C           CALL FMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)                FMFP 110
C                                                                       FMFP 120
C        DESCRIPTION OF PARAMETERS                                      FMFP 130
C           FUNCT  - USER-WRITTEN SUBROUTINE CONCERNING THE FUNCTION TO FMFP 140
C                    BE MINIMIZED. IT MUST BE OF THE FORM               FMFP 150
C                    SUBROUTINE FUNCTN(N,ARG,VAL,GRAD)                  FMFP 160
C                    AND MUST SERVE THE FOLLOWING PURPOSE               FMFP 170
C                    FOR EACH N-DIMENSIONAL ARGUMENT VECTOR  ARG,       FMFP 180
C                    FUNCTION VALUE AND GRADIENT VECTOR MUST BE COMPUTEDFMFP 190
C                    AND, ON RETURN, STORED IN VAL AND GRAD RESPECTIVELYFMFP 200
C              N     - NUMBER OF VARIABLES                              FMFP 210
C              X     - VECTOR OF DIMENSION N CONTAINING THE INITIAL     FMFP 220
C                      ARGUMENT WHERE THE ITERATION STARTS. ON RETURN,  FMFP 230
C                      X HOLDS THE ARGUMENT COORDINATING TO THE         FMFP 240
C                      COMPUTED MINIMUM FUNCTION VALUE                  FMFP 250
C              F     - SINGLE VARIABLE CONTAINING THE MINIMUM FUNCTION  FMFP 260
C                      VALUE ON RETURN, I.E. F=F(X).                    FMFP 270
C              G     - VECTOR OF DIMENSION N CONTAINING THE GRADIENT    FMFP 280
C                      VECTOR CORRESPONDING TO THE MINIMUM ON RETURN,   FMFP 290
C                      I.E. G=G(X).                                     FMFP 300
C              EST   - IS AN ESTIMATE OF THE MINIMUM FUNCTION VALUE.    FMFP 310
C              EPS   - TESTVALUE REPRESENTING THE EXPECTED ABSOLUTE ERROR,FMFP 320
C                      A REASONABLE CHOICE IS 10**(-K), I.E.            FMFP 330
C                      SOMEWHAT GREATER THAN 10**(-D), WHERE D IS THE   FMFP 340
C                      NUMBER OF SIGNIFICANT DIGITS IN FLOATING POINT   FMFP 350
C                      REPRESENTATION.                                  FMFP 360
C              LIMIT - MAXIMUM NUMBER OF ITERATIONS.                    FMFP 370
C              IER   - ERROR PARAMETER                                  FMFP 380
C                      IER = 0 MEANS CONVERGENCE WAS OBTAINED           FMFP 390
C                      IER = 1 MEANS NO CONVERGENCE IN LIMIT ITERATIONS FMFP 400
C                      IER =-1 MEANS ERRORS IN GRADIENT CALCULATION     FMFP 410
C                      IER = 2 MEANS LINEAR SEARCH TECHNIQUE INDICATES  FMFP 420
C                      IT IS LIKELY THAT THERE EXISTS NO MINIMUM.       FMFP 430
C              H     - WORKING STORAGE OF DIMENSION N*(N+7)/2.          FMFP 440
C                                                                       FMFP 450
C        REMARKS                                                        FMFP 460
C           I) THE SUBROUTINE NAME REPLACING THE DUMMY ARGUMENT  FUNCT  FMFP 470
C              MUST BE DECLARED AS EXTERNAL IN THE CALLING PROGRAM.     FMFP 480
C           II) IER IS SET TO 2 IF , STEPPING IN ONE OF THE COMPUTED    FMFP 490
C               DIRECTIONS, THE FUNCTION WILL NEVER INCREASE WITHIN     FMFP 500
C               A TOLERABLE RANGE OF ARGUMENT.                          FMFP 510
C               IER = 2 MAY OCCUR ALSO IF THE INTERVAL WHERE F          FMFP 520
C               INCREASES IS SMALL AND THE INITIAL ARGUMENT WAS         FMFP 530
C               RELATIVELY FAR AWAY FROM THE MINIMUM SUCH THAT THE      FMFP 540
C               MINIMUM WAS OVERLEAPED. THIS IS DUE TO THE SEARCH       FMFP 550
C               TECHNIQUE WHICH DOUBLES THE STEPSIZE UNTIL A POINT      FMFP 560
C               IS FOUND WHERE THE FUNCTION INCREASES.                  FMFP 570
C                                                                       FMFP 580
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FMFP 590
C           FUNCT                                                       FMFP 600
C                                                                       FMFP 610
C        METHOD                                                         FMFP 620
C           THE METHOD IS DESCRIBED IN THE FOLLOWING ARTICLE            FMFP 630
C           R. FLETCHER AND M.J.D. POWELL, A RAPID DESCENT METHOD FOR   FMFP 640
C           MINIMIZATION,                                               FMFP 650
C           COMPUTER JOURNAL VOL.6, ISS. 2, 1963, PP.163-168.           FMFP 660
C                                                                       FMFP 670
C     ..................................................................FMFP 680
C                                                                       FMFP 690
      SUBROUTINE FMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)                FMFP 700
C                                                                       FMFP 710
C        DIMENSIONED DUMMY VARIABLES                                    FMFP 720
      DIMENSION H(1),X(1),G(1)                                          FMFP 730
C                                                                       FMFP 740
C        COMPUTE FUNCTION VALUE AND GRADIENT VECTOR FOR INITIAL ARGUMENTFMFP 750
      CALL FUNCT(N,X,F,G)                                               FMFP 760
C                                                                       FMFP 770
C        RESET ITERATION COUNTER AND GENERATE IDENTITY MATRIX           FMFP 780
      IER=0                                                             FMFP 790
      KCLAT=0                                                           FMFP 800
      A2=N+N                                                            FMFP 810
      A3=A2+N                                                           FMFP 820
      A31=A3+1                                                          FMFP 830
    1 K=A31                                                             FMFP 840
      DO 4 J=1,N                                                        FMFP 850
      H(K)=1.                                                           FMFP 860
      AJ=N-J                                                            FMFP 870
      IF(AJ)5,5,2                                                       FMFP 880
    2 DO 3 L=1,AJ                                                       FMFP 890
      KL=K+L                                                            FMFP 900
    3 H(KL)=0.                                                          FMFP 910
    4 K=KL+1                                                            FMFP 920
C                                                                       FMFP 930
C        START ITERATION LOOP                                           FMFP 940
    5 KCLAT=KCLAT+1                                                     FMFP 950
C                                                                       FMFP 960
C        SAVE FUNCTION VALUE, ARGUMENT VECTOR AND GRADIENT VECTOR       FMFP 970
      OLDF=F                                                            FMFP 980
      DO 6 J=1,N                                                        FMFP 990
      K=N+J                                                             FMFP1000
      H(K)=G(J)                                                         FMFP1010
      K=K+N                                                             FMFP1020
    6 H(K)=X(J)                                                         FMFP1030
C                                                                       FMFP1040
C        DETERMINE DIRECTION VECTOR H                                   FMFP1050
      K=J+N3                                                            FMFP1060
      T=0.                                                              FMFP1070
      DO 8 L=1,N                                                        FMFP1080
      T=T-G(L)*H(K)                                                     FMFP1090
      K=K+1                                                             FMFP1100
    8 H(K)=T                                                            FMFP1110
C                                                                       FMFP1120
C        CHECK WHETHER FUNCTION WILL DECREASE STEPPING ALONG H.         FMFP1130
      DY=0.                                                             FMFP1140
      HARP=0.                                                           FMFP1150
      GARP=0.                                                           FMFP1160
C                                                                       FMFP1170
C           CALCULATE DIRECTIONAL DERIVATIVE AND TESTVALUES FOR DIRECTIONFMFP1180
C           VECTOR H AND GRADIENT VECTOR G.                             FMFP1190
      DO 10 J=1,N                                                       FMFP1200
      HARP=HARP+ABS(H(J))                                               FMFP1210
      GARP=GARP+ABS(G(J))                                               FMFP1220
   10 DY=DY+H(J)*G(J)                                                   FMFP1230
C                                                                       FMFP1240
C           REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DIRECTIONALFMFP1250
C           DERIVATIVE APPEARS TO BE POSITIVE OR ZERO.                  FMFP1260
      IF(DY)11,51,51                                                    FMFP1270
C                                                                       FMFP1280
C           REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DIRECTION FMFP1290
C           VECTOR H IS SMALL COMPARED TO GRADIENT VECTOR G.            FMFP1300
   11 IF(HARP/GARP-EPS)51,51,12                                         FMFP1310
C                                                                       FMFP1320
C           SEARCH MINIMUM ALONG DIRECTION H                            FMFP1330
C                                                                       FMFP1340
C           SEARCH ALONG H FOR POSITIVE DIRECTIONAL DERIVATIVE          FMFP1350
   12 FY=F                                                              FMFP1360
      ALFA=2.*(EST-F)/DY                                                FMFP1370
      APREC=1.                                                          FMFP1380
C                                                                       FMFP1390
C           USE ESTIMATE FOR STEPSIZE ONLY IF IT IS POSITIVE AND LESS THAN FMFP1400
C           1. OTHERWISE TAKE 1. AS STEPSIZE                            FMFP1410
      IF(ALFA)15,15,13                                                  FMFP1420
   13 IF(ALFA-APREC)14,15,15                                            FMFP1430
   14 APREC=ALFA                                                        FMFP1440
   15 ALFA=0.                                                           FMFP1450
C                                                                       FMFP1460
C           SAVE FUNCTION AND DERIVATIVE VALUES FOR OLD ARGUMENT        FMFP1470
   16 FX=FY                                                             FMFP1480
      DX=DY                                                             FMFP1490
C                                                                       FMFP1500
C           STEP ARGUMENT ALONG H                                       FMFP1510
      DO 17 I=1,N                                                       FMFP1520
   17 X(I)=X(I)+APREC*H(I)                                              FMFP1530
C                                                                       FMFP1540
C           COMPUTE FUNCTION VALUE AND GRADIENT FOR NEW ARGUMENT        FMFP1550
      CALL FUNCT(N,X,F,G)                                               FMFP1560
      FY=F                                                              FMFP1570
C                                                                       FMFP1580
C           COMPUTE DIRECTIONAL DERIVATIVE DY FOR NEW ARGUMENT.  TERMINATEFMFP1590
C           SEARCH, IF DY IS POSITIVE. IF DY IS ZERO THE MINIMUM IS FOUNDFMFP1600
      DY=0.                                                             FMFP1610
      DO 18 I=1,N                                                       FMFP1620
   18 DY=DY+G(I)*H(I)                                                   FMFP1630
      IF(DY)19,36,22                                                    FMFP1640
C                                                                       FMFP1650
C           TERMINATE SEARCH ALSO IF THE FUNCTION VALUE INDICATES THAT  FMFP1660
C           A MINIMUM HAS BEEN PASSED                                   FMFP1670
   19 IF(FY-FX)20,22,22                                                 FMFP1680
C                                                                       FMFP1690
C           REPEAT SEARCH AND DOUBLE STEPSIZE FOR FURTHER SEARCHES      FMFP1700
   20 APREC=APREC+ALFA                                                  FMFP1710
      ALFA=APREC                                                        FMFP1720
C           END OF SEARCH LOOP                                          FMFP1730
C                                                                       FMFP1740
C           TERMINATE IF THE CHANGE IN ARGUMENT GETS VERY LARGE         FMFP1750
      IF(HARP*APREC-1.E10)16,16,21                                      FMFP1760
C                                                                       FMFP1770
C           LINEAR SEARCH TECHNIQUE INDICATES THAT NO MINIMUM EXISTS    FMFP1780
   21 IER=2                                                             FMFP1790
      RETURN                                                            FMFP1800
C                                                                       FMFP1810
C           INTERPOLATE CUBICALLY IN THE INTERVAL DEFINED BY THE SEARCH FMFP1820
C           ABOVE AND COMPUTE THE ARGUMENT X FOR WHICH THE INTERPOLATION FMFP1830
C           POLYNOMIAL IS MINIMIZED                                     FMFP1840
   22 T=0.                                                              FMFP1850
   23 IF(APREC)24,24,24                                                 FMFP1860
   24 Z=3.*(F)-FY)/APREC+DX+DY                                          FMFP1870
      ALFA=APREC*(ABS(Z),ABS(DX),ABS(DY))                               FMFP1880
      CALFA=Z/ALFA                                                      FMFP1890
      CALFA=CALFA*CALFA-DX/ALFA*DY/ALFA                                 FMFP1900
      IF(CALFA)251,25,25                                                FMFP1910
   25 W=ALFA*SQRT(CALFA)                                                FMFP1920
      ALFA=DY-DX+W+W                                                    FMFP1930
      IF(ALFA) 25C,251,25C                                              FMFP1940
  25C ALFA=(DY-Z+W)/ALFA                                                FMFP1950
      GO TO 252                                                         FMFP1960
  251 ALFA=(Z+DY-W)/(Z+DX+Z+DY)                                         FMFP1970
  252 ALFA=ALFA*APREC                                                   FMFP1971
      DO 26 I=1,N                                                       FMFP1972
   26 X(I)=X(I)+(T-ALFA)*H(I)                                           FMFP1973
C                                                                       FMFP1974
C           TERMINATE, IF THE VALUE OF THE ACTUAL FUNCTION AT X IS LESS FMFP1975
C           THAN THE FUNCTION VALUES AT THE INTERVAL ENDS. OTHERWISE REDUCEFMFP1980
C           THE INTERVAL BY CHOOSING ONE END-POINT EQUAL TO X AND REPEAT FMFP1990
C           THE INTERPOLATION. WHICH END-POINT IS CHOOSEN DEPENDS ON THE FMFP2000
C           VALUE OF THE FUNCTION AND ITS GRADIENT AT X                 FMFP2010
C                                                                       FMFP2020
      CALL FUNCT(N,X,F,G)                                               FMFP2030
      IF(F-FX)27,27,28                                                  FMFP2040
   27 IF(F-FY)36,36,28                                                  FMFP2050
   28 CALFA=0.                                                          FMFP2060
      DO 29 I=1,N                                                       FMFP2070
   29 CALFA=CALFA+G(I)*H(I)                                             FMFP2080
      IF(CALFA)30,33,33                                                 FMFP2090
   30 IF(F-FX)32,31,33                                                  FMFP2100
   31 IF(DX-CALFA)32,36,32                                              FMFP2110
   32 FY=F                                                              FMFP2120
      DY=CALFA                                                          FMFP2130
      T=ALFA                                                            FMFP2140
      APREC=ALFA                                                        FMFP2150
      GO TO 23                                                          FMFP2160
   33 IF(FY-F)35,34,35                                                  FMFP2170
   34 IF(DY-CALFA)35,36,35                                              FMFP2180
   35 FY=F                                                              FMFP2190
      DY=CALFA                                                          FMFP2200
      APREC=APREC-ALFA                                                  FMFP2210
      GO TO 22                                                          FMFP2220
C                                                                       FMFP2230
C           TERMINATE, IF FUNCTION HAS NOT DECREASED DURING LAST ITERATIONFMFP2240
   36 IF(OLDF-F+EPS)51,36,36                                            FMFP2250
C                                                                       FMFP2260
C           COMPUTE DIFFERENCE VECTORS OF ARGUMENT AND GRADIENT FROM    FMFP2270
C           TWO CONSECUTIVE ITERATIONS                                  FMFP2280
   36 DO 37 J=1,N                                                       FMFP2290
      K=N+J                                                             FMFP2300
      H(K)=G(J)-H(K)                                                    FMFP2310
      K=N+K                                                             FMFP2320
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   37 P(K)=X(J)-P(K)                                                    FMFP2370
C                                                                       FMFP2380
C        TEST LENGTH OF ARGUMENT DIFFERENCE VECTOR AND DIRECTION VECTOR FMFP2390
C        IF AT LEAST N ITERATIONS HAVE BEEN EXECUTED. TERMINATE, IF     FMFP2400
C        BOTH ARE LESS THAN  EPS                                        FMFP2410
      IER=0                                                             FMFP2420
      IF(KCLAT-N)42,39,39                                               FMFP2430
   39 T=0.                                                              FMFP2440
      Z=0.                                                              FMFP2450
      DO 40 J=1,N                                                       FMFP2460
      K=N+J                                                             FMFP2470
      W=P(K)                                                            FMFP2480
      K=K+N                                                             FMFP2490
      T=T+ZES(P(K))                                                     FMFP2500
   40 Z=Z+W*P(K)                                                        FMFP2510
      IF(SNRM-EPS)41,41,42                                              FMFP2520
   41 IF(T-EPS)26,26,42                                                 FMFP2530
C                                                                       FMFP2540
C        TERMINATE, IF NUMBER OF ITERATIONS WOULD EXCEED  LIMIT         FMFP2550
   42 IF(KCLAT-LIMIT)43,50,50                                           FMFP2560
C                                                                       FMFP2570
C        PREPARE UPDATING OF MATRIX P                                   FMFP2580
   43 ALFA=0.                                                           FMFP2590
      DO 47 J=1,N                                                       FMFP2600
      K=J+N2                                                            FMFP2610
      W=0.                                                              FMFP2620
      DO 46 L=1,N                                                       FMFP2630
      KL=N+L                                                            FMFP2640
      W=W+P(KL)*H(K)                                                    FMFP2650
      IF(L-J)44,45,45                                                   FMFP2660
   44 K=K+N-L                                                           FMFP2670
      GO TO 46                                                          FMFP2680
   45 K=K+1                                                             FMFP2690
   46 CONTINUE                                                          FMFP2700
      K=N+J                                                             FMFP2710
      ALFA=ALFA+W*P(K)                                                  FMFP2720
   47 P(J)=W                                                            FMFP2730
C                                                                       FMFP2740
C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF RESULTS      FMFP2750
C        ARE NOT SATISFACTORY                                           FMFP2760
      IF(2*ALFA)48,1,48                                                 FMFP2770
C                                                                       FMFP2780
C        UPDATE MATRIX P                                                FMFP2790
   48 K=N2I                                                             FMFP2800
      DO 49 L=1,N                                                       FMFP2810
      KL=N2+L                                                           FMFP2820
      DO 49 J=L,N                                                       FMFP2830
      KJ=N2+J                                                           FMFP2840
      P(K)=P(K)+P(KL)*P(KJ)/Z-P(L)*P(J)/ALFA                            FMFP2850
   49 K=K+1                                                             FMFP2860
      GO TO 5                                                           FMFP2870
C        END OF ITERATION LOOP                                          FMFP2880
C                                                                       FMFP2890
C        NO CONVERGENCE AFTER  LIMIT  ITERATIONS                        FMFP2900
   50 IER=1                                                             FMFP2910
      RETURN                                                            FMFP2920
C                                                                       FMFP2930
C        RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                   FMFP2940
   51 DO 52 J=1,N                                                       FMFP2950
      K=N2+J                                                            FMFP2960
   52 X(J)=P(K)                                                         FMFP2970
      CALL FUNCT(N,X,F,G)                                               FMFP2980
C                                                                       FMFP2990
C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DERIVATIVE   FMFP3000
C        FAILS TO BE SUFFICIENTLY SMALL                                 FMFP3010
      IF(GAMM-EPS)55,55,53                                              FMFP3020
C                                                                       FMFP3030
C        TEST FOR REPEATED FAILURE OF ITERATION                         FMFP3040
   53 IF(IER)56,54,54                                                   FMFP3050
   54 IER=-1                                                            FMFP3060
      GOTO 1                                                            FMFP3070
   55 IER=0                                                             FMFP3080
   56 RETURN                                                            FMFP3090
      END                                                               FMFP3100
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C                                                                       DFMF  10
C     ------------------------------------------------------------------DFMF  20
C                                                                       DFMF  30
C        SUBROUTINE DFMFP                                               DFMF  40
C                                                                       DFMF  50
C        PURPOSE                                                        DFMF  60
C           TO FIND A LOCAL MINIMUM OF A FUNCTION OF SEVERAL VARIABLES  DFMF  70
C           BY THE METHOD OF FLETCHER AND POWELL                        DFMF  80
C                                                                       DFMF  90
C        USAGE                                                          DFMF 100
C           CALL DFMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)               DFMF 110
C                                                                       DFMF 120
C        DESCRIPTION OF PARAMETERS                                      DFMF 130
C           FUNCT  - USER-WRITTEN SUBROUTINE CONCERNING THE FUNCTION TO DFMF 140
C                    BE MINIMIZED. IT MUST BE OF THE FORM               DFMF 150
C                    SUBROUTINE FUNCT(N,ARG,VAL,GRAD)                   DFMF 160
C                    AND MUST SERVE THE FOLLOWING PURPOSE               DFMF 170
C                    FOR EACH N-DIMENSIONAL ARGUMENT VECTOR  ARG,       DFMF 180
C                    FUNCTION VALUE AND GRADIENT VECTOR MUST BE COMPUTEDDFMF 190
C                    AND, ON RETURN, STORED IN VAL AND GRAD RESPECTIVELYDFMF 200
C                    ARG,VAL AND GRAD MUST BE OF DOUBLE PRECISION.      DFMF 210
C              N     - NUMBER OF VARIABLES                              DFMF 220
C              X     - VECTOR OF DIMENSION N CONTAINING THE INITIAL     DFMF 230
C                      ARGUMENT WHERE THE ITERATION STARTS. ON RETURN,  DFMF 240
C                      X HOLDS THE ARGUMENT CORRESPONDING TO THE        DFMF 250
C                      COMPUTED MINIMUM FUNCTION VALUE                  DFMF 260
C                      DOUBLE PRECISION VECTOR.                         DFMF 270
C              F     - SINGLE VARIABLE CONTAINING THE MINIMUM FUNCTION  DFMF 280
C                      VALUE ON RETURN, I.E. F=F(X).                    DFMF 290
C                      DOUBLE PRECISION VARIABLE.                       DFMF 300
C              G     - VECTOR OF DIMENSION N CONTAINING THE GRADIENT    DFMF 310
C                      VECTOR CORRESPONDING TO THE MINIMUM ON RETURN,   DFMF 320
C                      I.E. G=G(X).                                     DFMF 330
C                      DOUBLE PRECISION VECTOR.                         DFMF 340
C              EST   - IS AN ESTIMATE OF THE MINIMUM FUNCTION VALUE.     DFMF 350
C                      SINGLE PRECISION VARIABLE.                       DFMF 360
C              EPS   - TESTVALUE REPRESENTING THE EXPECTED ABSOLUTE ERROR.DFMF 370
C                      A REASONABLE CHOICE IS 10**(-16), I.E.           DFMF 380
C                      SOMEWHAT GREATER THAN 10**(-D), WHERE D IS THE   DFMF 390
C                      NUMBER OF SIGNIFICANT DIGITS IN FLOATING POINT   DFMF 400
C                      REPRESENTATION.                                  DFMF 410
C                      SINGLE PRECISION VARIABLE.                       DFMF 420
C              LIMIT - MAXIMUM NUMBER OF ITERATIONS.                    DFMF 430
C              IER   - ERROR PARAMETER                                  DFMF 440
C                      IER = 0 MEANS CONVERGENCE WAS OBTAINED           DFMF 450
C                      IER = 1 MEANS NO CONVERGENCE IN LIMIT ITERATIONS DFMF 460
C                      IER =-1 MEANS ERRORS IN GRADIENT CALCULATION     DFMF 470
C                      IER = 2 MEANS LINEAR SEARCH TECHNIQUE INDICATES  DFMF 480
C                      IT IS LIKELY THAT THERE EXISTS NO MINIMUM.       DFMF 490
C              H     - WORKING STORAGE OF DIMENSION N*(N+7)/2.          DFMF 500
C                      DOUBLE PRECISION ARRAY.                          DFMF 510
C                                                                       DFMF 520
C        REMARKS                                                        DFMF 530
C           1) THE SUBROUTINE NAME REPLACING THE DUMMY ARGUMENT  FUNCT  DFMF 540
C              MUST BE DECLARED AS EXTERNAL IN THE CALLING PROGRAM.     DFMF 550
C           2) IER IS SET TO 2 IF , STEPPING IN ONE OF THE COMPUTED     DFMF 560
C              DIRECTIONS, THE FUNCTION WILL NEVER INCREASE WITHIN      DFMF 570
C              A TOLERABLE RANGE OF ARGUMENT.                           DFMF 580
C              IER = 2 MAY OCCUR ALSO IF THE INTERVAL WHERE F           DFMF 590
C              INCREASES IS SMALL AND THE INITIAL ARGUMENT WAS          DFMF 600
C              RELATIVELY FAR AWAY FROM THE MINIMUM SUCH THAT THE       DFMF 610
C              MINIMUM WAS OVERLEAPED. THIS IS DUE TO THE SEARCH        DFMF 620
C              TECHNIQUE WHICH DOUBLES THE STEPSIZE UNTIL A POINT       DFMF 630
C              IS FOUND WHERE THE FUNCTION INCREASES.                   DFMF 640
C                                                                       DFMF 650
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DFMF 660
C           FUNCT                                                       DFMF 670
C                                                                       DFMF 680
C        METHOD                                                         DFMF 690
C           THE METHOD IS DESCRIBED IN THE FOLLOWING ARTICLE            DFMF 700
C           R. FLETCHER AND M.J.D. POWELL, A RAPID DESCENT METHOD FOR   DFMF 710
C           MINIMIZATION.                                               DFMF 720
C           COMPUTER JOURNAL VOL.6, ISS. 2, 1963, PP.163-168.           DFMF 730
C                                                                       DFMF 740
C     ------------------------------------------------------------------DFMF 750
C                                                                       DFMF 760
      SUBROUTINE DFMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)               DFMF 770
C                                                                       DFMF 780
C        DIMENSIONED DUMMY VARIABLES                                    DFMF 790
      DIMENSION H(1),X(1),G(1)                                          DFMF 800
      DOUBLE PRECISION X,F,FX,FY,DLEF,HARM,GARM,H,G,DX,DY,ALFA,DALFA,   DFMF 810
     1APEGA,T,Z,W                                                       DFMF 820
C                                                                       DFMF 830
C        COMPUTE FUNCTION VALUE AND GRADIENT VECTOR FOR INITIAL ARGUMENTDFMF 840
      CALL FUNCT(N,X,F,G)                                               DFMF 850
C                                                                       DFMF 860
C        RESET ITERATION COUNTER AND GENERATE IDENTITY MATRIX           DFMF 870
      IER=0                                                             DFMF 880
      KCLAT=0                                                           DFMF 890
      N2=N+N                                                            DFMF 900
      N3=N2+N                                                           DFMF 910
      N31=N3+1                                                          DFMF 920
    1 K=N31                                                             DFMF 930
      DO 4 J=1,N                                                        DFMF 940
      H(K)=1.0D0                                                        DFMF 950
      NJ=N-J                                                            DFMF 960
      IF(NJ)5,5,2                                                       DFMF 970
    2 DO 3 L=1,NJ                                                       DFMF 980
      KL=K+L                                                            DFMF 990
    3 H(KL)=0.0D0                                                       DFMF1000
    4 K=KL+1                                                            DFMF1010
C                                                                       DFMF1020
C        START ITERATION LOOP                                           DFMF1030
    5 KCLAT=KCLAT+1                                                     DFMF1040
C                                                                       DFMF1050
C        SAVE FUNCTION VALUE, ARGUMENT VECTOR AND GRADIENT VECTOR       DFMF1060
      OLDF=F                                                            DFMF1070
      DO 6 J=1,N                                                        DFMF1080
      K=N+J                                                             DFMF1090
      H(K)=G(J)                                                         DFMF1100
      K=K+N                                                             DFMF1110
    6 H(K)=X(J)                                                         DFMF1120
C                                                                       DFMF1130
C        DETERMINE DIRECTION VECTOR H                                   DFMF1140
      K=J+N3                                                            DFMF1150
      T=0.0D0                                                           DFMF1160
      DO 8 L=1,N                                                        DFMF1170
      T=T-G(L)*H(K)                                                     DFMF1180
      IF(L-J)8,7,7                                                      DFMF1190
    7 K=K+N-L                                                           DFMF1200
      GO TO 8                                                           DFMF1210
    8 K=K+1                                                             DFMF1220
      CONTINUE                                                          DFMF1230
      H(J)=T                                                            DFMF1240
C                                                                       DFMF1250
C        CHECK WHETHER FUNCTION WILL DECREASE STEPPING ALONG H.         DFMF1260
      DY=0.0D0                                                          DFMF1270
      HARM=0.0D0                                                        DFMF1280
      GARM=0.0D0                                                        DFMF1290
C                                                                       DFMF1300
C        CALCULATE DIRECTIONAL DERIVATIVE AND TESTVALUES FOR DIRECTION  DFMF1310
C        VECTOR H AND GRADIENT VECTOR G.                                DFMF1320
      DO 10 J=1,N                                                       DFMF1330
      HARM=HARM+DABS(H(J))                                              DFMF1340
      GARM=GARM+DABS(G(J))                                              DFMF1350
   10 DY=DY+H(J)*G(J)                                                   DFMF1360
C                                                                       DFMF1370
C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DIRECTIONAL  DFMF1380
C        DERIVATIVE APPEARS TO BE POSITIVE OR ZERO.                     DFMF1390
      IF(DY)11,51,51                                                    DFMF1400
C                                                                       DFMF1410
C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DIRECTION    DFMF1420
C        VECTOR H IS SMALL COMPARED TO GRADIENT VECTOR G.               DFMF1430
   11 IF(HARM/GARM-EPS)51,51,12                                         DFMF1440
C                                                                       DFMF1450
C        SEARCH MINIMUM ALONG DIRECTION H                               DFMF1460
C                                                                       DFMF1470
C        SEARCH ALONG H FOR POSITIVE DIRECTIONAL DERIVATIVE             DFMF1480
   12 FY=F                                                              DFMF1490
      ALFA=2.0D0*(EST-F)/DY                                             DFMF1500
      APEGA=1.0D0                                                       DFMF1510
C                                                                       DFMF1520
C        USE ESTIMATE FOR STEPSIZE ONLY IF IT IS POSITIVE AND LESS THAN DFMF1530
C        1. OTHERWISE TAKE 1. AS STEPSIZE                               DFMF1540
      IF(ALFA)15,15,13                                                  DFMF1550
   13 IF(ALFA-APEGA)14,15,15                                            DFMF1560
   14 APEGA=ALFA                                                        DFMF1570
   15 ALFA=0.0D0                                                        DFMF1580
C                                                                       DFMF1590
C        SAVE FUNCTION AND DERIVATIVE VALUES FOR OLD ARGUMENT           DFMF1600
   16 FX=FY                                                             DFMF1610
      DX=DY                                                             DFMF1620
C                                                                       DFMF1630
C        STEP ARGUMENT ALONG H                                          DFMF1640
      DO 17 I=1,N                                                       DFMF1650
   17 X(I)=X(I)+APEGA*H(I)                                              DFMF1660
C                                                                       DFMF1670
C        COMPUTE FUNCTION VALUE AND GRADIENT FOR NEW ARGUMENT           DFMF1680
      CALL FUNCT(N,X,F,G)                                               DFMF1690
      FY=F                                                              DFMF1700
C                                                                       DFMF1710
C        COMPUTE DIRECTIONAL DERIVATIVE DY FOR NEW ARGUMENT.  TERMINATE DFMF1720
C        SEARCH, IF DY IS POSITIVE. IF DY IS ZERO THE MINIMUM IS FOUND  DFMF1730
      DY=0.0D0                                                          DFMF1740
      DO 18 I=1,N                                                       DFMF1750
   18 DY=DY+G(I)*H(I)                                                   DFMF1760
      IF(DY)15,36,22                                                    DFMF1770
C                                                                       DFMF1780
C        TERMINATE SEARCH ALSO IF THE FUNCTION VALUE INDICATES THAT     DFMF1790
C        A MINIMUM HAS BEEN PASSED                                      DFMF1800
   19 IF(FY-FX)20,20,22                                                 DFMF1810
C                                                                       DFMF1820
C        REPEAT SEARCH AND DOUBLE STEPSIZE FOR FURTHER SEARCHES         DFMF1830
   20 APEGA=APEGA+ALFA                                                  DFMF1840
      ALFA=APEGA                                                        DFMF1850
C        END OF SEARCH LOOP                                             DFMF1860
C                                                                       DFMF1870
```

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C        TERMINATE IF THE CHANGE IN ARGUMENT GETS VERY LARGE                    DFMF1880
         IF(ABS(P*APBCA)-1.E10)16,16,21                                         DFMF1890
C                                                                               DFMF1900
C        LINEAR SEARCH TECHNIQUE INDICATES THAT NO MINIMUM EXISTS               DFMF1910
   21    IER=2                                                                  DFMF1920
         RETURN                                                                 DFMF1930
C                                                                               DFMF1940
C           INTERPOLATE CUBICALLY IN THE INTERVAL DEFINED BY THE SEARCH         DFMF1950
C           ABOVE AND COMPUTE THE ARGUMENT X FOR WHICH THE INTERPOLATION        DFMF1960
C           POLYNOMIAL IS MINIMIZED                                             DFMF1970
   22    T=C.CC                                                                 DFMF1980
   23    IF(APBCA)24,36,24                                                      DFMF1990
   24    Z=3.CC*(FA-FY)/APBCA+GX+GY                                             DFMF2000
         ALFA=CMAX1(ABS(Z),ABS(GX),ABS(GY))                                     DFMF2010
         CALFA=Z/ALFA                                                           DFMF2020
         CALFA=CALFA*CALFA-GX/ALFA*GY/ALFA                                      DFMF2030
         IF(CALFA)51,25,25                                                      DFMF2040
   25    W=ALFA*CSQRT(CALFA)                                                    DFMF2050
         ALFA=GY-GX+W                                                           DFMF2060
         IF(ALFA) 25C,251,25C                                                   DFMF2061
  25C    ALFA=(GY-GX+W)/ALFA                                                    DFMF2062
         GO TO 252                                                              DFMF2063
  251    ALFA=(Z+GY-W)/(Z+GX+Z+GY)                                              DFMF2064
  252    ALFA=ALFA*APBCA                                                        DFMF2065
         DO 26 I=1,N                                                            DFMF2070
   26    X(I)=X(I)+(T-ALFA)*P(I)                                                DFMF2080
C                                                                               DFMF2090
C           TERMINATE, IF THE VALUE OF THE ACTUAL FUNCTION AT X IS LESS         DFMF2100
C           THAN THE FUNCTION VALUES AT THE INTERVAL ENDS. OTHERWISE REDUCE     DFMF2110
C           THE INTERVAL BY CHOOSING ONE END-POINT EQUAL TO X AND REPEAT        DFMF2120
C           THE INTERPOLATION. WHICH END-POINT IS CHOSEN DEPENDS ON THE         DFMF2130
C           VALUE OF THE FUNCTION AND ITS GRADIENT AT X                         DFMF2140
C                                                                               DFMF2150
         CALL FUNCTN(N,X,F,G)                                                   DFMF2160
         IF(F-FA)27,27,28                                                       DFMF2170
   27    IF(F-FY)36,36,26                                                       DFMF2180
   28    CALFA=C.CC                                                             DFMF2190
         DO 29 I=1,N                                                            DFMF2200
   29    CALFA=CALFA+G(I)*P(I)                                                  DFMF2210
         IF(CALFA)3C,33,33                                                      DFMF2220
   3C    IF(F-FA)32,31,33                                                       DFMF2230
   31    IF(GX-CALFA)32,36,32                                                   DFMF2240
   32    FX=F                                                                   DFMF2250
         GX=CALFA                                                               DFMF2260
         T=ALFA                                                                 DFMF2270
         APBCA=ALFA                                                             DFMF2280
         GO TO 23                                                               DFMF2290
   33    IF(FY-F)35,34,35                                                       DFMF2300
   34    IF(GY-CALFA)35,36,35                                                   DFMF2310
   35    FY=F                                                                   DFMF2320
         GY=CALFA                                                               DFMF2330
         APBCA=APBCA-ALFA                                                       DFMF2340
         GO TO 22                                                               DFMF2350
C                                                                               DFMF2360
C           TERMINATE, IF FUNCTION HAS NOT DECREASED DURING LAST ITERATION      DFMF2370
   36    IF(CLOF-F+EPS)351,38,38                                                DFMF2380
C                                                                               DFMF2390
C           COMPUTE DIFFERENCE VECTORS OF ARGUMENT AND GRADIENT FROM            DFMF2400
C           TWO CONSECUTIVE ITERATIONS                                          DFMF2410
   36    DO 37 J=1,N                                                            DFMF2420
         K=N+J                                                                  DFMF2430
         P(K)=G(J)-P(K)                                                         DFMF2440
         K=N+K                                                                  DFMF2450
   37    P(K)=X(J)-P(K)                                                         DFMF2460
C                                                                               DFMF2470
C           TEST LENGTH OF ARGUMENT DIFFERENCE VECTOR AND DIRECTION VECTOR      DFMF2480
C           IF AT LEAST N ITERATIONS HAVE BEEN EXECUTED. TERMINATE, IF          DFMF2490
C           BOTH ARE LESS THAN  EPS                                             DFMF2500
         IER=C                                                                  DFMF2510
         IF(KCLAT-N)42,39,39                                                    DFMF2520
   39    T=C.CC                                                                 DFMF2530
         Z=C.CC                                                                 DFMF2540
         DO 4C J=1,N                                                            DFMF2550
         K=N+J                                                                  DFMF2560
         W=P(K)                                                                 DFMF2570
         K=K+N                                                                  DFMF2580
         T=T+ABS(P(K))                                                          DFMF2590
   4C    Z=Z+W*P(K)                                                             DFMF2600
         IF(T-APP-EPS)41,41,42                                                  DFMF2610
   41    IF(T-EPS)56,56,42                                                      DFMF2620
C                                                                               DFMF2630
C           TERMINATE, IF NUMBER OF ITERATIONS WOULD EXCEED  LIMIT              DFMF2640
   42    IF(KCLAT-LIMIT)43,5C,5C                                                DFMF2650
C                                                                               DFMF2660
C           PREPARE UPDATING OF MATRIX P                                        DFMF2670
   43    ALFA=C.CC                                                              DFMF2680
         DO 47 J=1,N                                                            DFMF2690
         K=J+N2                                                                 DFMF2700
         W=C.CC                                                                 DFMF2710
         DO 46 L=1,N                                                            DFMF2720
         KL=N+L                                                                 DFMF2730
         W=W+P(KL)*P(K)                                                         DFMF2740
         IF(L-J)44,45,45                                                        DFMF2750
   44    K=K+N-L                                                                DFMF2760
         GO TO 46                                                               DFMF2770
   45    K=K+1                                                                  DFMF2780
   46    CONTINUE                                                               DFMF2790
         K=N+J                                                                  DFMF2800
         ALFA=ALFA+W*P(K)                                                       DFMF2810
   47    P(J)=W                                                                 DFMF2820
C                                                                               DFMF2830
C           REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF RESULTS           DFMF2840
C           ARE NOT SATISFACTORY                                                DFMF2850
         IF(Z*ALFA)48,1,48                                                      DFMF2860
C                                                                               DFMF2870
C           UPDATE MATRIX P                                                     DFMF2880
   48    K=N2                                                                   DFMF2890
         DO 49 L=1,N                                                            DFMF2900
         KL=N2+L                                                                DFMF2910
         DO 49 J=L,N                                                            DFMF2920
         KJ=N2+J                                                                DFMF2930
         P(K)=P(K)+P(KL)*P(KJ)/Z-P(L)*P(J)/ALFA                                 DFMF2940
   49    K=K+1                                                                  DFMF2950
         GO TO 5                                                                DFMF2960
C           END OF ITERATION LOOP                                               DFMF2970
C                                                                               DFMF2980
C        NO CONVERGENCE AFTER  LIMIT  ITERATIONS                                DFMF2990
   5C    IER=1                                                                  DFMF3000
         RETURN                                                                 DFMF3010
C                                                                               DFMF3020
C           RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                        DFMF3030
   51    DO 52 J=1,N                                                            DFMF3040
         K=N2+J                                                                 DFMF3050
   52    X(J)=P(K)                                                              DFMF3060
         CALL FUNCTN(N,X,F,G)                                                   DFMF3070
C                                                                               DFMF3080
C           REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DERIVATIVE        DFMF3090
C           FAILS TO BE SUFFICIENTLY SMALL                                      DFMF3100
      IF(GAPP-EPS)55,55,53                                                      DFMF3110
C        TEST FOR REPEATED FAILURE OF ITERATION                                 DFMF3120
   53 IF(IER)56,54,54                                                           DFMF3130
   54 IER=-1                                                                    DFMF3140
      GOTO 1                                                                    DFMF3150
   55 IER=0                                                                     DFMF3160
   56 RETURN                                                                    DFMF3170
      END                                                                       DFMF3180
                                                                                DFMF3190
```

Subroutines FMCG and DFMCG

These subroutines perform the calculation of an unconstrained minimum of a function of several variables using conjugate gradients. The underlying method is described in the article by R. Fletcher and C. M. Reeves, "Function minimization by conjugate gradients", Computer Journal, vol. 7, no. 2, 1964, pp. 149-154.

It is assumed that the function f(x) of the n variables $x_1, \ldots, x_n$ may be computed, together with its gradient g(x) for any point $x = \begin{pmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{pmatrix}$. In the neighborhood of the required minimum x_{min} the function f(x) is approximated closely by the first three terms of its Taylor expansion, giving

$$f(x) = f(x_{min}) + \frac{1}{2}(x - x_{min})^T G(x_{min})(x - x_{min})$$

since $g(x_{min}) = 0$. The quantity $G(x_{min})$ means the matrix of second-order partial derivatives taken at the point x_{min}.

From the Taylor expansion, the gradient is seen to be approximately:

$$g(x) = G(x_{min}) \cdot (x - x_{min})$$

The condition for the gradient to vanish is:

$$G(x_{min}) \cdot x = G(x_{min}) \cdot x_{min}$$

For solution of these equations, directions $h^{(0)}$, $h^{(1)}$, ... are generated such that $h^{(i+1)}$ is a linear combination of $-g^{(i+1)}(x^{(i+1)})$ and $h^{(0)}$, $h^{(1)}$, ..., $h^{(i)}$, so that G-orthogonality is satisfied, that is, $h^{(i)T} Gh^{(j)} = 0$ for $i \neq j$.

An easy calculation gives the following results. If a sequence of successive linear searches in directions $h^{(0)} = -g^{(0)}$, $h^{(i+1)} = -g^{(i+1)} + \beta_i \cdot h^{(i)}$ is performed with:

$$\beta_i = \frac{(g^{(i+1)}, g^{(i+1)})}{(g^{(i)}, g^{(i)})}, \quad x^{(i+1)} = x^{(i)} + t_i h^{(i)} \quad \text{and}$$

$$(g^{(i+1)}, h^{(i)}) = 0$$

then this process is guaranteed to locate the minimum of a quadratic function in n iterations at most. For general functions the process is iterative rather than n-step. (This is true even for quadratic functions due to roundoff errors.)

Strategy for termination of the successive linear searches is as follows:

1. If the change of the argument is very small, and at least n + 1 iterations have been performed, the search for the minimum is terminated.

2. If the function value has not decreased in the last linear search, the minimization is terminated.

3. If the number of iterations exceeds an upper bound furnished by the user, further calculation is bypassed, and an error code is set to 1 indicating poor convergence.

4. If one of the successive linear searches indicates that no constrained minimum exists, further calculation is bypassed, and the error code is set to 2 indicating that it is likely that no minimum exists.

5. After each cycle of n + 1 iterations, the next iteration is in the direction of steepest descent.

The linear search technique used in subroutines FMCG and DFMCG is described in the writeup for subroutines FMFP and DFMFP.

```
C                                                                       FMCG  10
C     ******************************************************************FMCG  20
C                                                                       FMCG  30
C        SUBROUTINE FMCG                                                FMCG  40
C                                                                       FMCG  50
C        PURPOSE                                                        FMCG  60
C           TO FIND A LOCAL MINIMUM OF A FUNCTION OF SEVERAL VARIABLES  FMCG  70
C           BY THE METHOD OF CONJUGATE GRADIENTS                        FMCG  80
C                                                                       FMCG  90
C        USAGE                                                          FMCG 100
C           CALL FMCG(IFUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)               FMCG 110
C                                                                       FMCG 120
C        DESCRIPTION OF PARAMETERS                                      FMCG 130
C           FUNCT  - USER-WRITTEN SUBROUTINE CONCERNING THE FUNCTION TO FMCG 140
C                    BE MINIMIZED. IT MUST BE OF THE FORM               FMCG 150
C                    SUBROUTINE FUNCTN(ARG,VAL,GRAD)                    FMCG 160
C                    AND MUST SERVE THE FOLLOWING PURPOSE               FMCG 170
C                    FOR EACH N-DIMENSIONAL ARGUMENT VECTOR  ARG,       FMCG 180
C                    FUNCTION VALUE AND GRADIENT VECTOR MUST BE COMPUTEDFMCG 190
C                    AND, ON RETURN, STORED IN VAL AND GRAD RESPECTIVELYFMCG 200
C              N     - NUMBER OF VARIABLES                              FMCG 210
C              X     - VECTOR OF DIMENSION N CONTAINING THE INITIAL     FMCG 220
C                      ARGUMENT WHERE THE ITERATION STARTS. ON RETURN,  FMCG 230
C                      X HOLDS THE ARGUMENT CORRESPONDING TO THE        FMCG 240
C                      COMPUTED MINIMUM FUNCTION VALUE                  FMCG 250
C              F     - SINGLE VARIABLE CONTAINING THE MINIMUM FUNCTION  FMCG 260
C                      VALUE ON RETURN, I.E. F=F(X).                    FMCG 270
C              G     - VECTOR OF DIMENSION N CONTAINING THE GRADIENT    FMCG 280
C                      VECTOR CORRESPONDING TO THE MINIMUM ON RETURN,   FMCG 290
C                      I.E. G=G(X).                                     FMCG 300
C              EST   - IS AN ESTIMATE OF THE MINIMUM FUNCTION VALUE.    FMCG 310
C              EPS   - TESTVALUE REPRESENTING THE EXPECTED ABSOLUTE ERROR.FMCG 320
C                      A REASONABLE CHOICE IS 10**(-E), I.E.            FMCG 330
C                      SOMEWHAT GREATER THAN 10**(-C), WHERE C IS THE   FMCG 340
C                      NUMBER OF SIGNIFICANT DIGITS IN FLOATING POINT   FMCG 350
C                      REPRESENTATION.                                  FMCG 360
C              LIMIT - MAXIMUM NUMBER OF ITERATIONS.                    FMCG 370
C              IER   - ERROR PARAMETER                                  FMCG 380
C                      IER = 0 MEANS CONVERGENCE WAS OBTAINED           FMCG 390
C                      IER = 1 MEANS NO CONVERGENCE IN LIMIT ITERATIONS FMCG 400
C                      IER =-1 MEANS ERRORS IN GRADIENT CALCULATION     FMCG 410
C                      IER = 2 MEANS LINEAR SEARCH TECHNIQUE INDICATES  FMCG 420
C                      IT IS LIKELY THAT THERE EXISTS NO MINIMUM.       FMCG 430
C              H     - WORKING STORAGE OF DIMENSION 2*N.                FMCG 440
C                                                                       FMCG 450
C        REMARKS                                                        FMCG 460
C           1) THE SUBROUTINE NAME REPLACING THE DUMMY ARGUMENT  FUNCT  FMCG 470
C              MUST BE DECLARED AS EXTERNAL IN THE CALLING PROGRAM.     FMCG 480
C           2) IER IS SET TO 2 IF , STEPPING IN ONE OF THE COMPUTED     FMCG 490
C              DIRECTIONS, THE FUNCTION WILL NEVER INCREASE WITHIN      FMCG 500
C              A TOLERABLE RANGE OF ARGUMENT.                           FMCG 510
C              IER = 2 MAY OCCUR ALSO IF THE INTERVAL WHERE F           FMCG 520
C              INCREASES IS SMALL AND THE INITIAL ARGUMENT WAS          FMCG 530
C              RELATIVELY FAR AWAY FROM THE MINIMUM SUCH THAT THE       FMCG 540
C              MINIMUM WAS OVERLEAPED. THIS IS DUE TO THE SEARCH        FMCG 550
C              TECHNIQUE WHICH DOUBLES THE STEPSIZE UNTIL A POINT       FMCG 560
C              IS FOUND WHERE THE FUNCTION INCREASES.                   FMCG 570
C                                                                       FMCG 580
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FMCG 590
C           FUNCT                                                       FMCG 600
C                                                                       FMCG 610
C        METHOD                                                         FMCG 620
C           THE METHOD IS DESCRIBED IN THE FOLLOWING ARTICLE            FMCG 630
C           R.FLETCHER AND C.M.REEVES, FUNCTION MINIMIZATION BY         FMCG 640
C           CONJUGATE GRADIENTS.                                        FMCG 650
C           COMPUTER JOURNAL VOL.7, ISS.2, 1964, PP.149-154.            FMCG 660
C                                                                       FMCG 670
C     ******************************************************************FMCG 680
C                                                                       FMCG 690
      SUBROUTINE FMCG(IFUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)               FMCG 700
C                                                                       FMCG 710
C        DIMENSIONED DUMMY VARIABLES                                    FMCG 720
      DIMENSION X(1),G(1),H(1)                                          FMCG 730
C                                                                       FMCG 740
C                                                                       FMCG 750
C        COMPUTE FUNCTION VALUE AND GRADIENT VECTOR FOR INITIAL ARGUMENTFMCG 760
      CALL IFUNCT(N,X,F,G)                                              FMCG 770
C                                                                       FMCG 780
C        RESET ITERATION COUNTER                                        FMCG 790
      KOUNT=0                                                           FMCG 800
      IER=0                                                             FMCG 810
      N1=N+1                                                            FMCG 820
C                                                                       FMCG 830
C        START ITERATION CYCLE FOR EVERY N+1 ITERATIONS                 FMCG 840
    1 DO 43 II=1,N1                                                     FMCG 850
C                                                                       FMCG 860
C        STEP ITERATION COUNTER AND SAVE FUNCTION VALUE                 FMCG 870
      KOUNT=KOUNT+1                                                     FMCG 880
      OLDF=F                                                            FMCG 890
C                                                                       FMCG 900
C        COMPUTE SQUARE OF GRADIENT AND TERMINATE IF ZERO               FMCG 910
      GNRM=0.                                                           FMCG 920
      DO 2 J=1,N                                                        FMCG 930
    2 GNRM=GNRM+G(J)*G(J)                                               FMCG 940
      IF(GNRM)46,46,3                                                   FMCG 950
C                                                                       FMCG 960
C        EACH TIME THE ITERATION LOOP IS EXECUTED , THE FIRST STEP WILL FMCG 970
C        BE IN DIRECTION OF STEEPEST DESCENT                            FMCG 980
    3 IF(II-1)4,4,6                                                     FMCG 990
    4 DO 5 J=1,N                                                        FMCG1000
    5 H(J)=-G(J)                                                        FMCG1010
      GO TO 8                                                           FMCG1020
C                                                                       FMCG1030
C        FURTHER DIRECTION VECTORS H WILL BE CHOOSEN CORRESPONDING      FMCG1040
C        TO THE CONJUGATE GRADIENT METHOD                               FMCG1050
    6 BETA=GNRM/OLDG                                                    FMCG1060
      DO 7 J=1,N                                                        FMCG1070
    7 H(J)=BETA*H(J)-G(J)                                               FMCG1080
C                                                                       FMCG1090
C        COMPUTE TESTVALUE FOR DIRECTIONAL VECTOR AND DIRECTIONAL       FMCG1100
C        DERIVATIVE                                                     FMCG1110
    8 GY=0.                                                             FMCG1120
      HNRM=0.                                                           FMCG1130
      DO 9 J=1,N                                                        FMCG1140
      H=J+N                                                             FMCG1150
C                                                                       FMCG1160
C        SAVE ARGUMENT VECTOR                                           FMCG1170
      H(K)=X(J)                                                         FMCG1180
      HNRM=HNRM+ABS(H(J))                                               FMCG1190
    9 GY=GY+H(J)*G(J)                                                   FMCG1200
C                                                                       FMCG1210
C        CHECK WHETHER FUNCTION WILL DECREASE STEPPING ALONG H AND      FMCG1220
C        SKIP LINEAR SEARCH ROUTINE IF NOT                              FMCG1230
      IF(GY)10,42,42                                                    FMCG1240
C                                                                       FMCG1250
C        COMPUTE SCALE FACTOR USED IN LINEAR SEARCH SUBROUTINE          FMCG1260
   10 SNRM=1./HNRM                                                      FMCG1270
C                                                                       FMCG1280
C        SEARCH MINIMUM ALONG DIRECTION H                               FMCG1290
C                                                                       FMCG1300
C        SEARCH ALONG H FOR POSITIVE DIRECTIONAL DERIVATIVE             FMCG1310
      FY=F                                                              FMCG1320
      ALFA=2.*(EST-F)/GY                                                FMCG1330
      ABSCA=SNRM                                                        FMCG1340
C                                                                       FMCG1350
C        USE ESTIMATE FOR STEPSIZE ONLY IF IT IS POSITIVE AND LESS THAN FMCG1360
C        SNRM, OTHERWISE TAKE SNRM AS STEPSIZE.                         FMCG1370
      IF(ALFA)13,13,11                                                  FMCG1380
   11 IF(ALFA-ABSCA)12,13,13                                            FMCG1390
   12 ABSCA=ALFA                                                        FMCG1400
   13 ALFA=0.                                                           FMCG1410
C                                                                       FMCG1420
C        SAVE FUNCTION AND DERIVATIVE VALUES FOR OLD ARGUMENT           FMCG1430
   14 FX=FY                                                             FMCG1440
      GX=GY                                                             FMCG1450
C                                                                       FMCG1460
C        STEP ARGUMENT ALONG H                                          FMCG1470
      DO 15 I=1,N                                                       FMCG1480
   15 X(I)=X(I)+ABSCA*H(I)                                              FMCG1490
C                                                                       FMCG1500
C        COMPUTE FUNCTION VALUE AND GRADIENT FOR NEW ARGUMENT           FMCG1510
      CALL IFUNCT(N,X,F,G)                                              FMCG1520
      FY=F                                                              FMCG1530
C                                                                       FMCG1540
C        COMPUTE DIRECTIONAL DERIVATIVE GY FOR NEW ARGUMENT.  TERMINATE FMCG1550
C        SEARCH, IF GY POSITIVE. IF GY IS ZERO THE MINIMUM IS FOUND     FMCG1560
      GY=0.                                                             FMCG1570
      DO 16 I=1,N                                                       FMCG1580
   16 GY=GY+G(I)*H(I)                                                   FMCG1590
      IF(GY)17,38,2C                                                    FMCG1600
C                                                                       FMCG1610
C        TERMINATE SEARCH ALSO IF THE FUNCTION VALUE INDICATES THAT     FMCG1620
C        A MINIMUM HAS BEEN PASSED                                      FMCG1630
   17 IF(FY-FX)18,2C,2C                                                 FMCG1640
C                                                                       FMCG1650
C        REPEAT SEARCH AND DOUBLE STEPSIZE FOR FURTHER SEARCHES         FMCG1660
   18 ABSCA=ABSCA+ALFA                                                  FMCG1670
      ALFA=ABSCA                                                        FMCG1680
C                                                                       FMCG1690
C        TERMINATE IF THE CHANGE IN ARGUMENT GETS VERY LARGE            FMCG1700
      IF(SNRM*ABSCA-1.E1C)14,14,19                                      FMCG1710
C                                                                       FMCG1720
C        LINEAR SEARCH TECHNIQUE INDICATES THAT NO MINIMUM EXISTS       FMCG1730
   19 IER=2                                                             FMCG1740
C                                                                       FMCG1741
C        RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                   FMCG1742
      F=OLDF                                                            FMCG1743
      DO 1CC J=1,N                                                      FMCG1744
      G(J)=H(J)                                                         FMCG1745
      K=N+J                                                             FMCG1746
  1CC X(J)=H(K)                                                         FMCG1747
      RETURN                                                            FMCG1750
C        END OF SEARCH LOOP                                             FMCG1760
C                                                                       FMCG1770
C        INTERPOLATE CUBICALLY IN THE INTERVAL DEFINED BY THE SEARCH    FMCG1780
C        ABOVE AND COMPUTE THE ARGUMENT X FOR WHICH THE INTERPOLATION   FMCG1790
C        POLYNOMIAL IS MINIMIZED                                        FMCG1800
C                                                                       FMCG1810
   2C T=0.                                                              FMCG1820
   21 IF(ABSCA)22,38,22                                                 FMCG1830
   22 Z=3.*(F)-FY)/ABSCA+GX+GY                                          FMCG1840
      ALFA=ABSCA*(ABS(Z)+ABS(GX)+ABS(GY))                               FMCG1850
      GALFA=Z/ALFA                                                      FMCG1860
      GALFA=GALFA*(GALFA-GX/ALFA+GY/ALFA                                FMCG1870
      IF(GALFA)23,23,27                                                 FMCG1880
C                                                                       FMCG1890
C        RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                   FMCG1900
   23 DO 24 J=1,N                                                       FMCG1910
      K=N+J                                                             FMCG1920
   24 X(J)=H(K)                                                         FMCG1930
      CALL IFUNCT(N,X,F,G)                                              FMCG1940
C                                                                       FMCG1950
C        TEST FOR REPEATED FAILURE OF ITERATION                         FMCG1960
   25 IF(IER)47,26,47                                                   FMCG1970
   26 IER=-1                                                            FMCG1980
      GOTO 1                                                            FMCG1990
   27 H=ALFA*SQRT(GALFA)                                                FMCG2000
      ALFA=GY-GX+H                                                      FMCG2010
      IF(ALFA)27C,271,27C                                               FMCG2011
  27C ALFA=(GY-GX+H)/ALFA                                               FMCG2012
      GO TO 272                                                         FMCG2013
  271 ALFA=(Z+GY-H)/(Z+GX+Z+GY)                                         FMCG2014
  272 ALFA=ALFA*ABSCA                                                   FMCG2015
      DO 28 I=1,N                                                       FMCG2020
   28 X(I)=X(I)+(T-ALFA)*H(I)                                           FMCG2030
C                                                                       FMCG2040
C        TERMINATE, IF THE VALUE OF THE ACTUAL FUNCTION AT X IS LESS    FMCG2050
C        THAN THE FUNCTION VALUES AT THE INTERVAL ENDS. OTHERWISE REDUCEFMCG2060
C        THE INTERVAL BY CHOOSING ONE END-POINT EQUAL TO X AND REPEAT   FMCG2070
C        THE INTERPOLATION.  WHICH END-POINT IS CHOOSEN DEPENDS ON THE  FMCG2080
C        VALUE OF THE FUNCTION AND ITS GRADIENT AT X                    FMCG2090
C                                                                       FMCG2100
      CALL IFUNCT(N,X,F,G)                                              FMCG2110
      IF(F-FX)25,25,3C                                                  FMCG2120
   25 IF(F-FY)3E,3E,3C                                                  FMCG2130
C                                                                       FMCG2140
C        COMPUTE DIRECTIONAL DERIVATIVE                                 FMCG2150
   3C GALFA=0.                                                          FMCG2160
      DO 31 I=1,N                                                       FMCG2170
   31 GALFA=GALFA+G(I)*H(I)                                             FMCG2180
      IF(GALFA)32,35,35                                                 FMCG2190
   32 IF(F-FX)34,33,35                                                  FMCG2200
   33 IF(GX-GALFA)34,3E,34                                              FMCG2210
   34 FX=F                                                              FMCG2220
      GX=GALFA                                                          FMCG2230
      T=ALFA                                                            FMCG2240
      ABSCA=ALFA                                                        FMCG2250
      GO TO 21                                                          FMCG2260
   35 IF(FY-F)37,3E,37                                                  FMCG2270
   3E IF(GY-GALFA)37,3E,37                                              FMCG2280
   37 FY=F                                                              FMCG2290
      GY=GALFA                                                          FMCG2300
      ABSCA=ABSCA-ALFA                                                  FMCG2310
      GO TO 2C                                                          FMCG2320
C                                                                       FMCG2330
C        TERMINATE, IF FUNCTION HAS NOT DECREASED DURING LAST ITERATION FMCG2340
C        OTHERWISE SAVE GRADIENT NORM                                   FMCG2350
   3E IF(OLDF-F+EPS)39,25,39                                            FMCG2360
   39 OLDG=GNRM                                                         FMCG2370
C                                                                       FMCG2380
C        COMPUTE DIFFERENCE OF NEW AND OLD ARGUMENT VECTOR              FMCG2390
      T=0.                                                              FMCG2400
      DO 4C J=1,N                                                       FMCG2410
      K=J+N                                                             FMCG2420
      H(K)=X(J)-H(K)                                                    FMCG2430
   4C T=T+ABS(H(K))                                                     FMCG2440
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C                                                                       FMCG2450
C       TEST LENGTH OF DIFFERENCE VECTOR IF AT LEAST N+1 ITERATIONS     FMCG2460
C       HAVE BEEN EXECUTED. TERMINATE, IF LENGTH IS LESS THAN EPS       FMCG2470
      IF(KCUNT-N)42,41,41                                               FMCG2480
   41 IF(T-EPS)45,45,42                                                 FMCG2490
C                                                                       FMCG2500
C       TERMINATE, IF NUMBER OF ITERATIONS WOULD EXCEED  LIMIT          FMCG2510
   42 IF(KCUNT-LIMIT)43,44,44                                           FMCG2520
   43 IER=0                                                             FMCG2530
C       END OF ITERATION CYCLE                                          FMCG2540
C                                                                       FMCG2550
C       START NEXT ITERATION CYCLE                                      FMCG2560
      GO TO 1                                                           FMCG2570
C                                                                       FMCG2580
C       NO CONVERGENCE AFTER  LIMIT  ITERATIONS                         FMCG2590
   44 IER=1                                                             FMCG2600
      IF(GAMM-EPS)46,46,47                                              FMCG2610
C                                                                       FMCG2620
C       TEST FOR SUFFICIENTLY SMALL GRADIENT                            FMCG2630
   45 IF(GAMM-EPS)46,46,25                                              FMCG2640
   46 IER=0                                                             FMCG2650
   47 RETURN                                                            FMCG2660
      END                                                               FMCG2670
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C                                                                       DFMC  10
C     ****************************************************************DFMC  20
C                                                                       DFMC  30
C       SUBROUTINE DFPMC                                                DFMC  40
C                                                                       DFMC  50
C       PURPOSE                                                         DFMC  60
C          TO FIND A LOCAL MINIMUM OF A FUNCTION OF SEVERAL VARIABLES   DFMC  70
C          BY THE METHOD OF CONJUGATE GRADIENTS                         DFMC  80
C                                                                       DFMC  90
C       USAGE                                                           DFMC 100
C          CALL DFPMC(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)                DFMC 110
C                                                                       DFMC 120
C       DESCRIPTION OF PARAMETERS                                       DFMC 130
C          FUNCT  - USER-WRITTEN SUBROUTINE CONCERNING THE FUNCTION TO  DFMC 140
C                   BE MINIMIZED. IT MUST BE OF THE FORM                DFMC 150
C                   SUBROUTINE FUNCT(N,ARG,VAL,GRAD)                    DFMC 160
C                   AND MUST SERVE THE FOLLOWING PURPOSE                DFMC 170
C                   FOR EACH N-DIMENSIONAL ARGUMENT VECTOR  ARG,        DFMC 180
C                   FUNCTION VALUE AND GRADIENT VECTOR MUST BE COMPUTEDDFMC 190
C                   AND, ON RETURN, STORED IN VAL AND GRAD RESPECTIVELYDFMC 200
C                   ARG,VAL AND GRAD MUST BE OF DOUBLE PRECISION.       DFMC 210
C          N      - NUMBER OF VARIABLES                                DFMC 220
C          X      - VECTOR OF DIMENSION N CONTAINING THE INITIAL       DFMC 230
C                   ARGUMENT WHERE THE ITERATION STARTS. ON RETURN,     DFMC 240
C                   X HOLDS THE ARGUMENT CORRESPONDING TO THE           DFMC 250
C                   COMPUTED MINIMUM FUNCTION VALUE                     DFMC 260
C                   DOUBLE PRECISION VECTOR.                            DFMC 270
C          F      - SINGLE VARIABLE CONTAINING THE MINIMUM FUNCTION    DFMC 280
C                   VALUE ON RETURN, I.E. F=F(X).                       DFMC 290
C                   DOUBLE PRECISION VARIABLE.                          DFMC 300
C          G      - VECTOR OF DIMENSION N CONTAINING THE GRADIENT      DFMC 310
C                   VECTOR CORRESPONDING TO THE MINIMUM ON RETURN,      DFMC 320
C                   I.E. G=G(X).                                        DFMC 330
C                   DOUBLE PRECISION VECTOR.                            DFMC 340
C          EST    - IS AN ESTIMATE OF THE MINIMUM FUNCTION VALUE.      DFMC 350
C                   SINGLE PRECISION VARIABLE.                          DFMC 360
C          EPS    - TESTVALUE REPRESENTING THE EXPECTED ABSOLUTE ERROR.DFMC 370
C                   A REASONABLE CHOICE IS 10**(-10), I.E.              DFMC 380
C                   SOMEWHAT GREATER THAN 10**(-D), WHERE D IS THE      DFMC 390
C                   NUMBER OF SIGNIFICANT DIGITS IN FLOATING POINT      DFMC 400
C                   REPRESENTATION.                                     DFMC 410
C                   SINGLE PRECISION VARIABLE.                          DFMC 420
C          LIMIT  - MAXIMUM NUMBER OF ITERATIONS.                      DFMC 430
C          IER    - ERROR PARAMETER                                    DFMC 440
C                   IER = 0 MEANS CONVERGENCE HAS OBTAINED              DFMC 450
C                   IER = 1 MEANS NO CONVERGENCE IN LIMIT ITERATIONS    DFMC 460
C                   IER =-1 MEANS ERRORS IN GRADIENT CALCULATION        DFMC 470
C                   IER = 2 MEANS LINEAR SEARCH TECHNIQUE INDICATES     DFMC 480
C                   IT IS LIKELY THAT THERE EXISTS NO MINIMUM.          DFMC 490
C          H      - WORKING STORAGE OF DIMENSION 2*N.                  DFMC 500
C                   DOUBLE PRECISION ARRAY.                             DFMC 510
C                                                                       DFMC 520
C       REMARKS                                                         DFMC 530
C          I) THE SUBROUTINE NAME REPLACING THE DUMMY ARGUMENT  FUNCT   DFMC 540
C             MUST BE DECLARED AS EXTERNAL IN THE CALLING PROGRAM.      DFMC 550
C          II) IER IS SET TO 2 IF , STEPPING IN ONE OF THE COMPUTED     DFMC 560
C              DIRECTIONS, THE FUNCTION WILL NEVER INCREASE WITHIN      DFMC 570
C              A TOLERABLE RANGE OF ARGUMENT.                           DFMC 580
C              IER = 2 MAY OCCUR ALSO IF THE INTERVAL WHERE F           DFMC 590
C              INCREASES IS SMALL AND THE INITIAL ARGUMENT WAS          DFMC 600
C              RELATIVELY FAR AWAY FROM THE MINIMUM SUCH THAT THE       DFMC 610
C              MINIMUM WAS OVERLEAPED. THIS IS DUE TO THE SEARCH        DFMC 620
C              TECHNIQUE WHICH DOUBLES THE STEPSIZE UNTIL A POINT       DFMC 630
C              IS FOUND WHERE THE FUNCTION INCREASES.                   DFMC 640
C                                                                       DFMC 650
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DFMC 660
C          FUNCT                                                        DFMC 670
C                                                                       DFMC 680
C       METHOD                                                          DFMC 690
C          THE METHOD IS DESCRIBED IN THE FOLLOWING ARTICLE             DFMC 700
C          R.FLETCHER AND C.M.REEVES, FUNCTION MINIMIZATION BY          DFMC 710
C          CONJUGATE GRADIENTS,                                         DFMC 720
C          COMPUTER JOURNAL VOL.7, ISS.2, 1964, PP.149-154.             DFMC 730
C                                                                       DFMC 740
C     ****************************************************************DFMC 750
C                                                                       DFMC 760
      SUBROUTINE DFPMC(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)               DFMC 770
C                                                                       DFMC 780
C       DIMENSIONED DUMMY VARIABLES                                     DFMC 790
      DIMENSION X(1),G(1),H(1)                                          DFMC 800
      DOUBLE PRECISION X,G,GNRM,H,HNRM,F,FX,FY,CLDF,CLDG,SNRM,AMBDA,    DFMC 810
     1ALFA,CALFA,T,Z,W,CX,CY                                            DFMC 820
C                                                                       DFMC 830
C       COMPUTE FUNCTION VALUE AND GRADIENT VECTOR FOR INITIAL ARGUMENTDFMC 840
      CALL FUNCT(N,X,F,G)                                               DFMC 850
C                                                                       DFMC 860
C       RESET ITERATION COUNTER                                         DFMC 870
      KCUNT=0                                                           DFMC 880
      IER=0                                                             DFMC 890
      N1=N+1                                                            DFMC 900
C                                                                       DFMC 910
C       START ITERATION CYCLE FOR EVERY N+1 ITERATIONS                  DFMC 920
    1 DO 43 II=1,N1                                                     DFMC 930
C                                                                       DFMC 940
C       STEP ITERATION COUNTER AND SAVE FUNCTION VALUE                  DFMC 950
      KCUNT=KCUNT+1                                                     DFMC 960
      CLDF=F                                                            DFMC 970
C                                                                       DFMC 980
C       COMPUTE SQUARE OF GRADIENT AND TERMINATE IF ZERO                DFMC 990
      GAMM=0.DO                                                         DFMC1000
      DO 2 J=1,N                                                        DFMC1010
    2 GAMM=GAMM+G(J)*G(J)                                               DFMC1020
      IF(GAMM)46,46,3                                                   DFMC1030
C                                                                       DFMC1040
C       EACH TIME THE ITERATION LOOP IS EXECUTED , THE FIRST STEP WILL  DFMC1050
C       BE IN DIRECTION OF STEEPEST DESCENT                             DFMC1060
    3 IF(II-1)4,4,6                                                     DFMC1070
    4 DO 5 J=1,N                                                        DFMC1080
    5 H(J)=-G(J)                                                        DFMC1090
      GO TO 8                                                           DFMC1100
C                                                                       DFMC1110
C       FURTHER DIRECTION VECTORS H WILL BE CHOOSEN CORRESPONDING       DFMC1120
C       TO THE CONJUGATE GRADIENT METHOD                                DFMC1130
    6 AMBDA=GAMM/CLDG                                                   DFMC1140
      DO 7 J=1,N                                                        DFMC1150
    7 H(J)=AMBDA*H(J)-G(J)                                              DFMC1160
C                                                                       DFMC1170
C       COMPUTE TESTVALUE FOR DIRECTIONAL VECTOR AND DIRECTIONAL        DFMC1180
C       DERIVATIVE                                                      DFMC1190
    8 CY=0.DO                                                           DFMC1200
      HNRM=0.DO                                                         DFMC1210
      DO 9 J=1,N                                                        DFMC1220
      K=J+N                                                             DFMC1230
C                                                                       DFMC1240
C       SAVE ARGUMENT VECTOR                                            DFMC1250
      H(K)=X(J)                                                         DFMC1260
      HNRM=HNRM+DABS(H(J))                                              DFMC1270
    9 CY=CY+H(J)*G(J)                                                   DFMC1280
C                                                                       DFMC1290
C       CHECK WHETHER FUNCTION WILL DECREASE STEPPING ALONG H AND       DFMC1300
C       SKIP LINEAR SEARCH ROUTINE IF NOT                               DFMC1310
      IF(CY)10,42,42                                                    DFMC1320
C                                                                       DFMC1330
C       COMPUTE SCALE FACTOR USED IN LINEAR SEARCH SUBROUTINE           DFMC1340
   10 SNRM=1.DO/HNRM                                                    DFMC1350
C                                                                       DFMC1360
C       SEARCH MINIMUM ALONG DIRECTION H                                DFMC1370
C                                                                       DFMC1380
C       SEARCH ALONG H FOR POSITIVE DIRECTIONAL DERIVATIVE              DFMC1390
      FY=F                                                              DFMC1400
      ALFA=2.DO*(EST-F)/CY                                              DFMC1410
      AMBDA=SNRM                                                        DFMC1420
C                                                                       DFMC1430
C       USE ESTIMATE FOR STEPSIZE ONLY IF IT IS POSITIVE AND LESS THAN  DFMC1440
C       SNRM. OTHERWISE TAKE SNRM AS STEPSIZE.                          DFMC1450
      IF(ALFA)13,13,11                                                  DFMC1460
   11 IF(ALFA-AMBDA)12,13,13                                            DFMC1470
   12 AMBDA=ALFA                                                        DFMC1480
   13 ALFA=0.DO                                                         DFMC1490
C                                                                       DFMC1500
C       SAVE FUNCTION AND DERIVATIVE VALUES FOR OLD ARGUMENT            DFMC1510
   14 FX=FY                                                             DFMC1520
      CX=CY                                                             DFMC1530
C                                                                       DFMC1540
C       STEP ARGUMENT ALONG H                                           DFMC1550
      DO 15 I=1,N                                                       DFMC1560
   15 X(I)=X(I)+AMBDA*H(I)                                              DFMC1570
C                                                                       DFMC1580
C       COMPUTE FUNCTION VALUE AND GRADIENT FOR NEW ARGUMENT            DFMC1590
      CALL FUNCT(N,X,F,G)                                               DFMC1600
      FY=F                                                              DFMC1610
C                                                                       DFMC1620
C       COMPUTE DIRECTIONAL DERIVATIVE CY FOR NEW ARGUMENT.  TERMINATE DFMC1630
C       SEARCH, IF CY POSITIVE. IF CY IS ZERO THE MINIMUM IS FOUND      DFMC1640
      CY=0.DO                                                           DFMC1650
      DO 16 I=1,N                                                       DFMC1660
   16 CY=CY+G(I)*H(I)                                                   DFMC1670
      IF(CY)17,38,20                                                    DFMC1680
C                                                                       DFMC1690
C       TERMINATE SEARCH ALSO IF THE FUNCTION VALUE INDICATES THAT      DFMC1700
C       A MINIMUM HAS BEEN PASSED                                       DFMC1710
   17 IF(FY-FX)18,20,20                                                 DFMC1720
C                                                                       DFMC1730
C       REPEAT SEARCH AND DOUBLE STEPSIZE FOR FURTHER SEARCHES          DFMC1740
   18 AMBDA=AMBDA+ALFA                                                  DFMC1750
      ALFA=AMBDA                                                        DFMC1760
C                                                                       DFMC1770
C       TERMINATE IF THE CHANGE IN ARGUMENT GETS VERY LARGE             DFMC1780
      IF(GAMM*AMBDA-0.1D0)14,14,19                                      DFMC1790
C                                                                       DFMC1800
C       LINEAR SEARCH TECHNIQUE INDICATES THAT NO MINIMUM EXISTS        DFMC1810
   19 IER=2                                                             DFMC1820
C                                                                       DFMC1821
C       RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                    DFMC1822
      F=OLDF                                                            DFMC1823
      DO 100 J=1,N                                                      DFMC1824
      G(J)=H(J)                                                         DFMC1825
      K=N+J                                                             DFMC1826
  100 X(J)=H(K)                                                         DFMC1827
      GETLRA                                                            DFMC1830
C       END OF SEARCH LOOP                                              DFMC1840
C                                                                       DFMC1850
C       INTERPOLATE CUBICALLY IN THE INTERVAL DEFINED BY THE SEARCH     DFMC1860
C       ABOVE AND COMPUTE THE ARGUMENT X FOR WHICH THE INTERPOLATION    DFMC1870
C       POLYNOMIAL IS MINIMIZED                                         DFMC1880
C                                                                       DFMC1890
   20 T=0.                                                              DFMC1900
   21 IF(AMBDA)22,38,22                                                 DFMC1910
   22 Z=3.DO*(F-FY)/AMBDA+CX+CY                                         DFMC1920
      ALFA=DMAX1(DABS(Z),DABS(CX),DABS(CY))                             DFMC1930
      CALFA=Z/ALFA                                                      DFMC1940
      CALFA=CALFA*(CALFA-CX/ALFA*CY/ALFA                                DFMC1950
      IF(CALFA)23,23,27                                                 DFMC1960
C                                                                       DFMC1970
C       RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                    DFMC1980
   23 DO 24 J=1,N                                                       DFMC1990
      K=N+J                                                             DFMC2000
   24 X(J)=H(K)                                                         DFMC2010
      CALL FUNCT(N,X,F,G)                                               DFMC2020
C                                                                       DFMC2030
C       TEST FOR REPEATED FAILURE OF ITERATION                          DFMC2040
   25 IF(IER)47,26,47                                                   DFMC2050
   26 IER=-1                                                            DFMC2060
      GOTO 1                                                            DFMC2070
   27 W=ALFA*DSQRT(CALFA)                                               DFMC2080
      ALFA=CY-CX+W+W                                                    DFMC2090
      IF(ALFA)270,271,270                                               DFMC2091
  270 ALFA=(CY-CX+W)/ALFA                                               DFMC2092
      GO TO 272                                                         DFMC2093
  271 ALFA=(CX+CY-W)/(2.DO*CX+2.DO*CY)                                  DFMC2094
  272 ALFA=ALFA*AMBDA                                                   DFMC2095
      DO 28 I=1,N                                                       DFMC2100
   28 X(I)=X(I)+(ET-ALFA)*H(I)                                          DFMC2110
C                                                                       DFMC2120
```

```
C        TERMINATE, IF THE VALUE OF THE ACTUAL FUNCTION AT X IS LESS     DFMC2130
C        THAN THE FUNCTION VALUES AT THE INTERVAL ENDS. OTHERWISE REDUCEDFMC2140
C        THE INTERVAL BY CHOOSING ONE END-POINT EQUAL TO X AND REPEAT    DFMC2150
C        THE INTERPOLATION.  WHICH END-POINT IS CHOOSEN DEPENDS ON THE   DFMC2160
C        VALUE OF THE FUNCTION AND ITS GRADIENT AT X                     DFMC2170
C                                                                        DFMC2180
      CALL FUNCTN(N,X,F,G)                                               DFMC2190
      IF(F-FX)25,25,30                                                   DFMC2200
   29 IF(F-FY)38,38,30                                                   DFMC2210
C                                                                        DFMC2220
C        COMPUTE DIRECTIONAL DERIVATIVE                                  DFMC2230
   30 CALFA=0.00                                                         DFMC2240
      DO 31 I=1,N                                                        DFMC2250
   31 CALFA=CALFA+G(I)*H(I)                                              DFMC2260
      IF(CALFA)32,35,35                                                  DFMC2270
   32 IF(F-FX)34,33,35                                                   DFMC2280
   33 IF(DX-CALFA)34,38,34                                               DFMC2290
   34 FX=F                                                              DFMC2300
      DX=CALFA                                                           DFMC2310
      T=ALFA                                                             DFMC2320
      APREC=ALFA                                                         DFMC2330
      GO TO 21                                                           DFMC2340
   35 IF(FY-F)37,36,37                                                   DFMC2350
   36 IF(DY-CALFA)37,38,37                                               DFMC2360
   37 FY=F                                                              DFMC2370
      DY=CALFA                                                           DFMC2380
      APREC=APREC-ALFA                                                   DFMC2390
      GO TO 22                                                           DFMC2400
C                                                                        DFMC2410
C        TERMINATE, IF FUNCTION HAS NOT DECREASED DURING LAST ITERATION  DFMC2420
C        OTHERWISE SAVE GRADIENT NORM                                    DFMC2430
   38 IF(CLOF-F+EPS)15,25,25                                             DFMC2440
   39 CLOG=GNRM                                                         DFMC2450
C                                                                        DFMC2460
C        COMPUTE DIFFERENCE OF NEW AND OLD ARGUMENT VECTOR               DFMC2470
      I=0.00                                                             DFMC2480
      DO 40 J=1,N                                                        DFMC2490
      K=J+N                                                              DFMC2500
      H(K)=X(J)-H(K)                                                     DFMC2510
   40 T=T+DABS(H(K))                                                     DFMC2520
C                                                                        DFMC2530
C        TEST LENGTH OF DIFFERENCE VECTOR IF AT LEAST N+1 ITERATIONS     DFMC2540
C        HAVE BEEN EXECUTED. TERMINATE, IF LENGTH IS LESS THAN EPS       DFMC2550
      IF(KCNT-N)42,41,41                                                 DFMC2560
   41 IF(T-EPS)45,45,42                                                  DFMC2570
C                                                                        DFMC2580
C        TERMINATE, IF NUMBER OF ITERATIONS WOULD EXCEED  LIMIT          DFMC2590
   42 IF(KCNT-LIMIT)43,43,44                                             DFMC2600
   43 IER=0                                                             DFMC2610
C        END OF ITERATION CYCLE                                          DFMC2620
C                                                                        DFMC2630
C        START NEXT ITERATION CYCLE                                      DFMC2640
      GO TO 1                                                            DFMC2650
C                                                                        DFMC2660
C        NO CONVERGENCE AFTER  LIMIT  ITERATIONS                         DFMC2670
   44 IER=1                                                             DFMC2680
      IF(GNRM-EPS)46,46,47                                               DFMC2690
C                                                                        DFMC2700
C        TEST FOR SUFFICIENTLY SMALL GRADIENT                            DFMC2710
   45 IF(GNRM-EPS)46,46,25                                               DFMC2720
   46 IER=0                                                             DFMC2730
   47 RETURN                                                            DFMC2740
      END                                                                DFMC2750
```

PERMUTATIONS

Let n be a positive integer and let $N = \{1, \ldots, n\}$. A permutation on N is a one-one function from N onto N. In what follows, all permutations will be on N.

Suppose P and Q are permutations. We define a new permutation $R = Q \cdot P$ by $R(j) = (Q \cdot P)(j) = Q(P(j))$ for $j \in N$. Note that in general $P \cdot Q \neq Q \cdot P$, although $\cdot$ is associative. The operation $\cdot$ is ordinary function composition. The identity permutation is the identity function I on N, defined by $I(j) = j$ for $j \in N$. An inverse of a permutation P is a permutation P^{-1} with the property that $P \cdot P^{-1} = P^{-1} \cdot P = I$. It is easily proved that every permutation has a unique inverse; indeed, if P is a permutation, its inverse P^{-1} is given by $P^{-1}(j) = s$ where s is such that $P(s) = j$, $j \in N$. Note also that if P and Q are permutations, $(Q \cdot P)^{-1} = P^{-1} \cdot Q^{-1}$. The conjugate of Q by P is the permutation $P \cdot Q \cdot P^{-1}$.

A transposition is a permutation that moves at most two elements of N; that is, T is a transposition if and only if integers i and j exist such that $T(k) = k$ for $k \neq i, j$. It may easily be proved that every permutation can be written as a product $T_1 \cdot T_2 \cdot \ldots \cdot T_n$ of transpositions where for $i = 1, \ldots, n$ there exists $k_i \in N$ such that:

$$T_i(j) = \begin{cases} k_i & \text{if } j = i \\ i & \text{if } j = k_i \\ j & \text{if } j \neq i, k_i \end{cases}$$

Every transposition is its own inverse.

If P is a permutation, we will identify P and the symbol

$$\begin{pmatrix} 1 & 2 & \ldots & n \\ p_1 & p_2 & \cdots & p_n \end{pmatrix}$$

where

$$p_i = P(i) \text{ for } i = 1, \ldots, n.$$

At times we will also identify the permutation P and the vector $(p_1, \ldots, p_n)$. Whenever this is the case we will write "... permutation $P = (p_1, \ldots, p_n)$ ...", or "permutation vector $P = (p_1, \ldots, p_n)$".

Similarly, if T is the transposition given by:

$$T(j) = \begin{cases} j & \text{if } j \neq i, k \\ i & \text{if } j = k \\ k & \text{if } j = i \end{cases}$$

then we identify T and the symbol (i, k). (This leads to no difficulty if $n = 2$, since in this case all permutations are also transpositions.)

We note above that any permutation P can be written as a product $T_1 \cdot \ldots \cdot T_n$ of transpositions of a certain form. In the new notation we have $P = (1, t_1) \cdot \ldots \cdot (n, t_n)$, $t_i \in N$, $i = 1, \ldots, n$. The t_i are generally not distinct. At times we will identify the product $(1, t_1) \cdot \ldots \cdot (n, t_n)$ and the vector $(t_1, \ldots, t_n)$. Whenever this identification is meant we will write "... transposition vector $P = (t_1, \ldots, t_n)$".

Permutations can be used to induce rearrangements of ordered collections of objects. The convention that we will use is illustrated by the following example. Suppose that A is an m by n matrix and C_i is the i^{th} column of A for $i = 1, \ldots, n$. If the permutation $P = (p_1, \ldots, p_n)$ is applied to the columns of A, there results the m by n matrix A' whose p_i^{th} column, C_{p_i}, is C_i for $i = 1, \ldots, n$.

Examples

Suppose $n = 5$, and let P and Q be the permutations given by:

$P(1) = 3$ $P(2) = 1$ $P(3) = 5$ $P(4) = 2$ $P(5) = 4$

and

$Q(1) = 1$ $Q(2) = 3$ $Q(3) = 5$ $Q(4) = 2$ $Q(5) = 4$

Then P and Q may also be written as:

$$P = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 1 & 5 & 2 & 4 \end{pmatrix} \quad \text{and} \quad Q = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 5 & 2 & 4 \end{pmatrix}$$

or as the permutation vectors:

$$P = (3, 1, 5, 2, 4) \quad \text{and} \quad Q = (1, 3, 5, 2, 4)$$

Now:

$$Q \cdot P = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 5 & 2 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 1 & 5 & 2 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 5 & 1 & 4 & 3 & 2 \end{pmatrix}$$

while:

$$P \cdot Q = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 1 & 5 & 2 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 5 & 2 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 3 & 5 & 4 & 1 & 2 \end{pmatrix}$$

P^{-1} is the permutation given by

$$P^{-1}(1)=2 \quad P^{-1}(2)=4 \quad P^{-1}(3)=1 \quad P^{-1}(4)=5$$

$$P^{-1}(5)=3$$

or

$$P^{-1}=\begin{pmatrix}1&2&3&4&5\\2&4&1&5&3\end{pmatrix}$$

or the permutation vector P = (2,4,1,5,3).

We now write P as a product of transpositions in the standard form defined above. We have:

$$P=\begin{pmatrix}1&2&3&4&5\\3&1&5&2&4\end{pmatrix}=(1,3)\cdot\begin{pmatrix}1&2&3&4&5\\1&3&5&2&4\end{pmatrix}$$

$$=(1,3)\cdot\left[(2,3)\cdot\begin{pmatrix}1&2&3&4&5\\1&2&5&3&4\end{pmatrix}\right]$$

$$=(1,3)\cdot(2,3)\cdot$$

$$\left[(3,5)\cdot\begin{pmatrix}1&2&3&4&5\\1&2&3&5&4\end{pmatrix}\right]$$

$$=(1,3)\cdot(2,3)\cdot(3,5)\cdot$$

$$\left[(4,5)\cdot\begin{pmatrix}1&2&3&4&5\\1&2&3&4&5\end{pmatrix}\right]$$

$$=(1,3)\cdot(2,3)\cdot(3,5)\cdot(4,5)\cdot(5,5).$$

Hence P is equivalent to the transposition vector (3,3,5,5,5).

Subroutine PPRCN

Subroutine PPRCN computes the permutation vector that is the composition of two given permutation vectors, and the permutation vector that is the conjugate of a given permutation vector by another permutation vector. (See the general discussion for definitions and notation.)

1. Mathematical background

Suppose that IP1 = $(p_1,\ldots,p_n)$ and IP2 = $(q_1,\ldots,q_n)$ are permutation vectors on $N=\{1,\ldots,n\}$.

a. The composition IP3 = IP2•IP1 of IP1 and IP2 is given by IP3 = $(r_1,\ldots,r_n)$ where $r_i = q_{p_i}$ for $i = 1,\ldots,n$.

b. The conjugate IP3 = IP1•IP2•$IP1^{-1}$ of IP2 by IP1 is given by IP3 = $(r_1,\ldots,r_n)$ where $r_{p_i} = p_{q_i}$ for $i=1,\ldots,n$.

2. Programming considerations

Depending on whether the input parameter IPAR is nonnegative or negative, subroutine PPRCN computes either the composition of IP1 and IP2 or the conjugate of IP2 by IP1.

Subroutine PERM is used to check that n is positive and that IP1 and IP2 are permutation vectors on N. If n is not positive or if IP1 and IP2 are not both permutation vectors on N, computation is terminated as soon as the error is detected, and the error parameter IER is set to -1 or 1, respectively. If there is no error, IER is set to zero.

The computation of the resulting vector IP3 proceeds as follows.

a. If IPAR is nonnegative, for each i, i = 1,..., n, IP3(i) is set to IP2(IP1(i)).

b. If IPAR is negative, initially subroutine PERM is used to compute $IP1^{-1}$, which is stored in IP3. Then, for i = 1,...,n, IP3(i) is set to IP1 (IP2 (IP3(i))).

IP3 cannot have the same storage allocation as IP1 or IP2. IP1 and IP2 are returned unchanged.

```
C
C     ..................................................................PPRC  10
C                                                                      PPRC  20
C        SUBROUTINE PPRCN                                              PPRC  30
C                                                                      PPRC  40
C        PURPOSE                                                       PPRC  50
C           TO COMPUTE, GIVEN TWO PERMUTATION VECTORS IP1 AND IP2, THE PPRC  60
C           COMPOSITION IP2(IP1) AND THE CONJUGATE IP1(IP2(IP1 INVERSE))PPRC  80
C           OF IP2 BY IP1.  (SEE THE GENERAL DISCUSSION FOR DEFINITIONS PPRC  90
C           AND NOTATION.)                                             PPRC 100
C                                                                      PPRC 110
C        USAGE                                                         PPRC 120
C           CALL PPRCN(IP1,IP2,IP3,N,IPAR,IER)                         PPRC 130
C                                                                      PPRC 140
C        DESCRIPTION OF PARAMETERS                                     PPRC 150
C           IP1  - GIVEN PERMUTATION VECTOR (DIMENSION N)              PPRC 160
C           IP2  - GIVEN PERMUTATION VECTOR (DIMENSION N)              PPRC 170
C           IP3  - RESULTING PERMUTATION VECTOR (DIMENSION N)          PPRC 180
C           N    - DIMENSION OF VECTORS IP1, IP2 AND IP3               PPRC 190
C           IPAR - INPUT PARAMETER                                     PPRC 200
C                  IPAR NON-NEGATIVE - COMPUTE IP2(IP1)                PPRC 210
C                  IPAR NEGATIVE     - COMPUTE IP1(IP2(IP1 INVERSE))   PPRC 220
C           IER  - RESULTING ERROR PARAMETER                           PPRC 230
C                  IER=-1  -  N IS NOT POSITIVE                        PPRC 240
C                  IER= 0  -  NO ERROR                                 PPRC 250
C                  IER= 1  -  IP1 AND IP2 ARE NOT BOTH PERMUTATION     PPRC 260
C                             VECTORS ON 1,...,N                       PPRC 270
C                                                                      PPRC 280
C        REMARKS                                                       PPRC 290
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.              PPRC 300
C           (2)  IF IER=1, THEN COMPUTATION HAS BEEN UNSUCCESSFUL DUE TOPPRC 310
C                ERROR AND THE PARTIAL RESULTS FOUND IN IP2 ARE USELESS.PPRC 320
C           (3)  IP3 CANNOT HAVE THE SAME STORAGE ALLOCATION AS IP1 OR PPRC 330
C                IP2.                                                  PPRC 340
C                                                                      PPRC 350
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 PPRC 360
C           PERM                                                       PPRC 370
C                                                                      PPRC 380
C        METHOD                                                        PPRC 390
C           SUBROUTINE PERM IS USED TO CHECK THAT IP1 AND IP2 ARE PERMU-PPRC 400
C           TATION VECTORS.  IF IP2(IP1) IS COMPUTED, IP3(I) IS SET TO PPRC 410
C           IP2(IP1(I)) FOR I=1,...,N.  IF IP1(IP2(IP1 INVERSE)) IS    PPRC 420
C           COMPUTED, FIRST IP3 IS SET TO IP1 INVERSE BY SUBROUTINE PERMPPRC 430
C           AND THEN IP3(I) IS SET TO IP1(IP2(IP3(I))) FOR I=1,...,N.  PPRC 440
C                                                                      PPRC 450
C     ..................................................................PPRC 460
      SUBROUTINE PPRCN(IP1,IP2,IP3,N,IPAR,IER)                         PPRC 470
C                                                                      PPRC 480
C                                                                      PPRC 490
      DIMENSION IP1(1),IP2(1),IP3(1)                                   PPRC 500
C                                                                      PPRC 510
C        CHECK THAT N IS POSITIVE AND THAT IP2 IS A PERMUTATION VECTOR PPRC 520
      CALL PERM(IP2,IP3,N,-1,IER)                                      PPRC 530
C                                                                      PPRC 540
C        TEST IER TO SEE IF THERE IS AN ERROR                          PPRC 550
      IF(IER)7,1,7                                                     PPRC 560
C                                                                      PPRC 570
C        CHECK THAT IP1 IS A PERMUTATION VECTOR AND COMPUTE IP1 INVERSEPPRC 580
    1 CALL PERM(IP1,IP3,N,-1,IER)                                      PPRC 590
C                                                                      PPRC 600
C        TEST IER TO SEE IF THERE IS AN ERROR                          PPRC 610
      IF(IER)7,2,7                                                     PPRC 620
C                                                                      PPRC 630
C
C                                                                      PPRC 640
C        TEST IPAR FOR THE DESIRED OPERATION                           PPRC 650
    2 IF(IPAR)3,5,5                                                    PPRC 660
C                                                                      PPRC 670
C        COMPUTE IP1(IP2(IP1 INVERSE))                                 PPRC 680
    3 DO 4 I=1,N                                                       PPRC 690
      K=IP3(I)                                                         PPRC 700
      J=IP2(K)                                                         PPRC 710
    4 IP3(I)=IP1(J)                                                    PPRC 720
      RETURN                                                           PPRC 730
C                                                                      PPRC 740
C        COMPUTE IP2(IP1)                                              PPRC 750
    5 DO 6 I=1,N                                                       PPRC 760
      K=IP1(I)                                                         PPRC 770
    6 IP3(I)=IP2(K)                                                    PPRC 780
    7 RETURN                                                           PPRC 790
      END                                                              PPRC 800
```

Subroutine PERM

Subroutine PERM computes the permutation vector that is the inverse of a given permutation vector, the permutation vector that is equivalent to a given transposition vector, and a transposition vector that is equivalent to a given permutation vector. (See the general discussion for definitions and notation.)

1. Mathematical background

Let $N = \{1, \ldots, n\}$.

a. If $IP1 = (p_1, \ldots, p_n)$ is a permutation vector on N, its inverse, IP2, is given by $IP2 = (r_1, \ldots, r_n)$ where $r_{p_i} = i$ for $i = 1, \ldots, n$.

b. Let $IP1 = (t_1, \ldots, t_n)$ be a transposition vector on N. The computation of the permutation vector that is equivalent to IP1 is based on the identity:

$$\begin{pmatrix} 1 & \ldots & n \\ s_1 & \ldots & s_n \end{pmatrix} \cdot (i, v_i) = \begin{pmatrix} 1 & \ldots & i & \ldots & v_i & \ldots & n \\ s_1 & \ldots & s_{v_i} & \ldots & s_i & \ldots & s_n \end{pmatrix} \tag{1}$$

Applying (1) for $i = 1, \ldots, n$ to the right-hand side of the identity

$$(1, t_1) \cdot \ldots \cdot (n, t_n) = \begin{pmatrix} 1 & \ldots & n \\ 1 & \ldots & n \end{pmatrix} \cdot (1, t_1) \cdot \ldots \cdot (n, t_n)$$

there results

$$(1, t_1) \cdot \ldots \cdot (n, t_n) = \begin{pmatrix} 1 & \ldots & n \\ q_1 & \ldots & q_n \end{pmatrix}$$

The desired permutation vector, IP2, is $IP2 = (q_1, \ldots, q_n)$.

c. Let $IP1 = (p_1, \ldots, p_n)$ be a permutation vector on N. The computation of a transposition vector that is equivalent to IP1 is based on the identity:

$$\begin{pmatrix} 1 & \ldots & n \\ & & \\ s_1 & \ldots & s_n \end{pmatrix} = (i, s_i) \cdot \begin{pmatrix} 1 & \ldots & i & \ldots & k & \ldots & n \\ & & & & & & \\ s_1 & \ldots & i & \ldots & s_i & \ldots & s_n \end{pmatrix} \tag{2}$$

for $i = 1, \ldots, n$ where for each i, k is such that $p_k = i$. Using (2) with i successively $1, \ldots, n$ we may write:

$$\begin{pmatrix} 1 & \ldots & n \\ & & \\ p_1 & \ldots & p_n \end{pmatrix} = (1, t_1) \cdot \ldots \cdot (n, t_n) \cdot \begin{pmatrix} 1 & \ldots & n \\ & & \\ 1 & \ldots & n \end{pmatrix}$$

$$= (1, t_1) \cdot \ldots \cdot (n, t_n)$$

for some $t_i \in N$. The desired transposition vector is IP2=($t_1, \ldots, t_n$).

2. Programming considerations

Depending on whether the input parameter IPAR is negative, zero, or positive, subroutine PERM performs the computation described above in 1a, 1b, or 1c, respectively.

If n is not positive, there is no computation and the error parameter IER is set to -1. If IPAR is not zero and IP1 is not a permutation vector on N, or if IPAR is zero and IP1 is not a transposition vector on N, computation is terminated as soon as the error is detected and IER is set to 1. If there is no error, IER is set to zero.

The computation of the resulting vector IP2 proceeds as follows.

a. If IPAR is negative, for each i, i=1,...,n, IP2(IP1(i)) is set to i.

b. If IPAR is zero, initially IP2(i) is set to i for i=1,...,n, and then for i=1,...,n in that order, IP2(i) and IP2(IP1(i)) are interchanged.

c. If IPAR is positive, initially IP1 is moved to IP2, and then the following two steps are repeated for i successively 1,...,n:

(1) Find the smallest j ≥ i such that IP2(j)=i.

(2) Set IP2(j) to IP2(i).

IP2 cannot have the same storage allocation as IP1. IP1 is returned unchanged.

```
C                                                                       PERM  10
C     ...................................................................PERM  20
C                                                                       PERM  30
C        SUBROUTINE PERM                                                PERM  40
C                                                                       PERM  50
C        PURPOSE                                                        PERM  60
C           TO COMPUTE THE PERMUTATION VECTOR THAT IS INVERSE TO A GIVENPERM  70
C           PERMUTATION VECTOR, THE PERMUTATION VECTOR THAT IS EQUIVA- PERM  80
C           LENT TO A GIVEN TRANSPOSITION VECTOR AND A TRANSPOSITION   PERM  90
C           VECTOR THAT IS EQUIVALENT TO A GIVEN PERMUTATION VECTOR.   PERM 100
C           (SEE THE GENERAL DISCUSSION FOR DEFINITIONS AND NOTATION.) PERM 110
C                                                                       PERM 120
C        USAGE                                                          PERM 130
C           CALL PERM(IP1,IP2,N,IPAR,IER)                               PERM 140
C                                                                       PERM 150
C        DESCRIPTION OF PARAMETERS                                      PERM 160
C           IP1  - GIVEN PERMUTATION OR TRANSPOSITION VECTOR            PERM 170
C                  (DIMENSION N)                                        PERM 180
C           IP2  - RESULTING PERMUTATION OR TRANSPOSITION VECTOR        PERM 190
C                  (DIMENSION N)                                        PERM 200
C           N    - DIMENSION OF VECTORS IP1 AND IP2                     PERM 210
C           IPAR - INPUT PARAMETER                                      PERM 220
C                  IPAR NEGATIVE - COMPUTE THE PERMUTATION VECTOR IP2   PERM 230
C                                  THAT IS THE INVERSE OF THE PERMUTA-  PERM 240
C                                  TION VECTOR IP1                      PERM 250
C                  IPAR = ZERO   - COMPUTE THE PERMUTATION VECTOR IP2   PERM 260
C                                  THAT IS EQUIVALENT TO THE TRANSPOSI- PERM 270
C                                  TION VECTOR IP1                      PERM 280
C                  IPAR POSITIVE - COMPUTE A TRANSPOSITION VECTOR IP2   PERM 290
C                                  THAT IS EQUIVALENT TO THE PERMUTATIONPERM 300
C                                  VECTOR IP1                           PERM 310
C           IER  - RESULTING ERROR PARAMETER                            PERM 320
C                  IER=-1 -  N IS NOT POSITIVE                          PERM 330
C                  IER= 0 -  NO ERROR                                   PERM 340
C                  IER= 1 -  IP1 IS EITHER NOT A PERMUTATION VECTOR OR  PERM 350
C                            NOT A TRANSPOSITION VECTOR ON 1,...,N,     PERM 360
C                            DEPENDING ON WHETHER IPAR IS NON-ZERO OR   PERM 370
C                            ZERO, RESPECTIVELY                         PERM 380
C                                                                       PERM 390
C        REMARKS                                                        PERM 400
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               PERM 410
C           (2)  IF IER=1, THEN COMPUTATION HAS BEEN UNSUCCESSFUL DUE TOPERM 420
C                ERROR AND THE PARTIAL RESULTS FOUND IN IP2 ARE USELESS.PERM 430
C           (3)  IP2 CANNOT HAVE THE SAME STORAGE ALLOCATION AS IP1.    PERM 440
C                                                                       PERM 450
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PERM 460
C           NONE                                                        PERM 470
C                                                                       PERM 480
C        METHOD                                                         PERM 490
C           (1)  IPAR NEGATIVE - FOR EACH I, I=1,...,N, IP2(IP1(I)) IS  PERM 500
C                                SET TO I.                              PERM 510
C           (2)  IPAR = ZERO   - INITIALLY IP2(I) IS SET TO I FOR       PERM 520
C                                I=1,...,N.  THEN, FOR I=1,...,N IN THATPERM 530
C                                ORDER, IP2(I) AND IP2(IP1(I)) ARE      PERM 540
C                                INTERCHANGED.                          PERM 550
C           (3)  IPAR POSITIVE - INITIALLY IP1 IS MOVED TO IP2.  THEN   PERM 560
C                                THE FOLLOWING TWO STEPS ARE REPEATED   PERM 570
C                                FOR I SUCCESSIVELY EQUAL TO 1,...,N.   PERM 580
C                                (A) FIND THE SMALLEST J GREATER THAN ORPERM 590
C                                    EQUAL TO I SUCH THAT IP2(J)=I.     PERM 600
C                                (B) SET IP2(J) TO IP2(I).              PERM 610
C                                                                       PERM 620
C     ...................................................................PERM 630
```

```
C                                                                       PERM 640
      SUBROUTINE PERM(IP1,IP2,N,IPAR,IER)                               PERM 650
C                                                                       PERM 660
C                                                                       PERM 670
      DIMENSION IP1(1),IP2(1)                                           PERM 680
C                                                                       PERM 690
C        TEST DIMENSION                                                 PERM 700
      IF(N)19,19,1                                                      PERM 710
C                                                                       PERM 720
C        TEST IPAR TO DETERMINE WHETHER IP1 IS TO BE INTERPRETED AS     PERM 730
C        A PERMUTATION VECTOR OR AS A TRANSPOSITION VECTOR              PERM 740
    1 IF(IPAR)2,13,2                                                    PERM 750
C                                                                       PERM 760
C        CHECK THAT IP1 IS A PERMUTATION VECTOR AND COMPUTE IP1 INVERSE PERM 770
    2 DO 3 I=1,N                                                        PERM 780
    3 IP2(I)=0                                                          PERM 790
      DO 6 I=1,N                                                        PERM 800
      K=IP1(I)                                                          PERM 810
      IF(K-N)4,5,20                                                     PERM 820
    4 IF(K)20,20,5                                                      PERM 830
    5 IF(IP2(K))20,6,20                                                 PERM 840
    6 IP2(K)=I                                                          PERM 850
C                                                                       PERM 860
C        TEST IPAR FOR THE DESIRED OPERATION                            PERM 870
      IF(IPAR)12,7,7                                                    PERM 880
C                                                                       PERM 890
C        COMPUTE TRANSPOSITION VECTOR IP2 FOR PERMUTATION VECTOR IP1    PERM 900
    7 DO 8 I=1,N                                                        PERM 910
    8 IP2(I)=IP1(I)                                                     PERM 920
      NN=N-1                                                            PERM 930
      IF(NN)12,12,9                                                     PERM 940
    9 DO 11 I=1,NN                                                      PERM 950
      DO 10 J=1,NN                                                      PERM 960
      IF(IP2(J)-I)10,11,10                                              PERM 970
   10 CONTINUE                                                          PERM 980
      J=N                                                               PERM 990
   11 IP2(J)=IP2(I)                                                     PERM1000
C                                                                       PERM1010
C        NORMAL RETURN - NO ERROR                                       PERM1020
C                                                                       PERM1030
   12 IER=0                                                             PERM1040
      RETURN                                                            PERM1050
C                                                                       PERM1060
C        COMPUTE PERMUTATION VECTOR IP2 FOR TRANSPOSITION VECTOR IP1    PERM1070
   13 DO 14 I=1,N                                                       PERM1080
   14 IP2(I)=I                                                          PERM1090
      DO 18 I=1,N                                                       PERM1100
      K=IP1(I)                                                          PERM1110
      IF(K-I)15,18,16                                                   PERM1120
   15 IF(K)20,20,17                                                     PERM1130
   16 IF(N-K)20,17,17                                                   PERM1140
   17 J=IP2(I)                                                          PERM1150
      IP2(I)=IP2(K)                                                     PERM1160
      IP2(K)=J                                                          PERM1170
   18 CONTINUE                                                          PERM1180
      GO TO 12                                                          PERM1190
C                                                                       PERM1200
C        ERROR RETURN - N IS NOT POSITIVE                               PERM1210
   19 IER=-1                                                            PERM1220
      RETURN                                                            PERM1230
C                                                                       PERM1240
C        ERROR RETURN - IP1 IS EITHER NOT A PERMUTATION VECTOR          PERM1250
C                       OR NOT A TRANSPOSITION VECTOR                   PERM1260
   20 IER=1                                                             PERM1270
      RETURN                                                            PERM1280
      END
```

Subroutines TEAS and DTEAS

The problem is to assign a scalar value S to a given sequence $x_1, x_2, x_3, \ldots$. In case of convergence of the sequence, S should be the limit. The Epsilon algorithm possibly increases the speed of convergence and determines an approximate value FIN of S in terms of the given members of the finite sequence $x_1, x_2, x_3, \ldots, x_N$.

1. Theoretical background

The value FIN is calculated by means of the Epsilon algorithm (see Figure 16).

The first column (with superscript 1) is identical to the given sequence:

$$x_i^{(1)} = x_i \qquad (i = 1, 2, 3, \ldots)$$

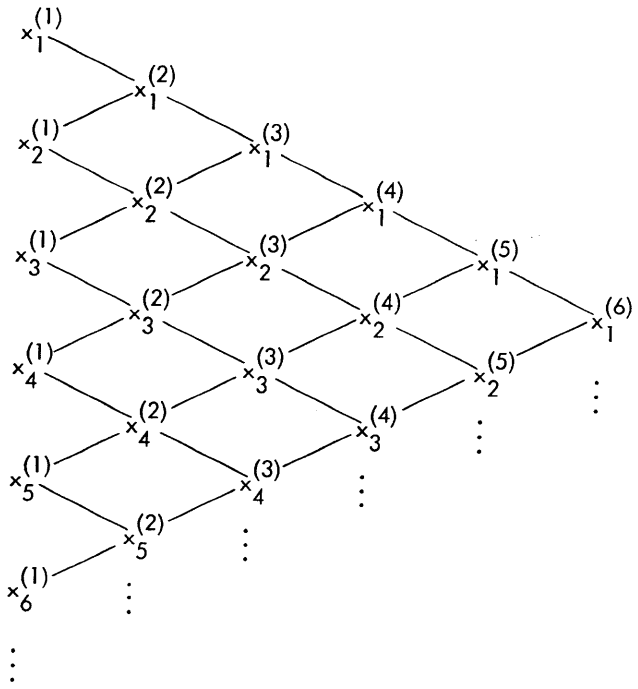


Figure 16. The complete Epsilon array

The values in the third column (with superscript 3) are derived from three consecutive members of the sequence; for example, $x_2^{(3)}$ is derived from $x_2^{(1)}$, $x_3^{(1)}$ and $x_4^{(1)}$. Generally, the column with superscript $2k + 1$ ($k = 1, 2, 3, \ldots$) contains quantities derived from $2k + 1$ consecutive members of the sequence. The intermediate values with even superscripts are auxiliary quantities.

The Epsilon algorithm is based on the following relationship:

$$x_i^{(k)} = x_{i+1}^{(k-2)} + \frac{1}{x_{i+1}^{(k-1)} - x_i^{(k-1)}} \qquad \begin{matrix}(k = 2, 3, 4, \ldots) \\ (i = 1, 2, 3, \ldots)\end{matrix} \qquad (1)$$

$$x_i^{(o)} = 0$$

With this fundamental relationship the complete Epsilon array shown in Figure 16 is built up from left to right.

2. Programming considerations

Subroutines TEAS and DTEAS generate only the first five columns of the complete Epsilon array; this E-2 transformation is used in an iterative way. Within one iteration the quantities in the upward diagonals are computed in a DO-loop by means of the algorithmic relationship (1). This process requires six auxiliary storage boxes (W1, W2, W3, W4, W5, W6).

The values in the fifth column $x_1^{(5)}, x_2^{(5)}, \ldots, x_{NEW-4}^{(5)}$ are successively stored in x(1), x(2), ..., x(NEW-4) as long as they are finite.

If a term $x_k^{(5)}$ in the fifth column becomes formally infinite, the values $x_1^{(5)}$ up to $x_k^{(5)}$ are cancelled and $x_{k+1}^{(5)}$ is stored in x(1), $x_{k+2}^{(5)}$ in x(2), and so on. Hence, after one iteration no component of the transformed vector x becomes infinite except possibly the last.

Consecutive equal terms in the column with superscript k(k=1, 2, 3) are reproduced in the column with superscript k+2. The basic mesh of the E-2 transformation is shown in Figure 17.

As a nonlinear algorithm the E-2 transformation is sensitive to roundoff errors; therefore special procedures are incorporated to avoid undue loss of accuracy:

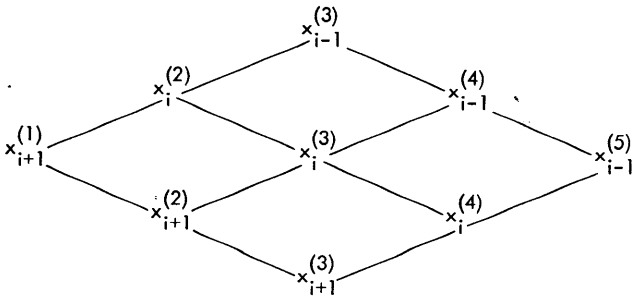


Figure 17. Basic mesh of the E-2 transformation

a. If there is an intolerable loss of significance in the calculation of a term in the third or fifth column, TEAS or DTEAS transfers out of the diagonal loop and uses for further calculation only those components of vector x, which have already been transformed.

b. If two consecutive quantities in the second column $x_i^{(2)}$ and $x_{i+1}^{(2)}$ (see Figure 17) are nearly equal, $x_i^{(3)}$ is large and ill-determined. Therefore, if:

$$\left| x_{i+1}^{(2)} - x_i^{(2)} \right| \leqq 10^{-4} \cdot \left| x_{i+1}^{(2)} \right| \quad \text{in single precision or}$$

$$\left| x_{i+1}^{(2)} - x_i^{(2)} \right| \leqq 10^{-12} \cdot \left| x_{i+1}^{(2)} \right| \quad \text{in double precision} \qquad (2)$$

subroutine TEAS or DTEAS calculates the iterated member of the sequence $x_{i-1}^{(5)}$ with a singular rule:

$$x_{i-1}^{(5)} = \frac{x_i^{(3)} \cdot W7}{1 + W7} \qquad (3)$$

where $$W7 = \frac{x_{i+1}^{(3)}}{x_i^{(3)} - x_{i+1}^{(3)}} + \frac{x_{i-1}^{(3)}}{x_i^{(3)} - x_{i-1}^{(3)}} - \frac{x_{i+1}^{(1)}}{x_i^{(3)} - x_{i+1}^{(1)}}$$

This requires two more auxiliary storage locations W7 and T.

c. If $x_i^{(2)}$ and $x_{i+1}^{(2)}$ are exactly equal, $x_i^{(3)}$ becomes infinite, and the singular rule for the Epsilon algorithm is simply:

$$x_{i-1}^{(5)} = x_{i+1}^{(3)} + x_{i-1}^{(3)} - x_{i+1}^{(1)} \qquad (4)$$

d. If three or more consecutive terms in the second column are equal, singular rule (4) cannot be applied; the corresponding iterated members of the sequence in the fifth column become formally infinite.

Iteration is terminated if one of the following conditions holds true:

a. Three times in succession the relative difference between neighboring transformed terms $X(I) = x_i$ is not greater than EPS; that is,

$$\left| x_i - x_{i+1} \right| \leqq EPS \cdot \left| x_{i+1} \right| \qquad (i = k, k+1, k+2) \qquad (5)$$

In case $\left| x_{i+1} \right| \leqq 1$, the relative difference (5) is replaced by the absolute

$$\left| x_i - x_{i+1} \right| \leqq EPS \qquad (i = k, k+1, k+2) \qquad (6)$$

b. The number of the transformed members of sequence (NEW-IMIN) is less than six.

In the first case x_{k+2} is returned as result value FIN, and IER = 0 as the error parameter. In the second case the values IER = 1 and FIN = x_1 are returned.

Some remarks are in order. First, the user must specify N--that is, the dimension of the input vector x--so that the character of the infinite sequence is recognizable. Second, subroutine TEAS or DTEAS works satisfactorily if the convergence of the given sequence is a geometric one; that is,

$$x_n - S = A \cdot \lambda^n + O(\lambda^n), \qquad |\lambda| < 1 \qquad (7)$$

For reference see:

(1) Shanks, Algorithm 215, CACM 1963, no. 11, p. 662.

(2) P. Wynn, "Singular Rules for certain nonlinear Algorithms," BIT vol. 3, 1963, pp. 175 - 195.

```
C                                                                       TEAS  10
C     ...................................................................TEAS  20
C                                                                       TEAS  30
C        SUBROUTINE TEAS                                                TEAS  40
C                                                                       TEAS  50
C        PURPOSE                                                        TEAS  60
C           CALCULATE THE LIMIT OF A GIVEN SEQUENCE BY MEANS OF THE     TEAS  70
C           EPSILON-ALGORITHM.                                          TEAS  80
C                                                                       TEAS  90
C        USAGE                                                          TEAS 100
C           CALL TEAS(X,N,FIN,EPS,IER)                                  TEAS 110
C                                                                       TEAS 120
C        DESCRIPTION OF PARAMETERS                                      TEAS 130
C           X      - VECTOR WHOSE COMPONENTS ARE TERMS OF THE GIVEN     TEAS 140
C                    SEQUENCE. ON RETURN THE COMPONENTS OF VECTOR X     TEAS 150
C                    ARE DESTROYED.                                     TEAS 160
C           N      - DIMENSION OF INPUT VECTOR X.                       TEAS 170
C           FIN    - RESULTANT SCALAR CONTAINING ON RETURN THE LIMIT    TEAS 180
C                    OF THE GIVEN SEQUENCE.                             TEAS 190
C           EPS    - AN INPUT VALUE, WHICH SPECIFIES THE UPPER BOUND    TEAS 200
C                    OF THE RELATIVE (ABSOLUTE) ERROR IF THE COMPONENTS TEAS 210
C                    OF X ARE ABSOLUTELY GREATER (LESS) THAN ONE.       TEAS 220
C                    CALCULATION IS TERMINATED AS SOON AS THREE TIMES INTEAS 230
C                    SUCCESSION THE RELATIVE (ABSOLUTE) DIFFERENCE      TEAS 240
C                    BETWEEN NEIGHBOURING TERMS IS NOT GREATER THAN EPS.TEAS 250
C           IER    - RESULTANT ERROR PARAMETER CODED IN THE FOLLOWING   TEAS 260
C                    FORM                                               TEAS 270
C                      IER=0  - NO ERROR                                TEAS 280
C                      IER=1  - REQUIRED ACCURACY NOT REACHED WITH      TEAS 290
C                               MAXIMAL NUMBER OF ITERATIONS            TEAS 300
C                      IER=-1 - INTEGER N IS LESS THAN TEN.             TEAS 310
C                                                                       TEAS 320
C        REMARKS                                                        TEAS 330
C           NO ACTION BESIDES ERROR MESSAGE IN CASE N LESS THAN TEN.    TEAS 340
C           THE CHARACTER OF THE GIVEN INFINITE SEQUENCE MUST BE        TEAS 350
C           RECOGNIZABLE BY THOSE N COMPONENTS OF THE INPUT VECTOR X.   TEAS 360
C                                                                       TEAS 370
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  TEAS 380
C           NONE                                                        TEAS 390
C                                                                       TEAS 400
C        METHOD                                                         TEAS 410
C           THE CONVERGENCE OF THE GIVEN SEQUENCE IS ACCELERATED BY     TEAS 420
C           MEANS OF THE E(2)-TRANSFORMATION, USED IN AN ITERATIVE WAY. TEAS 430
C           FOR REFERENCE, SEE                                          TEAS 440
C           ALGORITHM 215,SHANKS, CACM 1963, NO. 11, PP. 662. AND       TEAS 450
C           P. WYNN, SINGULAR RULES FOR CERTAIN NON-LINEAR ALGORITHMS   TEAS 460
C           BIT VOL. 3, 1963, PP. 175-195.                              TEAS 470
C                                                                       TEAS 480
C     ...................................................................TEAS 490
C                                                                       TEAS 500
      SUBROUTINE TEAS(X,N,FIN,EPS,IER)                                  TEAS 510
C                                                                       TEAS 520
      DIMENSION X(1)                                                    TEAS 530
C                                                                       TEAS 540
C        TEST ON WRONG INPUT PARAMETER N                                TEAS 550
C                                                                       TEAS 560
      NEW=N                                                             TEAS 570
      IF(NEW-10)1,2,2                                                   TEAS 580
    1 IER=-1                                                            TEAS 590
      RETURN                                                            TEAS 600
C                                                                       TEAS 610
C        CALCULATE INITIAL VALUES FOR THE EPSILON ARRAY                 TEAS 620
C                                                                       TEAS 630
    2 ISW1=0                                                            TEAS 640
      ISW2=0                                                            TEAS 650
      W1=1.E38                                                          TEAS 660
      W7=X(4)-X(3)                                                      TEAS 670
      IF(W7)3,4,3                                                       TEAS 680
    3 W1=1./W7                                                          TEAS 690
C                                                                       TEAS 700
    4 W5=1.E38                                                          TEAS 710
      W7=X(2)-X(1)                                                      TEAS 720
      IF(W7)5,6,5                                                       TEAS 730
    5 W5=1./W7                                                          TEAS 740
C                                                                       TEAS 750
    6 W4=X(3)-X(2)                                                      TEAS 760
      IF(W4)9,7,9                                                       TEAS 770
    7 W4=1.E38                                                          TEAS 780
      T=X(2)                                                            TEAS 790
      W2=X(3)                                                           TEAS 800
    8 W3=1.E38                                                          TEAS 810
      GO TO 17                                                          TEAS 820
C                                                                       TEAS 830
    9 W4=1./W4                                                          TEAS 840
C                                                                       TEAS 850
      T=1.E38                                                           TEAS 860
      W7=W4-W5                                                          TEAS 870
      IF(W7)10,11,10                                                    TEAS 880
   10 T=X(2)+1./W7                                                      TEAS 890
C                                                                       TEAS 900
   11 W2=W1-W4                                                          TEAS 910
      IF(W2)15,12,15                                                    TEAS 920
   12 W2=1.E38                                                          TEAS 930
      IF(T-1.E38)13,14,14                                               TEAS 940
   13 ISW2=1                                                            TEAS 950
   14 W3=W4                                                             TEAS 960
      GO TO 17                                                          TEAS 970
C                                                                       TEAS 980
   15 W2=X(3)+1./W2                                                     TEAS 990
      W7=W2-T                                                           TEAS1000
      IF(W7)16,8,16                                                     TEAS1010
   16 W3=W4+1./W7                                                       TEAS1020
C                                                                       TEAS1030
   17 ISW1=ISW2                                                         TEAS1040
      ISW2=0                                                            TEAS1050
      IMIN=4                                                            TEAS1060
C                                                                       TEAS1070
C        CALCULATE DIAGONALS OF THE EPSILON ARRAY IN A DO-LOOP          TEAS1080
C                                                                       TEAS1090
      DO 40 I=5,NEW                                                     TEAS1100
      IAUS=I-IMIN                                                       TEAS1110
      W4=1.E38                                                          TEAS1120
      W5=X(I-1)                                                         TEAS1130
      W7=X(I)-X(I-1)                                                    TEAS1140
      IF(W7)18,24,18                                                    TEAS1150
   18 W4=1./W7                                                          TEAS1160
C                                                                       TEAS1170
      IF(W1-1.E38)19,25,25                                              TEAS1180
   19 W6=W4-W1                                                          TEAS1190
C                                                                       TEAS1200
C        TEST FOR NECESSITY OF A SINGULAR RULE                          TEAS1210
C                                                                       TEAS1220
      IF(ABS(W6)-ABS(W4)*1.E-4)20,20,22                                 TEAS1230
   20 ISW2=1                                                            TEAS1240
      IF(W6)22,21,22                                                    TEAS1250
   21 W5=1.E38                                                          TEAS1260
      W6=W1                                                             TEAS1270
      IF(W2-1.E38)28,26,26                                              TEAS1280
   22 W5=X(I-1)+1./W6                                                   TEAS1290
C                                                                       TEAS1300
C        FIRST TEST FOR LOSS OF SIGNIFICANCE                            TEAS1310
C                                                                       TEAS1320
      IF(ABS(W5)-ABS(X(I-1))*1.E-5)23,24,24                             TEAS1330
   23 IF(W5)36,24,36                                                    TEAS1340
C                                                                       TEAS1350
   24 W7=W5-W2                                                          TEAS1360
      IF(W7)27,25,27                                                    TEAS1370
   25 W6=1.E38                                                          TEAS1380
   26 ISW2=0                                                            TEAS1390
      X(IAUS)=W2                                                        TEAS1400
      GO TO 37                                                          TEAS1410
   27 W6=W1+1./W7                                                       TEAS1420
   28 IF(ISW1-1)33,29,29                                                TEAS1430
C                                                                       TEAS1440
C        CALCULATE X(IAUS) WITH HELP OF SINGULAR RULE                   TEAS1450
C                                                                       TEAS1460
   29 IF(W2-1.E38)30,32,32                                              TEAS1470
   30 W7=W5/(W2-W5)+T/(W2-T)+X(I-2)/(X(I-2)-W2)                         TEAS1480
      IF(1.+W7)31,38,31                                                 TEAS1490
   31 X(IAUS)=W7*W2/(1.+W7)                                             TEAS1500
      GO TO 39                                                          TEAS1510
C                                                                       TEAS1520
   32 X(IAUS)=W5+T-X(I-2)                                               TEAS1530
      GO TO 39                                                          TEAS1540
C                                                                       TEAS1550
   33 W7=W6-W3                                                          TEAS1560
      IF(W7)34,38,34                                                    TEAS1570
   34 X(IAUS)=W2+1./W7                                                  TEAS1580
C                                                                       TEAS1590
C        SECOND TEST FOR LOSS OF SIGNIFICANCE                           TEAS1600
C                                                                       TEAS1610
      IF(ABS(X(IAUS))-ABS(W2)*1.E-5)35,37,37                            TEAS1620
   35 IF(X(IAUS))36,37,36                                               TEAS1630
C                                                                       TEAS1640
   36 NEW=IAUS-1                                                        TEAS1650
      ISW2=0                                                            TEAS1660
      GO TO 41                                                          TEAS1670
C                                                                       TEAS1680
   37 IF(W2-1.E38)39,38,38                                              TEAS1690
   38 X(IAUS)=1.E38                                                     TEAS1700
      IMIN=I                                                            TEAS1710
C                                                                       TEAS1720
   39 W1=W4                                                             TEAS1730
      T=W2                                                              TEAS1740
      W2=W5                                                             TEAS1750
      W3=W6                                                             TEAS1760
      ISW1=ISW2                                                         TEAS1770
   40 ISW2=0                                                            TEAS1780
C                                                                       TEAS1790
      NEW=NEW-IMIN                                                      TEAS1800
C                                                                       TEAS1810
C        TEST FOR ACCURACY                                              TEAS1820
C                                                                       TEAS1830
   41 IEND=NEW-1                                                        TEAS1840
      DO 47 I=1,IEND                                                    TEAS1850
      W1=ABS(X(I)-X(I+1))                                               TEAS1860
      W2=ABS(X(I+1))                                                    TEAS1870
      IF(W1-EPS)44,44,42                                                TEAS1880
   42 IF(W2-1.)46,46,43                                                 TEAS1890
   43 IF(W1-EPS*W2)44,44,46                                             TEAS1900
   44 ISW2=ISW2+1                                                       TEAS1910
      IF(3-ISW2)45,45,47                                                TEAS1920
   45 FIN=X(I)                                                          TEAS1930
      IER=0                                                             TEAS1940
      RETURN                                                            TEAS1950
C                                                                       TEAS1960
   46 ISW2=0                                                            TEAS1970
   47 CONTINUE                                                          TEAS1980
C                                                                       TEAS1990
      IF(NEW-6)48,2,2                                                   TEAS2000
   48 FIN=X(NEW)                                                        TEAS2010
      IER=1                                                             TEAS2020
      RETURN                                                            TEAS2030
      END                                                               TEAS2040
```

```
C                                                                       DTEA  10
C     ..................................................................DTEA  20
C                                                                       DTEA  30
C        SUBROUTINE DTEAS                                               DTEA  40
C                                                                       DTEA  50
C        PURPOSE                                                        DTEA  60
C           CALCULATE THE LIMIT OF A GIVEN SEQUENCE BY MEANS OF THE     DTEA  70
C           EPSILON-ALGORITHM.                                          DTEA  80
C                                                                       DTEA  90
C        USAGE                                                          DTEA 100
C           CALL DTEAS(X,N,FIN,EPS,IER)                                 DTEA 110
C                                                                       DTEA 120
C        DESCRIPTION OF PARAMETERS                                      DTEA 130
C           X      - DOUBLE PRECISION VECTOR WHOSE COMPONENTS ARE TERMS DTEA 140
C                    OF THE GIVEN SEQUENCE. ON RETURN THE COMPONENTS OF DTEA 150
C                    VECTOR X ARE DESTROYED.                            DTEA 160
C           N      - DIMENSION OF INPUT VECTOR X.                      DTEA 170
C           FIN    - RESULTANT SCALAR IN DOUBLE PRECISION CONTAINING ON DTEA 180
C                    RETURN THE LIMIT OF THE GIVEN SEQUENCE.            DTEA 190
C           EPS    - SINGLE PRECISION INPUT VALUE, WHICH SPECIFIES THE DTEA 200
C                    UPPER BOUND OF THE RELATIVE (ABSOLUTE) ERROR IF THEDTEA 210
C                    COMPONENTS OF X ARE ABSOLUTELY GREATER (LESS) THAN DTEA 220
C                    ONE.                                               DTEA 230
C                    CALCULATION IS TERMINATED AS SOON AS THREE TIMES INDTEA 240
C                    SUCCESSION THE RELATIVE (ABSOLUTE) DIFFERENCE      DTEA 250
C                    BETWEEN NEIGHBOURING TERMS IS NOT GREATER THAN EPS.DTEA 260
C           IER    - RESULTANT ERROR PARAMETER CODED IN THE FOLLOWING  DTEA 270
C                    FORM                                               DTEA 280
C                     IER=0  - NO ERROR                                 DTEA 290
C                     IER=1  - REQUIRED ACCURACY NOT REACHED WITH       DTEA 300
C                              MAXIMAL NUMBER OF ITERATIONS             DTEA 310
C                     IER=-1 - INTEGER N IS LESS THAN TEN.              DTEA 320
C                                                                       DTEA 330
C        REMARKS                                                        DTEA 340
C           NO ACTION BESIDES ERROR MESSAGE IN CASE N LESS THAN TEN.    DTEA 350
C           THE CHARACTER OF THE GIVEN INFINITE SEQUENCE MUST BE        DTEA 360
C           RECOGNIZABLE BY THOSE N COMPONENTS OF THE INPUT VECTOR X.   DTEA 370
C                                                                       DTEA 380
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTEA 390
C           NONE                                                        DTEA 400
C                                                                       DTEA 410
C        METHOD                                                         DTEA 420
C           THE CONVERGENCE OF THE GIVEN SEQUENCE IS ACCELERATED BY     DTEA 430
C           MEANS OF THE E(2)-TRANSFORMATION, USED IN AN ITERATIVE WAY. DTEA 440
C           FOR REFERENCE, SEE                                          DTEA 450
C           ALGORITHM 215,SHANKS, CACM 1963, NO. 11, PP. 662. AND       DTEA 460
C           P. WYNN, SINGULAR RULES FOR CERTAIN NON-LINEAR ALGORITHMS   DTEA 470
C           BIT VOL. 3, 1963, PP. 175-195.                              DTEA 480
C                                                                       DTEA 490
C     ..................................................................DTEA 500
C                                                                       DTEA 510
      SUBROUTINE DTEAS(X,N,FIN,EPS,IER)                                 DTEA 520
C                                                                       DTEA 530
      DIMENSION X(1)                                                    DTEA 540
      DOUBLE PRECISION X,FIN,W1,W2,W3,W4,W5,W6,W7,T                     DTEA 550
C                                                                       DTEA 560
C        TEST ON WRONG INPUT PARAMETER N                                DTEA 570
C                                                                       DTEA 580
      NEW=N                                                             DTEA 590
      IF(NEW-10)1,1,2                                                   DTEA 600
    1 IER=-1                                                            DTEA 610
      RETURN                                                            DTEA 620
C                                                                       DTEA 630
C        CALCULATE INITIAL VALUES FOR THE EPSILON ARRAY                 DTEA 640
C                                                                       DTEA 650
    2 ISW1=0                                                            DTEA 660
      ISW2=0                                                            DTEA 670
      W1=1.D38                                                          DTEA 680
      W7=X(4)-X(3)                                                      DTEA 690
      IF(W7)3,4,3                                                       DTEA 700
    3 W1=1.D0/W7                                                        DTEA 710
C                                                                       DTEA 720
    4 W5=1.D38                                                          DTEA 730
      W7=X(2)-X(1)                                                      DTEA 740
      IF(W7)5,6,5                                                       DTEA 750
    5 W5=1.D0/W7                                                        DTEA 760
C                                                                       DTEA 770
    6 W4=X(3)-X(2)                                                      DTEA 780
      IF(W4)9,7,9                                                       DTEA 790
    7 W4=1.D38                                                          DTEA 800
      T=X(2)                                                            DTEA 810
      W2=X(3)                                                           DTEA 820
    8 W3=1.D38                                                          DTEA 830
      GO TO 17                                                          DTEA 840
C                                                                       DTEA 850
    9 W4=1.D0/W4                                                        DTEA 860
C                                                                       DTEA 870
      T=1.D38                                                           DTEA 880
      W7=W4-W5                                                          DTEA 890
      IF(W7)10,11,10                                                    DTEA 900
   10 T=X(2)+1.D0/W7                                                    DTEA 910
C                                                                       DTEA 920
   11 W2=W1-W4                                                          DTEA 930
      IF(W2)15,12,15                                                    DTEA 940
   12 W2=1.D38                                                          DTEA 950
      IF(T-1.D38)13,14,14                                               DTEA 960
   13 ISW2=1                                                            DTEA 970
   14 W3=W4                                                             DTEA 980
      GO TO 17                                                          DTEA 990
C                                                                       DTEA1000
   15 W2=X(3)+1.D0/W2                                                   DTEA1010
      W7=W2-T                                                           DTEA1020
      IF(W7)16,8,16                                                     DTEA1030
   16 W3=W4+1.D0/W7                                                     DTEA1040
C                                                                       DTEA1050
   17 ISW1=ISW2                                                         DTEA1060
      ISW2=0                                                            DTEA1070
      IMIN=4                                                            DTEA1080
C                                                                       DTEA1090
C        CALCULATE DIAGONALS OF THE EPSILON ARRAY IN A DO-LOOP          DTEA1100
C                                                                       DTEA1110
      DO 40 I=5,NEW                                                     DTEA1120
      IAUS=I-IMIN                                                       DTEA1130
      W4=1.D38                                                          DTEA1140
      W5=X(I-1)                                                         DTEA1150
      W7=X(I)-X(I-1)                                                    DTEA1160
      IF(W7)18,24,18                                                    DTEA1170
   18 W4=1.D0/W7                                                        DTEA1180
C                                                                       DTEA1190
      IF(W1-1.D38)19,25,25                                              DTEA1200
   19 W6=W4-W1                                                          DTEA1210
C                                                                       DTEA1220
C        TEST FOR NECESSITY OF A SINGULAR RULE                          DTEA1230
C                                                                       DTEA1240
      IF(DABS(W6)-DABS(W4)*1.D-12)20,20,22                              DTEA1250
   20 ISW2=1                                                            DTEA1260
      IF(W6)22,21,22                                                    DTEA1270
   21 W5=1.D38                                                          DTEA1280
      W6=W1                                                             DTEA1290
      IF(W2-1.D38)28,26,26                                              DTEA1300
   22 W5=X(I-1)+1.D0/W6                                                 DTEA1310
C                                                                       DTEA1320
C        FIRST TEST FOR LOSS OF SIGNIFICANCE                            DTEA1330
C                                                                       DTEA1340
      IF(DABS(W5)-DABS(X(I-1))*1.D-10)23,24,24                          DTEA1350
   23 IF(W5)36,24,36                                                    DTEA1360
C                                                                       DTEA1370
   24 W7=W5-W2                                                          DTEA1380
      IF(W7)27,25,27                                                    DTEA1390
   25 W6=1.D38                                                          DTEA1400
   26 ISW2=0                                                            DTEA1410
      X(IAUS)=W2                                                        DTEA1420
      GO TO 37                                                          DTEA1430
   27 W6=W1+1.D0/W7                                                     DTEA1440
   28 IF(ISW1-1)33,29,29                                                DTEA1450
C                                                                       DTEA1460
C        CALCULATE X(IAUS) WITH HELP OF SINGULAR RULE                   DTEA1470
C                                                                       DTEA1480
   29 IF(W2-1.D38)30,32,32                                              DTEA1490
   30 W7=W5/(W2-W5)+T/(W2-T)+X(I-2)/(X(I-2)-W2)                         DTEA1500
      IF(1.D0+W7)31,38,31                                               DTEA1510
   31 X(IAUS)=W7*W2/(1.D0+W7)                                           DTEA1520
      GO TO 39                                                          DTEA1530
C                                                                       DTEA1540
   32 X(IAUS)=W5+T-X(I-2)                                               DTEA1550
      GO TO 39                                                          DTEA1560
C                                                                       DTEA1570
   33 W7=W6-W3                                                          DTEA1580
      IF(W7)34,38,34                                                    DTEA1590
   34 X(IAUS)=W2+1.D0/W7                                                DTEA1600
C                                                                       DTEA1610
C        SECOND TEST FOR LOSS OF SIGNIFICANCE                           DTEA1620
C                                                                       DTEA1630
      IF(DABS(X(IAUS))-DABS(W2)*1.D-10)35,37,37                         DTEA1640
   35 IF(X(IAUS))36,37,36                                               DTEA1650
C                                                                       DTEA1660
   36 NEW=IAUS-1                                                        DTEA1670
      ISW2=0                                                            DTEA1680
      GO TO 41                                                          DTEA1690
C                                                                       DTEA1700
   37 IF(W2-1.D38)39,38,38                                              DTEA1710
   38 X(IAUS)=1.D38                                                     DTEA1720
      IMIN=I                                                            DTEA1730
C                                                                       DTEA1740
   39 W1=W4                                                             DTEA1750
      T=W2                                                              DTEA1760
      W2=W5                                                             DTEA1770
      W3=W6                                                             DTEA1780
      ISW1=ISW2                                                         DTEA1790
   40 ISW2=0                                                            DTEA1800
C                                                                       DTEA1810
      NEW=NEW-IMIN                                                      DTEA1820
C                                                                       DTEA1830
C        TEST FOR ACCURACY                                              DTEA1840
C                                                                       DTEA1850
   41 IEND=NEW-1                                                        DTEA1860
      DO 47 I=1,IEND                                                    DTEA1870
      HE1=DABS(X(I)-X(I+1))                                             DTEA1880
      HE2=DABS(X(I+1))                                                  DTEA1890
      IF(HE1-EPS)44,44,42                                               DTEA1900
   42 IF(HE2-1.)46,46,43                                                DTEA1910
   43 IF(HE1-EPS*HE2)44,44,46                                           DTEA1920
   44 ISW2=ISW2+1                                                       DTEA1930
      IF(3-ISW2)45,45,47                                                DTEA1940
   45 FIN=X(I)                                                          DTEA1950
      IER=0                                                             DTEA1960
      RETURN                                                            DTEA1970
C                                                                       DTEA1980
   46 ISW2=0                                                            DTEA1990
   47 CONTINUE                                                          DTEA2000
C                                                                       DTEA2010
      IF(NEW-6)48,2,2                                                   DTEA2020
   48 FIN=X(NEW)                                                        DTEA2030
      IER=1                                                             DTEA2040
      RETURN                                                            DTEA2050
      END                                                               DTEA2060
```

Subroutines TEUL and DTEUL

These subroutines calculate the sum value of the series $\sum_{k=1}^{\infty} F_k$ by means of a refined Euler transformation.

The following abbreviations are used:

$$\Delta^0 F_i = F_i$$

$$\Delta^1 F_i = \frac{1}{2}\left[F_i + F_{i+1}\right]$$

$$\Delta^2 F_i = \frac{1}{2}\left[\Delta F_i + \Delta F_{i+1}\right] = \frac{1}{4}\left[F_i + 2F_{i+1} + F_{i+2}\right]$$

$$\Delta^3 F_i = \frac{1}{2}\left[\Delta^2 F_i + \Delta^2 F_{i+1}\right] = \frac{1}{8}\left[F_i + 3F_{i+1} + 3F_{i+2} + F_{i+3}\right]$$

Generally:

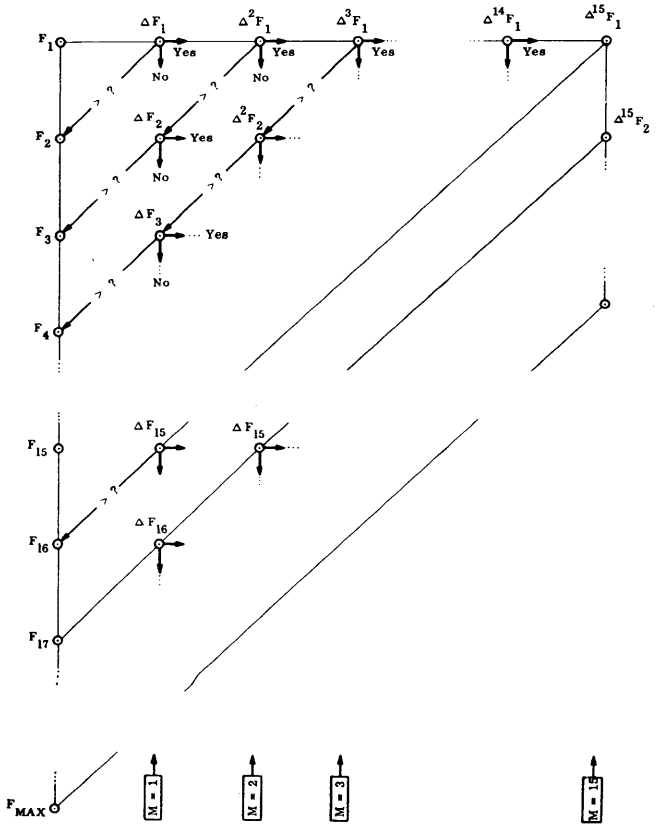
$$\Delta^m F_i = \frac{1}{2}\left[\Delta^{m-1} F_i + \Delta^{m-1} F_{i+1}\right] = \frac{1}{2^m}\left[F_i + \binom{m}{1} F_{i+1} + \binom{m}{2} F_{i+2} + \ldots + \binom{m}{m-1} F_{i+m-1} + \binom{m}{m} F_{i+m}\right]$$

Euler transformation means that the given infinite series will be transformed as follows:

$$\sum_{k=1}^{\infty} F_k = \frac{1}{2}\left[F_1 + \Delta F_1 + \Delta^2 F_1 + \Delta^3 F_1 + \Delta^4 F_1 + \ldots\right]$$

The transformed series will converge whenever the given series does, and to the same sum. It may even converge when the parent series does not; in this case the sum is called the Euler sum of the parent series.

A refined Euler transformation is explained by means of the following diagram.



The computation is done in this way. First the absolute value $|\Delta F_1|$ is compared with $|F_2|$ (see diagram). In case $|\Delta F_1| < |F_2|$, the value $\frac{1}{2}(\Delta F_1)$ is added to the initial value $\frac{1}{2}F_1$ (the beginning of the Euler transformation). Then $|\Delta^2 F_1|$ is compared with $|\Delta F_2|$ (see "YES" in diagram).

In case $|\Delta F_1| \geq |F_2|$, the value ΔF_1 is added to $\frac{1}{2}F_1$ and, as next $|\Delta F_2|$, is compared with $|F_3|$ (see "NO"). This means that F_1 is added unchanged, and the Euler transformation is delayed for one term, and so forth.

If in this sequence of comparisons $|\Delta^i F_k| < |\Delta^{i-1} F_{k+1}|$ is generally true, the value $\frac{1}{2}(\Delta^i F_k)$ is added to the current sum in the sense of the Euler transformation. If it is not true, the value $\Delta^i F_k$ is added and the Euler transformation is delayed for one term--that is, the terms F_1, F_2, ..., F_k are added unchanged, and the transformation actually starts with term F_{k+1}.

The highest term in the scheme of calculation may be $\Delta^{15} F_i$ ($i = 1, 2, 3, \ldots,$ MAX-15), in case MAX > 15. Hence a maximum of fourteen terms of the series may be transformed in succession by Euler. If the procedure is not terminated up to this point, the index of the transformed terms is raised by 1, and a further unchanged term is added.

The last term of the parent series which may be used by the computation is F_{MAX}.

The procedure is terminated if with five successive terms of the series the relative change of the sum value is less than EPS, or if MAX terms of the series were used for calculation.

For reference see:

(1.) F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York/Toronto/London, 1956, pp. 155 - 160.

(2.) P. Naur, "Report on the Algorithmic Language ALGOL 60", CACM, vol. 3, no. 5 (1960), pp. 311.


```
C                                                                       TEUL  10
C  ....................................................................TEUL  20
C                                                                       TEUL  30
C     SUBROUTINE TEUL                                                   TEUL  40
C                                                                       TEUL  50
C     PURPOSE                                                           TEUL  60
C        COMPUTE THE SUM OF FCT(K) FOR K FROM ONE UP TO INFINITY.       TEUL  70
C                                                                       TEUL  80
C     USAGE                                                             TEUL  90
C        CALL TEUL(FCT,SUM,MAX,EPS,IER)                                 TEUL 100
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.                  TEUL 110
C                                                                       TEUL 120
C     DESCRIPTION OF PARAMETERS                                         TEUL 130
C        FCT    - NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.         TEUL 140
C                 IT COMPUTES THE K-TH TERM OF THE SERIES TO ANY       TEUL 150
C                 GIVEN INDEX K.                                       TEUL 160
C        SUM    - RESULTANT VALUE CONTAINING ON RETURN THE SUM OF      TEUL 170
C                 THE GIVEN SERIES.                                    TEUL 180
C        MAX    - INPUT VALUE, WHICH SPECIFIES THE MAXIMAL NUMBER      TEUL 190
C                 OF TERMS OF THE SERIES THAT ARE RESPECTED.           TEUL 200
C        EPS    - INPUT VALUE, WHICH SPECIFIES THE UPPER BOUND OF      TEUL 210
C                 THE RELATIVE ERROR.                                  TEUL 220
C                 SUMMATION IS STOPPED AS SOON AS FIVE TIMES IN        TEUL 230
C                 SUCCESSION THE ABSOLUTE VALUE OF THE TERMS OF THE    TEUL 240
C                 TRANSFORMED SERIES ARE FOUND TO BE LESS THAN         TEUL 250
C                 EPS*(ABSOLUTE VALUE OF CURRENT SUM).                 TEUL 260
C        IER    - RESULTANT ERROR PARAMETER CODED IN THE FOLLOWING     TEUL 270
C                 FORM                                                 TEUL 280
C                  IER=0  - NO ERROR                                   TEUL 290
C                  IER=1  - REQUIRED ACCURACY NOT REACHED WITH         TEUL 300
C                           MAXIMAL NUMBER OF TERMS                    TEUL 310
C                  IER=-1 - THE INTEGER MAX IS LESS THAN ONE.          TEUL 320
C                                                                       TEUL 330
C     REMARKS                                                           TEUL 340
C        NO ACTION BESIDES ERROR MESSAGE IN CASE MAX LESS THAN ONE.     TEUL 350
C                                                                       TEUL 360
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     TEUL 370
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(K) MUST BE FURNISHED      TEUL 380
C        BY THE USER.                                                   TEUL 390
C                                                                       TEUL 400
C     METHOD                                                            TEUL 410
C        EVALUATION IS DONE BY MEANS OF A SUITABLY REFINED EULER        TEUL 420
C        TRANSFORMATION. FOR REFERENCE, SEE                             TEUL 430
C        F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,            TEUL 440
C        MCGRAW/HILL, NEW YORK/TORONTO/LONDON, 1956, PP.155-160, AND    TEUL 450
C        P. NAUR, REPORT ON THE ALGORITHMIC LANGUAGE ALGOL 60,          TEUL 460
C        CACM, VOL.3, ISS.5 (1960), PP.311.                             TEUL 470
C                                                                       TEUL 480
C  ....................................................................TEUL 490
C                                                                       TEUL 500
      SUBROUTINE TEUL (FCT,SUM,MAX,EPS,IER)                             TEUL 510
C                                                                       TEUL 520
      DIMENSION Y(15)                                                   TEUL 530
C                                                                       TEUL 540
C        TEST ON WRONG INPUT PARAMETER MAX                              TEUL 550
C                                                                       TEUL 560
      IF(MAX)1,1,2                                                      TEUL 570
    1 IER=-1                                                            TEUL 580
      GOTO 12                                                           TEUL 590
C                                                                       TEUL 600
C        INITIALIZE EULER TRANSFORMATION                                TEUL 610
C                                                                       TEUL 620
    2 IER=1                                                             TEUL 630
      I=1                                                               TEUL 640
      M=1                                                               TEUL 650
      N=1                                                               TEUL 660
      Y(1)=FCT(N)                                                       TEUL 670
      SUM=Y(1)*.5                                                       TEUL 680
C                                                                       TEUL 690
C        START EULER-LOOP                                               TEUL 700
C                                                                       TEUL 710
    3 J=0                                                               TEUL 720
    4 I=I+1                                                             TEUL 730
      IF(I-MAX)5,5,12                                                   TEUL 740
    5 N=I                                                               TEUL 750
      AMN=FCT(N)                                                        TEUL 760
      DO 6 K=1,M                                                        TEUL 770
      AMP=(AMN+Y(K))*.5                                                 TEUL 780
      Y(K)=AMN                                                          TEUL 790
    6 AMN=AMP                                                           TEUL 800
C                                                                       TEUL 810
C        CHECK EULER TRANSFORMATION                                     TEUL 820
C                                                                       TEUL 830
      IF(ABS(AMN)-ABS(Y(M)))7,9,9                                       TEUL 840
    7 IF(M-15)8,9,9                                                     TEUL 850
    8 M=M+1                                                             TEUL 860
      Y(M)=AMN                                                          TEUL 870
      AMN=.5*AMN                                                        TEUL 880
C                                                                       TEUL 890
C        UPDATE SUM                                                     TEUL 900
C                                                                       TEUL 910
    9 SUM=SUM+AMN                                                       TEUL 920
      IF(ABS(AMN)-EPS*ABS(SUM))10,10,3                                  TEUL 930
C                                                                       TEUL 940
C        TEST END OF PROCEDURE                                          TEUL 950
C                                                                       TEUL 960
   10 J=J+1                                                             TEUL 970
      IF(J-5)4,11,11                                                    TEUL 980
   11 IER=0                                                             TEUL 990
   12 RETURN                                                            TEUL1000
      END                                                               TEUL1010
```

```
C                                                                       DTEU  10
C ...................................................................DTEU  20
C                                                                       DTEU  30
C     SUBROUTINE DTEUL                                                  DTEU  40
C                                                                       DTEU  50
C     PURPOSE                                                           DTEU  60
C        COMPUTE THE SUM OF FCT(K) FOR K FROM ONE UP TO INFINITY.       DTEU  70
C                                                                       DTEU  80
C     USAGE                                                             DTEU  90
C        CALL DTEUL(FCT,SUM,MAX,EPS,IER)                                DTEU 100
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.                  DTEU 110
C                                                                       DTEU 120
C     DESCRIPTION OF PARAMETERS                                         DTEU 130
C        FCT    - NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION         DTEU 140
C                 SUBPROGRAM USED. IT COMPUTES THE K-TH TERM OF THE     DTEU 150
C                 SERIES TO ANY GIVEN INDEX K.                          DTEU 160
C        SUM    - RESULTANT VALUE IN DOUBLE PRECISION CONTAINING ON     DTEU 170
C                 RETURN THE SUM OF THE GIVEN SERIES.                   DTEU 180
C        MAX    - INPUT VALUE, WHICH SPECIFIES THE MAXIMAL NUMBER       DTEU 190
C                 OF TERMS OF THE SERIES THAT ARE RESPECTED.            DTEU 200
C        EPS    - SINGLE PRECISION INPUT VALUE, WHICH SPECIFIES THE     DTEU 210
C                 UPPER BOUND OF THE RELATIVE ERROR.                    DTEU 220
C                 SUMMATION IS STOPPED AS SOON AS FIVE TIMES IN         DTEU 230
C                 SUCCESSION THE ABSOLUTE VALUE OF THE TERMS OF THE     DTEU 240
C                 TRANSFORMED SERIES ARE FOUND TO BE LESS THAN          DTEU 250
C                 EPS*(ABSOLUTE VALUE OF CURRENT SUM).                  DTEU 260
C        IER    - RESULTANT ERROR PARAMETER CODED IN THE FOLLOWING      DTEU 270
C                 FORM                                                  DTEU 280
C                  IER=0  - NO ERROR                                    DTEU 290
C                  IER=1  - REQUIRED ACCURACY NOT REACHED WITH          DTEU 300
C                           MAXIMAL NUMBER OF TERMS                     DTEU 310
C                  IER=-1 - THE INTEGER MAX IS LESS THAN ONE.           DTEU 320
C                                                                       DTEU 330
C     REMARKS                                                           DTEU 340
C        NO ACTION BESIDES ERROR MESSAGE IN CASE MAX LESS THAN ONE.     DTEU 350
C                                                                       DTEU 360
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DTEU 370
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(K) MUST BE FURNISHED      DTEU 380
C        BY THE USER.                                                   DTEU 390
C                                                                       DTEU 400
C     METHOD                                                            DTEU 410
C        EVALUATION IS DONE BY MEANS OF A SUITABLY REFINED EULER        DTEU 420
C        TRANSFORMATION. FOR REFERENCE, SEE                             DTEU 430
C        F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,            DTEU 440
C        MCGRAW/HILL, NEW YORK/TORONTO/LONDON, 1956, PP.155-160, AND    DTEU 450
C        P. NAUR, REPORT ON THE ALGORITHMIC LANGUAGE ALGOL 60,          DTEU 460
C        CACM, VOL.3, ISS.5 (1960), PP.311.                             DTEU 470
C                                                                       DTEU 480
C ...................................................................DTEU 490
C                                                                       DTEU 500
      SUBROUTINE DTEUL (FCT,SUM,MAX,EPS,IER)                            DTEU 510
C                                                                       DTEU 520
      DIMENSION Y(15)                                                   DTEU 530
      DOUBLE PRECISION FCT,SUM,Y,AMN,AMP                                DTEU 540
C                                                                       DTEU 550
C        TEST ON WRONG INPUT PARAMETER MAX                              DTEU 560
C                                                                       DTEU 570
      IF(MAX)1,1,2                                                      DTEU 580
    1 IER=-1                                                            DTEU 590
      GOTO 12                                                           DTEU 600
C                                                                       DTEU 610
C        INITIALIZE EULER TRANSFORMATION                                DTEU 620
C                                                                       DTEU 630
    2 IER=1                                                             DTEU 640
      I=1                                                               DTEU 650
      M=1                                                               DTEU 660
      N=1                                                               DTEU 670
      Y(1)=FCT(N)                                                       DTEU 680
      SUM=Y(1)*.500                                                     DTEU 690
C                                                                       DTEU 700
C        START EULER-LOOP                                               DTEU 710
C                                                                       DTEU 720
    3 J=0                                                               DTEU 730
    4 I=I+1                                                             DTEU 740
      IF(I-MAX)5,5,12                                                   DTEU 750
    5 N=I                                                               DTEU 760
      AMN=FCT(N)                                                        DTEU 770
      DO 6 K=1,M                                                        DTEU 780
      AMP=(AMN+Y(K))*.500                                               DTEU 790
      Y(K)=AMN                                                          DTEU 800
    6 AMN=AMP                                                           DTEU 810
C                                                                       DTEU 820
C        CHECK EULER TRANSFORMATION                                     DTEU 830
C                                                                       DTEU 840
      IF(DABS(AMN)-DABS(Y(M)))7,9,9                                     DTEU 850
    7 IF(M-15)8,9,9                                                     DTEU 860
    8 M=M+1                                                             DTEU 870
      Y(M)=AMN                                                          DTEU 880
      AMN=.500*AMN                                                      DTEU 890
C                                                                       DTEU 900
C        UPDATE SUM                                                     DTEU 910
C                                                                       DTEU 920
    9 SUM=SUM+AMN                                                       DTEU 930
      IF(ABS(SNGL(AMN))-EPS*ABS(SNGL(SUM)))10,10,3                      DTEU 940
C                                                                       DTEU 950
C        TEST END OF PROCEDURE                                          DTEU 960
C                                                                       DTEU 970
   10 J=J+1                                                             DTEU 980
      IF(J-5)4,11,11                                                    DTEU 990
   11 IER=0                                                             DTEU1000
   12 RETURN                                                            DTEU1010
      END                                                               DTEU1020
```

Subroutines ALI and DALI

These subroutines perform an Aitken-Lagrange interpolation. Given the table x_i, y_i ($i = 1, 2, \ldots, n$) of argument and function values stored in the two one-dimensional storage arrays ARG and VAL, the problem is to interpolate function value Y at the given point X. It is assumed that the table represents a single-valued function $y = y(x)$ which is suitable for approximation by a polynomial+, and that $|x_i - X| \geq |x_j - X|$ for $i > j$.++

Then, using the following formulas:

$$y_{1,2} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} y_1 & x_1 - X \\ y_2 & x_2 - X \end{vmatrix};$$

$$y_{1,3} = \frac{1}{x_3 - x_1} \cdot \begin{vmatrix} y_1 & x_1 - X \\ y_3 & x_3 - X \end{vmatrix},$$

$$y_{1,2,3} = \frac{1}{x_3 - x_2} \cdot \begin{vmatrix} y_{1,2} & x_2 - X \\ y_{1,3} & x_3 - X \end{vmatrix};$$

$$y_{1,4} = \frac{1}{x_4 - x_1} \cdot \begin{vmatrix} y_1 & x_1 - X \\ y_4 & x_4 - X \end{vmatrix},$$

$$y_{1,2,4} = \frac{1}{x_4 - x_2} \cdot \begin{vmatrix} y_{1,2} & x_2 - X \\ y_{1,4} & x_4 - X \end{vmatrix},$$

$$y_{1,2,3,4} = \frac{1}{x_4 - x_3} \cdot \begin{vmatrix} y_{1,2,3} & x_3 - X \\ y_{1,2,4} & x_4 - X \end{vmatrix};$$

.....,

it is possible to generate by row the triangular Aitken scheme shown in Figure 18.

x_1	y_1				
x_2	y_2	$y_{1,2}$			
x_3	y_3	$y_{1,3}$	$y_{1,2,3}$		
x_4	y_4	$y_{1,4}$	$y_{1,2,4}$	$y_{1,2,3,4}$	
⋮	⋮	⋮	⋮		
x_n	y_n	$y_{1,n}$	$y_{1,2,n}$	$y_{1,2,3,n}$	... $y_{1,2,3,\ldots,n}$

Figure 18. Aitken's scheme for Lagrange interpolation

All result values of row j can be stored in VAL(J). Thus, it is possible to generate the downward diagonal of Aitken's scheme in storage array VAL, using the machine-processable formula:

$$\text{VAL(J)} = \frac{\text{VAL(I)}*(\text{X-ARG(J)}) - \text{VAL(J)}*(\text{X-ARG(I)})}{\text{ARG(I)} - \text{ARG(J)}}$$

$$(\text{I} = 1, 2, \ldots, \text{J-1}) \qquad (1)$$

for J = 2, 3, ..., NDIM.

The procedure stops under the following conditions: if the difference of two successive values in the downward diagonal is absolutely less than a given tolerance ϵ (test starts at step J = 3), or if the absolute value of this difference stops diminishing, thus showing the influence of rounding errors (test starts at step J = 5, or for double-precision, J = 8), or if the procedure has worked through the whole triangular Aitken scheme, or if it discovers two table points with identical arguments.

Finally, Y is set equal to VAL(J) in case of monotonically decreasing absolute differences, or equal to VAL(J-1) if these differences start oscillating.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York/Toronto/London, 1956, pp. 49-50.

+This order in table x_i, y_i, ($i = 1, 2, \ldots, n$) could be generated by subroutines ATSG, ATSM, ATSE, DATSG, DATSM, DATSE.

++This means y(x) should be closely approximated by a polynomial of low degree which has the table points with arguments next to x as nodes.

```
C                                                                       ALI   10
C     ..................................................................ALI   20
C                                                                       ALI   30
C        SUBROUTINE ALI                                                 ALI   40
C                                                                       ALI   50
C        PURPOSE                                                        ALI   60
C           TO INTERPOLATE FUNCTION VALUE Y FOR A GIVEN ARGUMENT VALUE  ALI   70
C           X USING A GIVEN TABLE (ARG,VAL) OF ARGUMENT AND FUNCTION    ALI   80
C           VALUES.                                                     ALI   90
C                                                                       ALI  100
C        USAGE                                                          ALI  110
C           CALL ALI (X,ARG,VAL,Y,NDIM,EPS,IER)                         ALI  120
C                                                                       ALI  130
C        DESCRIPTION OF PARAMETERS                                      ALI  140
C           X      - THE ARGUMENT VALUE SPECIFIED BY INPUT.             ALI  150
C           ARG    - THE INPUT VECTOR (DIMENSION NDIM) OF ARGUMENT      ALI  160
C                    VALUES OF THE TABLE (NOT DESTROYED).               ALI  170
C           VAL    - THE INPUT VECTOR (DIMENSION NDIM) OF FUNCTION      ALI  180
C                    VALUES OF THE TABLE (DESTROYED).                   ALI  190
C           Y      - THE RESULTING INTERPOLATED FUNCTION VALUE.         ALI  200
C           NDIM   - AN INPUT VALUE WHICH SPECIFIES THE NUMBER OF       ALI  210
C                    POINTS IN TABLE (ARG,VAL).                         ALI  220
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS UPPER BOUND     ALI  230
C                    FOR THE ABSOLUTE ERROR.                            ALI  240
C           IER    - A RESULTING ERROR PARAMETER.                       ALI  250
C                                                                       ALI  260
C        REMARKS                                                        ALI  270
C           (1) TABLE (ARG,VAL) SHOULD REPRESENT A SINGLE-VALUED        ALI  280
C               FUNCTION AND SHOULD BE STORED IN SUCH A WAY, THAT THE   ALI  290
C               DISTANCES ABS(ARG(I)-X) INCREASE WITH INCREASING        ALI  300
C               SUBSCRIPT I. TO GENERATE THIS ORDER IN TABLE (ARG,VAL), ALI  310
C               SUBROUTINES ATSG, ATSM OR ATSE COULD BE USED IN A       ALI  320
C               PREVIOUS STAGE.                                         ALI  330
C           (2) NO ACTION BESIDES ERROR MESSAGE IN CASE NDIM LESS       ALI  340
C               THAN 1.                                                 ALI  350
C           (3) INTERPOLATION IS TERMINATED EITHER IF THE DIFFERENCE    ALI  360
C               BETWEEN TWO SUCCESSIVE INTERPOLATED VALUES IS           ALI  370
C               ABSOLUTELY LESS THAN TOLERANCE EPS, OR IF THE ABSOLUTE  ALI  380
C               VALUE OF THIS DIFFERENCE STOPS DIMINISHING, OR AFTER    ALI  390
C               (NDIM-1) STEPS. FURTHER IT IS TERMINATED IF THE         ALI  400
C               PROCEDURE DISCOVERS TWO ARGUMENT VALUES IN VECTOR ARG   ALI  410
C               WHICH ARE IDENTICAL. DEPENDENT ON THESE FOUR CASES,     ALI  420
C               ERROR PARAMETER IER IS CODED IN THE FOLLOWING FORM      ALI  430
C                IER=0 - IT WAS POSSIBLE TO REACH THE REQUIRED          ALI  440
C                        ACCURACY (NO ERROR).                           ALI  450
C                IER=1 - IT WAS IMPOSSIBLE TO REACH THE REQUIRED        ALI  460
C                        ACCURACY BECAUSE OF ROUNDING ERRORS.           ALI  470
C                IER=2 - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE    ALI  480
C                        NDIM IS LESS THAN 3, OR THE REQUIRED ACCURACY  ALI  490
C                        COULD NOT BE REACHED BY MEANS OF THE GIVEN     ALI  500
C                        TABLE. NDIM SHOULD BE INCREASED.               ALI  510
C                IER=3 - THE PROCEDURE DISCOVERED TWO ARGUMENT VALUES   ALI  520
C                        IN VECTOR ARG WHICH ARE IDENTICAL.             ALI  530
C                                                                       ALI  540
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ALI  550
C           NONE                                                        ALI  560
C                                                                       ALI  570
C        METHOD                                                         ALI  580
C           INTERPOLATION IS DONE BY MEANS OF AITKENS SCHEME OF         ALI  590
C           LAGRANGE INTERPOLATION. ON RETURN Y CONTAINS AN INTERPOLATEDALI  600
C           FUNCTION VALUE AT POINT X, WHICH IS IN THE SENSE OF REMARK  ALI  610
C           (3) OPTIMAL WITH RESPECT TO GIVEN TABLE. FOR REFERENCE, SEE ALI  620
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         ALI  630
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.49-50.       ALI  640
C                                                                       ALI  650
C     ..................................................................ALI  660
C                                                                       ALI  670
      SUBROUTINE ALI(X,ARG,VAL,Y,NDIM,EPS,IER)                          ALI  680
C                                                                       ALI  690
C                                                                       ALI  700
      DIMENSION ARG(1),VAL(1)                                           ALI  710
      IER=2                                                             ALI  720
      DELT2=0.                                                          ALI  730
      IF(NDIM-1)9,7,1                                                   ALI  740
C                                                                       ALI  750
C     START OF AITKEN-LOOP                                              ALI  760
    1 DO 6 J=2,NDIM                                                     ALI  770
      DELT1=DELT2                                                       ALI  780
      IEND=J-1                                                          ALI  790
      DO 2 I=1,IEND                                                     ALI  800
      H=ARG(I)-ARG(J)                                                   ALI  810
      IF(H)2,13,2                                                       ALI  820
    2 VAL(J)=(VAL(I)*(X-ARG(J))-VAL(J)*(X-ARG(I)))/H                    ALI  830
      DELT2=ABS(VAL(J)-VAL(IEND))                                       ALI  840
      IF(J-2)6,6,3                                                      ALI  850
    3 IF(DELT2-EPS)10,10,4                                              ALI  860
    4 IF(J-5)6,5,5                                                      ALI  870
    5 IF(DELT2-DELT1)6,11,11                                            ALI  880
    6 CONTINUE                                                          ALI  890
C     END OF AITKEN-LOOP                                                ALI  900
C                                                                       ALI  910
    7 J=NDIM                                                            ALI  920
    8 Y=VAL(J)                                                          ALI  930
    9 RETURN                                                            ALI  940
C                                                                       ALI  950
C     THERE IS SUFFICIENT ACCURACY WITHIN NDIM-1 ITERATION STEPS        ALI  960
   10 IER=0                                                             ALI  970
      GOTO 8                                                            ALI  980
C                                                                       ALI  990
C     TEST VALUE DELT2 STARTS OSCILLATING                               ALI 1000
   11 IER=1                                                             ALI 1010
   12 J=IEND                                                            ALI 1020
      GOTO 8                                                            ALI 1030
C                                                                       ALI 1040
C     THERE ARE TWO IDENTICAL ARGUMENT VALUES IN VECTOR ARG             ALI 1050
   13 IER=3                                                             ALI 1060
      GOTO 12                                                           ALI 1070
      END                                                               ALI 1080
```

```
C                                                                       DALI  10
C     ..................................................................DALI  20
C                                                                       DALI  30
C        SUBROUTINE DALI                                                DALI  40
C                                                                       DALI  50
C        PURPOSE                                                        DALI  60
C           TO INTERPOLATE FUNCTION VALUE Y FOR A GIVEN ARGUMENT VALUE  DALI  70
C           X USING A GIVEN TABLE (ARG,VAL) OF ARGUMENT AND FUNCTION    DALI  80
C           VALUES.                                                     DALI  90
C                                                                       DALI 100
C        USAGE                                                          DALI 110
C           CALL DALI (X,ARG,VAL,Y,NDIM,EPS,IER)                        DALI 120
C                                                                       DALI 130
C        DESCRIPTION OF PARAMETERS                                      DALI 140
C           X      - DOUBLE PRECISION ARGUMENT VALUE SPECIFIED BY INPUT.DALI 150
C           ARG    - DOUBLE PRECISION INPUT VECTOR (DIMENSION NDIM) OF  DALI 160
C                    ARGUMENT VALUES OF THE TABLE (NOT DESTROYED).      DALI 170
C           VAL    - DOUBLE PRECISION INPUT VECTOR (DIMENSION NDIM) OF  DALI 180
C                    FUNCTION VALUES OF THE TABLE (DESTROYED).          DALI 190
C           Y      - RESULTING INTERPOLATED DOUBLE PRECISION FUNCTION   DALI 200
C                    VALUE.                                             DALI 210
C           NDIM   - AN INPUT VALUE WHICH SPECIFIES THE NUMBER OF       DALI 220
C                    POINTS IN TABLE (ARG,VAL).                         DALI 230
C           EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS   DALI 240
C                    UPPER BOUND FOR THE ABSOLUTE ERROR.                DALI 250
C                    FOR THE ABSOLUTE ERROR.                            DALI 260
C           IER    - A RESULTING ERROR PARAMETER.                       DALI 270
C                                                                       DALI 280
C        REMARKS                                                        DALI 290
C           (1) TABLE (ARG,VAL) SHOULD REPRESENT A SINGLE-VALUED        DALI 300
C               FUNCTION AND SHOULD BE STORED IN SUCH A WAY, THAT THE   DALI 310
C               DISTANCES ABS(ARG(I)-X) INCREASE WITH INCREASING        DALI 320
C               SUBSCRIPT I. TO GENERATE THIS ORDER IN TABLE (ARG,VAL), DALI 330
C               SUBROUTINES DATSG, DATSM OR DATSE COULD BE USED IN A    DALI 340
C               PREVIOUS STAGE.                                         DALI 350
C           (2) NO ACTION BESIDES ERROR MESSAGE IN CASE NDIM LESS       DALI 360
C               THAN 1.                                                 DALI 370
C           (3) INTERPOLATION IS TERMINATED EITHER IF THE DIFFERENCE    DALI 380
C               BETWEEN TWO SUCCESSIVE INTERPOLATED VALUES IS           DALI 390
C               ABSOLUTELY LESS THAN TOLERANCE EPS, OR IF THE ABSOLUTE  DALI 400
C               VALUE OF THIS DIFFERENCE STOPS DIMINISHING, OR AFTER    DALI 410
C               (NDIM-1) STEPS. FURTHER IT IS TERMINATED IF THE         DALI 420
C               PROCEDURE DISCOVERS TWO ARGUMENT VALUES IN VECTOR ARG   DALI 430
C               WHICH ARE IDENTICAL. DEPENDENT ON THESE FOUR CASES,     DALI 440
C               ERROR PARAMETER IER IS CODED IN THE FOLLOWING FORM      DALI 450
C                IER=0 - IT WAS POSSIBLE TO REACH THE REQUIRED          DALI 460
C                        ACCURACY (NO ERROR).                           DALI 470
C                IER=1 - IT WAS IMPOSSIBLE TO REACH THE REQUIRED        DALI 480
C                        ACCURACY BECAUSE OF ROUNDING ERRORS.           DALI 490
C                IER=2 - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE    DALI 500
C                        NDIM IS LESS THAN 3, OR THE REQUIRED ACCURACY  DALI 510
C                        COULD NOT BE REACHED BY MEANS OF THE GIVEN     DALI 520
C                        TABLE. NDIM SHOULD BE INCREASED.               DALI 530
C                IER=3 - THE PROCEDURE DISCOVERED TWO ARGUMENT VALUES   DALI 540
C                        IN VECTOR ARG WHICH ARE IDENTICAL.             DALI 550
C                                                                       DALI 560
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DALI 570
C           NONE                                                        DALI 580
C                                                                       DALI 590
C        METHOD                                                         DALI 600
C           INTERPOLATION IS DONE BY MEANS OF AITKENS SCHEME OF         DALI 610
C           LAGRANGE INTERPOLATION. ON RETURN Y CONTAINS AN INTERPOLATEDDALI 620
C           FUNCTION VALUE AT POINT X, WHICH IS IN THE SENSE OF REMARK  DALI 630
C           (3) OPTIMAL WITH RESPECT TO GIVEN TABLE. FOR REFERENCE, SEE DALI 640
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         DALI 650
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.49-50.       DALI 660
C                                                                       DALI 670
C     ..................................................................DALI 680
C                                                                       DALI 690
      SUBROUTINE DALI(X,ARG,VAL,Y,NDIM,EPS,IER)                         DALI 700
C                                                                       DALI 710
C                                                                       DALI 720
      DIMENSION ARG(1),VAL(1)                                           DALI 730
      DOUBLE PRECISION ARG,VAL,X,Y,H                                    DALI 740
      IER=2                                                             DALI 750
      DELT2=0.                                                          DALI 760
      IF(NDIM-1)9,7,1                                                   DALI 770
C                                                                       DALI 780
C     START OF AITKEN-LOOP                                              DALI 790
    1 DO 6 J=2,NDIM                                                     DALI 800
      DELT1=DELT2                                                       DALI 810
      IEND=J-1                                                          DALI 820
      DO 2 I=1,IEND                                                     DALI 830
      H=ARG(I)-ARG(J)                                                   DALI 840
      IF(H)2,13,2                                                       DALI 850
    2 VAL(J)=(VAL(I)*(X-ARG(J))-VAL(J)*(X-ARG(I)))/H                    DALI 860
      DELT2=DABS(VAL(J)-VAL(IEND))                                      DALI 870
      IF(J-2)6,6,3                                                      DALI 880
    3 IF(DELT2-EPS)10,10,4                                              DALI 890
    4 IF(J-8)6,5,5                                                      DALI 900
    5 IF(DELT2-DELT1)6,11,11                                            DALI 910
    6 CONTINUE                                                          DALI 920
C     END OF AITKEN-LOOP                                                DALI 930
C                                                                       DALI 940
    7 J=NDIM                                                            DALI 950
    8 Y=VAL(J)                                                          DALI 960
    9 RETURN                                                            DALI 970
C                                                                       DALI 980
C     THERE IS SUFFICIENT ACCURACY WITHIN NDIM-1 ITERATION STEPS        DALI 990
   10 IER=0                                                             DALI1000
      GOTO 8                                                            DALI1010
C                                                                       DALI1020
C     TEST VALUE DELT2 STARTS OSCILLATING                               DALI1030
   11 IER=1                                                             DALI1040
   12 J=IEND                                                            DALI1050
      GOTO 8                                                            DALI1060
C                                                                       DALI1070
C     THERE ARE TWO IDENTICAL ARGUMENT VALUES IN VECTOR ARG             DALI1080
   13 IER=3                                                             DALI1090
      GOTO 12                                                           DALI1100
      END                                                               DALI1110
```

Subroutines AHI and DAHI

These subroutines perform an Aitken-Hermite interpolation. Given the table x_i, y_i, y'_i (i = 1, 2, ..., n) of argument, function and derivative values, stored in the two one-dimensional storage arrays ARG and VAL, the problem is to interpolate function value Y at the given point X. It is assumed that the table represents a single-valued function y = y(x) which is suitable for approximation by a polynomial[+], and that it is stored as shown in Figure 19 (first and second column) with $|x_i - X| \geq |x_j - X|$ for i > j.[++]

Before starting Aitken's iteration scheme, the components of vector VAL (that is, function and derivative values) are replaced by interpolation values z_i of first order (third column). This is done by the following machine-processable formulas:

$$VAL(I) = Y + VAL(I+1) * H_1$$

$$(I = 1,3,5,\ldots,2 * NDIM-1) \qquad (1)$$

$$VAL(I+1) = Y + (VAL(I+2)-Y)\,\frac{H_1}{H_1 - H_2}$$

$$(I = 1,3,5,\ldots,2 * NDIM-3) \qquad (2)$$

with

$$Y = VAL(I),\quad H_1 = X - ARG(J-1),\quad H_2 = X - ARG(J)$$

and

$$J = \frac{I+1}{2} + 1 .$$

Now it is possible to generate successively the upward diagonals of the triangular Aitken scheme, using the following formulas:

$$z_{1,2} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} z_1 & x_1 - X \\ z_2 & x_2 - X \end{vmatrix} ;$$

$$z_{2,3} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} z_2 & x_1 - X \\ z_3 & x_2 - X \end{vmatrix} ,$$

$$z_{1,2,3} = \frac{1}{x_2 - x_1} \cdot \begin{vmatrix} z_{1,2} & x_1 - X \\ z_{2,3} & x_2 - X \end{vmatrix} ;$$

$$z_{3,4} = \frac{1}{x_3 - x_2} \cdot \begin{vmatrix} z_3 & x_2 - X \\ z_4 & x_3 - X \end{vmatrix} ,$$

$$z_{2,3,4} = \frac{1}{x_3 - x_1} \cdot \begin{vmatrix} z_{2,3} & x_1 - X \\ z_{3,4} & x_3 - X \end{vmatrix} ;$$

$$z_{1,2,3,4} = \frac{1}{x_3 - x_1} \cdot \begin{vmatrix} z_{1,2,3} & x_1 - X \\ z_{2,3,4} & x_3 - X \end{vmatrix} ;$$

.....

All result values of an upward diagonal can be stored in positions of vector VAL with decreasing subscripts, using the machine-processable formula:

$$VAL(K) = \frac{VAL(K)*(X-H_1) - VAL(K+1)*(X-ARG(L))}{ARG(L) - H_1}$$

$$(J = 1,2,\ldots,I) \qquad (3)$$

with

$$K = I + 1 - J,\quad M = \left[\frac{I+3}{2}\right],\quad L = \left[\frac{K+1}{2}\right]$$

and

$$H_1 = ARG(M)$$

for I = 1,2,...,2 * NDIM-2.

The procedure stops under the following circumstances: if the difference between two successive interpolated values VAL(1) is absolutely less than a given tolerance ε or if the absolute value of this difference stops diminishing, thus showing the influence of rounding errors (test starts at step i = 5, or for double-precision, i = 8), or if the procedure has worked through the whole triangular Aitken scheme, or if it discovers two table points with identical arguments.

[+]This order in table x_i, y_i, y_i (i = 1, 2, ..., n) could be generated by subroutines ATSG, ATSM, ATSE, DATSG, DATSM, DATSE.

[++]This means y(x) should be closely approximated by a polynomial of low degree which has the table points with arguments next to x as nodes and which has the specified derivative values in these nodes.

ARG(1) = x_1	VAL(1) = y_1	VAL(1) = z_1	$z_{1,2}$	$z_{1,2,3}$	$z_{1,2,3,4}$
	VAL(2) = y'_1	VAL(2) = z_2	$z_{2,3}$	$z_{2,3,4}$	
ARG(2) = x_2	VAL(3) = y_2	VAL(3) = z_3	$z_{3,4}$		
	VAL(4) = y'_2	VAL(4) = z_4			
...	...	...	...	...	...
ARG(NDIM) = x_n	VAL(2*NDIM-1) = y_n	VAL(2*NDIM-1) = z_{2n-1}			
	VAL(2*NDIM) = y'_n				

Figure 19. Aitken's scheme for Hermite interpolation

Finally, Y is set equal to VAL(1) in case of monotonically decreasing absolute differences, or to VAL(1) of the step before if these differences start oscillating.

For reference see:

(1) F. B. Hildebrand, Introduction to Numerical Analysis, McGraw Hill, New York/Toronto, London, 1956, pp. 49-50, 352-356.

(2) Gershinsky/Levine, "Aitken-Hermite Interpolation", JACM, vol. 11, iss. 3 (1964), pp. 352-356.

```
C                                                                       AHI   10
C     ..................................................................AHI   20
C                                                                       AHI   30
C        SUBROUTINE AHI                                                 AHI   40
C                                                                       AHI   50
C        PURPOSE                                                        AHI   60
C           TO INTERPOLATE FUNCTION VALUE Y FOR A GIVEN ARGUMENT VALUE  AHI   70
C           X USING A GIVEN TABLE (ARG,VAL) OF ARGUMENT, FUNCTION, AND  AHI   80
C           DERIVATIVE VALUES.                                          AHI   90
C                                                                       AHI  100
C        USAGE                                                          AHI  110
C           CALL AHI (X,ARG,VAL,Y,NDIM,EPS,IER)                         AHI  120
C                                                                       AHI  130
C        DESCRIPTION OF PARAMETERS                                      AHI  140
C           X      - THE ARGUMENT VALUE SPECIFIED BY INPUT.             AHI  150
C           ARG    - THE INPUT VECTOR (DIMENSION NDIM) OF ARGUMENT      AHI  160
C                    VALUES OF THE TABLE (NOT DESTROYED).               AHI  170
C           VAL    - THE INPUT VECTOR (DIMENSION 2*NDIM) OF FUNCTION    AHI  180
C                    AND DERIVATIVE VALUES OF THE TABLE (DESTROYED).    AHI  190
C                    FUNCTION AND DERIVATIVE VALUES MUST BE STORED IN   AHI  200
C                    PAIRS, THAT MEANS BEGINNING WITH FUNCTION VALUE AT AHI  210
C                    POINT ARG(1) EVERY FUNCTION VALUE MUST BE FOLLOWED AHI  220
C                    BY THE VALUE OF DERIVATIVE AT THE SAME POINT.      AHI  230
C           Y      - THE RESULTING INTERPOLATED FUNCTION VALUE.         AHI  240
C           NDIM   - AN INPUT VALUE WHICH SPECIFIES THE NUMBER OF       AHI  250
C                    POINTS IN TABLE (ARG,VAL).                         AHI  260
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS UPPER BOUND     AHI  270
C                    FOR THE ABSOLUTE ERROR.                            AHI  280
C           IER    - A RESULTING ERROR PARAMETER.                       AHI  290
C                                                                       AHI  300
C        REMARKS                                                        AHI  310
C           (1) TABLE (ARG,VAL) SHOULD REPRESENT A SINGLE-VALUED        AHI  320
C               FUNCTION AND SHOULD BE STORED IN SUCH A WAY, THAT THE   AHI  330
C               DISTANCES ABS(ARG(I)-X) INCREASE WITH INCREASING        AHI  340
C               SUBSCRIPT I. TO GENERATE THIS ORDER IN TABLE (ARG,VAL), AHI  350
C               SUBROUTINES ATSG, ATSM OR ATSE COULD BE USED IN A       AHI  360
C               PREVIOUS STAGE.                                         AHI  370
C           (2) NO ACTION BESIDES ERROR MESSAGE IN CASE NDIM LESS       AHI  380
C               THAN 1.                                                 AHI  390
C           (3) INTERPOLATION IS TERMINATED EITHER IF THE DIFFERENCE     AHI  400
C               BETWEEN TWO SUCCESSIVE INTERPOLATED VALUES IS           AHI  410
C               ABSOLUTELY LESS THAN TOLERANCE EPS, OR IF THE ABSOLUTE  AHI  420
C               VALUE OF THIS DIFFERENCE STOPS DIMINISHING, OR AFTER    AHI  430
C               (2*NDIM-2) STEPS. FURTHER IT IS TERMINATED IF THE       AHI  440
C               PROCEDURE DISCOVERS TWO ARGUMENT VALUES IN VECTOR ARG   AHI  450
C               WHICH ARE IDENTICAL. DEPENDENT ON THESE FOUR CASES,     AHI  460
C               ERROR PARAMETER IER IS CODED IN THE FOLLOWING FORM      AHI  470
C                IER=0 - IT WAS POSSIBLE TO REACH THE REQUIRED          AHI  480
C                        ACCURACY (NO ERROR).                           AHI  490
C                IER=1 - IT WAS IMPOSSIBLE TO REACH THE REQUIRED        AHI  500
C                        ACCURACY BECAUSE OF ROUNDING ERRORS.           AHI  510
C                IER=2 - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE    AHI  520
C                        NDIM IS LESS THAN 2, OR THE REQUIRED ACCURACY  AHI  530
C                        COULD NOT BE REACHED BY MEANS OF THE GIVEN     AHI  540
C                        TABLE. NDIM SHOULD BE INCREASED.               AHI  550
C                IER=3 - THE PROCEDURE DISCOVERED TWO ARGUMENT VALUES   AHI  560
C                        IN VECTOR ARG WHICH ARE IDENTICAL.             AHI  570
C                                                                       AHI  580
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  AHI  590
C           NONE                                                        AHI  600
C                                                                       AHI  610
C        METHOD                                                         AHI  620
C           INTERPOLATION IS DONE BY MEANS OF AITKENS SCHEME OF         AHI  630
C           HERMITE INTERPOLATION. ON RETURN Y CONTAINS AN INTERPOLATED AHI  640
C           FUNCTION VALUE AT POINT X, WHICH IS IN THE SENSE OF REMARK  AHI  650
C           (3) OPTIMAL WITH RESPECT TO GIVEN TABLE. FOR REFERENCE, SEE AHI  660
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         AHI  670
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.314-317, AND AHI  680
C           GERSHINSKY/LEVINE, AITKEN-HERMITE INTERPOLATION,            AHI  690
C           JACM, VOL.11, ISS.3 (1964), PP.352-356.                     AHI  700
C                                                                       AHI  710
C     ..................................................................AHI  720
C                                                                       AHI  730
      SUBROUTINE AHI(X,ARG,VAL,Y,NDIM,EPS,IER)                          AHI  740
C                                                                       AHI  750
C                                                                       AHI  760
      DIMENSION ARG(1),VAL(1)                                           AHI  770
      IER=2                                                             AHI  780
      H2=X-ARG(1)                                                       AHI  790
      IF(NDIM-1)2,1,3                                                   AHI  800
    1 Y=VAL(1)+VAL(2)*H2                                                AHI  810
    2 RETURN                                                            AHI  820
C                                                                       AHI  830
C     VECTOR ARG HAS MORE THAN 1 ELEMENT.                               AHI  840
C     THE FIRST STEP PREPARES VECTOR VAL SUCH THAT AITKEN SCHEME CAN BE AHI  850
C     USED.                                                             AHI  860
    3 I=1                                                               AHI  870
      DO 5 J=2,NDIM                                                     AHI  880
      H1=H2                                                             AHI  890
      H2=X-ARG(J)                                                       AHI  900
      Y=VAL(I)                                                          AHI  910
      VAL(I)=Y+VAL(I+1)*H1                                              AHI  920
      H=H1-H2                                                           AHI  930
      IF(H)4,13,4                                                       AHI  940
    4 VAL(I+1)=Y+(VAL(I+2)-Y)*H1/H                                      AHI  950
    5 I=I+2                                                             AHI  960
      VAL(I)=VAL(I)+VAL(I+1)*H2                                         AHI  970
C     END OF FIRST STEP                                                 AHI  980
C                                                                       AHI  990
C     PREPARE AITKEN SCHEME                                             AHI 1000
      DELT2=0.                                                          AHI 1010
      IEND=I-1                                                          AHI 1020
C                                                                       AHI 1030
C     START AITKEN-LOOP                                                 AHI 1040
      DO 9 I=1,IEND                                                     AHI 1050
      DELT1=DELT2                                                       AHI 1060
      Y=VAL(I)                                                          AHI 1070
      M=(I+3)/2                                                         AHI 1080
      H1=ARG(M)                                                         AHI 1090
      DO 6 J=1,I                                                        AHI 1100
      K=I+1-J                                                           AHI 1110
      L=(K+1)/2                                                         AHI 1120
      H=ARG(L)-H1                                                       AHI 1130
      IF(H)6,14,6                                                       AHI 1140
    6 VAL(K)=(VAL(K)*(X-H1)-VAL(K+1)*(X-ARG(L)))/H                      AHI 1150
      DELT2=ABS(Y-VAL(1))                                               AHI 1160
      IF(DELT2-EPS)11,11,7                                              AHI 1170
    7 IF(I-5)9,8,8                                                      AHI 1180
    8 IF(DELT2-DELT1)9,12,12                                            AHI 1190
    9 CONTINUE                                                          AHI 1200
C     END OF AITKEN-LOOP                                                AHI 1210
C                                                                       AHI 1220
   10 Y=VAL(1)                                                          AHI 1230
      RETURN                                                            AHI 1240
C                                                                       AHI 1250
C     THERE IS SUFFICIENT ACCURACY WITHIN 2*NDIM-2 ITERATION STEPS      AHI 1260
   11 IER=0                                                             AHI 1270
      GOTO 10                                                           AHI 1280
C                                                                       AHI 1290
C     TEST VALUE DELT2 STARTS OSCILLATING                               AHI 1300
   12 IER=1                                                             AHI 1310
      RETURN                                                            AHI 1320
C                                                                       AHI 1330
C     THERE ARE TWO IDENTICAL ARGUMENT VALUES IN VECTOR ARG             AHI 1340
   13 Y=VAL(1)                                                          AHI 1350
   14 IER=3                                                             AHI 1360
      RETURN                                                            AHI 1370
      END                                                               AHI 1380
```

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C                                                                       DAHI  10
C     ..................................................................DAHI  20
C                                                                       DAHI  30
C        SUBROUTINE DAHI                                                DAHI  40
C                                                                       DAHI  50
C        PURPOSE                                                        DAHI  60
C           TO INTERPOLATE FUNCTION VALUE Y FOR A GIVEN ARGUMENT VALUE  DAHI  70
C           X USING A GIVEN TABLE (ARG,VAL) OF ARGUMENT, FUNCTION, AND  DAHI  80
C           DERIVATIVE VALUES.                                          DAHI  90
C                                                                       DAHI 100
C        USAGE                                                          DAHI 110
C           CALL DAHI (X,ARG,VAL,Y,NDIM,EPS,IER)                        DAHI 120
C                                                                       DAHI 130
C        DESCRIPTION OF PARAMETERS                                      DAHI 140
C           X      - DOUBLE PRECISION ARGUMENT VALUE SPECIFIED BY INPUT.DAHI 150
C           ARG    - DOUBLE PRECISION INPUT VECTOR (DIMENSION NDIM) OF  DAHI 160
C                    ARGUMENT VALUES OF THE TABLE (NOT DESTROYED).      DAHI 170
C           VAL    - DOUBLE PRECISION INPUT VECTOR (DIMENSION 2*NDIM) OFDAHI 180
C                    FUNCTION AND DERIVATIVE VALUES OF THE TABLE (DES-  DAHI 190
C                    TROYED). FUNCTION AND DERIVATIVE VALUES MUST BE    DAHI 200
C                    STORED IN PAIRS, THAT MEANS BEGINNING WITH FUNCTIONDAHI 210
C                    VALUE AT POINT ARG(1) EVERY FUNCTION VALUE MUST BE DAHI 220
C                    FOLLOWED BY THE DERIVATIVE VALUE AT THE SAME POINT.DAHI 230
C           Y      - RESULTING INTERPOLATED DOUBLE PRECISION FUNCTION   DAHI 240
C                    VALUE.                                             DAHI 250
C           NDIM   - AN INPUT VALUE WHICH SPECIFIES THE NUMBER OF       DAHI 260
C                    POINTS IN TABLE (ARG,VAL).                         DAHI 270
C           EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS   DAHI 280
C                    UPPER BOUND FOR THE ABSOLUTE ERROR.                DAHI 290
C           IER    - A RESULTING ERROR PARAMETER.                       DAHI 300
C                                                                       DAHI 310
C        REMARKS                                                        DAHI 320
C           (1) TABLE (ARG,VAL) SHOULD REPRESENT A SINGLE-VALUED        DAHI 330
C               FUNCTION AND SHOULD BE STORED IN SUCH A WAY, THAT THE   DAHI 340
C               DISTANCES ABS(ARG(I)-X) INCREASE WITH INCREASING        DAHI 350
C               SUBSCRIPT I. TO GENERATE THIS ORDER IN TABLE (ARG,VAL), DAHI 360
C               SUBROUTINES DATSG, DATSM OR DATSE COULD BE USED IN A    DAHI 370
C               PREVIOUS STAGE.                                         DAHI 380
C           (2) NO ACTION BESIDES ERROR MESSAGE IN CASE NDIM LESS       DAHI 390
C               THAN 1.                                                 DAHI 400
C           (3) INTERPOLATION IS TERMINATED EITHER IF THE DIFFERENCE     DAHI 410
C               BETWEEN TWO SUCCESSIVE INTERPOLATED VALUES IS           DAHI 420
C               ABSOLUTELY LESS THAN TOLERANCE EPS, OR IF THE ABSOLUTE  DAHI 430
C               VALUE OF THIS DIFFERENCE STOPS DIMINISHING, OR AFTER    DAHI 440
C               (2*NDIM-2) STEPS. FURTHER IT IS TERMINATED IF THE       DAHI 450
C               PROCEDURE DISCOVERS TWO ARGUMENT VALUES IN VECTOR ARG   DAHI 460
C               WHICH ARE IDENTICAL. DEPENDENT ON THESE FOUR CASES,     DAHI 470
C               ERROR PARAMETER IER IS CODED IN THE FOLLOWING FORM      DAHI 480
C                IER=0 - IT WAS POSSIBLE TO REACH THE REQUIRED          DAHI 490
C                        ACCURACY (NO ERROR).                           DAHI 500
C                IER=1 - IT WAS IMPOSSIBLE TO REACH THE REQUIRED        DAHI 510
C                        ACCURACY BECAUSE OF ROUNDING ERRORS.           DAHI 520
C                IER=2 - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE    DAHI 530
C                        NDIM IS LESS THAN 2, OR THE REQUIRED ACCURACY  DAHI 540
C                        COULD NOT BE REACHED BY MEANS OF THE GIVEN     DAHI 550
C                        TABLE. NDIM SHOULD BE INCREASED.               DAHI 560
C                IER=3 - THE PROCEDURE DISCOVERED TWO ARGUMENT VALUES   DAHI 570
C                        IN VECTOR ARG WHICH ARE IDENTICAL.             DAHI 580
C                                                                       DAHI 590
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DAHI 600
C           NONE                                                        DAHI 610
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C                                                                       DAHI 620
C       METHOD                                                          DAHI 630
C          INTERPOLATION IS DONE BY MEANS OF AITKENS SCHEME OF          DAHI 640
C          HERMITE INTERPOLATION. ON RETURN Y CONTAINS AN INTERPOLATED  DAHI 650
C          FUNCTION VALUE AT POINT X, WHICH IS IN THE SENSE OF REMARK   DAHI 660
C          (3) OPTIMAL WITH RESPECT TO GIVEN TABLE. FOR REFERENCE, SEE  DAHI 670
C          F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,          DAHI 680
C          MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.314-317, AND  DAHI 690
C          GERSHINSKY/LEVINE, AITKEN-HERMITE INTERPOLATION,             DAHI 700
C          JACM, VOL.11, ISS.3 (1964), PP.352-356.                      DAHI 710
C                                                                       DAHI 720
C     ..................................................................DAHI 730
C                                                                       DAHI 740
      SUBROUTINE DAHI(X,ARG,VAL,Y,NDIM,EPS,IER)                         DAHI 750
C                                                                       DAHI 760
C                                                                       DAHI 770
      DIMENSION ARG(1),VAL(1)                                           DAHI 780
      DOUBLE PRECISION ARG,VAL,X,Y,H,H1,H2                              DAHI 790
      IER=2                                                             DAHI 800
      H2=X-ARG(1)                                                       DAHI 810
      IF(NDIM-1)2,1,3                                                   DAHI 820
    1 Y=VAL(1)+VAL(2)*H2                                                DAHI 830
    2 RETURN                                                            DAHI 840
C                                                                       DAHI 850
C     VECTOR ARG HAS MORE THAN 1 ELEMENT.                               DAHI 860
C     THE FIRST STEP PREPARES VECTOR VAL SUCH THAT AITKEN SCHEME CAN BE DAHI 870
C     USED.                                                             DAHI 880
    3 I=1                                                               DAHI 890
      DO 5 J=2,NDIM                                                     DAHI 900
      H1=H2                                                             DAHI 910
      H2=X-ARG(J)                                                       DAHI 920
      Y=VAL(I)                                                          DAHI 930
      VAL(I)=Y+VAL(I+1)*H1                                              DAHI 940
      H=H1-H2                                                           DAHI 950
      IF(H)4,13,4                                                       DAHI 960
    4 VAL(I+1)=Y+(VAL(I+2)-Y)*H1/H                                      DAHI 970
    5 I=I+2                                                             DAHI 980
      VAL(I)=VAL(I)+VAL(I+1)*H2                                         DAHI 990
C     END OF FIRST STEP                                                 DAHI1000
C                                                                       DAHI1010
C     PREPARE AITKEN SCHEME                                             DAHI1020
      DELT2=0.                                                          DAHI1030
      IEND=I-1                                                          DAHI1040
C                                                                       DAHI1050
C     START AITKEN-LOOP                                                 DAHI1060
      DO 9 I=1,IEND                                                     DAHI1070
      DELT1=DELT2                                                       DAHI1080
      Y=VAL(1)                                                          DAHI1090
      M=(I+3)/2                                                         DAHI1100
      H1=ARG(M)                                                         DAHI1110
      DO 6 J=1,I                                                        DAHI1120
      K=I+1-J                                                           DAHI1130
      L=(K+1)/2                                                         DAHI1140
      H=ARG(L)-H1                                                       DAHI1150
      IF(H)6,14,6                                                       DAHI1160
    6 VAL(K)=(VAL(K)*(X-H1)-VAL(K+1)*(X-ARG(L)))/H                      DAHI1170
      DELT2=DABS(Y-VAL(1))                                              DAHI1180
      IF(DELT2-EPS)11,11,7                                              DAHI1190
    7 IF(I-8)9,8,8                                                      DAHI1200
    8 IF(DELT2-DELT1)9,12,12                                            DAHI1210
    9 CONTINUE                                                          DAHI1220
C     END OF AITKEN-LOOP                                                DAHI1230
C                                                                       DAHI1240
   10 Y=VAL(1)                                                          DAHI1250
      RETURN                                                            DAHI1260
C                                                                       DAHI1270
C     THERE IS SUFFICIENT ACCURACY WITHIN 2*NDIM-2 ITERATION STEPS      DAHI1280
   11 IER=0                                                             DAHI1290
      GOTO 10                                                           DAHI1300
C                                                                       DAHI1310
C     TEST VALUE DELT2 STARTS OSCILLATING                               DAHI1320
   12 IER=1                                                             DAHI1330
      RETURN                                                            DAHI1340
C                                                                       DAHI1350
C     THERE ARE TWO IDENTICAL ARGUMENT VALUES IN VECTOR ARG             DAHI1360
   13 Y=VAL(1)                                                          DAHI1370
   14 IER=3                                                             DAHI1380
      RETURN                                                            DAHI1390
      END                                                               DAHI1400
```

Subroutines ACFI and DACFI

These subroutines perform a continued fraction interpolation. Given the table x_i, y_i (i = 1, 2, ..., n) of argument and function values, stored in the two one-dimensional storage arrays ARG and VAL, the problem is to interpolate function value Y at the given point X. It is assumed that the table represents a single-valued function y = y(x) which is suitable for approximation by a rational function[+], and that $|x_i - X| \geq x_j - X|$ for $i > j$.[++]

Then, using the following formulas:

$$y_{1,2} = \frac{x_2 - x_1}{y_2 - y_1};$$

$$y_{1,3} = \frac{x_3 - x_1}{y_3 - y_1}; \quad y_{1,2,3} = \frac{x_3 - x_2}{y_{1,3} - y_{1,2}};$$

$$y_{1,4} = \frac{x_4 - x_1}{y_4 - y_1}; \quad y_{1,2,4} = \frac{x_4 - x_2}{y_{1,4} - y_{1,2}};$$

$$y_{1,2,3,4} = \frac{x_4 - x_3}{y_{1,2,4} - y_{1,2,3}};$$

the triangular scheme of inverted differences shown in Figure 20 can be generated by row for the given table x_i, y_i.

All result values of row i can be stored in VAL(I). Thus, it is possible to generate the downward diagonal of the inverted differences scheme in storage array VAL, using the machine-processable formula:

$$\text{VAL(I)} = \frac{\text{ARG(I)} - \text{ARG(J)}}{\text{VAL(I)} - \text{VAL(J)}} \quad (\text{J} = 1, 2, \ldots, \text{I-1}) \qquad (1)$$

for I = 2, 3, ..., NDIM.

[+]This order in table x_i, y_i (i = 1, 2, ..., n) could be generated by subroutines ATSG, ATSM, ATSE, DATSG, DATSM, DATSE.

[++]This means y(x) should be closely approximated by a rational function, with numerator and denominator of low degree, which has the table points with arguments next to x as nodes.

x_1	y_1					
x_2	y_2	$y_{1,2}$				
x_3	y_3	$y_{1,3}$	$y_{1,2,3}$			
x_4	y_4	$y_{1,4}$	$y_{1,2,4}$			
.	.	.	.	$y_{1,2,3,4}$		
.	.	.	.	.		
.	.	.	.	.	...	
x_n	y_n	$y_{1,n}$	$y_{1,2,n}$	$y_{1,2,3,n}$		$y_{1,2,3,\ldots,n}$

Figure 20. Triangular scheme for fraction interpolation

If for J = I-1, VAL(I) is equal to the infinity element, table point ARG(I), VAL(I) (that is, x_i, y_i) gets interchanged with a table point ahead.

Now, after computation of each new component VAL(I), continued fraction interpolation generates the following set of parameters:

$$P_3 = VAL(I) * P_2 + (X - ARG(I-1)) * P_1 \qquad (2)$$

$$Q_3 = VAL(I) * Q_2 + (X - ARG(I-1)) * Q_1 \qquad (3)$$

and

$$Y = P_3/Q_3 \qquad (4)$$

starting with $P_1 = 1$, $P_2 = VAL(1)$, $Q_1 = 0$, $Q_2 = 1$. After having done this, it sets $P_1 = P_2$, $P_2 = P_3$, $Q_1 = Q_2$, $Q_2 = Q_3$ after each step.

The procedure stops under the following conditions: if the difference between two successive values of Y is absolutely less than a given tolerance ε, or if the absolute value of this difference starts oscillating (test of oscillating differences starts at step I = 8, or for double-precision, I = 10), or if I has become NDIM, or if the procedure discovers two table points with identical argument values.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill, New York/ Toronto/London, 1956, pp. 395-406.

```
C                                                                       ACFI  10
C     ..................................................................ACFI  20
C                                                                       ACFI  30
C        SUBROUTINE ACFI                                                ACFI  40
C                                                                       ACFI  50
C        PURPOSE                                                        ACFI  60
C           TO INTERPOLATE FUNCTION VALUE Y FOR A GIVEN ARGUMENT VALUE  ACFI  70
C           X USING A GIVEN TABLE (ARG,VAL) OF ARGUMENT AND FUNCTION    ACFI  80
C           VALUES.                                                     ACFI  90
C                                                                       ACFI 100
C        USAGE                                                          ACFI 110
C           CALL ACFI (X,ARG,VAL,Y,NDIM,EPS,IER)                        ACFI 120
C                                                                       ACFI 130
C        DESCRIPTION OF PARAMETERS                                      ACFI 140
C           X      - THE ARGUMENT VALUE SPECIFIED BY INPUT.             ACFI 150
C           ARG    - THE INPUT VECTOR (DIMENSION NDIM) OF ARGUMENT      ACFI 160
C                    VALUES OF THE TABLE (POSSIBLY DESTROYED).          ACFI 170
C           VAL    - THE INPUT VECTOR (DIMENSION NDIM) OF FUNCTION      ACFI 180
C                    VALUES OF THE TABLE (DESTROYED).                   ACFI 190
C           Y      - THE RESULTING INTERPOLATED FUNCTION VALUE.         ACFI 200
C           NDIM   - AN INPUT VALUE WHICH SPECIFIES THE NUMBER OF       ACFI 210
C                    POINTS IN TABLE (ARG,VAL).                         ACFI 220
C           EPS    - AN INPUT CONSTANT WHICH IS USED AS UPPER BOUND     ACFI 230
C                    FOR THE ABSOLUTE ERROR.                            ACFI 240
C           IER    - A RESULTING ERROR PARAMETER.                       ACFI 250
C                                                                       ACFI 260
C        REMARKS                                                        ACFI 270
C           (1) TABLE (ARG,VAL) SHOULD REPRESENT A SINGLE-VALUED        ACFI 280
C               FUNCTION AND SHOULD BE STORED IN SUCH A WAY, THAT THE   ACFI 290
C               DISTANCES ABS(ARG(I)-X) INCREASE WITH INCREASING        ACFI 300
C               SUBSCRIPT I. TO GENERATE THIS ORDER IN TABLE (ARG,VAL), ACFI 310
C               SUBROUTINES ATSG, ATSM OR ATSE COULD BE USED IN A       ACFI 320
C               PREVIOUS STAGE.                                         ACFI 330
C           (2) NO ACTION BESIDES ERROR MESSAGE IN CASE NDIM LESS       ACFI 340
C               THAN 1.                                                 ACFI 350
C           (3) INTERPOLATION IS TERMINATED EITHER IF THE DIFFERENCE    ACFI 360
C               BETWEEN TWO SUCCESSIVE INTERPOLATED VALUES IS           ACFI 370
C               ABSOLUTELY LESS THAN TOLERANCE EPS, OR IF THE ABSOLUTE  ACFI 380
C               VALUE OF THIS DIFFERENCE STOPS DIMINISHING, OR AFTER    ACFI 390
C               (NDIM-1) STEPS (THE NUMBER OF POSSIBLE STEPS IS         ACFI 400
C               DIMINISHED IF AT ANY STAGE INFINITY ELEMENT APPEARS IN  ACFI 410
C               THE DOWNWARD DIAGONAL OF INVERTED-DIFFERENCES-SCHEME    ACFI 420
C               AND IF IT IS IMPOSSIBLE TO ELIMINATE THIS INFINITY      ACFI 430
C               ELEMENT BY INTERCHANGING OF TABLE POINTS).              ACFI 440
C               FURTHER IT IS TERMINATED IF THE PROCEDURE DISCOVERS TWO  ACFI 450
C               ARGUMENT VALUES IN VECTOR ARG WHICH ARE IDENTICAL.      ACFI 460
C               DEPENDENT ON THESE FOUR CASES, ERROR PARAMETER IER IS   ACFI 470
C               CODED IN THE FOLLOWING FORM                             ACFI 480
C                  IER=0 - IT WAS POSSIBLE TO REACH THE REQUIRED        ACFI 490
C                          ACCURACY (NO ERROR).                         ACFI 500
C                  IER=1 - IT WAS IMPOSSIBLE TO REACH THE REQUIRED      ACFI 510
C                          ACCURACY BECAUSE OF ROUNDING ERRORS.         ACFI 520
C                  IER=2 - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE  ACFI 530
C                          NDIM IS LESS THAN 2, OR THE REQUIRED ACCURACY ACFI 540
C                          COULD NOT BE REACHED BY MEANS OF THE GIVEN   ACFI 550
C                          TABLE. NDIM SHOULD BE INCREASED.             ACFI 560
C                  IER=3 - THE PROCEDURE DISCOVERED TWO ARGUMENT VALUES ACFI 570
C                          IN VECTOR ARG WHICH ARE IDENTICAL.           ACFI 580
C                                                                       ACFI 590
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ACFI 600
C           NONE                                                        ACFI 610
C                                                                       ACFI 620
C        METHOD                                                         ACFI 630
C           INTERPOLATION IS DONE BY CONTINUED FRACTIONS AND INVERTED-   ACFI 640
C           DIFFERENCES-SCHEME. ON RETURN Y CONTAINS AN INTERPOLATED     ACFI 650
C           FUNCTION VALUE AT POINT X, WHICH IS IN THE SENSE OF REMARK   ACFI 660
C           (3) OPTIMAL WITH RESPECT TO GIVEN TABLE. FOR REFERENCE, SEE  ACFI 670
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,          ACFI 680
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.395-406.      ACFI 690
C                                                                       ACFI 700
C     ..................................................................ACFI 710
C                                                                       ACFI 720
      SUBROUTINE ACFI(X,ARG,VAL,Y,NDIM,EPS,IER)                         ACFI 730
C                                                                       ACFI 740
C                                                                       ACFI 750
      DIMENSION ARG(1),VAL(1)                                           ACFI 760
      IER=2                                                             ACFI 770
      IF(NDIM)20,20,1                                                   ACFI 780
    1 Y=VAL(1)                                                          ACFI 790
      DELT2=0.                                                          ACFI 800
      IF(NDIM-1)20,20,2                                                 ACFI 810
C                                                                       ACFI 820
C     PREPARATIONS FOR INTERPOLATION LOOP                               ACFI 830
    2 P2=1.                                                             ACFI 840
      P3=Y                                                              ACFI 850
      Q2=0.                                                             ACFI 860
      Q3=1.                                                             ACFI 870
C                                                                       ACFI 880
C                                                                       ACFI 890
C     START INTERPOLATION LOOP                                          ACFI 900
      DO 16 I=2,NDIM                                                    ACFI 910
      II=0                                                              ACFI 920
      P1=P2                                                             ACFI 930
      P2=P3                                                             ACFI 940
      Q1=Q2                                                             ACFI 950
      Q2=Q3                                                             ACFI 960
      Z=Y                                                               ACFI 970
      DELT1=DELT2                                                       ACFI 980
      JEND=I-1                                                          ACFI 990
C                                                                       ACFI1000
C     COMPUTATION OF INVERTED DIFFERENCES                               ACFI1010
    3 AUX=VAL(I)                                                        ACFI1020
      DO 10 J=1,JEND                                                    ACFI1030
      H=VAL(I)-VAL(J)                                                   ACFI1040
      IF(ABS(H)-1.E-6*ABS(VAL(I)))4,4,9                                 ACFI1050
    4 IF(ARG(I)-ARG(J))5,17,5                                           ACFI1060
    5 IF(J-JEND)8,6,6                                                   ACFI1070
C                                                                       ACFI1080
C     INTERCHANGE ROW I WITH ROW I+II                                   ACFI1090
    6 II=II+1                                                           ACFI1100
      III=I+II                                                          ACFI1110
      IF(III-NDIM)7,7,19                                                ACFI1120
    7 VAL(I)=VAL(III)                                                   ACFI1130
      VAL(III)=AUX                                                      ACFI1140
      AUX=ARG(I)                                                        ACFI1150
      ARG(I)=ARG(III)                                                   ACFI1160
      ARG(III)=AUX                                                      ACFI1170
      GOTO 3                                                            ACFI1180
C                                                                       ACFI1190
C     COMPUTATION OF VAL(I) IN CASE VAL(I)=VAL(J) AND J LESS THAN I-1   ACFI1200
    8 VAL(I)=1.E75                                                      ACFI1210
      GOTO 10                                                           ACFI1220
C                                                                       ACFI1230
C     COMPUTATION OF VAL(I) IN CASE VAL(I) NOT EQUAL TO VAL(J)          ACFI1240
    9 VAL(I)=(ARG(I)-ARG(J))/H                                          ACFI1250
   10 CONTINUE                                                          ACFI1260
C     INVERTED DIFFERENCES ARE COMPUTED                                 ACFI1270
C                                                                       ACFI1280
C     COMPUTATION OF NEW Y                                              ACFI1290
      P3=VAL(I)*P2+(X-ARG(I-1))*P1                                      ACFI1300
      Q3=VAL(I)*Q2+(X-ARG(I-1))*Q1                                      ACFI1310
      IF(Q3)11,12,11                                                    ACFI1320
   11 Y=P3/Q3                                                           ACFI1330
      GOTO 13                                                           ACFI1340
   12 Y=1.E75                                                           ACFI1350
   13 DELT2=ABS(Z-Y)                                                    ACFI1360
      IF(DELT2-EPS)19,19,14                                             ACFI1370
   14 IF(I-8)16,15,15                                                   ACFI1380
   15 IF(DELT2-DELT1)16,18,18                                           ACFI1390
   16 CONTINUE                                                          ACFI1400
C     END OF INTERPOLATION LOOP                                         ACFI1410
C                                                                       ACFI1420
C                                                                       ACFI1430
      RETURN                                                            ACFI1440
C                                                                       ACFI1450
C     THERE ARE TWO IDENTICAL ARGUMENT VALUES IN VECTOR ARG             ACFI1460
   17 IER=3                                                             ACFI1470
      RETURN                                                            ACFI1480
C                                                                       ACFI1490
C     TEST VALUE DELT2 STARTS OSCILLATING                               ACFI1500
   18 Y=Z                                                               ACFI1510
      IER=1                                                             ACFI1520
      RETURN                                                            ACFI1530
C                                                                       ACFI1540
C     THERE IS SATISFACTORY ACCURACY WITHIN NDIM-1 STEPS                ACFI1550
   19 IER=0                                                             ACFI1560
   20 RETURN                                                            ACFI1570
      END                                                               ACFI1580
```

```
C                                                                       DACF  10
C*********************************************************************DACF  20
C                                                                       DACF  30
C     SUBROUTINE DACFI                                                  DACF  40
C                                                                       DACF  50
C     PURPOSE                                                           DACF  60
C        TO INTERPOLATE FUNCTION VALUE Y FOR A GIVEN ARGUMENT VALUE     DACF  70
C        X USING A GIVEN TABLE (ARG,VAL) OF ARGUMENT AND FUNCTION       DACF  80
C        VALUES.                                                        DACF  90
C                                                                       DACF 100
C     USAGE                                                             DACF 110
C        CALL DACFI (X,ARG,VAL,Y,NDIM,EPS,IER)                          DACF 120
C                                                                       DACF 130
C     DESCRIPTION OF PARAMETERS                                         DACF 140
C        X      - DOUBLE PRECISION ARGUMENT VALUE SPECIFIED BY INPUT.   DACF 150
C        ARG    - DOUBLE PRECISION INPUT VECTOR (DIMENSION NDIM) OF     DACF 160
C                 ARGUMENT VALUES OF THE TABLE (POSSIBLY DESTROYED).   DACF 170
C        VAL    - DOUBLE PRECISION INPUT VECTOR (DIMENSION NDIM) OF     DACF 180
C                 FUNCTION VALUES OF THE TABLE (DESTROYED).            DACF 190
C        Y      - RESULTING INTERPOLATED DOUBLE PRECISION FUNCTION      DACF 200
C                 VALUE.                                               DACF 210
C        NDIM   - AN INPUT VALUE WHICH SPECIFIES THE NUMBER OF          DACF 220
C                 POINTS IN TABLE (ARG,VAL).                           DACF 230
C        EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS      DACF 240
C                 UPPER BOUND FOR THE ABSOLUTE ERROR.                  DACF 250
C        IER    - A RESULTING ERROR PARAMETER.                          DACF 260
C                                                                       DACF 270
C     REMARKS                                                           DACF 280
C        (1) TABLE (ARG,VAL) SHOULD REPRESENT A SINGLE-VALUED           DACF 290
C            FUNCTION AND SHOULD BE STORED IN SUCH A WAY, THAT THE      DACF 300
C            DISTANCES ABS(ARG(I)-X) INCREASE WITH INCREASING           DACF 310
C            SUBSCRIPT I. TO GENERATE THIS ORDER IN TABLE (ARG,VAL),    DACF 320
C            SUBROUTINES DATSG, DATSM OR DATSE COULD BE USED IN A       DACF 330
C            PREVIOUS STAGE.                                            DACF 340
C        (2) NO ACTION BESIDES ERROR MESSAGE IN CASE NDIM LESS          DACF 350
C            THAN 1.                                                    DACF 360
C        (3) INTERPOLATION IS TERMINATED EITHER IF THE DIFFERENCE       DACF 370
C            BETWEEN TWO SUCCESSIVE INTERPOLATED VALUES IS              DACF 380
C            ABSOLUTELY LESS THAN TOLERANCE EPS, OR IF THE ABSOLUTE     DACF 390
C            VALUE OF THIS DIFFERENCE STOPS DIMINISHING, OR AFTER       DACF 400
C            (NDIM-1) STEPS (THE NUMBER OF POSSIBLE STEPS IS            DACF 410
C            DIMINISHED IF AT ANY STAGE INFINITY ELEMENT APPEARS IN     DACF 420
C            THE DOWNWARD DIAGONAL OF INVERTED-DIFFERENCES-SCHEME       DACF 430
C            AND IF IT IS IMPOSSIBLE TO ELIMINATE THIS INFINITY         DACF 440
C            ELEMENT BY INTERCHANGING OF TABLE POINTS).                 DACF 450
C            FURTHER IT IS TERMINATED IF THE PROCEDURE DISCOVERS TWO     DACF 460
C            ARGUMENT VALUES IN VECTOR ARG WHICH ARE IDENTICAL.         DACF 470
C            DEPENDENT ON THESE FOUR CASES, ERROR PARAMETER IER IS      DACF 480
C            CODED IN THE FOLLOWING FORM                                DACF 490
C             IER=0 - IT WAS POSSIBLE TO REACH THE REQUIRED             DACF 500
C                     ACCURACY (NO ERROR).                              DACF 510
C             IER=1 - IT WAS IMPOSSIBLE TO REACH THE REQUIRED           DACF 520
C                     ACCURACY BECAUSE OF ROUNDING ERRORS.              DACF 530
C             IER=2 - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE       DACF 540
C                     NDIM IS LESS THAN 2, OR THE REQUIRED ACCURACY     DACF 550
C                     COULD NOT BE REACHED BY MEANS OF THE GIVEN        DACF 560
C                     TABLE. NDIM SHOULD BE INCREASED.                  DACF 570
C             IER=3 - THE PROCEDURE DISCOVERED TWO ARGUMENT VALUES      DACF 580
C                     IN VECTOR ARG WHICH ARE IDENTICAL.                DACF 590
C                                                                       DACF 600
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DACF 610
C        NONE                                                           DACF 620
C                                                                       DACF 630
C     METHOD                                                            DACF 640
C        INTERPOLATION IS DONE BY CONTINUED FRACTIONS AND INVERTED-     DACF 650
C        DIFFERENCES-SCHEME. ON RETURN Y CONTAINS AN INTERPOLATED       DACF 660
C        FUNCTION VALUE AT POINT X, WHICH IS IN THE SENSE OF REMARK     DACF 670
C        (3) OPTIMAL WITH RESPECT TO GIVEN TABLE. FOR REFERENCE, SEE    DACF 680
C        F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,            DACF 690
C        MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.395-406.        DACF 700
C                                                                       DACF 710
C*********************************************************************DACF 720
C                                                                       DACF 730
      SUBROUTINE DACFI(X,ARG,VAL,Y,NDIM,EPS,IER)                        DACF 740
C                                                                       DACF 750
C                                                                       DACF 760
      DIMENSION ARG(1),VAL(1)                                           DACF 770
      DOUBLE PRECISION ARG,VAL,X,Y,Z,P1,P2,P3,Q1,Q2,Q3,AUX,H            DACF 780
      IER=2                                                             DACF 790
      IF(NDIM)20,20,1                                                   DACF 800
    1 Y=VAL(1)                                                          DACF 810
      DELT2=0.                                                          DACF 820
      IF(NDIM-1)20,20,2                                                 DACF 830
C                                                                       DACF 840
C     PREPARATIONS FOR INTERPOLATION LOOP                               DACF 850
    2 P2=1.D0                                                           DACF 860
      P3=Y                                                              DACF 870
      Q2=0.D0                                                           DACF 880
      Q3=1.D0                                                           DACF 890
C                                                                       DACF 900
C                                                                       DACF 910
C     START INTERPOLATION LOOP                                          DACF 920
      DO 16 I=2,NDIM                                                    DACF 930
      II=0                                                              DACF 940
      P1=P2                                                             DACF 950
      P2=P3                                                             DACF 960
      Q1=Q2                                                             DACF 970
      Q2=Q3                                                             DACF 980
      Z=Y                                                               DACF 990
      DELT1=DELT2                                                       DACF1000
      JEND=I-1                                                          DACF1010
C                                                                       DACF1020
C     COMPUTATION OF INVERTED DIFFERENCES                               DACF1030
    3 AUX=VAL(I)                                                        DACF1040
      DO 10 J=1,JEND                                                    DACF1050
      H=VAL(I)-VAL(J)                                                   DACF1060
      IF(DABS(H)-1.D-13*DABS(VAL(I)))4,4,9                              DACF1070
    4 IF(ARG(I)-ARG(J))5,17,5                                           DACF1080
    5 IF(J-JEND)8,6,6                                                   DACF1090
C                                                                       DACF1100
C     INTERCHANGE ROW I WITH ROW I+II                                   DACF1110
    6 II=II+1                                                           DACF1120
      III=I+II                                                          DACF1130
      IF(III-NDIM)7,7,19                                                DACF1140
    7 VAL(I)=VAL(III)                                                   DACF1150
      VAL(III)=AUX                                                      DACF1160
      AUX=ARG(I)                                                        DACF1170
      ARG(I)=ARG(III)                                                   DACF1180
      ARG(III)=AUX                                                      DACF1190
      GOTO 3                                                            DACF1200
C                                                                       DACF1210
C     COMPUTATION OF VAL(I) IN CASE VAL(I)=VAL(J) AND J LESS THAN I-1   DACF1220
    8 VAL(I)=1.D75                                                      DACF1230
      GOTO 10                                                           DACF1240
C                                                                       DACF1250
C     COMPUTATION OF VAL(I) IN CASE VAL(I) NOT EQUAL TO VAL(J)          DACF1260
    9 VAL(I)=(ARG(I)-ARG(J))/H                                          DACF1270
   10 CONTINUE                                                          DACF1280
C     INVERTED DIFFERENCES ARE COMPUTED                                 DACF1290
C                                                                       DACF1300
C     COMPUTATION OF NEW Y                                              DACF1310
      P3=VAL(I)*P2+(X-ARG(I-1))*P1                                      DACF1320
      Q3=VAL(I)*Q2+(X-ARG(I-1))*Q1                                      DACF1330
      IF(Q3)11,12,11                                                    DACF1340
   11 Y=P3/Q3                                                           DACF1350
      GOTO 13                                                           DACF1360
   12 Y=1.D75                                                           DACF1370
   13 DELT2=DABS(Z-Y)                                                   DACF1380
      IF(DELT2-EPS)19,19,14                                             DACF1390
   14 IF(I-10)16,15,15                                                  DACF1400
   15 IF(DELT2-DELT1)16,18,18                                           DACF1410
   16 CONTINUE                                                          DACF1420
C     END OF INTERPOLATION LOOP                                         DACF1430
C                                                                       DACF1440
C                                                                       DACF1450
C     RETURN                                                            DACF1460
C                                                                       DACF1470
C     THERE ARE TWO IDENTICAL ARGUMENT VALUES IN VECTOR ARG             DACF1480
   17 IER=3                                                             DACF1490
      RETURN                                                            DACF1500
C                                                                       DACF1510
C     TEST VALUE DELT2 STARTS OSCILLATING                               DACF1520
   18 Y=Z                                                               DACF1530
      IER=1                                                             DACF1540
      RETURN                                                            DACF1550
C                                                                       DACF1560
C     THERE IS SATISFACTORY ACCURACY WITHIN NDIM-1 STEPS                DACF1570
   19 IER=0                                                             DACF1580
   20 RETURN                                                            DACF1590
      END                                                               DACF1600
```

These subroutines perform a table selection out of a given general table.

Given a search argument x and a general table z_i, f_i (i = 1, 2, ..., irow) stored in two vectors Z and F (in case icol = 1), or z_i, f_i, f_i' (i = 1, 2, ..., irow) stored in vector Z and the two columns of matrix F (in case icol = 2); the problem is to select those n ($\leq$ irow) points z_{i_j}, f_{i_j} or z_{i_j}, f_{i_j}, f'_{i_j} (j = 1, 2, ..., n), respectively, which are next to x and to store their coordinates in two vectors ARG and VAL so that the distances $|x - z_{i_j}|$ increase with increasing subscript j. This problem may arise when using interpolation subroutines ALI, AHI, ACFI, DALI, DAHI, DACFI. The table for the case icol = 1 is shown in Figure 21, and that for case icol = 2 in Figure 22.

Selection is done in two parts. In the first part, auxiliary vector WORK with components $z_i - x$ (i = 1, 2, ..., irow) is generated and its greatest component, $\max_i |z_i - x|$, is stored in an auxiliary storage location. In each of the n steps of the second part the subscript i_j of the smallest component of vector WORK is searched for. Afterwards this component is replaced by a number greater than $\max_i |z_i - x|$.

Then, z_{i_j} goes into the storage location ARG(J) and:

In case icol = 1 -- f_{i_j} into the storage location VAL(J)

In case icol = 2 -- f_{i_j} into the storage location VAL(2 * J - 1) and f'_{i_j} into the storage location VAL(2 * J)

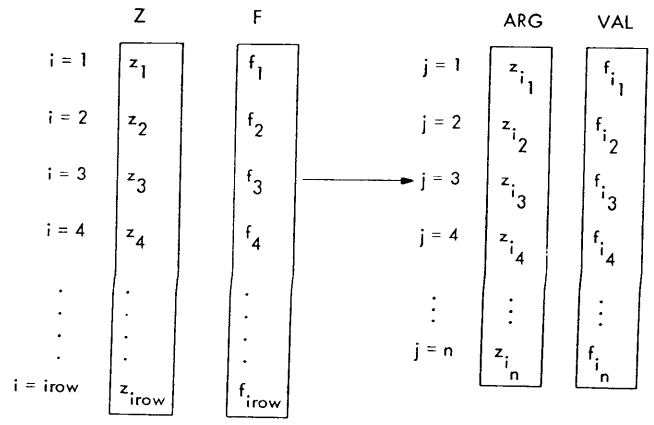


Figure 21. Table selection in case icol=1

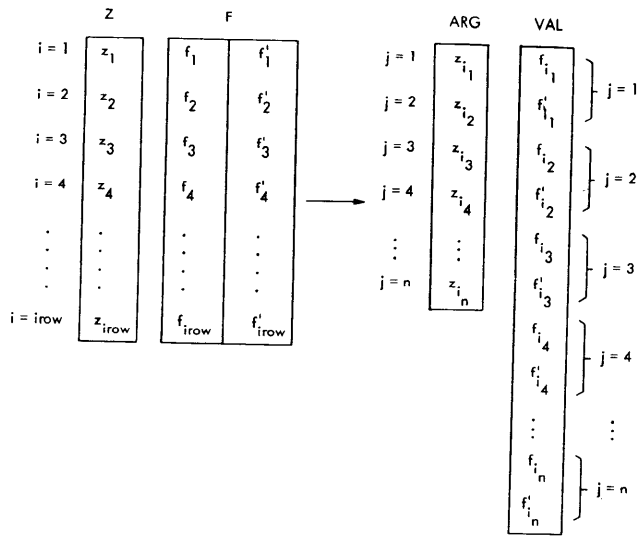


Figure 22. Table selection in case icol=2

If (by an error of the user) the dimension n of the table to be selected is greater than the dimension irow of the given table, the procedure selects only a maximum table of irow points. In order to avoid errors in further work with table (ARG, VAL), the user ought to check the correspondence between the selected table and its dimension by comparison of n and irow. This test may be done before or after calling subroutine ATSG or DATSG.

```
C                                                                       ATSG  10
C     ...................................................................ATSG  20
C                                                                       ATSG  30
C       SUBROUTINE ATSG                                                 ATSG  40
C                                                                       ATSG  50
C       PURPOSE                                                         ATSG  60
C          NDIM POINTS OF A GIVEN GENERAL TABLE ARE SELECTED AND        ATSG  70
C          ORDERED SUCH THAT ABS(ARG(I)-X).GE.ABS(ARG(J)-X) IF I.GT.J.  ATSG  80
C                                                                       ATSG  90
C       USAGE                                                           ATSG 100
C          CALL ATSG (X,Z,F,WORK,IROW,ICOL,ARG,VAL,NDIM)                ATSG 110
C                                                                       ATSG 120
C       DESCRIPTION OF PARAMETERS                                       ATSG 130
C          X      - THE SEARCH ARGUMENT.                                ATSG 140
C          Z      - THE VECTOR OF ARGUMENT VALUES (DIMENSION IROW).     ATSG 150
C          F      - IN CASE ICOL=1, F IS THE VECTOR OF FUNCTION VALUES  ATSG 160
C                   (DIMENSION IROW).                                   ATSG 170
C                   IN CASE ICOL=2, F IS AN IROW BY 2 MATRIX. THE FIRSTATSG 180
C                   COLUMN SPECIFIES THE VECTOR OF FUNCTION VALUES AND  ATSG 190
C                   THE SECOND THE VECTOR OF DERIVATIVES.               ATSG 200
C          WORK   - A WORKING STORAGE (DIMENSION IROW).                 ATSG 210
C          IROW   - THE DIMENSION OF VECTORS Z AND WORK AND OF EACH     ATSG 220
C                   COLUMN IN MATRIX F.                                 ATSG 230
C          ICOL   - THE NUMBER OF COLUMNS IN F (I.E. 1 OR 2).           ATSG 240
C          ARG    - THE RESULTING VECTOR OF SELECTED AND ORDERED       ATSG 250
C                   ARGUMENT VALUES (DIMENSION NDIM).                   ATSG 260
C          VAL    - THE RESULTING VECTOR OF SELECTED FUNCTION VALUES    ATSG 270
C                   (DIMENSION NDIM) IN CASE ICOL=1. IN CASE ICOL=2,    ATSG 280
C                   VAL IS THE VECTOR OF FUNCTION AND DERIVATIVE VALUESATSG 290
C                   (DIMENSION 2*NDIM) WHICH ARE STORED IN PAIRS (I.E.  ATSG 300
C                   EACH FUNCTION VALUE IS FOLLOWED BY ITS DERIVATIVE   ATSG 310
C                   VALUE).                                             ATSG 320
C          NDIM   - THE NUMBER OF POINTS WHICH MUST BE SELECTED OUT OF  ATSG 330
C                   THE GIVEN TABLE (Z,F).                              ATSG 340
C                                                                       ATSG 350
C       REMARKS                                                         ATSG 360
C          NO ACTION IN CASE IROW LESS THAN 1.                          ATSG 370
C          IF INPUT VALUE NDIM IS GREATER THAN IROW, THE PROGRAM        ATSG 380
C          SELECTS ONLY A MAXIMUM TABLE OF IROW POINTS.  THEREFORE THE  ATSG 390
C          USER OUGHT TO CHECK CORRESPONDENCE BETWEEN TABLE (ARG,VAL)   ATSG 400
C          AND ITS DIMENSION BY COMPARISON OF NDIM AND IROW, IN ORDER   ATSG 410
C          TO GET CORRECT RESULTS IN FURTHER WORK WITH TABLE (ARG,VAL).  ATSG 420
C          THIS TEST MAY BE DONE BEFORE OR AFTER CALLING                ATSG 430
C          SUBROUTINE ATSG.                                             ATSG 440
C          SUBROUTINE ATSG ESPECIALLY CAN BE USED FOR GENERATING THE    ATSG 450
C          TABLE (ARG,VAL) NEEDED IN SUBROUTINES ALI, AHI, AND ACFI.    ATSG 460
C                                                                       ATSG 470
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   ATSG 480
C          NONE                                                         ATSG 490
C                                                                       ATSG 500
C       METHOD                                                          ATSG 510
C          SELECTION IS DONE BY GENERATING THE VECTOR WORK WITH         ATSG 520
C          COMPONENTS WORK(I)=ABS(Z(I)-X) AND AT EACH OF THE NDIM STEPSATSG 530
C          (OR IROW STEPS IF NDIM IS GREATER THAN IROW)                 ATSG 540
C          SEARCHING FOR THE SUBSCRIPT OF THE SMALLEST COMPONENT, WHICHATSG 550
C          IS AFTERWARDS REPLACED BY A NUMBER GREATER THAN              ATSG 560
C          MAX(WORK(I)).                                                ATSG 570
```

```
C                                                                       ATSG 580
C     ..................................................................ATSG 590
C                                                                       ATSG 600
      SUBROUTINE ATSG(X,Z,F,WORK,IROW,ICOL,ARG,VAL,NDIM)                ATSG 610
C                                                                       ATSG 620
C                                                                       ATSG 630
      DIMENSION Z(1),F(1),WORK(1),ARG(1),VAL(1)                         ATSG 640
      IF(IROW)11,11,1                                                   ATSG 650
    1 N=NDIM                                                            ATSG 660
C     IF N IS GREATER THAN IROW, N IS SET EQUAL TO IROW.                ATSG 670
      IF(N-IROW)3,3,2                                                   ATSG 680
    2 N=IROW                                                            ATSG 690
C                                                                       ATSG 700
C     GENERATION OF VECTOR WORK AND COMPUTATION OF ITS GREATEST ELEMENT.ATSG 710
C                                                                       ATSG 720
    3 B=0.                                                              ATSG 730
      DO 5 I=1,IROW                                                     ATSG 740
      DELTA=ABS(Z(I)-X)                                                 ATSG 750
      IF(DELTA-B)5,5,4                                                  ATSG 760
    4 B=DELTA                                                           ATSG 770
    5 WORK(I)=DELTA                                                     ATSG 780
C                                                                       ATSG 790
C     GENERATION OF TABLE (ARG,VAL)                                     ATSG 800
      B=B+1.                                                            ATSG 810
      DO 10 J=1,N                                                       ATSG 820
      DELTA=B                                                           ATSG 830
      DO 7 I=1,IROW                                                     ATSG 840
      IF(WORK(I)-DELTA)6,7,7                                            ATSG 850
    6 II=I                                                              ATSG 860
      DELTA=WORK(I)                                                     ATSG 870
    7 CONTINUE                                                          ATSG 880
      ARG(J)=Z(II)                                                      ATSG 890
      IF(ICOL-1)8,9,8                                                   ATSG 900
    8 VAL(2*J-1)=F(II)                                                  ATSG 910
      III=II+IROW                                                       ATSG 920
      VAL(2*J)=F(III)                                                   ATSG 930
      GOTO 10                                                           ATSG 940
    9 VAL(J)=F(II)                                                      ATSG 950
   10 WORK(II)=B                                                        ATSG 960
   11 RETURN                                                            ATSG 970
      END
```

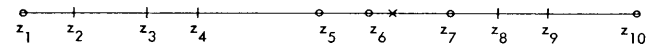
```
C                                                                       DTSG  10
C     ..................................................................DTSG  20
C                                                                       DTSG  30
      SUBROUTINE DATSG                                                  DTSG  40
C                                                                       DTSG  50
C     PURPOSE                                                           DTSG  60
C        NDIM POINTS OF A GIVEN GENERAL TABLE ARE SELECTED AND          DTSG  70
C        ORDERED SUCH THAT ABS(ARG(I)-X).GE.ABS(ARG(J)-X) IF I.GT.J.    DTSG  80
C                                                                       DTSG  90
C     USAGE                                                             DTSG 100
C        CALL DATSG (X,Z,F,WORK,IROW,ICOL,ARG,VAL,NDIM)                 DTSG 110
C                                                                       DTSG 120
C     DESCRIPTION OF PARAMETERS                                         DTSG 130
C        X      - DOUBLE PRECISION SEARCH ARGUMENT.                     DTSG 140
C        Z      - DOUBLE PRECISION VECTOR OD ARGUMENT VALUES            DTSG 150
C                 (DIMENSION IROW).                                     DTSG 160
C        F      - IN CASE ICOL=1, F IS THE DOUBLE PRECISION VECTOR      DTSG 170
C                 OF FUNCTION VALUES (DIMENSION IROW).                  DTSG 180
C                 IN CASE ICOL=2, F IS A DOUBLE PRECISION IROW BY 2     DTSG 190
C                 MATRIX. THE FIRST COLUMN SPECIFIES VECTOR OF FUNC-    DTSG 200
C                 TION VALUES AND THE SECOND VECTOR OF DERIVATIVES.     DTSG 210
C        WORK   - DOUBLE PRECISION WORKING STORAGE (DIMENSION IROW).    DTSG 220
C        IROW   - THE DIMENSION OF VECTORS Z AND WORK AND OF EACH       DTSG 230
C                 COLUMN IN MATRIX F.                                   DTSG 240
C        ICOL   - THE NUMBER OF COLUMNS IN F (I.E. 1 OR 2).             DTSG 250
C        ARG    - RESULTING DOUBLE PRECISION VECTOR OF SELECTED AND     DTSG 260
C                 ORDERED ARGUMENT VALUES (DIMENSION NDIM).             DTSG 270
C        VAL    - RESULTING DOUBLE PRECISION VECTOR OF SELECTED         DTSG 280
C                 FUNCTION VALUES (DIMENSION NDIM) IN CASE ICOL=1.      DTSG 290
C                 IN CASE ICOL=2, VAL IS THE DOUBLE PRECISION VECTOR    DTSG 300
C                 OF FUNCTION AND DERIVATIVE VALUES (DIMENSION          DTSG 310
C                 2*NDIM) WHICH ARE STORED IN PAIRS (I.E. EACH FUNC-    DTSG 320
C                 TION VALUE IS FOLLOWED BY ITS DERIVATIVE VALUE).      DTSG 330
C        NDIM   - THE NUMBER OF POINTS WHICH MUST BE SELECTED OUT OF    DTSG 340
C                 THE GIVEN TABLE (Z,F).                                DTSG 350
C                                                                       DTSG 360
C     REMARKS                                                           DTSG 370
C        NO ACTION IN CASE IROW LESS THAN 1.                            DTSG 380
C        IF INPUT VALUE NDIM IS GREATER THAN IROW, THE PROGRAM          DTSG 390
C        SELECTS ONLY A MAXIMUM TABLE OF IROW POINTS.  THEREFORE THE    DTSG 400
C        USER OUGHT TO CHECK CORRESPONDENCE BETWEEN TABLE (ARG,VAL)     DTSG 410
C        AND ITS DIMENSION BY COMPARISON OF NDIM AND IROW, IN ORDER     DTSG 420
C        TO GET CORRECT RESULTS IN FURTHER WORK WITH TABLE (ARG,VAL).   DTSG 430
C        THIS TEST MAY BE DONE BEFORE OR AFTER CALLING                  DTSG 440
C        SUBROUTINE DATSG.                                              DTSG 450
C        SUBROUTINE DATSG ESPECIALLY CAN BE USED FOR GENERATING THE     DTSG 460
C        TABLE (ARG,VAL) NEEDED IN SUBROUTINES DALI, DAHI, AND DACFI.   DTSG 470
C                                                                       DTSG 480
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DTSG 490
C        NONE                                                           DTSG 500
C                                                                       DTSG 510
C     METHOD                                                            DTSG 520
C        SELECTION IS DONE BY GENERATING THE VECTOR WORK WITH           DTSG 530
C        COMPONENTS WORK(I)=ABS(Z(I)-X) AND AT EACH OF THE NDIM STEPS   DTSG 540
C        (OR IROW STEPS IF NDIM IS GREATER THAN IROW)                   DTSG 550
C        SEARCHING FOR THE SUBSCRIPT OF THE SMALLEST COMPONENT, WHICH   DTSG 560
C        IS AFTERWARDS REPLACED BY A NUMBER GREATER THAN                DTSG 570
C        MAX(WORK(I)).                                                  DTSG 580
C                                                                       DTSG 590
C     ..................................................................DTSG 600
C                                                                       DTSG 610
      SUBROUTINE DATSG(X,Z,F,WORK,IROW,ICOL,ARG,VAL,NDIM)               DTSG 620
C                                                                       DTSG 630
C                                                                       DTSG 640
      DIMENSION Z(1),F(1),WORK(1),ARG(1),VAL(1)                         DTSG 650
      DOUBLE PRECISION X,Z,F,WORK,ARG,VAL,B,DELTA                       DTSG 660
      IF(IROW)11,11,1                                                   DTSG 670
    1 N=NDIM                                                            DTSG 680
C     IF N IS GREATER THAN IROW, N IS SET EQUAL TO IROW.                DTSG 690
      IF(N-IROW)3,3,2                                                   DTSG 700
    2 N=IROW                                                            DTSG 710
C                                                                       DTSG 720
C     GENERATION OF VECTOR WORK AND COMPUTATION OF ITS GREATEST ELEMENT.DTSG 730
    3 B=0.D0                                                            DTSG 740
      DO 5 I=1,IROW                                                     DTSG 750
      DELTA=DABS(Z(I)-X)                                                DTSG 760
      IF(DELTA-B)5,5,4                                                  DTSG 770
    4 B=DELTA                                                           DTSG 780
    5 WORK(I)=DELTA                                                     DTSG 790
C                                                                       DTSG 800
C     GENERATION OF TABLE (ARG,VAL)                                     DTSG 810
      B=B+1.D0                                                          DTSG 820
      DO 10 J=1,N                                                       DTSG 830
      DELTA=B                                                           DTSG 840
      DO 7 I=1,IROW                                                     DTSG 850
      IF(WORK(I)-DELTA)6,7,7                                            DTSG 860
    6 II=I                                                              DTSG 870
      DELTA=WORK(I)                                                     DTSG 880
    7 CONTINUE                                                          DTSG 890
      ARG(J)=Z(II)                                                      DTSG 900
      IF(ICOL-1)8,9,8                                                   DTSG 910
    8 VAL(2*J-1)=F(II)                                                  DTSG 920
      III=II+IROW                                                       DTSG 930
      VAL(2*J)=F(III)                                                   DTSG 940
      GOTO 10                                                           DTSG 950
    9 VAL(J)=F(II)                                                      DTSG 960
   10 WORK(II)=B                                                        DTSG 970
   11 RETURN                                                            DTSG 980
      END                                                               DTSG 990
```

These subroutines perform a table selection out of a given monotonic table. They have the same function as subroutines ATSG and DATSG with the difference that the given table is stored with monotonically increasing or decreasing arguments z_i.

Selection is done in two parts. In the first part, argument z_i next to search argument x is searched for by "binary search". This procedure (in case irow = 10) is shown in Figure 23.

The second part starts at z_{i_1}. At each of the n steps, the procedure decides by comparison of distances if the next step has to go to the right or to the left. Care must be taken that none of the selected subscripts i_j becomes greater than irow or less than one. Thus, in case n = 5, the sequence of argument values becomes $z_{i_1} = z_6$, $z_{i_2} = z_7$, $z_{i_3} = z_5$, $z_{i_4} = z_8$, $z_{i_5} = z_9$. The selected table is stored in the same way as in subroutine ATSG or DATSG.

If (by an error of the user) the dimension n of the table to be selected is greater than the dimension irow of the given table, the procedure selects only a maximum table of irow points. In order to avoid errors in further work with table (ARG, VAL), the user ought to check the correspondence between the selected table and its dimension by comparison of n and irow. This test may be done before or after calling subroutine ATSM or DATSM.



(1) x lies between z_1 and z_{10}.

(2) x lies between z_5 and z_{10}.

(3) x lies between z_5 and z_7.

(4) x lies between z_6 and z_7.

(5) Comparison of the two distances $|z_6 - x|$ and $|z_7 - x|$ shows that z_6 is next to x.

Figure 23. Binary search for argument z_i(irow=10)

```
C
C     ..................................................................ATSM  10
C                                                                      ATSM  20
C        SUBROUTINE ATSM                                               ATSM  30
C                                                                      ATSM  40
C        PURPOSE                                                       ATSM  50
C           NDIM POINTS OF A GIVEN TABLE WITH MONOTONIC ARGUMENTS ARE  ATSM  60
C           SELECTED AND ORDERED SUCH THAT                             ATSM  70
C           ABS(ARG(I)-X).GE.ABS(ARG(J)-X) IF I.GT.J.                  ATSM  80
C                                                                      ATSM  90
C        USAGE                                                         ATSM 100
C           CALL ATSM (X,Z,F,IROW,ICOL,ARG,VAL,NDIM)                   ATSM 110
C                                                                      ATSM 120
C        DESCRIPTION OF PARAMETERS                                     ATSM 130
C           X      - THE SEARCH ARGUMENT.                              ATSM 140
C           Z      - THE VECTOR OF ARGUMENT VALUES (DIMENSION IROW).   ATSM 150
C                    THE ARGUMENT VALUES MUST BE STORED IN INCREASING  ATSM 160
C                    OR DECREASING SEQUENCE.                           ATSM 170
C           F      - IN CASE ICOL=1, F IS THE VECTOR OF FUNCTION VALUES ATSM 180
C                    (DIMENSION IROW).                                 ATSM 190
C                    IN CASE ICOL=2, F IS AN IROW BY 2 MATRIX. THE FIRSTATSM 200
C                    COLUMN SPECIFIES THE VECTOR OF FUNCTION VALUES AND ATSM 210
C                    THE SECOND THE VECTOR OF DERIVATIVES.             ATSM 220
C           IROW   - THE DIMENSION OF VECTOR Z AND OF EACH COLUMN      ATSM 230
C                    IN MATRIX F.                                      ATSM 240
C           ICOL   - THE NUMBER OF COLUMNS IN F (I.E. 1 OR 2).         ATSM 250
C           ARG    - THE RESULTING VECTOR OF SELECTED AND ORDERED      ATSM 260
C                    ARGUMENT VALUES (DIMENSION NDIM).                 ATSM 270
C           VAL    - THE RESULTING VECTOR OF SELECTED FUNCTION VALUES  ATSM 280
C                    (DIMENSION NDIM) IN CASE ICOL=1. IN CASE ICOL=2,  ATSM 290
C                    VAL IS THE VECTOR OF FUNCTION AND DERIVATIVE VALUESATSM 300
C                    (DIMENSION 2*NDIM) WHICH ARE STORED IN PAIRS (I.E.ATSM 310
C                    EACH FUNCTION VALUE IS FOLLOWED BY ITS DERIVATIVE ATSM 320
C                    VALUE).                                           ATSM 330
C           NDIM   - THE NUMBER OF POINTS WHICH MUST BE SELECTED OUT OF ATSM 340
C                    THE GIVEN TABLE (Z,F).                            ATSM 350
C                                                                      ATSM 360
C        REMARKS                                                       ATSM 370
C           NO ACTION IN CASE IROW LESS THAN 1.                        ATSM 380
C           IF INPUT VALUE NDIM IS GREATER THAN IROW, THE PROGRAM      ATSM 390
C           SELECTS ONLY A MAXIMUM TABLE OF IROW POINTS. THEREFORE THE ATSM 400
C           USER OUGHT TO CHECK CORRESPONDENCE BETWEEN TABLE (ARG,VAL) ATSM 410
C           AND ITS DIMENSION BY COMPARISON OF NDIM AND IROW, IN ORDER ATSM 420
C           TO GET CORRECT RESULTS IN FURTHER WORK WITH TABLE (ARG,VAL).ATSM 430
C           THIS TEST MAY BE DONE BEFORE OR AFTER CALLING              ATSM 440
C           SUBROUTINE ATSM.                                           ATSM 450
C           SUBROUTINE ATSM ESPECIALLY CAN BE USED FOR GENERATING THE  ATSM 460
C           TABLE (ARG,VAL) NEEDED IN SUBROUTINES ALI, AHI, AND ACFI.  ATSM 470
C                                                                      ATSM 480
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 ATSM 490
C           NONE                                                       ATSM 500
C                                                                      ATSM 510
C        METHOD                                                        ATSM 520
C           SELECTION IS DONE BY SEARCHING THE SUBSCRIPT J OF THAT     ATSM 530
C           ARGUMENT, WHICH IS NEXT TO X (BINARY SEARCH).              ATSM 540
C           AFTERWARDS NEIGHBOURING ARGUMENT VALUES ARE TESTED AND     ATSM 550
C           SELECTED IN THE ABOVE SENSE.                               ATSM 560
C                                                                      ATSM 570
C     ..................................................................ATSM 580
C                                                                      ATSM 590
      SUBROUTINE ATSM(X,Z,F,IROW,ICOL,ARG,VAL,NDIM)                    ATSM 600
C                                                                      ATSM 610
C                                                                      ATSM 620
      DIMENSION Z(1),F(1),ARG(1),VAL(1)                                ATSM 630
C                                                                      ATSM 640
C     CASE IROW=1 IS CHECKED OUT                                       ATSM 650
      IF(IROW-1)23,21,1                                                ATSM 660
    1 N=NDIM                                                           ATSM 670
C                                                                      ATSM 680
C     IF N IS GREATER THAN IROW, N IS SET EQUAL TO IROW.               ATSM 690
      IF(N-IROW)3,3,2                                                  ATSM 700
    2 N=IROW                                                           ATSM 710
C                                                                      ATSM 720
C     CASE IROW.GE.2                                                   ATSM 730
C     SEARCHING FOR SUBSCRIPT J SUCH THAT Z(J) IS NEXT TO X.           ATSM 740
    3 IF(Z(IROW)-Z(1))5,4,4                                            ATSM 750
    4 J=IROW                                                           ATSM 760
      I=1                                                              ATSM 770
      GOTO 6                                                           ATSM 780
    5 I=IROW                                                           ATSM 790
      J=1                                                              ATSM 800
    6 K=(J+I)/2                                                        ATSM 810
      IF(X-Z(K))7,7,8                                                  ATSM 820
    7 J=K                                                              ATSM 830
      GOTO 9                                                           ATSM 840
    8 I=K                                                              ATSM 850
    9 IF(IABS(J-I)-1)10,10,6                                           ATSM 860
   10 IF(ABS(Z(J)-X)-ABS(Z(I)-X))12,12,11                              ATSM 870
   11 J=I                                                              ATSM 880
C                                                                      ATSM 890
C     TABLE SELECTION                                                  ATSM 900
   12 K=J                                                              ATSM 910
      JL=0                                                             ATSM 920
      JR=0                                                             ATSM 930
      DO 20 I=1,N                                                      ATSM 940
      ARG(I)=Z(K)                                                      ATSM 950
      IF(ICOL-1)14,14,13                                               ATSM 960
   13 VAL(2*I-1)=F(K)                                                  ATSM 970
      KK=K+IROW                                                        ATSM 980
      VAL(2*I)=F(KK)                                                   ATSM 990
      GOTO 15                                                          ATSM1000
   14 VAL(I)=F(K)                                                      ATSM1010
   15 JJR=J+JR                                                         ATSM1020
      IF(JJR-IROW)16,18,18                                             ATSM1030
   16 JJL=J-JL                                                         ATSM1040
      IF(JJL-1)19,19,17                                                ATSM1050
   17 IF(ABS(Z(JJR+1)-X)-ABS(Z(JJL-1)-X))19,19,18                      ATSM1060
   18 JL=JL+1                                                          ATSM1070
      K=J-JL                                                           ATSM1080
      GOTO 20                                                          ATSM1090
   19 JR=JR+1                                                          ATSM1100
      K=J+JR                                                           ATSM1110
   20 CONTINUE                                                         ATSM1120
      RETURN                                                           ATSM1130
C                                                                      ATSM1140
C     CASE IROW=1                                                      ATSM1150
   21 ARG(1)=Z(1)                                                      ATSM1160
      VAL(1)=F(1)                                                      ATSM1170
      IF(ICOL-2)23,22,23                                               ATSM1180
   22 VAL(2)=F(2)                                                      ATSM1190
   23 RETURN                                                           ATSM1200
      END                                                              ATSM1210
                                                                       ATSM1220
```

```
C                                                                       DTSM  10
C     ...................................................................DTSM  20
C                                                                       DTSM  30
C        SUBROUTINE DATSM                                               DTSM  40
C                                                                       DTSM  50
C        PURPOSE                                                        DTSM  60
C           NDIM POINTS OF A GIVEN TABLE WITH MONOTONIC ARGUMENTS ARE   DTSM  70
C           SELECTED AND ORDERED SUCH THAT                              DTSM  80
C           ABS(ARG(I)-X).GE.ABS(ARG(J)-X) IF I.GT.J.                   DTSM  90
C                                                                       DTSM 100
C        USAGE                                                          DTSM 110
C           CALL DATSM (X,Z,F,IROW,ICOL,ARG,VAL,NDIM)                   DTSM 120
C                                                                       DTSM 130
C        DESCRIPTION OF PARAMETERS                                      DTSM 140
C           X      - DOUBLE PRECISION SEARCH ARGUMENT.                  DTSM 150
C           Z      - DOUBLE PRECISION VECTOR OF ARGUMENT VALUES (DIMEN- DTSM 160
C                    SION IROW). THE ARGUMENT VALUES MUST BE STORED IN  DTSM 170
C                    INCREASING OR DECREASING SEQUENCE.                 DTSM 180
C           F      - IN CASE ICOL=1, F IS THE DOUBLE PRECISION VECTOR   DTSM 190
C                    OF FUNCTION VALUES (DIMENSION IROW).               DTSM 200
C                    IN CASE ICOL=2, F IS A DOUBLE PRECISION IROW BY 2  DTSM 210
C                    MATRIX. THE FIRST COLUMN SPECIFIES VECTOR OF FUNC- DTSM 220
C                    TION VALUES AND THE SECOND VECTOR OF DERIVATIVES.  DTSM 230
C           IROW   - THE DIMENSION OF VECTOR Z AND OF EACH COLUMN       DTSM 240
C                    IN MATRIX F.                                       DTSM 250
C           ICOL   - THE NUMBER OF COLUMNS IN F (I.E. 1 OR 2).          DTSM 260
C           ARG    - RESULTING DOUBLE PRECISION VECTOR OF SELECTED AND  DTSM 270
C                    ORDERED ARGUMENT VALUES (DIMENSION NDIM).          DTSM 280
C           VAL    - RESULTING DOUBLE PRECISION VECTOR OF SELECTED      DTSM 290
C                    FUNCTION VALUES (DIMENSION NDIM) IN CASE ICOL=1.   DTSM 300
C                    IN CASE ICOL=2, VAL IS THE DOUBLE PRECISION VECTOR DTSM 310
C                    OF FUNCTION AND DERIVATIVE VALUES (DIMENSION       DTSM 320
C                    2*NDIM) WHICH ARE STORED IN PAIRS (I.E. EACH FUNC- DTSM 330
C                    TION VALUE IS FOLLOWED BY ITS DERIVATIVE VALUE).   DTSM 340
C           NDIM   - THE NUMBER OF POINTS WHICH MUST BE SELECTED OUT OF DTSM 350
C                    THE GIVEN TABLE (Z,F).                             DTSM 360
C                                                                       DTSM 370
C        REMARKS                                                        DTSM 380
C           NO ACTION IN CASE IROW LESS THAN 1.                         DTSM 390
C           IF INPUT VALUE NDIM IS GREATER THAN IROW, THE PROGRAM       DTSM 400
C           SELECTS ONLY A MAXIMUM TABLE OF IROW POINTS. THEREFORE THE  DTSM 410
C           USER OUGHT TO CHECK CORRESPONDENCE BETWEEN TABLE (ARG,VAL)  DTSM 420
C           AND ITS DIMENSION BY COMPARISON OF NDIM AND IROW, IN ORDER  DTSM 430
C           TO GET CORRECT RESULTS IN FURTHER WORK WITH TABLE (ARG,VAL). DTSM 440
C           THIS TEST MAY BE DONE BEFORE OR AFTER CALLING               DTSM 450
C           SUBROUTINE DATSM.                                           DTSM 460
C           SUBROUTINE DATSM ESPECIALLY CAN BE USED FOR GENERATING THE  DTSM 470
C           TABLE (ARG,VAL) NEEDED IN SUBROUTINES DALI, DAHI, AND DACFI.DTSM 480
C                                                                       DTSM 490
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTSM 500
C           NONE                                                        DTSM 510
C                                                                       DTSM 520
C        METHOD                                                         DTSM 530
C           SELECTION IS DONE BY SEARCHING THE SUBSCRIPT J OF THAT      DTSM 540
C           ARGUMENT, WHICH IS NEXT TO X (BINARY SEARCH).               DTSM 550
C           AFTERWARDS NEIGHBOURING ARGUMENT VALUES ARE TESTED AND      DTSM 560
C           SELECTED IN THE ABOVE SENSE.                                DTSM 570
C                                                                       DTSM 580
C     ...................................................................DTSM 590
C                                                                       DTSM 600
      SUBROUTINE DATSM(X,Z,F,IROW,ICOL,ARG,VAL,NDIM)                    DTSM 610
C                                                                       DTSM 620
C                                                                       DTSM 630
      DIMENSION Z(1),F(1),ARG(1),VAL(1)                                 DTSM 640
      DOUBLE PRECISION X,Z,F,ARG,VAL                                    DTSM 650
C                                                                       DTSM 660
C     CASE IROW=1 IS CHECKED OUT                                        DTSM 670
      IF(IROW-1)23,21,1                                                 DTSM 680
    1 N=NDIM                                                            DTSM 690
C                                                                       DTSM 700
C     IF N IS GREATER THAN IROW, N IS SET EQUAL TO IROW.                DTSM 710
      IF(N-IROW)3,3,2                                                   DTSM 720
    2 N=IROW                                                            DTSM 730
C                                                                       DTSM 740
C     CASE IROW.GE.2                                                    DTSM 750
C     SEARCHING FOR SUBSCRIPT J SUCH THAT Z(J) IS NEXT TO X.            DTSM 760
    3 IF(Z(IROW)-Z(1))5,4,4                                             DTSM 770
    4 J=IROW                                                            DTSM 780
      I=1                                                               DTSM 790
      GOTO 6                                                            DTSM 800
    5 I=IROW                                                            DTSM 810
      J=1                                                               DTSM 820
    6 K=(J+I)/2                                                         DTSM 830
      IF(X-Z(K))7,7,8                                                   DTSM 840
    7 J=K                                                               DTSM 850
      GOTO 9                                                            DTSM 860
    8 I=K                                                               DTSM 870
    9 IF(IABS(J-I)-1)10,10,6                                            DTSM 880
   10 IF(DABS(Z(J)-X)-DABS(Z(I)-X))12,12,11                             DTSM 890
   11 J=I                                                               DTSM 900
C                                                                       DTSM 910
C     TABLE SELECTION                                                   DTSM 920
   12 K=J                                                               DTSM 930
      JL=0                                                              DTSM 940
      JR=0                                                              DTSM 950
      DO 20 I=1,N                                                       DTSM 960
      ARG(I)=Z(K)                                                       DTSM 970
      IF(ICOL-1)14,14,13                                                DTSM 980
   13 VAL(2*I-1)=F(K)                                                   DTSM 990
      KK=K+IROW                                                         DTSM1000
      VAL(2*I)=F(KK)                                                    DTSM1010
      GOTO 15                                                           DTSM1020
   14 VAL(I)=F(K)                                                       DTSM1030
   15 JJR=J+JR                                                          DTSM1040
      IF(JJR-IROW)16,18,18                                              DTSM1050
   16 JJL=J-JL                                                          DTSM1060
      IF(JJL-1)19,19,17                                                 DTSM1070
   17 IF(DABS(Z(JJR+1)-X)-DABS(Z(JJL-1)-X))19,19,18                     DTSM1080
   18 JL=JL+1                                                           DTSM1090
      K=J-JL                                                            DTSM1100
      GOTO 20                                                           DTSM1110
   19 JR=JR+1                                                           DTSM1120
      K=J+JR                                                            DTSM1130
   20 CONTINUE                                                          DTSM1140
      RETURN                                                            DTSM1150
C                                                                       DTSM1160
C     CASE IROW=1                                                       DTSM1170
   21 ARG(1)=Z(1)                                                       DTSM1180
      VAL(1)=F(1)                                                       DTSM1190
      IF(ICOL-2)23,22,23                                                DTSM1200
   22 VAL(2)=F(2)                                                       DTSM1210
   23 RETURN                                                            DTSM1220
      END                                                               DTSM1230
```

Subroutines ATSE and DATSE

These subroutines perform a table selection out of a given equidistant table. They have the same function as subroutines ATSG and DATSG with the difference that the given table is stored with equidistant arguments. Instead of vector Z of argument values, subroutines ATSE and DATSE need only the starting argument z_s and the increment of arguments dz.

Selection is done in two parts. In the first part, the subscript i_1 of the argument next to search argument x is computed, using the formula

$$i_1 = \left[\frac{x - z_s}{dz} + 1.5 \right]$$

where [a] means "integer part of a".

The second part starts at z_{i_1} and goes one step to the left (right), one to the right (left), and so on until all n arguments are selected. Care must be taken that none of the selected subscripts i_j becomes greater than irow or less than one. In the example shown in Figure 24, the sequence (z_{i_j}) becomes

$z_{i_1} = z_6$, $z_{i_2} = z_5$, $z_{i_3} = z_7$, $z_{i_4} = z_4$, $z_{i_5} = z_8$, $z_{i_6} = z_3$, $z_{i_7} = z_2$.

The selected table is stored in the same way as in subroutine ATSG or DATSG.

If, by a user error, the dimension n of the table to be selected is greater than the dimension irow of the given table, the procedure selects only a maximum table of irow points. In order to avoid errors in further work with table (ARG, VAL), the user ought to check the correspondence between the selected table and its dimension by comparison of n and irow. This test may be done before or after calling subroutine ATSE or DATSE.

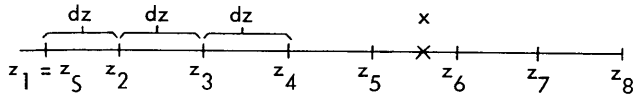


Figure 24. Generation of sequence (z_{i_j}) in case irow=8, n=7

```
C                                                                       ATSE  10
C     ...................................................................ATSE  20
C                                                                       ATSE  30
C        SUBROUTINE ATSE                                                ATSE  40
C                                                                       ATSE  50
C        PURPOSE                                                        ATSE  60
C           NDIM POINTS OF A GIVEN TABLE WITH EQUIDISTANT ARGUMENTS ARE ATSE  70
C           SELECTED AND ORDERED SUCH THAT                              ATSE  80
C           ABS(ARG(I)-X).GE.ABS(ARG(J)-X) IF I.GT.J.                   ATSE  90
C                                                                       ATSE 100
C        USAGE                                                          ATSE 110
C           CALL ATSE (X,ZS,DZ,F,IROW,ICOL,ARG,VAL,NDIM)                ATSE 120
C                                                                       ATSE 130
C        DESCRIPTION OF PARAMETERS                                      ATSE 140
C           X      - THE SEARCH ARGUMENT.                               ATSE 150
C           ZS     - THE STARTING VALUE OF ARGUMENTS.                   ATSE 160
C           DZ     - THE INCREMENT OF ARGUMENT VALUES.                  ATSE 170
C           F      - IN CASE ICOL=1, F IS THE VECTOR OF FUNCTION VALUES ATSE 180
C                    (DIMENSION IROW).                                  ATSE 190
C                    IN CASE ICOL=2, F IS AN IROW BY 2 MATRIX. THE FIRSTATSE 200
C                    COLUMN SPECIFIES THE VECTOR OF FUNCTION VALUES AND ATSE 210
C                    THE SECOND THE VECTOR OF DERIVATIVES.              ATSE 220
C           IROW   - THE DIMENSION OF EACH COLUMN IN MATRIX F.          ATSE 230
C           ICOL   - THE NUMBER OF COLUMNS IN F (I.E. 1 OR 2).          ATSE 240
C           ARG    - THE RESULTING VECTOR OF SELECTED AND ORDERED       ATSE 250
C                    ARGUMENT VALUES (DIMENSION NDIM).                  ATSE 260
C           VAL    - THE RESULTING VECTOR OF SELECTED FUNCTION VALUES   ATSE 270
C                    (DIMENSION NDIM) IN CASE ICOL=1. IN CASE ICOL=2,   ATSE 280
C                    VAL IS THE VECTOR OF FUNCTION AND DERIVATIVE VALUESATSE 290
C                    (DIMENSION 2*NDIM) WHICH ARE STORED IN PAIRS (I.E. ATSE 300
C                    EACH FUNCTION VALUE IS FOLLOWED BY ITS DERIVATIVE  ATSE 310
C                    VALUE).                                            ATSE 320
C           NDIM   - THE NUMBER OF POINTS WHICH MUST BE SELECTED OUT OF ATSE 330
C                    THE GIVEN TABLE.                                   ATSE 340
C                                                                       ATSE 350
C        REMARKS                                                        ATSE 360
C           NO ACTION IN CASE IROW LESS THAN 1.                         ATSE 370
C           IF INPUT VALUE NDIM IS GREATER THAN IROW, THE PROGRAM       ATSE 380
C           SELECTS ONLY A MAXIMUM TABLE OF IROW POINTS.  THEREFORE THE ATSE 390
C           USER OUGHT TO CHECK CORRESPONDENCE BETWEEN TABLE (ARG,VAL)  ATSE 400
C           AND ITS DIMENSION BY COMPARISON OF NDIM AND IROW, IN ORDER  ATSE 410
C           TO GET CORRECT RESULTS IN FURTHER WORK WITH TABLE (ARG,VAL).ATSE 420
C           THIS TEST MAY BE DONE BEFORE OR AFTER CALLING               ATSE 430
C           SUBROUTINE ATSE.                                            ATSE 440
C           SUBROUTINE ATSE ESPECIALLY CAN BE USED FOR GENERATING THE   ATSE 450
C           TABLE (ARG,VAL) NEEDED IN SUBROUTINES ALI, AHI, AND ACFI.   ATSE 460
C                                                                       ATSE 470
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ATSE 480
C           NONE                                                        ATSE 490
C                                                                       ATSE 500
C        METHOD                                                         ATSE 510
C           SELECTION IS DONE BY COMPUTING THE SUBSCRIPT J OF THAT      ATSE 520
C           ARGUMENT, WHICH IS NEXT TO X.                               ATSE 530
C           AFTERWARDS NEIGHBOURING ARGUMENT VALUES ARE TESTED AND      ATSE 540
C           SELECTED IN THE ABOVE SENSE.                                ATSE 550
C                                                                       ATSE 560
C     ...................................................................ATSE 570
C                                                                       ATSE 580
      SUBROUTINE ATSE(X,ZS,DZ,F,IROW,ICOL,ARG,VAL,NDIM)                 ATSE 590
C                                                                       ATSE 600
C                                                                       ATSE 610
      DIMENSION F(1),ARG(1),VAL(1)                                      ATSE 620
      IF(IROW-1)19,17,1                                                 ATSE 630
C                                                                       ATSE 640
C     CASE DZ=0 IS CHECKED OUT                                          ATSE 650
    1 IF(DZ)2,17,2                                                      ATSE 660
    2 N=NDIM                                                            ATSE 670
C                                                                       ATSE 680
C     IF N IS GREATER THAN IROW, N IS SET EQUAL TO IROW.                ATSE 690
      IF(N-IROW)4,4,3                                                   ATSE 700
    3 N=IROW                                                            ATSE 710
C                                                                       ATSE 720
C     COMPUTATION OF STARTING SUBSCRIPT J.                              ATSE 730
    4 J=(X-ZS)/DZ+1.5                                                   ATSE 740
      IF(J)5,5,6                                                        ATSE 750
    5 J=1                                                               ATSE 760
    6 IF(J-IROW)8,8,7                                                   ATSE 770
    7 J=IROW                                                            ATSE 780
C                                                                       ATSE 790
C     GENERATION OF TABLE ARG,VAL IN CASE DZ.NE.0.                      ATSE 800
    8 II=J                                                              ATSE 810
      JL=0                                                              ATSE 820
      JR=0                                                              ATSE 830
      DO 16 I=1,N                                                       ATSE 840
      ARG(I)=ZS+FLOAT(II-1)*DZ                                          ATSE 850
      IF(ICOL-2)9,10,10                                                 ATSE 860
    9 VAL(I)=F(II)                                                      ATSE 870
      GOTO 11                                                           ATSE 880
   10 VAL(2*I-1)=F(II)                                                  ATSE 890
      III=II+IROW                                                       ATSE 900
      VAL(2*I)=F(III)                                                   ATSE 910
   11 IF(J+JR-IROW)12,15,12                                             ATSE 920
   12 IF(J-JL-1)13,14,13                                                ATSE 930
   13 IF((ARG(I)-X)*DZ)14,15,15                                         ATSE 940
   14 JR=JR+1                                                           ATSE 950
      II=J+JR                                                           ATSE 960
      GOTO 16                                                           ATSE 970
   15 JL=JL+1                                                           ATSE 980
      II=J-JL                                                           ATSE 990
   16 CONTINUE                                                          ATSE1000
      RETURN                                                            ATSE1010
C                                                                       ATSE1020
C     CASE DZ=0                                                         ATSE1030
   17 ARG(1)=ZS                                                         ATSE1040
      VAL(1)=F(1)                                                       ATSE1050
      IF(ICOL-2)19,19,18                                                ATSE1060
   18 VAL(2)=F(2)                                                       ATSE1070
   19 RETURN                                                            ATSE1080
      END                                                               ATSE1090
```

```
C                                                                       DTSE  10
C     ...................................................................DTSE  20
C                                                                       DTSE  30
C        SUBROUTINE DATSE                                               DTSE  40
C                                                                       DTSE  50
C        PURPOSE                                                        DTSE  60
C           NDIM POINTS OF A GIVEN TABLE WITH EQUIDISTANT ARGUMENTS ARE DTSE  70
C           SELECTED AND ORDERED SUCH THAT                              DTSE  80
C           ABS(ARG(I)-X).GE.ABS(ARG(J)-X) IF I.GT.J.                   DTSE  90
C                                                                       DTSE 100
C        USAGE                                                          DTSE 110
C           CALL DATSE (X,ZS,DZ,F,IROW,ICOL,ARG,VAL,NDIM)               DTSE 120
C                                                                       DTSE 130
C        DESCRIPTION OF PARAMETERS                                      DTSE 140
C           X      - DOUBLE PRECISION SEARCH ARGUMENT.                  DTSE 150
C           ZS     - DOUBLE PRECISION STARTING VALUE OF ARGUMENTS.      DTSE 160
C           DZ     - DOUBLE PRECISION INCREMENT OF ARGUMENT VALUES.     DTSE 170
C           F      - IN CASE ICOL=1, F IS THE DOUBLE PRECISION VECTOR   DTSE 180
C                    OF FUNCTION VALUES (DIMENSION IROW).               DTSE 190
C                    IN CASE ICOL=2, F IS A DOUBLE PRECISION IROW BY 2  DTSE 200
C                    MATRIX. THE FIRST COLUMN SPECIFIES VECTOR OF FUNC- DTSE 210
C                    TION VALUES AND THE SECOND VECTOR OF DERIVATIVES.  DTSE 220
C           IROW   - THE DIMENSION OF EACH COLUMN IN MATRIX F.          DTSE 230
C           ICOL   - THE NUMBER OF COLUMNS IN F (I.E. 1 OR 2).          DTSE 240
C           ARG    - RESULTING DOUBLE PRECISION VECTOR OF SELECTED AND  DTSE 250
C                    ORDERED ARGUMENT VALUES (DIMENSION NDIM).          DTSE 260
C           VAL    - RESULTING DOUBLE PRECISION VECTOR OF SELECTED      DTSE 270
C                    FUNCTION VALUES (DIMENSION NDIM) IN CASE ICOL=1.   DTSE 280
C                    IN CASE ICOL=2, VAL IS THE DOUBLE PRECISION VECTOR DTSE 290
C                    OF FUNCTION AND DERIVATIVE VALUES (DIMENSION       DTSE 300
C                    2*NDIM) WHICH ARE STORED IN PAIRS (I.E. EACH FUNC- DTSE 310
C                    TION VALUE IS FOLLOWED BY ITS DERIVATIVE VALUE).   DTSE 320
C           NDIM   - THE NUMBER OF POINTS WHICH MUST BE SELECTED OUT OF DTSE 330
C                    THE GIVEN TABLE.                                   DTSE 340
C                                                                       DTSE 350
C        REMARKS                                                        DTSE 360
C           NO ACTION IN CASE IROW LESS THAN 1.                         DTSE 370
C           IF INPUT VALUE NDIM IS GREATER THAN IROW, THE PROGRAM       DTSE 380
C           SELECTS ONLY A MAXIMUM TABLE OF IROW POINTS.  THEREFORE THE DTSE 390
C           USER OUGHT TO CHECK CORRESPONDENCE BETWEEN TABLE (ARG,VAL)  DTSE 400
C           AND ITS DIMENSION BY COMPARISON OF NDIM AND IROW, IN ORDER  DTSE 410
C           TO GET CORRECT RESULTS IN FURTHER WORK WITH TABLE (ARG,VAL).DTSE 420
C           THIS TEST MAY BE DONE BEFORE OR AFTER CALLING               DTSE 430
C           SUBROUTINE DATSE.                                           DTSE 440
C           SUBROUTINE DATSE ESPECIALLY CAN BE USED FOR GENERATING THE  DTSE 450
C           TABLE (ARG,VAL) NEEDED IN SUBROUTINES DALI, DAHI, AND DACFI.DTSE 460
C                                                                       DTSE 470
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTSE 480
C           NONE                                                        DTSE 490
C                                                                       DTSE 500
C        METHOD                                                         DTSE 510
C           SELECTION IS DONE BY COMPUTING THE SUBSCRIPT J OF THAT      DTSE 520
C           ARGUMENT, WHICH IS NEXT TO X.                               DTSE 530
C           AFTERWARDS NEIGHBOURING ARGUMENT VALUES ARE TESTED AND      DTSE 540
C           SELECTED IN THE ABOVE SENSE.                                DTSE 550
C                                                                       DTSE 560
C     ...................................................................DTSE 570
C                                                                       DTSE 580
      SUBROUTINE DATSE(X,ZS,DZ,F,IROW,ICOL,ARG,VAL,NDIM)                DTSE 590
C                                                                       DTSE 600
C                                                                       DTSE 610
      DIMENSION F(1),ARG(1),VAL(1)                                      DTSE 620
      DOUBLE PRECISION X,ZS,DZ,F,ARG,VAL                                DTSE 630
      IF(IROW-1)19,17,1                                                 DTSE 640
C                                                                       DTSE 650
C     CASE DZ=0 IS CHECKED OUT                                          DTSE 660
    1 IF(DZ)2,17,2                                                      DTSE 670
    2 N=NDIM                                                            DTSE 680
C                                                                       DTSE 690
C     IF N IS GREATER THAN IROW, N IS SET EQUAL TO IROW.                DTSE 700
      IF(N-IROW)4,4,3                                                   DTSE 710
    3 N=IROW                                                            DTSE 720
C                                                                       DTSE 730
C     COMPUTATION OF STARTING SUBSCRIPT J.                              DTSE 740
    4 J=(X-ZS)/DZ+1.500                                                 DTSE 750
      IF(J)5,5,6                                                        DTSE 760
    5 J=1                                                               DTSE 770
    6 IF(J-IROW)8,8,7                                                   DTSE 780
    7 J=IROW                                                            DTSE 790
C                                                                       DTSE 800
C     GENERATION OF TABLE ARG,VAL IN CASE DZ.NE.0.                      DTSE 810
    8 II=J                                                              DTSE 820
      JL=0                                                              DTSE 830
      JR=0                                                              DTSE 840
      DO 16 I=1,N                                                       DTSE 850
      ARG(I)=ZS+DFLOAT(II-1)*DZ                                         DTSE 860
      IF(ICOL-2)9,10,10                                                 DTSE 870
    9 VAL(I)=F(II)                                                      DTSE 880
      GOTO 11                                                           DTSE 890
   10 VAL(2*I-1)=F(II)                                                  DTSE 900
      III=II+IROW                                                       DTSE 910
      VAL(2*I)=F(III)                                                   DTSE 920
   11 IF(J+JR-IROW)12,15,12                                             DTSE 930
   12 IF(J-JL-1)13,14,13                                                DTSE 940
   13 IF((ARG(I)-X)*DZ)14,15,15                                         DTSE 950
   14 JR=JR+1                                                           DTSE 960
      II=J+JR                                                           DTSE 970
      GOTO 16                                                           DTSE 980
   15 JL=JL+1                                                           DTSE 990
      II=J-JL                                                           DTSE1000
   16 CONTINUE                                                          DTSE1010
      RETURN                                                            DTSE1020
C                                                                       DTSE1030
C     CASE DZ=0                                                         DTSE1040
   17 ARG(1)=ZS                                                         DTSE1050
      VAL(1)=F(1)                                                       DTSE1060
      IF(ICOL-2)19,19,18                                                DTSE1070
   18 VAL(2)=F(2)                                                       DTSE1080
   19 RETURN                                                            DTSE1090
      END                                                               DTSE1100
```

Subroutine SG13 and DSG13

These subroutines compute a vector $Z = (z_1, \ldots, z_n)$ of smoothed function values, given vectors $X = (x_1, \ldots, x_n)$ of argument values and $Y = (y_1, \ldots, y_n)$ of corresponding function values. Except at the endpoints x_1 and x_n, each smoothed value z_i is obtained by evaluating at x_i the least-squares polynomial of degree 1 relevant to the three successive points (x_{i-1}, y_{i-1}), (x_i, y_i), and (x_{i+1}, y_{i+1}).

1. Mathematical background

For $i = 3, \ldots, n$ we must find m_i and b_i such that

$$w_i(x) = m_i x + b_i \tag{1}$$

gives the least-squares fit to the points (x_{i-1}, y_{i-2}), (x_{i-1}, y_{i-1}), and (x_i, y_i). The problem, then, is to minimize

$$F(m_i, b_i) = \sum_{k=0}^{2} \left[w_i(x_{i-k}) - y_{i-k} \right]^2$$

This minimum will occur when

$$\frac{\partial F}{\partial b_i} = 0 \text{ and } \frac{\partial F}{\partial m_i} = 0 \tag{2}$$

Now

$$\left.\begin{aligned} \frac{\partial F}{\partial b_i} &= 2 \sum_{k=0}^{2} \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \text{and} \\ \frac{\partial F}{\partial m_i} &= 2 \sum_{k=0}^{2} x_{i-k} \left[w_i(x_{i-k}) - y_{i-k} \right] \end{aligned}\right\} \tag{3}$$

Solving equations (2) and (3) yields:

$$m_i = \frac{\sum_{k=0}^{2} x_{i-k}\, y_{i-k} - 1/3 \left(\sum_{k=0}^{2} x_{i-k} \right) \left(\sum_{k=0}^{2} y_{i-k} \right)}{\sum_{k=0}^{2} x_{i-k}^2 - 1/3 \left(\sum_{k=0}^{2} x_{i-k} \right)^2} \tag{4}$$

and

$$b_i = \frac{i}{3} \sum_{k=0}^{2} \left(y_{i-k} - m_i x_{i-k} \right) \tag{5}$$

Letting:

$$\left.\begin{aligned} \bar{y}_i &= \frac{i}{3} \sum_{k=0}^{2} y_{i-k}, \quad \bar{x}_i = \frac{i}{3} \sum_{k=0}^{2} x_{i-k}, \\ t_{i,k} &= x_{i-k} - \bar{x}_i \quad \text{and} \quad v_{i,k} = y_{i-k} - \bar{y}_i \end{aligned}\right\} \tag{6}$$

we may rewrite (4) and (5) as:

$$m_i = \frac{\sum_{k=0}^{2} t_{i,k}\, v_{i,k}}{\sum_{k=0}^{2} t_{i,k}^2} \tag{7}$$

and

$$b_i = \bar{y}_i - m_i \bar{x}_i \tag{8}$$

Using (8) in (1) gives

$$w_i(x) = m_i(x - \bar{x}_i) + \bar{y}_i$$

where m_i is as in (7).

The desired smoothed values z_i are given by:

$$z_i = \begin{cases} w_3(x_1) = m_3 t_{3,2} + \bar{y}_3 & \text{if } i=1 \\ w_{i+1}(x_i) = m_{i+1} t_{i+1,1} + \bar{y}_{i+1} & \text{if } i=2, \ldots, n-1 \\ w_n(x_n) = m_n t_{n,0} + \bar{y}_n & \text{if } i=n \end{cases} \tag{9}$$

2. Programming considerations

The subroutines compute the z_i in serial order according to (9). If $n<3$, there is no computation, and the error parameter IER is set to -1. Otherwise IER is set to zero at the end of the computation. The output vector Z can have the same storage allocation as X or Y.

For reference see Hildebrand, F. B., Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp 258-311.

```
C                                                                       SG13  10
C     ******************************************************************SG13  20
C                                                                       SG13  30
C        SUBROUTINE SG13                                                SG13  40
C                                                                       SG13  50
C        PURPOSE                                                        SG13  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN       SG13  70
C           VECTORS OF ARGUMENT VALUES AND CORRESPONDING FUNCTION       SG13  80
C           VALUES.                                                     SG13  90
C                                                                       SG13 100
C        USAGE                                                          SG13 110
C           CALL SG13(X,Y,Z,NDIM,IER)                                   SG13 120
C                                                                       SG13 130
C        DESCRIPTION OF PARAMETERS                                      SG13 140
C           X      -  GIVEN VECTOR OF ARGUMENT VALUES (DIMENSION NDIM)  SG13 150
C           Y      -  GIVEN VECTOR OF FUNCTION VALUES CORRESPONDING TO X SG13 160
C                     (DIMENSION NDIM)                                  SG13 170
C           Z      -  RESULTING VECTOR OF SMOOTHED FUNCTION VALUES      SG13 180
C                     (DIMENSION NDIM)                                  SG13 190
C           NDIM   -  DIMENSION OF VECTORS X,Y,AND Z                    SG13 200
C           IER    -  RESULTING ERROR PARAMETER                         SG13 210
C                     IER = -1  - NDIM IS LESS THAN 3                   SG13 220
C                     IER =  0  - NO ERROR                              SG13 230
C                                                                       SG13 240
C        REMARKS                                                        SG13 250
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               SG13 260
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS X OR Y.  IF  SG13 270
C                X OR Y IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.   SG13 280
C                                                                       SG13 290
C        SUBROUTINES AND SUBPROGRAMS REQUIRED                           SG13 300
C           NONE                                                        SG13 310
C                                                                       SG13 320
C        METHOD                                                         SG13 330
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), EACH SMOOTHED     SG13 340
C           VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE LEAST-     SG13 350
C           SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 3 SUCCESSIVE SG13 360
C           POINTS (X(I+K),Y(I+K)) K = -1,0,1.(SEE HILDEBRAND, F.B.,    SG13 370
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/SG13 380
C           TORONTO/LONDON, 1956, PP.258-311.)                          SG13 390
C                                                                       SG13 400
C     ******************************************************************SG13 410
C                                                                       SG13 420
      SUBROUTINE SG13(X,Y,Z,NDIM,IER)                                   SG13 430
C                                                                       SG13 440
C                                                                       SG13 450
      DIMENSION X(1),Y(1),Z(1)                                          SG13 460
C                                                                       SG13 470
C        TEST OF DIMENSION                                              SG13 480
      IF(NDIM-3)7,1,1                                                   SG13 490
C                                                                       SG13 500
C        START LOOP                                                     SG13 510
    1 DO 6 I=3,NDIM                                                     SG13 520
      XM=.33333333*(X(I-2)+X(I-1)+X(I))                                 SG13 530
      YM=.33333333*(Y(I-2)+Y(I-1)+Y(I))                                 SG13 540
      T1=X(I-2)-XM                                                      SG13 550
      T2=X(I-1)-XM                                                      SG13 560
      T3=X(I)-XM                                                        SG13 570
      XM=T1*T1+T2*T2+T3*T3                                              SG13 580
      IF(XM)3,3,2                                                       SG13 590
    2 XM=(T1*(Y(I-2)-YM)+T2*(Y(I-1)-YM)+T3*(Y(I)-YM))/XM                SG13 600
C                                                                       SG13 610
C        CHECK FIRST POINT                                              SG13 620
    3 IF(I-3)4,4,5                                                      SG13 630
    4 H=XM*T1+YM                                                        SG13 640
      5 Z(I-2)=H                                                        SG13 650
      6 H=XM*T2+YM                                                      SG13 660
C        END OF LOOP                                                    SG13 670
C                                                                       SG13 680
C        UPDATE LAST TWO COMPONENTS                                     SG13 690
      Z(NDIM-1)=H                                                       SG13 700
      Z(NDIM)=XM*T3+YM                                                  SG13 710
      IER=0                                                             SG13 720
      RETURN                                                            SG13 730
C                                                                       SG13 740
C        ERROR EXIT IN CASE NDIM IS LESS THAN 3                         SG13 750
    7 IER=-1                                                            SG13 760
      RETURN                                                            SG13 770
      END                                                               SG13 780
```

```
C                                                                       DSG1  10
C     ******************************************************************DSG1  20
C                                                                       DSG1  30
C        SUBROUTINE DSG13                                               DSG1  40
C                                                                       DSG1  50
C        PURPOSE                                                        DSG1  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN       DSG1  70
C           VECTORS OF ARGUMENT VALUES AND CORRESPONDING FUNCTION       DSG1  80
C           VALUES.                                                     DSG1  90
C                                                                       DSG1 100
C        USAGE                                                          DSG1 110
C           CALL DSG13(X,Y,Z,NDIM,IER)                                  DSG1 120
C                                                                       DSG1 130
C        DESCRIPTION OF PARAMETERS                                      DSG1 140
C           X      -  GIVEN VECTOR OF DOUBLE PRECISION ARGUMENT VALUES  DSG1 150
C                     (DIMENSION NDIM)                                  DSG1 160
C           Y      -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES  DSG1 170
C                     CORRESPONDING TO X (DIMENSION NDIM)               DSG1 180
C           Z      -  RESULTING VECTOR OF DOUBLE PRECISION SMOOTHED     DSG1 190
C                     FUNCTION VALUES (DIMENSION NDIM)                  DSG1 200
C           NDIM   -  DIMENSION OF VECTORS X,Y,AND Z                    DSG1 210
C           IER    -  RESULTING ERROR PARAMETER                         DSG1 220
C                     IER = -1  - NDIM IS LESS THAN 3                   DSG1 230
C                     IER =  0  - NO ERROR                              DSG1 240
C                                                                       DSG1 250
C        REMARKS                                                        DSG1 260
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               DSG1 270
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS X OR Y.  IF  DSG1 280
C                X OR Y IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.   DSG1 290
C                                                                       DSG1 300
C        SUBROUTINES AND SUBPROGRAMS REQUIRED                           DSG1 310
C           NONE                                                        DSG1 320
C                                                                       DSG1 330
C        METHOD                                                         DSG1 340
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), EACH SMOOTHED     DSG1 350
C           VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE LEAST-     DSG1 360
C           SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 3 SUCCESSIVE DSG1 370
C           POINTS (X(I+K),Y(I+K)) K = -1,0,1.(SEE HILDEBRAND, F.B.,    DSG1 380
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/DSG1 390
C           TORONTO/LONDON, 1956, PP.258-311.)                          DSG1 400
C                                                                       DSG1 410
C     ******************************************************************DSG1 420
C                                                                       DSG1 430
      SUBROUTINE DSG13(X,Y,Z,NDIM,IER)                                  DSG1 440
C                                                                       DSG1 450
C                                                                       DSG1 460
      DIMENSION X(1),Y(1),Z(1)                                          DSG1 470
      DOUBLE PRECISION X,Y,Z,XM,YM,T1,T2,T3,H                           DSG1 480
C                                                                       DSG1 490
C        TEST OF DIMENSION                                              DSG1 500
      IF(NDIM-3)7,1,1                                                   DSG1 510
C                                                                       DSG1 520
C        START LOOP                                                     DSG1 530
    1 DO 6 I=3,NDIM                                                     DSG1 540
      XM=.33333333333333333D0*(X(I-2)+X(I-1)+X(I))                     DSG1 550
      YM=.33333333333333333D0*(Y(I-2)+Y(I-1)+Y(I))                     DSG1 560
      T1=X(I-2)-XM                                                      DSG1 570
      T2=Y(I-1)-XM                                                      DSG1 580
      T3=X(I)-XM                                                        DSG1 590
      XM=T1*T1+T2*T2+T3*T3                                              DSG1 600
      IF(XM)3,3,2                                                       DSG1 610
    2 XM=(T1*(Y(I-2)-YM)+T2*(Y(I-1)-YM)+T3*(Y(I)-YM))/XM                DSG1 620
C                                                                       DSG1 630
C        CHECK FIRST POINT                                              DSG1 640
    3 IF(I-3)4,4,5                                                      DSG1 650
    4 H=XM*T1+YM                                                        DSG1 660
      5 Z(I-2)=H                                                        DSG1 670
      6 H=XM*T2+YM                                                      DSG1 680
C        END OF LOOP                                                    DSG1 690
C                                                                       DSG1 700
C        UPDATE LAST TWO COMPONENTS                                     DSG1 710
      Z(NDIM-1)=H                                                       DSG1 720
      Z(NDIM)=XM*T3+YM                                                  DSG1 730
      IER=0                                                             DSG1 740
      RETURN                                                            DSG1 750
C                                                                       DSG1 760
C        ERROR EXIT IN CASE NDIM IS LESS THAN 3                         DSG1 770
    7 IER=-1                                                            DSG1 780
      RETURN                                                            DSG1 790
      END                                                               DSG1 800
```

Subroutines SE13 and DSE13

These subroutines compute a vector $Z = (z_1, \ldots, z_n)$ of smoothed function values, given a vector $Y = (y_1, \ldots, y_n)$ of function values whose entries y_i correspond to n equidistantly spaced argument values x_i, with $x_i - x_{i-1} = h$ for $i = 2, \ldots, n$. Except at the endpoints x_1 and x_n, each smoothed value z_i is obtained by evaluating at x_i the least-squares polynomial of degree 1 relevant to the three successive points (x_{i+k}, y_{i+k}), $k = -1, 0, 1$.

1. Mathematical background

The procedure is exactly that described for subroutines SG13 and DSG13, but here we have the additional relation $x_i - x_{i-1} = h$, a constant, for $i = 2, \ldots, n$. This leads to the following expressions for the z_i:

$$z_i = \begin{cases} \frac{1}{6}(5y_1 + 2y_2 - y_3) & \text{if } i=1 \\ \frac{1}{3}(y_{i-1} + y_i + y_{i+1}) & \text{if } i=2,\ldots,n-1 \\ \frac{1}{6}(-y_{n-2} + 2y_{n-1} + 5y_n) & \text{if } i=n \end{cases} \quad (1)$$

2. Programming considerations

The subroutines compute the z_i in serial order according to (1). If $n < 3$, there is no computation, and the error parameter IER is set to -1. Otherwise IER is set to zero at the end of the computation. The output vector Z can have the same storage allocation as Y.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp 295-302.

```
C                                                                       SE13  10
C     ..................................................................SE13  20
C                                                                       SE13  30
C        SUBROUTINE SE13                                                SE13  40
C                                                                       SE13  50
C        PURPOSE                                                        SE13  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN A     SE13  70
C           VECTOR OF FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO       SE13  80
C           EQUIDISTANTLY SPACED ARGUMENT VALUES.                       SE13  90
C                                                                       SE13 100
C        USAGE                                                          SE13 110
C           CALL SE13(Y,Z,NDIM,IER)                                     SE13 120
C                                                                       SE13 130
C        DESCRIPTION OF PARAMETERS                                      SE13 140
C           Y      -  GIVEN VECTOR OF FUNCTION VALUES (DIMENSION NDIM)  SE13 150
C           Z      -  RESULTING VECTOR OF SMOOTHED FUNCTION VALUES      SE13 160
C                     (DIMENSION NDIM)                                  SE13 170
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      SE13 180
C           IER    -  RESULTING ERROR PARAMETER                         SE13 190
C                     IER = -1  - NDIM IS LESS THAN 3                   SE13 200
C                     IER =  0  - NO ERROR                              SE13 210
C                                                                       SE13 220
C        REMARKS                                                        SE13 230
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               SE13 240
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y     SE13 250
C                IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.          SE13 260
C                                                                       SE13 270
C        SUBROUTINES AND SUBPROGRAMS REQUIRED                           SE13 280
C           NONE                                                        SE13 290
C                                                                       SE13 300
C        METHOD                                                         SE13 310
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    SE13 320
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), EACH SMOOTHED     SE13 330
C           VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE LEAST-     SE13 340
C           SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 3 SUCCESSIVE SE13 350
C           POINTS (X(I+K),Y(I+K)) K = -1,0,1.  (SEE HILDEBRAND, F.B.,  SE13 360
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/ SE13 370
C           TORONTO/LONDON, 1956, PP. 295-302.)                         SE13 380
C                                                                       SE13 390
C     ..................................................................SE13 400
C                                                                       SE13 410
C                                                                       SE13 420
      SUBROUTINE SE13(Y,Z,NDIM,IER)                                     SE13 430
C                                                                       SE13 440
C                                                                       SE13 450
      DIMENSION Y(1),Z(1)                                               SE13 460
C                                                                       SE13 470
C        TEST OF DIMENSION                                              SE13 480
      IF(NDIM-3)3,1,1                                                   SE13 490
C                                                                       SE13 500
C        PREPARE LOOP                                                   SE13 510
    1 B=.1666667*(5.*Y(1)+Y(2)+Y(2)-Y(3))                               SE13 520
      C=.1666667*(5.*Y(NDIM)+Y(NDIM-1)+Y(NDIM-1)-Y(NDIM-2))             SE13 530
C                                                                       SE13 540
C        START LOOP                                                     SE13 550
      DO 2 I=3,NDIM                                                     SE13 560
      A=B                                                               SE13 570
      B=.3333333*(Y(I-2)+Y(I-1)+Y(I))                                   SE13 580
    2 Z(I-2)=A                                                          SE13 590
C        END OF LOOP                                                    SE13 600
C                                                                       SE13 610
C        UPDATE LAST TWO COMPONENTS                                     SE13 620
      Z(NDIM-1)=B                                                       SE13 630
      Z(NDIM)=C                                                         SE13 640
      IER=0                                                             SE13 650
      RETURN                                                            SE13 660
C                                                                       SE13 670
C        ERROR EXIT IN CASE NDIM IS LESS THAN 3                         SE13 680
    3 IER=-1                                                            SE13 690
      RETURN                                                            SE13 700
      END
```

```
C                                                                       DE13  10
C     ..................................................................DE13  20
C                                                                       DE13  30
C        SUBROUTINE DSE13                                               DE13  40
C                                                                       DE13  50
C        PURPOSE                                                        DE13  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN A     DE13  70
C           VECTOR OF FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO       DE13  80
C           EQUIDISTANTLY SPACED ARGUMENT VALUES.                       DE13  90
C                                                                       DE13 100
C        USAGE                                                          DE13 110
C           CALL DSE13(Y,Z,NDIM,IER)                                    DE13 120
C                                                                       DE13 130
C        DESCRIPTION OF PARAMETERS                                      DE13 140
C           Y      -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES  DE13 150
C                     (DIMENSION NDIM)                                  DE13 160
C           Z      -  RESULTING VECTOR OF DOUBLE PRECISION SMOOTHED     DE13 170
C                     FUNCTION VALUES (DIMENSION NDIM)                  DE13 180
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      DE13 190
C           IER    -  RESULTING ERROR PARAMETER                         DE13 200
C                     IER = -1  - NDIM IS LESS THAN 3                   DE13 210
C                     IER =  0  - NO ERROR                              DE13 220
C                                                                       DE13 230
C        REMARKS                                                        DE13 240
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               DE13 250
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y     DE13 260
C                IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.          DE13 270
C                                                                       DE13 280
C        SUBROUTINES AND SUBPROGRAMS REQUIRED                           DE13 290
C           NONE                                                        DE13 300
C                                                                       DE13 310
C        METHOD                                                         DE13 320
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    DE13 330
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), EACH SMOOTHED     DE13 340
C           VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE LEAST-     DE13 350
C           SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 3 SUCCESSIVE DE13 360
C           POINTS (X(I+K),Y(I+K)) K = -1,0,1.  (SEE HILDEBRAND, F.B.,  DE13 370
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/ DE13 380
C           TORONTO/LONDON, 1956, PP. 295-302.)                         DE13 390
C                                                                       DE13 400
C     ..................................................................DE13 410
C                                                                       DE13 420
      SUBROUTINE DSE13(Y,Z,NDIM,IER)                                    DE13 430
C                                                                       DE13 440
      DIMENSION Y(1),Z(1)                                               DE13 450
      DOUBLE PRECISION Y,Z,A,B,C                                        DE13 460
C                                                                       DE13 470
C        TEST OF DIMENSION                                              DE13 480
      IF(NDIM-3)3,1,1                                                   DE13 490
C                                                                       DE13 500
C        PREPARE LOOP                                                   DE13 510
    1 B=.16666666666666670D0*(5.D0*Y(1)+Y(2)+Y(2)-Y(3))                 DE13 520
      C=.16666666666666667D0*(5.D0*Y(NDIM)+Y(NDIM-1)+Y(NDIM-1)-Y(NDIM-2)) DE13 530
C                                                                       DE13 540
C        START LOOP                                                     DE13 550
      DO 2 I=3,NDIM                                                     DE13 560
      A=B                                                               DE13 570
      B=.33333333333333300D0*(Y(I-2)+Y(I-1)+Y(I))                       DE13 580
    2 Z(I-2)=A                                                          DE13 590
C        END OF LOOP                                                    DE13 600
C                                                                       DE13 610
C        UPDATE LAST TWO COMPONENTS                                     DE13 620
      Z(NDIM-1)=B                                                       DE13 630
      Z(NDIM)=C                                                         DE13 640
      IER=0                                                             DE13 650
      RETURN                                                            DE13 660
C                                                                       DE13 670
C        ERROR EXIT IN CASE NDIM IS LESS THAN 3                         DE13 680
    3 IER=-1                                                            DE13 690
      RETURN                                                            DE13 700
      END                                                               DE13 710
```

Subroutines SE15 and DSE15

These subroutines compute a vector $Z = (z_1, \ldots, z_n)$ of smoothed function values, given a vector $Y = (y_1, \ldots, y_n)$ of function values whose entries y_i correspond to n equidistantly spaced argument values x_i with $x_i - x_{i-1} = h$ for $i = 2, \ldots, n$. Except at the points x_1, x_2, x_{n-1}, and x_n, each smoothed value z_i is obtained by evaluating at x_i the least-squares polynomial of degree 1 relevant to the five successive points (x_{i+k}, y_{i+k}), $k = -2, -1, \ldots, 2$.

1. Mathematical background

For $i = 5, \ldots, n$ we find m_i and b_i such that

$$w_i(x) = m_i x + b_i \tag{1}$$

gives the least-squares fit to the points (x_{i-k}, y_{i-k}), $k=0, \ldots, 4$. The problem, then, is to minimize

$$F(m_i, b_i) = \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right]^2$$

This minimum will occur when

$$\frac{\partial F}{\partial b_i} = 0 \quad \text{and} \quad \frac{\partial F}{\partial m_i} = 0 \tag{2}$$

Now

$$\frac{\partial F}{\partial b_i} = 2 \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right]$$

and

$$\frac{\partial F}{\partial m_i} = 2 \sum_{k=0}^{4} x_{i-k} \left[w_i(x_{i-k}) - y_{i-k} \right] \tag{3}$$

Solving equations (2) and (3) yields:

$$m_i = \frac{\sum_{k=0}^{4} x_{i-k} y_{i-k} - \frac{1}{5} \left(\sum_{k=0}^{4} x_{i-k} \right) \left(\sum_{k=0}^{4} y_{i-k} \right)}{\sum_{k=0}^{4} x_{i-k}^2 - \frac{1}{5} \left(\sum_{k=0}^{4} x_{i-k} \right)^2} \tag{4}$$

and

$$b_i = \frac{1}{5} \sum_{k=0}^{4} \left[y_{i-k} - m_i x_{i-k} \right] \tag{5}$$

Using the fact that $x_j - x_{j-1} = h$, a constant, for $j = 2, \ldots, n$, (4) and (5) may be rewritten as

$$m_i = \frac{1}{10h} (2y_i + y_{i-1} - y_{i-3} - 2y_{i-4}) \tag{6}$$

and

$$b_i = \frac{1}{5} \sum_{k=0}^{4} y_{i-k} - m_i x_{i-2} \tag{7}$$

Using (7) in (1) yields

$$w_i(x) = m_i(x - x_{i-2}) + \frac{1}{5} (y_{i-4} + \ldots + y_i)$$

The desired smoothed function values z_i are given by:

$$z_i = \begin{cases} w_5(x_1) = \frac{1}{5} (3y_1 + 2y_2 + y_3 - y_5) & i=1 \\ w_5(x_2) = \frac{1}{10} (4y_1 + 3y_2 + 2y_3 + y_4) & i=2 \\ w_{i+2}(x_i) = \frac{1}{5} (y_{i-2} + y_{i-1} + y_i + y_{i+1} + y_{i+2}) & i=3, \ldots, n-2 \\ w_n(x_{n-1}) = \frac{1}{10} (y_{n-3} + 2y_{n-2} + 3y_{n-1} + 4y_n) & i=n-1 \\ w_n(x_n) = \frac{1}{5} (-y_{n-4} + y_{n-2} + 2y_{n-1} + 3y_n) & i=n \end{cases} \tag{8}$$

2. Programming considerations

The subroutines compute the z_i in serial order according to (8). If $n < 5$, there is no computation, and the error parameter IER is set to -1. Otherwise IER is set to zero at the end of the computation. The output vector Z can have the same storage allocation as Y.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp 295-302.

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C                                                                       SE15  10
C     ..................................................................SE15  20
C                                                                       SE15  30
C        SUBROUTINE SE15                                                SE15  40
C                                                                       SE15  50
C        PURPOSE                                                        SE15  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN A     SE15  70
C           VECTOR OF FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO       SE15  80
C           EQUIDISTANTLY SPACED ARGUMENT VALUES.                       SE15  90
C                                                                       SE15 100
C        USAGE                                                          SE15 110
C           CALL SE15(Y,Z,NDIM,IER)                                     SE15 120
C                                                                       SE15 130
C        DESCRIPTION OF PARAMETERS                                      SE15 140
C           Y      -  GIVEN VECTOR OF FUNCTION VALUES (DIMENSION NDIM)  SE15 150
C           Z      -  RESULTING VECTOR OF SMOOTHED FUNCTION VALUES      SE15 160
C                     (DIMENSION NDIM)                                  SE15 170
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      SE15 180
C           IER    -  RESULTING ERROR PARAMETER                         SE15 190
C                     IER = -1  - NDIM IS LESS THAN 5                   SE15 200
C                     IER =  0  - NO ERROR                              SE15 210
C                                                                       SE15 220
C        REMARKS                                                        SE15 230
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               SE15 240
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y IS   SE15 250
C                DISTINCT FROM Z, THEN IT IS NOT DESTROYED.             SE15 260
C                                                                       SE15 270
C        SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED                   SE15 280
C           NONE                                                        SE15 290
C                                                                       SE15 300
C        METHOD                                                         SE15 310
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    SE15 320
C           EXCEPT AT THE POINTS X(1),X(2),X(NDIM-1) AND X(NDIM), EACH  SE15 330
C           SMOOTHED VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE   SE15 340
C           LEAST-SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 5      SE15 350
C           SUCCESSIVE POINTS (X(I+K),Y(I+K)) K = -2,-1,...,2.  (SEE    SE15 360
C           HILDEBRAND, F.B., INTRODUCTION TO NUMERICAL ANALYSIS.       SE15 370
C           MC GRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP. 295-302.)  SE15 380
C                                                                       SE15 390
C     ..................................................................SE15 400
C                                                                       SE15 410
      SUBROUTINE SE15(Y,Z,NDIM,IER)                                     SE15 420
C                                                                       SE15 430
C                                                                       SE15 440
      DIMENSION Y(1),Z(1)                                               SE15 450
C                                                                       SE15 460
C        TEST OF DIMENSION                                              SE15 470
      IF(NDIM-5)3,1,1                                                   SE15 480
C                                                                       SE15 490
C        PREPARE LOOP                                                   SE15 500
    1 A=Y(1)+Y(1)                                                       SE15 510
      C=Y(2)+Y(2)                                                       SE15 520
      B=.2*(A+Y(1)+C+Y(3)-Y(5))                                         SE15 530
      C=.1*(A+A+C+Y(2)+Y(3)+Y(3)+Y(4))                                  SE15 540
C                                                                       SE15 550
C        START LOOP                                                     SE15 560
      DO 2 I=5,NDIM                                                     SE15 570
      A=B                                                               SE15 580
      B=C                                                               SE15 590
      C=.2*(Y(I-4)+Y(I-3)+Y(I-2)+Y(I-1)+Y(I))                           SE15 600
    2 Z(I-4)=A                                                          SE15 610
C        END OF LOOP                                                    SE15 620
C                                                                       SE15 630
C        UPDATE LAST FOUR COMPONENTS                                    SE15 640
      A=Y(NDIM)+Y(NDIM)                                                 SE15 650
      A=.1*(A+A+Y(NDIM-1)+Y(NDIM-1)+Y(NDIM-1)+Y(NDIM-2)+Y(NDIM-2)       SE15 660
     1      +Y(NDIM-3))                                                 SE15 670
      Z(NDIM-3)=B                                                       SE15 680
      Z(NDIM-2)=C                                                       SE15 690
      Z(NDIM-1)=A                                                       SE15 700
      Z(NDIM)=A+A-C                                                     SE15 710
      IER=0                                                             SE15 720
      RETURN                                                            SE15 730
C                                                                       SE15 740
C        ERROR EXIT IN CASE NDIM IS LESS THAN 5                         SE15 750
    3 IER=-1                                                            SE15 760
      RETURN                                                            SE15 770
      END                                                               SE15 780
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C                                                                       DE15  10
C     ..................................................................DE15  20
C                                                                       DE15  30
C        SUBROUTINE DSE15                                               DE15  40
C                                                                       DE15  50
C        PURPOSE                                                        DE15  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN A     DE15  70
C           VECTOR OF FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO       DE15  80
C           EQUIDISTANTLY SPACED ARGUMENT VALUES.                       DE15  90
C                                                                       DE15 100
C        USAGE                                                          DE15 110
C           CALL DSE15(Y,Z,NDIM,IER)                                    DE15 120
C                                                                       DE15 130
C        DESCRIPTION OF PARAMETERS                                      DE15 140
C           Y      -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES  DE15 150
C                     (DIMENSION NDIM)                                  DE15 160
C           Z      -  RESULTING VECTOR OF DOUBLE PRECISION SMOOTHED     DE15 170
C                     FUNCTION VALUES (DIMENSION NDIM)                  DE15 180
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      DE15 190
C           IER    -  RESULTING ERROR PARAMETER                         DE15 200
C                     IER = -1  - NDIM IS LESS THAN 5                   DE15 210
C                     IER =  0  - NO ERROR                              DE15 220
C                                                                       DE15 230
C        REMARKS                                                        DE15 240
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               DE15 250
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y IS   DE15 260
C                DISTINCT FROM Z, THEN IT IS NOT DESTROYED.             DE15 270
C                                                                       DE15 280
C        SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED                   DE15 290
C           NONE                                                        DE15 300
C                                                                       DE15 310
C        METHOD                                                         DE15 320
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    DE15 330
C           EXCEPT AT THE POINTS X(1),X(2),X(NDIM-1) AND X(NDIM), EACH  DE15 340
C           SMOOTHED VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE   DE15 350
C           LEAST-SQUARES POLYNOMIAL OF DEGREE 1 RELEVANT TO THE 5      DE15 360
C           SUCCESSIVE POINTS (X(I+K),Y(I+K)) K = -2,-1,...,2.  (SEE    DE15 370
C           HILDEBRAND, F.B., INTRODUCTION TO NUMERICAL ANALYSIS.       DE15 380
C           MC GRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP. 295-302.)  DE15 390
C                                                                       DE15 400
C     ..................................................................DE15 410
C                                                                       DE15 420
      SUBROUTINE DSE15(Y,Z,NDIM,IER)                                    DE15 430
C                                                                       DE15 440
C                                                                       DE15 450
      DIMENSION Y(1),Z(1)                                               DE15 460
      DOUBLE PRECISION Y,Z,A,B,C                                        DE15 470
C                                                                       DE15 480
C        TEST OF DIMENSION                                              DE15 490
      IF(NDIM-5)3,1,1                                                   DE15 500
C                                                                       DE15 510
C        PREPARE LOOP                                                   DE15 520
    1 A=Y(1)+Y(1)                                                       DE15 530
      C=Y(2)+Y(2)                                                       DE15 540
      B=.2D0*(A+Y(1)+C+Y(3)-Y(5))                                       DE15 550
      C=.1D0*(A+A+C+Y(2)+Y(3)+Y(3)+Y(4))                                DE15 560
C                                                                       DE15 570
C        START LOOP                                                     DE15 580
      DO 2 I=5,NDIM                                                     DE15 590
      A=B                                                               DE15 600
      B=C                                                               DE15 610
      C=.2D0*(Y(I-4)+Y(I-3)+Y(I-2)+Y(I-1)+Y(I))                         DE15 620
    2 Z(I-4)=A                                                          DE15 630
C        END OF LOOP                                                    DE15 640
C                                                                       DE15 650
C        UPDATE LAST FOUR COMPONENTS                                    DE15 660
      A=Y(NDIM)+Y(NDIM)                                                 DE15 670
      A=.1D0*(A+A+Y(NDIM-1)+Y(NDIM-1)+Y(NDIM-1)+Y(NDIM-2)+Y(NDIM-2)     DE15 680
     1      +Y(NDIM-3))                                                 DE15 690
      Z(NDIM-3)=B                                                       DE15 700
      Z(NDIM-2)=C                                                       DE15 710
      Z(NDIM-1)=A                                                       DE15 720
      Z(NDIM)=A+A-C                                                     DE15 730
      IER=0                                                             DE15 740
      RETURN                                                            DE15 750
C                                                                       DE15 760
C        ERROR EXIT IN CASE NDIM IS LESS THAN 5                         DE15 770
    3 IER=-1                                                            DE15 780
      RETURN                                                            DE15 790
      END                                                               DE15 800
```

Subroutine SE35 and DSE35

These subroutines compute a vector $Z = (z_1, \ldots, z_n)$ of smoothed function values, given a vector $Y = (y_1, \ldots, y_n)$ of function values whose entries y_i correspond to n equidistantly spaced argument values x_i, with $x_i - x_{i-1} = h$ for $i = 2, \ldots, n$. Except at the points x_1, x_2, x_{n-1}, and x_n, each smoothed value z_i is obtained by evaluating at x_i the least-squares polynomial of degree 3 relevant to the five successive points (x_{i+k}, y_{i+k}), $k = -2, -1, \ldots, 2$.

1. Mathematical background

For $i = 5, \ldots, n$ we must find a_i, b_i, c_i, and d_i such that

$$w_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i \qquad (1)$$

gives the least-squares fit to the points (x_{i-k}, y_{i-k}), $k = 0, \ldots, 4$.

The problem, thus, is to minimize

$$F(a_i, b_i, c_i, d_i) = \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right]^2 \qquad (2)$$

The minimum will occur when

$$\frac{\partial F}{\partial a_i} = \frac{\partial F}{\partial b_i} = \frac{\partial F}{\partial c_i} = \frac{\partial F}{\partial d_i} = 0$$

Now:

$$\left.\begin{aligned} \frac{\partial F}{\partial a_i} &= 2 \sum_{k=0}^{4} x_{i-k}^3 \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \frac{\partial F}{\partial b_i} &= 2 \sum_{k=0}^{4} x_{i-k}^2 \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \frac{\partial F}{\partial c_i} &= 2 \sum_{k=0}^{4} x_{i-k} \left[w_i(x_{i-k}) - y_{i-k} \right] \\ \frac{\partial F}{\partial d_i} &= 2 \sum_{k=0}^{4} \left[w_i(x_{i-k}) - y_{i-k} \right] \end{aligned}\right\} \qquad (3)$$

Solving (2) and (3) for a_i, b_i, c_i, and d_i, with $x_i - x_{i-1} = h$, we get:

$$a_i = A_i$$

$$b_i = -3 A_i x_{i-2} + B_i$$

$$c_i = 3 A_i x_{i-2}^2 - 2 B_i x_{i-2} + C_i$$

$$d_i = -A_i x_{i-2}^3 + B_i x_{i-2}^2 - C_i x_{i-2} + D_i + \bar{y}_i$$

where:

$$\bar{y}_i = \frac{1}{5} \sum_{k=0}^{4} y_{i-k}$$

$$A_i = -\frac{1}{12 h^3} (y_{i-4} - 2y_{i-3} + 2y_{i-1} - y_i)$$

$$B_i = \frac{1}{14 h^2} (4y_{i-4} + y_{i-3} + y_{i-1} + 4y_i - 10 \bar{y}_i)$$

$$C_i = \frac{1}{12h} (y_{i-4} - 8y_{i-3} + 8y_{i-1} - y_i)$$

$$D_i = -\frac{1}{7} (4y_{i-4} + y_{i-3} + y_{i-1} + 4y_i - 10 \bar{y}_i)$$

Finally, the desired smoothed values z_i are given by:

$$z_i = \left\{ \begin{array}{ll} w_5(x_1) = y_1 - \frac{1}{70} \delta^4 y_3 & \text{if } i=1 \\ w_5(x_2) = y_2 + \frac{2}{35} \delta^4 y_3 & \text{if } i=2 \\ w_{i+2}(x_i) = y_i - \frac{3}{35} \delta^4 y_i & \text{if } i=3, \ldots, n-2 \\ w_n(x_{n-1}) = y_{n-1} + \frac{2}{35} \delta^4 y_{n-2} & \text{if } i=n-1 \\ w_n(x_n) = y_n - \frac{1}{70} \delta^4 y_{n-2} & \text{if } i=n \end{array} \right\} \qquad (4)$$

where

$$\delta^4 y_i = y_{i-2} - 4 y_{i-1} + 6y_i - 4y_{i+1} + y_{i+2}$$

for $i=3, \ldots, n-2$

2. Programming considerations

These subroutines compute the z_i in serial order according to (4). If $n < 5$, there is no computation, and the error parameter IER is set to -1. Otherwise IER is set to zero at the end of the computation. The output vector Z can have the same storage allocation as Y.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 295-302.

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C                                                                       SE35  10
C     ..................................................................SE35  20
C                                                                       SE35  30
C        SUBROUTINE SE35                                                SE35  40
C                                                                       SE35  50
C        PURPOSE                                                        SE35  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN A     SE35  70
C           VECTOR OF FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO       SE35  80
C           EQUIDISTANTLY SPACED ARGUMENT VALUES.                       SE35  90
C                                                                       SE35 100
C        USAGE                                                          SE35 110
C           CALL SE35(Y,Z,NDIM,IER)                                     SE35 120
C                                                                       SE35 130
C        DESCRIPTION OF PARAMETERS                                      SE35 140
C           Y      -  GIVEN VECTOR OF FUNCTION VALUES (DIMENSION NDIM)  SE35 150
C           Z      -  RESULTING VECTOR OF SMOOTHED FUNCTION VALUES      SE35 160
C                     (DIMENSION NDIM)                                  SE35 170
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      SE35 180
C           IER    -  RESULTING ERROR PARAMETER                         SE35 190
C                     IER = -1  - NDIM IS LESS THAN 5                   SE35 200
C                     IER =  0  - NO ERROR                              SE35 210
C                                                                       SE35 220
C        REMARKS                                                        SE35 230
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               SE35 240
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y IS  SE35 250
C                DISTINCT FROM Z, THEN IT IS NOT DESTROYED.             SE35 260
C                                                                       SE35 270
C        SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED                   SE35 280
C           NONE                                                        SE35 290
C                                                                       SE35 300
C        METHOD                                                         SE35 310
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    SE35 320
C           EXCEPT AT THE POINTS X(1),X(2),X(NDIM-1) AND X(NDIM), EACH  SE35 330
C           SMOOTHED VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE   SE35 340
C           LEAST-SQUARES POLYNOMIAL OF DEGREE 3 RELEVANT TO THE 5      SE35 350
C           SUCCESSIVE POINTS (X(I+K),Y(I+K)) K = -2,-1,...,2.  (SEE    SE35 360
C           HILDEBRAND, F.B., INTRODUCTION TO NUMERICAL ANALYSIS,       SE35 370
C           MC GRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP. 295-302.)  SE35 380
C                                                                       SE35 390
C     ..................................................................SE35 400
C                                                                       SE35 410
      SUBROUTINE SE35(Y,Z,NDIM,IER)                                     SE35 420
C                                                                       SE35 430
C                                                                       SE35 440
      DIMENSION Y(1),Z(1)                                               SE35 450
C                                                                       SE35 460
C        TEST OF DIMENSION                                              SE35 470
      IF(NDIM-5)6,1,1                                                   SE35 480
C                                                                       SE35 490
C        PREPARE LOOP                                                   SE35 500
    1 B=Y(1)                                                            SE35 510
      C=Y(2)                                                            SE35 520
C                                                                       SE35 530
C        START LOOP                                                     SE35 540
      DO 3 I=5,NDIM                                                     SE35 550
      A=B                                                               SE35 560
      B=C                                                               SE35 570
      C=Y(I-2)                                                          SE35 580
C                                                                       SE35 590
C        GENERATE FOURTH CENTRAL DIFFERENCE                             SE35 600
      D=C-B-Y(I-1)                                                      SE35 610
      D=D+D+C                                                           SE35 620
      D=D+D+A+Y(I)                                                      SE35 630
C                                                                       SE35 640
C        CHECK FIRST TWO COMPONENTS                                     SE35 650
      IF(I-5)2,2,3                                                      SE35 660
    2 Z(1)=A-.01428571*D                                                SE35 670
      Z(2)=B+.05714286*D                                                SE35 680
    3 Z(I-2)=C-.08571429*D                                              SE35 690
C        END OF LOOP                                                    SE35 700
C                                                                       SE35 710
C        UPDATE LAST TWO COMPONENTS                                     SE35 720
      Z(NDIM-1)=Y(NDIM-1)+.05714286*D                                   SE35 730
      Z(NDIM)=Y(NDIM)-.01428571*D                                       SE35 740
      IER=0                                                             SE35 750
      RETURN                                                            SE35 760
C                                                                       SE35 770
C        ERROR EXIT IN CASE NDIM IS LESS THAN 5                         SE35 780
    4 IER=-1                                                            SE35 790
      RETURN                                                            SE35 800
      END                                                               SE35 810
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C                                                                       DSE3  10
C     ..................................................................DSE3  20
C                                                                       DSE3  30
C        SUBROUTINE DSE35                                               DSE3  40
C                                                                       DSE3  50
C        PURPOSE                                                        DSE3  60
C           TO COMPUTE A VECTOR OF SMOOTHED FUNCTION VALUES GIVEN A     DSE3  70
C           VECTOR OF FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO       DSE3  80
C           EQUIDISTANTLY SPACED ARGUMENT VALUES.                       DSE3  90
C                                                                       DSE3 100
C        USAGE                                                          DSE3 110
C           CALL DSE35(Y,Z,NDIM,IER)                                    DSE3 120
C                                                                       DSE3 130
C        DESCRIPTION OF PARAMETERS                                      DSE3 140
C           Y      -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES  DSE3 150
C                     (DIMENSION NDIM)                                  DSE3 160
C           Z      -  RESULTING VECTOR OF DOUBLE PRECISION SMOOTHED     DSE3 170
C                     FUNCTION VALUES (DIMENSION NDIM)                  DSE3 180
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      DSE3 190
C           IER    -  RESULTING ERROR PARAMETER                         DSE3 200
C                     IER = -1  - NDIM IS LESS THAN 5                   DSE3 210
C                     IER =  0  - NO ERROR                              DSE3 220
C                                                                       DSE3 230
C        REMARKS                                                        DSE3 240
C           (1)  IF IER=-1 THERE HAS BEEN NO COMPUTATION.               DSE3 250
C           (2)  Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y IS  DSE3 260
C                DISTINCT FROM Z, THEN IT IS NOT DESTROYED.             DSE3 270
C                                                                       DSE3 280
C        SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED                   DSE3 290
C           NONE                                                        DSE3 300
C                                                                       DSE3 310
C        METHOD                                                         DSE3 320
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    DSE3 330
C           EXCEPT AT THE POINTS X(1),X(2),X(NDIM-1) AND X(NDIM), EACH  DSE3 340
C           SMOOTHED VALUE Z(I) IS OBTAINED BY EVALUATING AT X(I) THE   DSE3 350
C           LEAST-SQUARES POLYNOMIAL OF DEGREE 3 RELEVANT TO THE 5      DSE3 360
C           SUCCESSIVE POINTS (X(I+K),Y(I+K)) K = -2,-1,...,2.  (SEE    DSE3 370
C           HILDEBRAND, F.B., INTRODUCTION TO NUMERICAL ANALYSIS,       DSE3 380
C           MC GRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP. 295-302.)  DSE3 390
C                                                                       DSE3 400
C     ..................................................................DSE3 410
C                                                                       DSE3 420
      SUBROUTINE DSE35(Y,Z,NDIM,IER)                                    DSE3 430
C                                                                       DSE3 440
C                                                                       DSE3 450
      DIMENSION Y(1),Z(1)                                               DSE3 460
      DOUBLE PRECISION Y,Z,A,B,C,D                                      DSE3 470
C                                                                       DSE3 480
C        TEST OF DIMENSION                                              DSE3 490
      IF(NDIM-5)4,1,1                                                   DSE3 500
C                                                                       DSE3 510
C        PREPARE LOOP                                                   DSE3 520
    1 B=Y(1)                                                            DSE3 530
      C=Y(2)                                                            DSE3 540
C                                                                       DSE3 550
C        START LOOP                                                     DSE3 560
      DO 3 I=5,NDIM                                                     DSE3 570
      A=B                                                               DSE3 580
      B=C                                                               DSE3 590
      C=Y(I-2)                                                          DSE3 600
C                                                                       DSE3 610
C        GENERATE FOURTH CENTRAL DIFFERENCE                             DSE3 620
      D=C-B-Y(I-1)                                                      DSE3 630
      D=D+D+C                                                           DSE3 640
      D=D+D+A+Y(I)                                                      DSE3 650
C                                                                       DSE3 660
C        CHECK FIRST TWO COMPONENTS                                     DSE3 670
      IF(I-5)2,2,3                                                      DSE3 680
    2 Z(1)=A-.014285714285714286D0*D                                    DSE3 690
      Z(2)=B+.057142857142857143D0*D                                    DSE3 700
    3 Z(I-2)=C-.085714285714285700*D                                    DSE3 710
C        END OF LOOP                                                    DSE3 720
C                                                                       DSE3 730
C        UPDATE LAST TWO COMPONENTS                                     DSE3 740
      Z(NDIM-1)=Y(NDIM-1)+.057142857142857143D0*D                       DSE3 750
      Z(NDIM)=Y(NDIM)-.014285714285714286D0*D                           DSE3 760
      IER=0                                                             DSE3 770
      RETURN                                                            DSE3 780
C                                                                       DSE3 790
C        ERROR EXIT IN CASE NDIM IS LESS THAN 5                         DSE3 800
    4 IER=-1                                                            DSE3 810
      RETURN                                                            DSE3 820
      END                                                               DSE3 830
```

Subroutine APFS and DAPFS

These subroutines compute the solution of the normal equations set up by subroutines APLL and DAPLL. This is the second step in the procedure for determining the least-squares fit of a given discrete function.

1. Mathematical background

Let $f(x)$, $g_i(x)$, $i=1, 2, \ldots, m$, and $w(x) > 0$ be functions defined for $x=x_1, x_2, \ldots, x_n$.

The problem is to determine the coefficients c_i of the linear combination

$$p(x) = \sum_{i=1}^{m} c_i g_i(x)$$

such that

$$e_m = \sum_{k=1}^{n} w(x_k) \left(f(x_k) - p(x_k)\right)^2 = \text{minimum} \qquad (1)$$

The necessary conditions

$$\frac{\partial e_m}{\partial c_i} = 0, \quad i=1, 2, \ldots, m \qquad (2)$$

form a system of m linear equations in m unknowns c_i.

To simplify the notation we introduce the following matrices:

$$X = \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_n \end{bmatrix}, \quad F = \begin{bmatrix} f(x_1) \\ \\ . \\ . \\ . \\ f(x_n) \end{bmatrix}, \quad W = \begin{bmatrix} w(x_1) & & & & \\ & w(x_2) & & & \\ & & . & & \\ & & & . & \\ & & & & w(x_n) \end{bmatrix},$$

$$c = \begin{bmatrix} c_1 \\ . \\ . \\ . \\ c_m \end{bmatrix}, \quad G = \begin{bmatrix} g_1(x_1) & . & . & g_1(x_n) \\ . & & & . \\ . & & & . \\ g_m(x_1) & . & . & g_m(x_n) \end{bmatrix}$$

Then we have

$$e_m = (F^T - C^T G)\, W\, (F - G^T C)$$

or, with $e_o = F^T W F$,

$$e_m = e_o - 2C^T GWF + C^T GWG^T C \qquad (1')$$

Using (1'), equations (2) may be written as

$$GWG^T C = GWF \qquad (2')$$

Combining (1') and (2') gives

$$e_o - e_m = C^T GWG^T C \qquad (3)$$

The normal equations (2') for the unknown vector C may be solved using Cholesky's method, since the coefficient matrix $A = GWG^T$ is obviously symmetric and is positive definite if all the fundamental functions $g_i(x)$ are linearly independent for the arguments x_i; that is, if the rows of G are linearly independent. Let $R = GWF$. Using Cholesky's method, A and R are replaced without additional storage requirements by T and $(T^T)^{-1}R$, where $A = T^T T$, and T is upper triangular.

Using these facts, an easy calculation shows

$$e_o - e_m = \left\| (T^T)^{-1} R \right\|^2$$

Introducing additional fundamental functions in the linear combination p(x) will not affect the first m rows and columns of A or the first m elements of R. Therefore, Cholesky's method gives a decomposition of $e_o - e_m$ into the separate components corresponding to individual degrees of freedom.

2. Programming considerations

All least-squares fits of dimension 1, 2, ..., m may be computed from the reduced normal equations $TC = (T^T)^{-1} R$. If the solutions are generated in the storage locations of T, there is no additional storage requirement.

Using the decomposition of $e_o - e_m$, the factorization may be terminated with dimension k if $e_k < \eta e_o$, giving the least-squares fit of dimension k which satisfies the user-specified precision (relative tolerance η). Due to rounding errors this will work only if η is approximately between 1 and 10^{-6} in single precision, and between 1 and 10^{-15} in double precision. Nevertheless, the square sum of residuals corresponding to a least-squares fit calculated in single or double precision may be as small as $e_o\, 10^{-12}$ or $e_o\, 10^{-30}$, respectively.

Due to rounding errors the square root method may break down if very small or negative pivot elements indicate a loss of significance. Therefore, all pivot elements are tested against the absolute value of EPS multiplied by the first diagonal element of A. If the kth pivot element is not greater than this internal test value, the normal equations are treated as if they had dimension k-1 only.

Let N1, N2 denote the following numbers:

N1 = the largest number less than or equal to m for which there is no indication of loss of significance

N2 = the smallest number less than or equal to m for which

$$e_{N2} \leq \left| \eta \, e_o \right|$$

Depending on the input parameter IOP, which specifies the operations to be performed, the dimension IRES (that is, the dimension of the subsystem of the normal equations used for calculation) is set to N1 if IOP is positive or zero, and to the smaller of the two numbers N1, N2 if IOP is negative.

The operations performed by APFS are:

IOP = 0 Compute the triangular factorization $A = T^T T$, $TC = (T^T)^{-1}R$ and e_{IRES} only.

IOP = ±1 In addition to the above, the least-squares fit of dimension IRES is computed and stored in column IRES of the triangular array WORK.

IOP = ±2 In addition to IOP = 0 calculations, all least-square fits of dimension 1 up to IRES are computed and stored in columns 1 up to IRES of the array WORK.

a. Storage allocation

Initially the symmetric coefficient matrix A is stored columnwise in compressed form in the triangular array WORK. It is followed immediately by the right-hand side vector R and a single location containing e_o initially and e_{IRES} on return. This storage scheme is generated by subroutine APLL.

b. Errors

The error parameter IER is set to -1 if a non-positive dimension m has been specified.

If IOP is positive or zero, IER is set to 1 in case of an indication of a loss of significance.

If IOP is negative, IER is set to 1 if the specified accuracy could not be reached, even with a fit of dimension IRES.

For reference see A. T. Berztiss, "Least-squares fitting of polynomials to irregularly spaced data", SIAM Review (1964), vol. 6, no. 3, pp 203-227.

```
C                                                                       APFS  10
C     ..................................................................APFS  20
C                                                                       APFS  30
C        SUBROUTINE APFS                                                APFS  40
C                                                                       APFS  50
C        PURPOSE                                                        APFS  60
C           PERFORM SYMMETRIC FACTORIZATION OF THE MATRIX OF THE NORMAL  APFS  70
C           EQUATIONS FOLLOWED BY CALCULATION OF THE LEAST SQUARES FIT  APFS  80
C           OPTIONALLY                                                  APFS  90
C                                                                       APFS 100
C        USAGE                                                          APFS 110
C           CALL APFS(WORK,IP,IRES,IOP,EPS,ETA,IER)                     APFS 120
C                                                                       APFS 130
C        DESCRIPTION OF PARAMETERS                                      APFS 140
C           WORK  - GIVEN SYMMETRIC COEFFICIENT MATRIX, STORED          APFS 150
C                   COMPRESSED, I.E UPPER TRIANGULAR PART COLUMNWISE.   APFS 160
C                   THE GIVEN RIGHT HAND SIDE OCCUPIES THE NEXT IP      APFS 170
C                   LOCATIONS IN WORK. THE VERY LAST COMPONENT OF WORK  APFS 180
C                   CONTAINS THE SQUARE SUM OF FUNCTION VALUES EO       APFS 190
C                   THIS SCHEME OF STORAGE ALLOCATION IS PRODUCED E.G.  APFS 200
C                   BY SUBROUTINE APLL.                                 APFS 210
C                   THE GIVEN MATRIX IS FACTORED IN THE FORM            APFS 220
C                   TRANSPOSE(T)*T AND THE GIVEN RIGHT HAND SIDE IS     APFS 230
C                   DIVIDED BY TRANSPOSE(T).                            APFS 240
C                   THE UPPER TRIANGULAR FACTOR T IS RETURNED IN WORK IFAPFS 250
C                   IOP EQUALS ZERO.                                    APFS 260
C                   IN CASE OF NONZERO IOP THE CALCULATED SOLUTIONS ARE APFS 270
C                   STORED IN THE COLUMNS OF TRIANGULAR ARRAY WORK OF   APFS 280
C                   CORRESPONDING DIMENSION AND EO  IS REPLACED BY THE  APFS 290
C                   SQUARE SUM OF THE ERRORS FOR FIT OF DIMENSION IRES. APFS 300
C                   THE TOTAL DIMENSION OF WORK IS (IP+1)*(IP+2)/2      APFS 310
C           IP    - NUMBER OF FUNDAMENTAL FUNCTIONS USED FOR LEAST      APFS 320
C                   SQUARES FIT                                         APFS 330
C           IRES  - DIMENSION OF CALCULATED LEAST SQUARES FIT.          APFS 340
C                   LET N1, N2, DENOTE THE FOLLOWING NUMBERS            APFS 350
C                   N1 = MAXIMAL DIMENSION FOR WHICH NO LOSS OF         APFS 360
C                        SIGNIFICANCE WAS INDICATED DURING FACTORIZATIONAPFS 370
C                   N2 = SMALLEST DIMENSION FOR WHICH THE SQUARE SUM OF APFS 380
C                        THE ERRORS DOES NOT EXCEED TEST=ABS(ETA*FSQ)   APFS 390
C                   THEN IRES=MIN0(IP,N1) IF IOP IS NONNEGATIVE         APFS 400
C                   AND  IRES=MIN0(IP,N1,N2) IF IOP IS NEGATIVE         APFS 410
C           IOP   - INPUT PARAMETER FOR SELECTION OF OPERATION          APFS 420
C                   IOP = 0 MEANS TRIANGULAR FACTORIZATION, DIVISION OF APFS 430
C                           THE RIGHT HAND SIDE BY TRANSPOSE(T) AND     APFS 440
C                           CALCULATION OF THE SQUARE SUM OF ERRORS IS  APFS 450
C                           PERFORMED ONLY                              APFS 460
C                   IOP = +1 OR -1 MEANS THE SOLUTION OF DIMENSION IRES APFS 470
C                           IS CALCULATED ADDITIONALLY                  APFS 480
C                   IOP = +2 OR -2 MEANS ALL SOLUTIONS FOR DIMENSION ONEAPFS 490
C                           UP TO IRES ARE CALCULATED ADDITIONALLY      APFS 500
C           EPS   - RELATIVE TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.APFS 510
C                   A SENSIBLE VALUE IS BETWEEN 1.E-3 AND 1.E-6         APFS 520
C           ETA   - RELATIVE TOLERANCE FOR TOLERATED SQUARE SUM OF      APFS 530
C                   ERRORS. A REALISTIC VALUE IS BETWEEN 1.E0 AND 1.E-6 APFS 540
C           IER   - RESULTANT ERROR PARAMETER                           APFS 550
C                   IER =-1 MEANS NONPOSITIVE IP                        APFS 560
C                   IER = 0 MEANS NO LOSS OF SIGNIFICANCE DETECTED      APFS 570
C                           AND SPECIFIED TOLERANCE OF ERRORS REACHED   APFS 580
C                   IER = 1 MEANS LOSS OF SIGNIFICANCE DETECTED OR      APFS 590
C                           SPECIFIED TOLERANCE OF ERROES NOT REACHED   APFS 600
C                                                                       APFS 610
C        REMARKS                                                        APFS 620
C           THE ABSOLUTE TOLERANCE USED INTERNALLY FOR TEST ON LOSS OF  APFS 630
C           SIGNIFICANCE IS TOL=ABS(EPS*WORK(1)).                       APFS 640
C           THE ABSOLUTE TOLERANCE USED INTERNALLY FOR THE SQUARE SUM OFAPFS 650
C           ERRORS IS ABS(ETA*FSQ).                                     APFS 660
C           IOP GREATER THAN 2 HAS THE SAME EFFECT AS IOP = 2.          APFS 670
C           IOP LESS THAN -2 HAS THE SAME EFFECT AS IOP =-2.            APFS 680
C           IRES = 0 MEANS THE ABSOLUTE VALUE OF EPS IS NOT LESS THAN   APFS 690
C           ONE AND/OR WORK(1) IS NOT POSITIVE AND/OR IP IS NOT POSITIVEAPFS 700
C                                                                       APFS 710
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  APFS 720
C           NONE                                                        APFS 730
C                                                                       APFS 740
C        METHOD                                                         APFS 750
C           CALCULATION OF THE LEAST SQUARES FITS IS DONE USING         APFS 760
C           CHOLESKYS SQUARE ROOT METHOD FOR SYMMETRIC FACTORIZATION.   APFS 770
C           THE INCORPORATED TEST ON LOSS OF SIGNIFICANCE MEANS EACH    APFS 780
C           RADICAND MUST BE GREATER THAN THE INTERNAL ABSOLUTE         APFS 790
C           TOLERANCE TOL=ABS(EPS*WORK(1)).                             APFS 800
C           IN CASE OF LOSS OF SIGNIFICANCE IN THE ABOVE SENSE ONLY A   APFS 810
C           SUBSYSTEM OF THE NORMAL EQUATIONS IS SOLVED.                APFS 820
C           IN CASE OF NEGATIVE IOP THE TRIANGULAR FACTORIZATION IS     APFS 830
C           TERMINATED PREMATURELY EITHER IF THE SQUARE SUM OF THE      APFS 840
C           ERRORS DOES NOT EXCEED ETA*FSQ OR IF THERE IS INDICATION    APFS 850
C           FOR LOSS OF SIGNIFICANCE                                    APFS 860
C                                                                       APFS 870
C     ..................................................................APFS 880
C                                                                       APFS 890
      SUBROUTINE APFS(WORK,IP,IRES,IOP,EPS,ETA,IER)                     APFS 900
C                                                                       APFS 910
C                                                                       APFS 920
C        DIMENSIONED DUMMY VARIABLES                                    APFS 930
      DIMENSION WORK(1)                                                 APFS 940
      IRES=0                                                            APFS 950
C                                                                       APFS 960
C        TEST OF SPECIFIED DIMENSION                                    APFS 970
      IF(IP)1,1,2                                                       APFS 980
C                                                                       APFS 990
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSION                      APFS1000
    1 IER=-1                                                            APFS1010
      RETURN                                                            APFS1020
C                                                                       APFS1030
C        INITIALIZE FACTORIZATION PROCESS                               APFS1040
    2 IPIV=0                                                            APFS1050
      IPP1=IP+1                                                         APFS1060
      IER=1                                                             APFS1070
      ITE=IP*IPP1/2                                                     APFS1080
      IEND=ITE+IPP1                                                     APFS1090
      TOL=ABS(EPS*WORK(1))                                              APFS1100
      TEST=ABS(ETA*WORK(IEND))                                          APFS1110
C                                                                       APFS1120
C        START LOOP OVER ALL ROWS OF WORK                               APFS1130
      DO 11 I=1,IP                                                      APFS1140
      IPIV=IPIV+I                                                       APFS1150
      JA=IPIV-IRES                                                      APFS1160
      JE=IPIV-1                                                         APFS1170
C                                                                       APFS1180
C        FORM SCALAR PRODUCT NEEDED TO MODIFY CURRENT ROW ELEMENTS      APFS1190
      JK=IPIV                                                           APFS1200
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```
      DO 9 K=1,IPP1                                                     APFS1210
      SUM=0.                                                            APFS1220
      IF(IRES)5,5,3                                                     APFS1230
    3 JK=JK-IRES                                                        APFS1240
      DO 4 J=JA,JE                                                      APFS1250
      SUM=SUM+WORK(J)*WORK(JK)                                          APFS1260
    4 JK=JK+1                                                           APFS1270
    5 IF(JK-IPIV)6,6,8                                                  APFS1280
C                                                                       APFS1290
C        TEST FOR LOSS OF SIGNIFICANCE                                  APFS1300
    6 SUM=WORK(IPIV)-SUM                                                APFS1310
      IF(SUM-TOL)12,12,7                                                APFS1320
    7 SUM=SQRT(SUM)                                                     APFS1330
      WORK(IPIV)=SUM                                                    APFS1340
      PIV=1./SUM                                                        APFS1350
      GOTO 9                                                            APFS1360
C                                                                       APFS1370
C        UPDATE OFF-DIAGONAL TERMS                                      APFS1380
    8 SUM=(WORK(JK)-SUM)*PIV                                            APFS1390
      WORK(JK)=SUM                                                      APFS1400
    9 JK=JK+K                                                           APFS1410
C                                                                       APFS1420
C        UPDATE SQUARE SUM OF ERRORS                                    APFS1430
      WORK(IEND)=WORK(IEND)-SUM*SUM                                     APFS1440
C                                                                       APFS1450
C        RECORD ADDRESS OF LAST PIVOT ELEMENT                           APFS1460
      IRES=IRES+1                                                       APFS1470
      IADR=IPIV                                                         APFS1480
C                                                                       APFS1490
C        TEST FOR TOLERABLE ERROR IF SPECIFIED                          APFS1500
      IF(IOP)10,11,11                                                   APFS1510
   10 IF(WORK(IEND)-TEST)13,13,11                                       APFS1520
   11 CONTINUE                                                          APFS1530
      IF(IOP)12,22,12                                                   APFS1540
C                                                                       APFS1550
C        PERFORM BACK SUBSTITUTION IF SPECIFIED                         APFS1560
   12 IF(IOP)14,23,14                                                   APFS1570
   13 IER=0                                                             APFS1580
   14 IPIV=IRES                                                         APFS1590
   15 IF(IPIV)23,23,16                                                  APFS1600
   16 SUM=0.                                                            APFS1610
      JA=ITE+IPIV                                                       APFS1620
      JJ=IADR                                                           APFS1630
      JK=IADR                                                           APFS1640
      K=IPIV                                                            APFS1650
      DO 19 I=1,IPIV                                                    APFS1660
      WORK(JK)=(WORK(JA)-SUM)/WORK(JJ)                                  APFS1670
      IF(K-1)20,20,17                                                   APFS1680
   17 JE=JJ-1                                                           APFS1690
      SUM=0.                                                            APFS1700
      DO 18 J=K,IPIV                                                    APFS1710
      SUM=SUM+WORK(JK)*WORK(JE)                                         APFS1720
      JK=JK+1                                                           APFS1730
   18 JE=JE+J                                                           APFS1740
      JK=JE-IPIV                                                        APFS1750
      JA=JA-1                                                           APFS1760
      JJ=JJ-K                                                           APFS1770
   19 K=K-1                                                             APFS1780
   20 IF(IOP/2)21,23,21                                                 APFS1790
   21 IADR=IADR-IPIV                                                    APFS1800
      IPIV=IPIV-1                                                       APFS1810
      GOTO 15                                                           APFS1820
C                                                                       APFS1830
C        NORMAL RETURN                                                  APFS1840
   22 IER=0                                                             APFS1850
   23 RETURN                                                            APFS1860
      END                                                               APFS1870
```

```
C                                                                       DAPF  10
C     ****************************************************************DAPF  20
C                                                                       DAPF  30
C        SUBROUTINE DAPFS                                               DAPF  40
C                                                                       DAPF  50
C        PURPOSE                                                        DAPF  60
C           PERFORM SYMMETRIC FACTORIZATION OF THE MATRIX OF THE NORMAL  DAPF  70
C           EQUATIONS FOLLOWED BY CALCULATION OF THE LEAST SQUARES FIT  DAPF  80
C           OPTIONALLY                                                  DAPF  90
C                                                                       DAPF 100
C        USAGE                                                          DAPF 110
C           CALL DAPFS(WORK,IP,IRES,IOP,EPS,ETA,IER)                    DAPF 120
C                                                                       DAPF 130
C        DESCRIPTION OF PARAMETERS                                      DAPF 140
C           WORK  - GIVEN SYMMETRIC COEFFICIENT MATRIX, STORED          DAPF 150
C                   COMPRESSED, I.E UPPER TRIANGULAR PART COLUMNWISE.   DAPF 160
C                   THE GIVEN RIGHT HAND SIDE OCCUPIES THE NEXT IP      DAPF 170
C                   LOCATIONS IN WORK. THE VERY LAST COMPONENT OF WORK  DAPF 180
C                   CONTAINS THE SQUARE SUM OF FUNCTION VALUES E0       DAPF 190
C                   THIS SCHEME OF STORAGE ALLOCATION IS PRODUCED E.G.  DAPF 200
C                   BY SUBROUTINE APLL.                                 DAPF 210
C                   THE GIVEN MATRIX IS FACTORED IN THE FORM            DAPF 220
C                   TRANSPOSE(T)*T AND THE GIVEN RIGHT HAND SIDE IS     DAPF 230
C                   DIVIDED BY TRANSPOSE(T).                            DAPF 240
C                   THE UPPER TRIANGULAR FACTOR T IS RETURNED IN WORK IFDAPF 250
C                   IOP EQUALS ZERO.                                    DAPF 260
C                   IN CASE OF NONZERO IOP THE CALCULATED SOLUTIONS ARE DAPF 270
C                   STORED IN THE COLUMNS OF TRIANGULAR ARRAY WORK OF   DAPF 280
C                   CORRESPONDING DIMENSION AND E0  IS REPLACED BY THE  DAPF 290
C                   SQUARE SUM OF THE ERRORS FOR FIT OF DIMENSION IRES. DAPF 300
C                   THE TOTAL DIMENSION OF WORK IS (IP+1)*(IP+2)/2      DAPF 310
C                   WORK MUST BE OF DOUBLE PRECISION                    DAPF 320
C              IP   - NUMBER OF FUNDAMENTAL FUNCTIONS USED FOR LEAST    DAPF 330
C                     SQUARES FIT                                       DAPF 340
C              IRES - DIMENSION OF CALCULATED LEAST SQUARES FIT.        DAPF 350
C                     LET N1, N2, DENOTE THE FOLLOWING NUMBERS          DAPF 360
C                     N1 = MAXIMAL DIMENSION FOR WHICH NO LOSS OF       DAPF 370
C                          SIGNIFICANCE WAS INDICATED DURING FACTORIZATIONDAPF 380
C                     N2 = SMALLEST DIMENSION FOR WHICH THE SQUARE SUM OF DAPF 390
C                          THE ERRORS DOES NOT EXCEED TEST=ABS(ETA*FSQ)  DAPF 400
C                     THEN IRES=MINO(IP,N1) IF IOP IS NONNEGATIVE       DAPF 410
C                     AND  IRES=MINO(IP,N1,N2) IF IOP IS NEGATIVE       DAPF 420
C              IOP  - INPUT PARAMETER FOR SELECTION OF OPERATION        DAPF 430
C                     IOP = 0 MEANS TRIANGULAR FACTORIZATION, DIVISION OF DAPF 440
C                             THE RIGHT HAND SIDE BY TRANSPOSE(T) AND   DAPF 450
C                             CALCULATION OF THE SQUARE SUM OF ERRORS IS DAPF 460
C                             PERFORMED ONLY                            DAPF 470
C                     IOP = +1 OR -1 MEANS THE SOLUTION OF DIMENSION IRES DAPF 480
C                             IS CALCULATED ADDITIONALLY                DAPF 490
C                     IOP = +2 OR -2 MEANS ALL SOLUTIONS FOR DIMENSION ONEDAPF 500
C                             UP TO IRES ARE CALCULATED ADDITIONALLY    DAPF 510
C              EPS  - FELATIVE TOLERANCE FOR TEST ON LOSS OF SIGNIFICANCE.DAPF 520
C                     A SENSIBLE VALUE IS BETWEEN 1.E-10 AND 1.E-15     DAPF 530
C              ETA  - RELATIVE TOLERANCE FOR TOLERATED SQUARE SUM OF     DAPF 540
C                     ERRORS. A REALISTIC VALUE IS BETWEEN 1.E0 AND 1.E-15DAPF 550
C              IER  - RESULTANT ERROR PARAMETER                         DAPF 560
C                     IER =-1 MEANS NONPOSITIVE IP                      DAPF 570
C                     IER = 0 MEANS NO LOSS OF SIGNIFICANCE DETECTED    DAPF 580
C                             AND SPECIFIED TOLERANCE OF ERRORS REACHED DAPF 590
C                     IER = 1 MEANS LOSS OF SIGNIFICANCE DETECTED OR    DAPF 600
C                             SPECIFIED TOLERANCE OF ERRORS NOT REACHED DAPF 610
C                                                                       DAPF 620
C        REMARKS                                                        DAPF 630
C           THE ABSOLUTE TOLERANCE USED INTERNALLY FOR TEST ON LOSS OF  DAPF 640
C           SIGNIFICANCE IS TOL=ABS(EPS*SNGL(WORK(1))).                 DAPF 650
C           THE ABSOLUTE TOLERANCE USED INTERNALLY FOR THE SQUARE SUM OFDAPF 660
C           ERRORS IS ABS(ETA*SNGL(FSQ)).                               DAPF 670
C           IOP GREATER THAN 2 HAS THE SAME EFFECT AS IOP = 2.          DAPF 680
C           IOP LESS THAN -2 HAS THE SAME EFFECT AS IOP =-2.            DAPF 690
C           IRES = 0 MEANS THE ABSOLUTE VALUE OF EPS IS NOT LESS THAN   DAPF 700
C           ONE AND/OR WORK(1) IS NOT POSITIVE AND/OR IP IS NOT POSITIVEDAPF 710
C                                                                       DAPF 720
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DAPF 730
C           NONE                                                        DAPF 740
C                                                                       DAPF 750
C        METHOD                                                         DAPF 760
C           CALCULATION OF THE LEAST SQUARES FITS IS DONE USING         DAPF 770
C           CHOLESKYS SQUARE ROOT METHOD FOR SYMMETRIC FACTORIZATION.   DAPF 780
C           THE INCORPORATED TEST ON LOSS OF SIGNIFICANCE MEANS EACH    DAPF 790
C           RADICAND MUST BE GREATER THAN THE INTERNAL ABSOLUTE         DAPF 800
C           TOLERANCE TOL.                                              DAPF 810
C           IN CASE OF LOSS OF SIGNIFICANCE IN THE ABOVE SENSE ONLY A   DAPF 820
C           SUBSYSTEM OF THE NORMAL EQUATIONS IS SOLVED.                DAPF 830
C           IN CASE OF NEGATIVE IOP THE TRIANGULAR FACTORIZATION IS     DAPF 840
C           TERMINATED PREMATURELY EITHER IF THE SQUARE SUM OF THE      DAPF 850
C           ERRORS DOES NOT EXCEED ETA*FSQ OR IF THERE IS INDICATION    DAPF 860
C           FOR LOSS OF SIGNIFICANCE                                    DAPF 870
C                                                                       DAPF 880
C     ****************************************************************DAPF 890
C                                                                       DAPF 900
      SUBROUTINE DAPFS(WORK,IP,IRES,IOP,EPS,ETA,IER)                    DAPF 910
C                                                                       DAPF 920
C                                                                       DAPF 930
C        DIMENSIONED DUMMY VARIABLES                                    DAPF 940
      DIMENSION WORK(1)                                                 DAPF 950
      DOUBLE PRECISION WORK,SUM,PIV                                     DAPF 960
      IRES=0                                                            DAPF 970
C                                                                       DAPF 980
C        TEST OF SPECIFIED DIMENSION                                    DAPF 990
      IF(IP)1,1,2                                                       DAPF1000
C                                                                       DAPF1010
C        ERROR RETURN IN CASE OF ILLEGAL DIMENSION                      DAPF1020
    1 IER=-1                                                            DAPF1030
      RETURN                                                            DAPF1040
C                                                                       DAPF1050
C        INITIALIZE FACTORIZATION PROCESS                               DAPF1060
    2 IPIV=0                                                            DAPF1070
      IPP1=IP+1                                                         DAPF1080
      IER=1                                                             DAPF1090
      ITE=IP*IPP1/2                                                     DAPF1100
      IEND=ITE+IPP1                                                     DAPF1110
      TOL=ABS(EPS*SNGL(WORK(1)))                                        DAPF1120
      TEST=ABS(ETA*SNGL(WORK(IEND)))                                    DAPF1130
C                                                                       DAPF1140
C        START LOOP OVER ALL ROWS OF WORK                               DAPF1150
      DO 11 I=1,IP                                                      DAPF1160
      IPIV=IPIV+I                                                       DAPF1170
      JA=IPIV-IRES                                                      DAPF1180
      JE=IPIV-1                                                         DAPF1190
C                                                                       DAPF1200
C        FORM SCALAR PRODUCT NEEDED TO MODIFY CURRENT ROW ELEMENTS      DAPF1210
      JK=IPIV                                                           DAPF1220
      DO 9 K=1,IPP1                                                     DAPF1230
      SUM=0.D0                                                          DAPF1240
      IF(IRES)5,5,3                                                     DAPF1250
    3 JK=JK-IRES                                                        DAPF1260
      DO 4 J=JA,JE                                                      DAPF1270
      SUM=SUM+WORK(J)*WORK(JK)                                          DAPF1280
    4 JK=JK+1                                                           DAPF1290
    5 IF(JK-IPIV)6,6,8                                                  DAPF1300
C                                                                       DAPF1310
C        TEST FOR LOSS OF SIGNIFICANCE                                  DAPF1320
    6 SUM=WORK(IPIV)-SUM                                                DAPF1330
      IF(SNGL(SUM)-TOL)12,12,7                                          DAPF1340
    7 SUM=DSQRT(SUM)                                                    DAPF1350
      WORK(IPIV)=SUM                                                    DAPF1360
      PIV=1.D0/SUM                                                      DAPF1370
      GOTO 9                                                            DAPF1380
C                                                                       DAPF1390
C        UPDATE OFF-DIAGONAL TERMS                                      DAPF1400
    8 SUM=(WORK(JK)-SUM)*PIV                                            DAPF1410
      WORK(JK)=SUM                                                      DAPF1420
    9 JK=JK+K                                                           DAPF1430
C                                                                       DAPF1440
C        UPDATE SQUARE SUM OF ERRORS                                    DAPF1450
      WORK(IEND)=WORK(IEND)-SUM*SUM                                     DAPF1460
C                                                                       DAPF1470
C        RECORD ADDRESS OF LAST PIVOT ELEMENT                           DAPF1480
      IRES=IRES+1                                                       DAPF1490
      IADR=IPIV                                                         DAPF1500
C                                                                       DAPF1510
C        TEST FOR TOLERABLE ERROR IF SPECIFIED                          DAPF1520
      IF(IOP)10,11,11                                                   DAPF1530
   10 IF(SNGL(WORK(IEND))-TEST)13,13,11                                 DAPF1540
   11 CONTINUE                                                          DAPF1550
      IF(IOP)12,22,12                                                   DAPF1560
C                                                                       DAPF1570
C        PERFORM BACK SUBSTITUTION IF SPECIFIED                         DAPF1580
   12 IF(IOP)14,23,14                                                   DAPF1590
   13 IER=0                                                             DAPF1600
   14 IPIV=IRES                                                         DAPF1610
   15 IF(IPIV)23,23,16                                                  DAPF1620
   16 SUM=0.D0                                                          DAPF1630
      JA=ITE+IPIV                                                       DAPF1640
      JJ=IADR                                                           DAPF1650
      JK=IADR                                                           DAPF1660
      K=IPIV                                                            DAPF1670
      DO 19 I=1,IPIV                                                    DAPF1680
      WORK(JK)=(WORK(JA)-SUM)/WORK(JJ)                                  DAPF1690
      IF(K-1)20,20,17                                                   DAPF1700
   17 JE=JJ-1                                                           DAPF1710
      SUM=0.D0                                                          DAPF1720
      DO 18 J=K,IPIV                                                    DAPF1730
      SUM=SUM+WORK(JK)*WORK(JE)                                         DAPF1740
      JK=JK+1                                                           DAPF1750
   18 JE=JE+J                                                           DAPF1760
      JK=JE-IPIV                                                        DAPF1770
      JA=JA-1                                                           DAPF1780
      JJ=JJ-K                                                           DAPF1790
   19 K=K-1                                                             DAPF1800
   20 IF(IOP/2)21,23,21                                                 DAPF1810
   21 IADR=IADR-IPIV                                                    DAPF1820
      IPIV=IPIV-1                                                       DAPF1830
      GOTO 15                                                           DAPF1840
C                                                                       DAPF1850
C        NORMAL RETURN                                                  DAPF1860
   22 IER=0                                                             DAPF1870
   23 RETURN                                                            DAPF1880
      END                                                               DAPF1890
```

Subroutine APCH and DAPCH

These subroutines set up the normal equations for a polynomial least-squares fit to a given discrete function. The solution of these equations is determined by subroutine APFS. The best fitting polynomial is computed in terms of its Chebyshev expansion.

1. Mathematical background

Let f(x) be a function defined for $x = x_1, x_2, \ldots x_n$.

The problem is to determine the coefficients of the polynomial

$$p(x) = \sum_{i=1}^{m} c_i x^{i-1}, \text{ such that}$$

$$\sum_{i=1}^{n} (f(x_i) - p(x_i))^2 = \text{minimum}$$

This problem leads to a system of linear equations AC = R where C is the vector of unknown coefficients, A is the m by m symmetric positive definite matrix with elements

$$a_{jk} = \sum_{i=1}^{n} x_i^{j-1} x_i^{k-1}$$

and R is the vector with elements

$$r_j = \sum_{i=1}^{n} f(x_i) x_i^{j-1}$$

If there is a weight w_i corresponding to each point $(x_i, f(x_i))$, the i^{th} term of the sums for the a_{jk} and r_j must be multiplied by w_i.

In practice the positive definite matrix A is badly ill-conditioned. Therefore, the straightforward method described above is feasible only for polynomials of low degree, about 3 or 4.

Use of Chebyshev polynomials instead of monomials results in a remarkable improvement of the condition of the normal equations, provided the arguments have a sensible distribution (for example, equidistant).

Let x_L and x_R denote the leftmost and rightmost arguments. By means of the linear transformation

$$t(x) = \frac{2x - (x_L + x_R)}{x_R - x_L} = x_D \cdot x + x_0$$

the argument range $x_L \le x \le x_R$ is reduced to the argument range $-1 \le t \le +1$.

The polynomial p(x) is calculated in the form of its Chebyshev expansion $p(x) = b_1 T_0(t) + b_2 T_1(t) + \ldots + b_m T_{m-1}(t)$, where $T_k(t)$ is the Chebyshev polynomial of degree k.

Then the vector B of the unknown coefficients b_i is a solution of the matrix equation AB = R, where A is an m by m symmetric positive definite matrix with elements

$$a_{jk} = \sum_{i=1}^{n} T_{j-1}(t(x_i)) T_{k-1}(t(x_i))$$

and R is a vector with elements

$$r_j = \sum_{i=1}^{n} T_{j-1}(t(x_i)) f(x_i)$$

The values of the Chebyshev polynomials for the argument t are calculated by means of the three-term recurrence equation:

$$T_k(t) = 2t \cdot T_{k-1}(t) - T_{k-2}(t); \quad k \ge 2$$

with starting values $T_0(t) = 1$, $T_1(t) = t$.

In setting up the matrix A, time is saved by using the identity $2T_j \cdot T_k = T_{j+k} + T_{j-k}$.

a. Remarks

The Chebyshev expansion of the polynomial p(x) gives a much better indication of the accuracy of the approximation than the coefficient vector of the polynomial itself. If the specified degree of the polynomial is too high, the last terms of the Chebyshev expansion will be uniformly small compared to the coefficients in front. The degree may be reduced by the number of small trailing coefficients without unduly enlarging the overall error.

An upper bound for the error introduced by neglecting the last terms of the Chebyshev expansion is given by the sum of the absolute values of these terms. Normally, transformation of the Chebyshev expansions in t(x) to ordinary polynomials in x results in severe loss of accuracy. Therefore, no attempt is made to return the polynomial expansions, which is no disadvantage since the Chebyshev expansion may be evaluated effectively for a specified argument x using subroutines CNPS and DCNPS with argument $t = x \cdot x_D + x_0$ and the calculated coefficient vector of the Chebyshev expansion.

The transformation of the calculated Chebyshev expansion to an ordinary polynomial may be accomplished using subroutines TCNP and DTCNP.

2. Programming considerations

Input arrays passed to subroutines APCH and DAPCH are DATI and WORK. DATI contains the given data set to be approximated, consisting of n argument values $x_1, \ldots, x_n$ followed by corresponding function values $f_1, \ldots, f_n$ and by corresponding weight values (if any). Constant weighting (value one) is implied if DATI (2n + 1) contains a nonpositive value.

Instead of arguments x_i, we use $t_i = x_i \cdot x_D + x_0$ for setting up the normal equations. The constants x_D and x_0 are returned as result values.

The normal equations are generated in the triangular array WORK. Only the upper triangular part of the symmetric coefficient matrix is generated and stored columnwise, followed immediately by the right-hand side and by the weighted square sum of function values.

This storage allocation scheme is required by subroutine APFS and DAPFS, which may be used for calculation of the solution of the normal equations. Exceptions are indicated by the error parameter IER, which is set to -1 if n and m are not both positive or if n is less than m, and to +1 if the arguments are coinciding; otherwise to zero, indicating successful operation.

```
C                                                                       APCH  10
C     ..................................................................APCH  20
C                                                                       APCH  30
C        SUBROUTINE APCH                                                APCH  40
C                                                                       APCH  50
C        PURPOSE                                                        APCH  60
C           SET UP NORMAL EQUATIONS OF LEAST SQUARES FIT IN TERMS OF    APCH  70
C           CHEBYSHEV POLYNOMIALS FOR A GIVEN DISCRETE FUNCTION         APCH  80
C                                                                       APCH  90
C        USAGE                                                          APCH 100
C           CALL APCH(DATI,N,IP,XC,XC,WORK,IER)                         APCH 110
C                                                                       APCH 120
C        DESCRIPTION OF PARAMETERS                                      APCH 130
C           DATI  - VECTOR OF DIMENSION 3*N (OR DIMENSION 2*N+1)        APCH 140
C                   CONTAINING THE GIVEN ARGUMENTS, FOLLOWED BY THE     APCH 150
C                   FUNCTION VALUES AND N (RESPECTIVELY 1) WEIGHT       APCH 160
C                   VALUES. THE CONTENT OF VECTOR DATI REMAINS          APCH 170
C                   UNCHANGED.                                          APCH 180
C           N     - NUMBER OF GIVEN POINTS                              APCH 190
C           IP    - DIMENSION OF LEAST SQUARES FIT, I.E. NUMBER OF      APCH 200
C                   CHEBYSHEV POLYNOMIALS USED AS FUNDAMENTAL FUNCTIONS APCH 210
C                   IP SHOULD NOT EXCEED N                              APCH 220
C           XC    - RESULTANT MULTIPLICATIVE CONSTANT FOR LINEAR        APCH 230
C                   TRANSFORMATION OF ARGUMENT RANGE                    APCH 240
C           XC    - RESULTANT ADDITIVE CONSTANT FOR LINEAR              APCH 250
C                   TRANSFORMATION OF ARGUMENT RANGE                    APCH 260
C           WORK  - WORKING STORAGE OF DIMENSION (IP+1)*(IP+2)/2        APCH 270
C                   ON RETURN WORK CONTAINS THE SYMMETRIC COEFFICIENT    APCH 280
C                   MATRIX OF THE NORMAL EQUATIONS IN COMPRESSED FORM    APCH 290
C                   FOLLOWED IMMEDIATELY BY RIGHT HAND SIDE             APCH 300
C                   AND SQUARE SUM OF FUNCTION VALUES                   APCH 310
C           IER   - RESULTING ERROR PARAMETER                           APCH 320
C                   IER =-1 MEANS FORMAL ERRORS IN DIMENSION            APCH 330
C                   IER = 0 MEANS NO ERRORS                             APCH 340
C                   IER = 1 MEANS COINCIDING ARGUMENTS                  APCH 350
C                                                                       APCH 360
C        REMARKS                                                        APCH 370
C           NO WEIGHTS ARE USED IF THE VALUE OF DATI(2*N+1) IS          APCH 380
C           NOT POSITIVE.                                               APCH 390
C           EXECUTION OF SUBROUTINE APCH IS A PREPARATORY STEP FOR      APCH 400
C           CALCULATION OF LEAST SQUARES FITS IN CHEBYSHEV POLYNOMIALS  APCH 410
C           IT SHOULD BE FOLLOWED BY EXECUTION OF SUBROUTINE APFS       APCH 420
C                                                                       APCH 430
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  APCH 440
C           NONE                                                        APCH 450
C                                                                       APCH 460
C        METHOD                                                         APCH 470
C           THE LEAST SQUARE FIT IS DETERMINED USING CHEBYSHEV          APCH 480
C           POLYNOMIALS AS FUNDAMENTAL FUNCTION SYSTEM.                 APCH 490
C           THE METHOD IS DISCUSSED IN THE ARTICLE                      APCH 500
C           A.T.BERZTISS, LEAST SQUARES FITTING TO IRREGULARLY SPACED   APCH 510
C           DATA, SIAM REVIEW, VOL.6, ISS.3, 1964, PP. 203-227.         APCH 520
C                                                                       APCH 530
C     ..................................................................APCH 540
      SUBROUTINE APCH(DATI,N,IP,XD,XC,WORK,IER)                         APCH 550
C                                                                       APCH 560
C                                                                       APCH 570
C       DIMENSIONED DUMMY VARIABLES                                     APCH 580
      DIMENSION DATI(1),WORK(1)                                         APCH 590
                                                                        APCH 600
C                                                                       APCH 610
C        CHECK FOR FORMAL ERRORS IN SPECIFIED DIMENSIONS                APCH 620
      IF(N-1)15,2C,1                                                    APCH 630
    1 IF(IP)15,19,2                                                     APCH 640
C                                                                       APCH 650
C        SEARCH SMALLEST AND LARGEST ARGUMENT                           APCH 660
    2 IF(IP-N)3,3,15                                                    APCH 670
    3 AA=DATI(1)                                                        APCH 680
      XC=AA                                                             APCH 690
      XE=C.                                                             APCH 700
      CC 7 I=1,N                                                        APCH 710
      XP=DATI(I)                                                        APCH 720
      IF(AA-XP)5,5,4                                                    APCH 730
    4 AA=XP                                                             APCH 740
    5 IF(XC-XP)6,7,7                                                    APCH 750
    6 XC=XP                                                             APCH 760
    7 CONTINUE                                                          APCH 770
C                                                                       APCH 780
C        INITIALIZE CALCULATION OF NORMAL EQUATIONS                     APCH 790
      XC=XC-XA                                                          APCH 800
      K=(IP*(IP+1))/2                                                   APCH 810
      IEND=K+IP+1                                                       APCH 820
      KT2=IP+IP                                                         APCH 830
      KT2P=KT2-1                                                        APCH 840
C                                                                       APCH 850
C        SET WORKING STORAGE AND RIGHT HAND SIDE TO ZERO                APCH 860
      CC 8 I=1,IP                                                       APCH 870
      J=KT2-I                                                           APCH 880
      WORK(J)=C.                                                        APCH 890
      WORK(I)=C.                                                        APCH 900
      K=K+I                                                             APCH 910
    8 WORK(K)=C.                                                        APCH 920
C                                                                       APCH 930
C        CHECK FOR DEGENERATE ARGUMENT RANGE                            APCH 940
      IF(XC)2C,2C,9                                                     APCH 950
C                                                                       APCH 960
C        CALCULATE CONSTANTS FOR REDUCTION OF ARGUMENTS                 APCH 970
    9 XC=-(XC+XA)/XC                                                    APCH 980
      XC=2./XC                                                          APCH 990
      SLP=C.                                                            APCH1000
C                                                                       APCH1010
C        START GREAT LOOP OVER ALL GIVEN POINTS                         APCH1020
      CC 15 I=1,N                                                       APCH1030
      T=DATI(I)*XC+XC                                                   APCH1040
      J=I+N                                                             APCH1050
      CF=DATI(J)                                                        APCH1060
C                                                                       APCH1070
C        CALCULATE AND STORE VALUES OF CHEBYSHEV POLYNOMIALS            APCH1080
C        FOR ARGUMENT T                                                 APCH1090
      XA=1.                                                             APCH1100
      XP=T                                                              APCH1110
      IF(DATI(2*N+1))11,11,10                                           APCH1120
   10 J=J+N                                                             APCH1130
      XA=DATI(J)                                                        APCH1140
      XP=T*XP                                                           APCH1150
   11 K=I+T                                                             APCH1160
      SLP=SLP+CF*CF*XA                                                  APCH1170
      CF=CF+CF                                                          APCH1180
      J=1                                                               APCH1190
   12 K=K+J                                                             APCH1200
      WORK(K)=WORK(K)+CF*XA                                             APCH1210
   13 WORK(J)=WORK(J)+XA                                                APCH1220
      IF(J-KT2P)14,15,15                                                APCH1230
   14 J=J+1                                                             APCH1240
      XE=T*XP-XA                                                        APCH1250
      XA=XP                                                             APCH1260
      XP=XE                                                             APCH1270
      IF(J-IP)12,12,13                                                  APCH1280
   15 CONTINUE                                                          APCH1290
      WORK(IEND)=SLP+SLP                                                APCH1300
C                                                                       APCH1310
C        CALCULATE MATRIX OF NORMAL EQUATIONS                           APCH1320
      LL=K                                                              APCH1330
      KK=KT2P                                                           APCH1340
      JJ=1                                                              APCH1350
      K=KK                                                              APCH1360
      CC 18 J=1,K                                                       APCH1370
      WORK(LL)=WORK(K)+WORK(JJ)                                         APCH1380
      LL=LL-1                                                           APCH1390
      IF(K-JJ)16,16,17                                                  APCH1400
   16 KK=KK-2                                                           APCH1410
      K=KK                                                              APCH1420
      JJ=1                                                              APCH1430
      GOTO 18                                                           APCH1440
   17 JJ=JJ+1                                                          APCH1450
      K=K-1                                                             APCH1460
   18 CONTINUE                                                          APCH1470
      IER=C                                                             APCH1480
      RETURN                                                            APCH1490
C                                                                       APCH1500
C        ERROR RETURN IN CASE OF FORMAL ERRORS                          APCH1510
   15 IER=-1                                                            APCH1520
      RETURN                                                            APCH1530
C                                                                       APCH1540
C        ERROR RETURN IN CASE OF COINCIDING ARGUMENTS                   APCH1550
   2C IER=1                                                             APCH1560
      RETURN                                                            APCH1570
      END                                                               APCH1580
```

```
C                                                                       DAPC  10
C     ..................................................................DAPC  20
C                                                                       DAPC  30
C        SUBROUTINE DAPCH                                               DAPC  40
C                                                                       DAPC  50
C        PURPOSE                                                        DAPC  60
C           SET UP NORMAL EQUATIONS OF LEAST SQUARES FIT IN TERMS OF    DAPC  70
C           CHEBYSHEV POLYNOMIALS FOR A GIVEN DISCRETE FUNCTION         DAPC  80
C                                                                       DAPC  90
C        USAGE                                                          DAPC 100
C           CALL DAPCH(DATI,N,IP,XD,XD,WORK,IER)                        DAPC 110
C                                                                       DAPC 120
C        DESCRIPTION OF PARAMETERS                                      DAPC 130
C           DATI  - VECTOR OF DIMENSION 3*N (OR DIMENSION 2*N+1)        DAPC 140
C                   CONTAINING THE GIVEN ARGUMENTS, FOLLOWED BY THE     DAPC 150
C                   FUNCTION VALUES AND N (RESPECTIVELY 1) WEIGHT       DAPC 160
C                   VALUES. THE CONTENT OF VECTOR DATI REMAINS          DAPC 170
C                   UNCHANGED.                                          DAPC 180
C                   DATI MUST BE OF DOUBLE PRECISION                    DAPC 190
C           N     - NUMBER OF GIVEN POINTS                              DAPC 200
C           IP    - DIMENSION OF LEAST SQUARES FIT, I.E. NUMBER OF      DAPC 210
C                   CHEBYSHEV POLYNOMIALS USED AS FUNDAMENTAL FUNCTIONS DAPC 220
C                   IP SHOULD NOT EXCEED N                              DAPC 230
C           XD    - RESULTANT MULTIPLICATIVE CONSTANT FOR LINEAR        DAPC 240
C                   TRANSFORMATION OF ARGUMENT RANGE                    DAPC 250
C                   XD MUST BE DOUBLE PRECISION                         DAPC 260
C           XD    - RESULTANT ADDITIVE CONSTANT FOR LINEAR              DAPC 270
C                   TRANSFORMATION OF ARGUMENT RANGE                    DAPC 280
C                   XD MUST BE DOUBLE PRECISION                         DAPC 290
C           WORK  - WORKING STORAGE OF DIMENSION (IP+1)*(IP+2)/2        DAPC 300
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C                   ON RETURN WORK CONTAINS THE SYMMETRIC COEFFICIENT   DAPC 310
C                   MATRIX OF THE NORMAL EQUATIONS IN COMPRESSED FORM   DAPC 320
C                   FOLLOWED IMMEDIATELY BY RIGHT HAND SIDE            DAPC 330
C                   AND SQUARE SUM OF FUNCTION VALUES                  DAPC 340
C                   WORK MUST BE OF DOUBLE PRECISION                   DAPC 350
C           IER   - RESULTING ERROR PARAMETER                          DAPC 360
C                   IER =-1 MEANS FORMAL ERRORS IN DIMENSION           DAPC 370
C                   IER = 0 MEANS NO ERRORS                            DAPC 380
C                   IER = 1 MEANS COINCIDING ARGUMENTS                 DAPC 390
C                                                                      DAPC 400
C       REMARKS                                                        DAPC 410
C          NO WEIGHTS ARE USED IF THE VALUE OF DATI(2*N+1) IS          DAPC 420
C          NOT POSITIVE.                                               DAPC 430
C          EXECUTION OF SUBROUTINE DAPCH IS A PREPARATORY STEP FOR     DAPC 440
C          CALCULATION OF LEAST SQUARES FITS IN CHEBYSHEV POLYNOMIALS  DAPC 450
C          IT SHOULD BE FOLLOWED BY EXECUTION OF SUBROUTINE DAPES      DAPC 460
C                                                                      DAPC 470
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DAPC 480
C          NONE                                                        DAPC 490
C                                                                      DAPC 500
C       METHOD                                                         DAPC 510
C          THE LEAST SQUARE FIT IS DETERMINED USING CHEBYSHEV          DAPC 520
C          POLYNOMIALS AS FUNDAMENTAL FUNCTION SYSTEM.                 DAPC 530
C          THE METHOD IS DISCUSSED IN THE ARTICLE                      DAPC 540
C          A.T.BERZTISS, LEAST SQUARES FITTING TO IRREGULARLY SPACED   DAPC 550
C          DATA, SIAM REVIEW, VOL.6, ISS.3, 1964, PP. 203-227.         DAPC 560
C                                                                      DAPC 570
C     ..................................................................DAPC 580
C                                                                      DAPC 590
      SUBROUTINE DAPCH(DATI,N,IP,XD,X0,WORK,IER)                       DAPC 600
C                                                                      DAPC 610
C                                                                      DAPC 620
C       DIMENSIONED DUMMY VARIABLES                                    DAPC 630
      DIMENSION DATI(1),WORK(1)                                        DAPC 640
      DOUBLE PRECISION DATI,WORK,XD,X0,XA,XE,XM,DF,T,SUM               DAPC 650
C                                                                      DAPC 660
C       CHECK FOR FORMAL ERRORS IN SPECIFIED DIMENSIONS                DAPC 670
      IF(N-1)19,20,1                                                   DAPC 680
    1 IF(IP)19,19,2                                                    DAPC 690
C                                                                      DAPC 700
C       SEARCH SMALLEST AND LARGEST ARGUMENT                           DAPC 710
    2 IF(IP-N)3,3,19                                                   DAPC 720
    3 XA=DATI(1)                                                       DAPC 730
      X0=XA                                                            DAPC 740
      XE=0.D0                                                          DAPC 750
      DO 7 I=1,N                                                       DAPC 760
      XM=DATI(I)                                                       DAPC 770
      IF(XA-XM)5,5,4                                                   DAPC 780
    4 XA=XM                                                            DAPC 790
    5 IF(X0-XM)6,7,7                                                   DAPC 800
    6 X0=XM                                                            DAPC 810
    7 CONTINUE                                                         DAPC 820
C                                                                      DAPC 830
C       INITIALIZE CALCULATION OF NORMAL EQUATIONS                     DAPC 840
      XD=X0-XA                                                         DAPC 850
      M=((IP*(IP+1))/2                                                 DAPC 860
      IEND=M+IP+1                                                      DAPC 870
      MT2=IP+IP                                                        DAPC 880
      MT2M=MT2-1                                                       DAPC 890
C                                                                      DAPC 900
C       SET WORKING STORAGE AND RIGHT HAND SIDE TO ZERO                DAPC 910
      DO 8 I=1,IP                                                      DAPC 920
      J=MT2-I                                                          DAPC 930
      WORK(J)=0.D0                                                     DAPC 940
      WORK(I)=0.D0                                                     DAPC 950
      K=M+I                                                            DAPC 960
    8 WORK(K)=0.D0                                                     DAPC 970
C                                                                      DAPC 980
C       CHECK FOR DEGENERATE ARGUMENT RANGE                            DAPC 990
      IF(XD)20,20,9                                                    DAPC1000
C                                                                      DAPC1010
C       CALCULATE CONSTANTS FOR REDUCTION OF ARGUMENTS                 DAPC1020
    9 X0=-(X0+XA)/XD                                                   DAPC1030
      XD=2.D0/XD                                                       DAPC1040
      SUM=0.D0                                                         DAPC1050
C                                                                      DAPC1060
C       START GREAT LOOP OVER ALL GIVEN POINTS                         DAPC1070
      DO 15 I=1,N                                                      DAPC1080
      T=DATI(I)*XD+X0                                                  DAPC1090
      J=I+N                                                            DAPC1100
      DF=DATI(J)                                                       DAPC1110
C                                                                      DAPC1120
C       CALCULATE AND STORE VALUES OF CHEBYSHEV POLYNOMIALS            DAPC1130
C       FOR ARGUMENT T                                                 DAPC1140
      XA=1.D0                                                          DAPC1150
      XM=T                                                             DAPC1160
      IF(DATI(2*N+1))11,11,10                                          DAPC1170
   10 J=J+N                                                            DAPC1180
      XA=DATI(J)                                                       DAPC1190
      XM=T*XA                                                          DAPC1200
   11 T=T+T                                                            DAPC1210
      SUM=SUM+DF*DF*XA                                                 DAPC1220
      DF=DF+DF                                                         DAPC1230
      J=1                                                              DAPC1240
   12 K=M+J                                                            DAPC1250
      WORK(K)=WORK(K)+DF*XA                                            DAPC1260
   13 WORK(J)=WORK(J)+XA                                               DAPC1270
      IF(J-MT2M)14,15,15                                               DAPC1280
   14 J=J+1                                                            DAPC1290
      XE=T*XM-XA                                                       DAPC1300
      XA=XM                                                            DAPC1310
      XM=XE                                                            DAPC1320
      IF(J-IP)12,12,13                                                 DAPC1330
   15 CONTINUE                                                         DAPC1340
      WORK(IEND)=SUM+SUM                                               DAPC1350
C                                                                      DAPC1360
C       CALCULATE MATRIX OF NORMAL EQUATIONS                           DAPC1370
      LL=M                                                             DAPC1380
      KK=MT2M                                                          DAPC1390
      JJ=1                                                             DAPC1400
      K=KK                                                             DAPC1410
      DO 18 J=1,M                                                      DAPC1420
      WORK(LL)=WORK(K)+WORK(JJ)                                        DAPC1430
      LL=LL-1                                                          DAPC1440
      IF(K-JJ)16,16,17                                                 DAPC1450
   16 KK=KK-2                                                          DAPC1460
      K=KK                                                             DAPC1470
      JJ=1                                                             DAPC1480
      GOTO 18                                                          DAPC1490
   17 JJ=JJ+1                                                          DAPC1500
      K=K-1                                                            DAPC1510
   18 CONTINUE                                                         DAPC1520
      IER=0                                                            DAPC1530
      RETURN                                                           DAPC1540
C                                                                      DAPC1550
C       ERROR RETURN IN CASE OF FORMAL ERRORS                          DAPC1560
   19 IER=-1                                                           DAPC1570
      RETURN                                                           DAPC1580
C                                                                      DAPC1590
C       ERROR RETURN IN CASE OF COINCIDING ARGUMENTS                   DAPC1600
   20 IER=1                                                            DAPC1610
      RETURN                                                           DAPC1620
      END                                                              DAPC1630
```

Subroutines ARAT and DARAT

These subroutines compute the best rational approximation $P(x)/Q(x)$ to a discrete function, $f(x)$, in the least-squares sense. The argument range should be the interval $[-1, +1]$.

Subroutines FRAT and DFRAT are an integral part of the procedure and have no independent meaning.

1. Mathematical background

Given positive integers ip, iq, and n, arguments x_i, function values f_i, and positive weights w_i, i=1, 2,...,n, the problem is to determine the coefficients of the polynomials

$$P(x) = p_1 + p_2 x + \ldots + p_{ip} x^{ip-1}$$

$$Q(x) = q_1 + q_2 x + \ldots + q_{iq} x^{iq-1}$$

such that

$$F = \sum_{i=1}^{n} w_i \left[f_i - \frac{P(x_i)}{Q(x_i)} \right]^2 = \text{minimum} \qquad (1)$$

A direct approach to the problem (1) leads to a system of nonlinear equations. Therefore the problem is reformulated in the following way.

Let $P_o(x)$ and $Q_o(x)$ be an approximate solution to (1). The problem is then to determine increments $\Delta P_o(x)$ and $\Delta Q_o(x)$ such that

$$F = \sum_{i=1}^{n} w_i \left[f_i - \frac{P_o(x_i) + \Delta P_o(x_i)}{Q_o(x_i) + \Delta Q_o(x_i)} \right]^2 = \text{minimum} \qquad (1')$$

Without loss of generality it may be assumed that the constant term of Q_o remains unchanged, that is that the constant term of ΔQ_o is zero, since numerator and denominator of the rational approximation are determined only up to a common factor.

Linearizing $\dfrac{P_o + \Delta P_o}{Q_o + \Delta Q_o}$ with respect to ΔP_o and ΔQ_o,

$$\frac{P_o + \Delta P_o}{Q_o + \Delta Q_o} \approx \frac{P_o}{Q_o} \left[1 + \frac{\Delta P_o}{P_o} - \frac{\Delta Q_o}{Q_o} \right] \qquad (2)$$

and using (2) in (1') gives the approximation $F \approx F_o$ where

$$F_o = \sum_{i=1}^{n} \frac{w_i}{Q_o(x_i)^2} \left[f_i Q_o(x_i) - P_o(x_i) - \Delta P_o(x_i) + \frac{P_o(x_i)}{Q_o(x_i)} \Delta Q_o(x_i) \right]^2$$

Defining

$$f_i^* = f_i Q_o(x_i) - P_o(x_i)$$

$$w_i^* = w_i / Q_o(x_i)^2$$

and a set of functions

$$g_k(x) = -\frac{P_o(x)}{Q_o(x)} x^k \qquad k = 1, 2, \ldots, iq-1$$

$$g_k(x) = x^{k-iq} \qquad k = iq, iq+1, \ldots, iq+ip-1$$

we may write

$$F_o = \sum_{i=1}^{n} w_i^* \left[f_i^* - g(x_i) \right]^2$$

where

$$g(x) = \sum_{i=1}^{m} c_i g_i(x) \qquad m = iq+ip-1$$

and the c_i are the coefficients of $\Delta Q_o(x)$ and $\Delta P_o(x)$:

$$\Delta Q_o(x) = \sum_{i=1}^{iq-1} c_i x^i$$

$$\Delta P_o(x) = \sum_{i=iq}^{m} c_i x^{i-iq}$$

Now the coefficients c_i are determined so that F_o = minimum. This is a problem of the type discussed in APLL with function values f_i^*, weights w_i^* and fundamental functions $g_i(x)$, and leads to a system of linear equations

$$AC = R$$

with symmetric positive semi-definite coefficient matrix A (see APLL writeup for a desciption of A and R).

In subroutine ARAT, APLL is used to set up the normal equations AC = R, and APFS is used to solve the system for the coefficient vector C.

Given a solution ΔP_o and ΔQ_o to the problem F_o = minimum, a new approximation is formed using

$$P_1 = P_o + \Delta P_o$$

$$Q_1 = Q_o + \Delta Q_o$$

In general, given approximations P_k and Q_k, increments ΔP_k and ΔQ_k are determined as indicated above, and the next approximations are

$$P_{k+1} = P_k + \Delta P_k$$

$$Q_{k+1} = Q_k + \Delta Q_k \qquad (3)$$

This process is started with some initial approximation (usually with $P_o(x) \equiv 0$, $Q_o(x) \equiv 1$) and is stopped when there is indication of convergence (see below).

a. Refinement of the calculation procedure

The above approach has several defects:

(1) There is no guarantee for improvement of the rational fit obtained with successive iterations if the initial approximation is not close enough to a true solution.

(2) Zeros may come into the denominator, causing a complete breakdown of the procedure.

(3) The normal equations of the linearized problem are badly ill-conditioned if monomials are used as fundamental functions.

The first difficulty is resolved using an approach suggested by D. Braess in reference (1). Let

$$S_k = \sum_{i=1}^{n} w_i \left[f_i - \frac{P_k(x_i)}{Q_k(x_i)} \right]^2$$

Then instead of using the relations (3) we use

$$P_{k+1} = P_k + r \Delta P_k$$

$$Q_{k+1} = Q_k + r \Delta Q_k$$

where the relaxation factor r is chosen so that S_{k+1} is close to a minimum when regarded as a function of r, and $S_{k+1} \leq S_k$. If this cannot be done, the error parameter IER is set to IER = 1, and the process is stopped. Choosing r sufficiently small also prevents zeros from entering the denominator.

The condition of the normal equations is improved remarkably by using Chebyshev polynomials $T_k(x)$ instead of monomials x^k as fundamental functions; that is, the numerator and denominator are calculated in terms of their Chebyshev expansions. The argument range is assumed to be (-1, +1).

If it turns out that the normal equations are still ill-conditioned, the diagonal elements of the coefficient matrix are slightly increased. This modification was suggested by D. W. Marquardt in reference (2). In this case again the calculated increment is modified by a relaxation factor r; but now r may take on values even greater than 1 if this does not imply zeros coming into the denominator.

b. Convergence

Let T_k denote the sum of the absolute values of the coefficients of $P_k(x)$ and $Q_k(x)$. Then, assuming that the Marquardt modification was not needed, the process is stopped if either

$$\frac{S_k - S_{k+1}}{S_{k+1}} \leq r\,\epsilon$$

or

$$\frac{|T_k - T_{k+1}|}{T_{k+1}} \leq r\,\epsilon$$

or

$$S_{k+1} \leq \eta\, T_{k+1}$$

Here $\epsilon = 10^{-5}$ and $\eta = 10^{-11}$. If the diagonal terms of the coefficient matrix of the normal equations were increased, only the last test is applied. If none of these conditions is met, the process is repeated until the maximum number of iterations k = LIMIT is reached (LIMIT is set to 20 in ARAT).

c. Remarks

(1) The user must specify the dimension of the denominator and of the numerator of the rational approximation he wants to calculate. The calculation procedure is somewhat sensitive to getting adequate dimensions. If the specified dimensions are unrealistically high, the calculation procedure may break down due to a very poor convergence. In this case it is best to repeat the calculation with decreased dimensions.

(2) The initial approximation which the user has the option to specify must be such that the denominator is free of zeros over the range of approximation (-1, +1). The standard initial approximation is $P(x) \equiv 0$ and $Q(x) \equiv 1$.

(3) The arguments of the given discrete functions should be reduced to the interval (-1, +1). Arguments absolutely greater than 1 cause error propagation in the calculation of Chebyshev polynomials and may produce dubious results.

(4) Numerical experience has shown that the dimensions used in single precision should not exceed 5, and in double precision should not be above 10.

(5) Transformation of Chebyshev expansions to ordinary polynomials normally results in severe loss of accuracy. Therefore, no attempt is made to return the polynomial coefficients. This transformation may be easily accomplished through subroutines TCNP and DTCNP. The calculated Chebyshev expansions may be evaluated for a specified argument using subroutines CNPS and DCNPS.

2. Programming considerations

Arrays passed to subroutines ARAT and DARAT are DATI, WORK, and P. DATI contains the given data set to be approximated, consisting of n arguments $x_1, \ldots, x_n$ followed by the corresponding function values $f_1, \ldots, f_n$ and by weights $w_1, \ldots, w_n$. Constant weighting (value one) is implied if DATI (2n + 1) contains a nonpositive value.

WORK is used as working storage. On return it contains the values of the numerator in WORK (n + 1) up to WORK (2n) and the values of the denominator in WORK (2n + 1) up to WORK (3n). The storage positions WORK (1) up to WORK (n) and WORK (3n + 1) up to WORK (4n) are used to record the current nonmoderated values of change of numerator and denominator respectively. The remaining (ip + iq)(ip + iq + 1) + 1 storage locations of WORK are used to store the normal equations in compressed form twice, in a working area as well as in a save area. This is necessary to avoid recalculation of the normal equations in case of an ill-conditioned coefficient matrix.

P is a vector of dimension ip + iq containing the calculated rational approximation on return. The coefficients of the Chebyshev expansion of the denominator are stored first, immediately followed by the coefficients of the Chebyshev expansion of the numerator. Coefficients are ordered from low to

high. P may also be used as an input array containing the initial approximation in terms of its Chebyshev expansions (with same ordering) optionally.

The normal equations are generated internally by means of subroutines APLL and DAPLL in the storage allocation scheme which is required by subroutines APFS and DAPFS. Subroutines FRAT and DFRAT are simply the interface between subroutines ARAT, DARAT and APLL, DAPLL used for handling the given data set and the specified fundamental functions.

The error parameter IER gives an indication of success or failure of the procedure.

IER = 0 The process converged in the sense mentioned above.

IER = -1 Formal error occurred in specified dimensions or initial approximations such as violation of any of the restrictions $n > 0$, $ip > 0$, $iq > 0$, $n \geq ip + iq$ or $Q_0(x) \neq 0$ on $(-1, 1)$. The latter could occur only if an optional initial approximation was used.

IER = 1 The Marquardt modification was tried LIMIT times without success, or a suitable relaxation factor could not be found.

IER = 2 The process has not converged after LIMIT steps.

In all cases where IER $\geq$ 0 there is a calculated approximation available, but only in the case IER = 0 is there strong indication that this approximation is close to the best rational fit in the least-squares sense.

For reference see:

(1) D. Braess, "Ueber Daempfung bei Minimalisierungsverfahren", Computing (1966) vol. 1, ed. 3, pp 264 - 272.

(2) D. W. Marquardt, "An algorithm for least-squares estimation of non-linear parameters", JSIAM (1963), vol. II, ed. 2, pp. 431— 441.

```
C                                                                       ARAT  10
C     ..................................................................ARAT  20
C                                                                       ARAT  30
C        SUBROUTINE ARAT                                                ARAT  40
C                                                                       ARAT  50
C        PURPOSE                                                        ARAT  60
C           CALCULATE BEST RATIONAL APPROXIMATION OF A DISCRETE         ARAT  70
C           FUNCTION IN THE LEAST SQUARES SENSE                         ARAT  80
C                                                                       ARAT  90
C        USAGE                                                          ARAT 100
C           CALL ARAT(DATI,N,WORK,P,IP,IQ,IER)                          ARAT 110
C                                                                       ARAT 120
C        DESCRIPTION OF PARAMETERS                                      ARAT 130
C           DATI  - TWODIMENSIONAL ARRAY WITH 3 COLUMNS AND N ROWS      ARAT 140
C                   THE FIRST COLUMN MUST CONTAIN THE GIVEN ARGUMENTS,  ARAT 150
C                   THE SECOND COLUMN THE GIVEN FUNCTION VALUES AND     ARAT 160
C                   THE THIRD COLUMN THE GIVEN WEIGHTS IF ANY.          ARAT 170
C                   IF NO WEIGHTS ARE TO BE USED THEN THE THIRD         ARAT 180
C                   COLUMN MAY BE DROPPED , EXCEPT THE FIRST ELEMENT    ARAT 190
C                   WHICH MUST CONTAIN A NONPOSITIVE VALUE              ARAT 200
C           N     - NUMBER OF NODES OF THE GIVEN DISCRETE FUNCTION      ARAT 210
C           WORK  - WORKING STORAGE WHICH IS OF DIMENSION              ARAT 220
C                   (IP+IQ)*(IP+IQ+1)+4*N+1 AT LEAST.                   ARAT 230
C                   ON RETURN THE VALUES OF THE NUMERATOR ARE CONTAINED ARAT 240
C                   IN WORK(N+1) UP TO WORK(2*N), WHILE THE VALUES OF   ARAT 250
C                   THE DENOMINATOR ARE STORED IN WORK(2*N+1) UP TO     ARAT 260
C                   WORK(3*N)                                           ARAT 270
C           P     - RESULTANT COEFFICIENT VECTOR OF DENOMINATOR AND     ARAT 280
C                   NUMERATOR. THE DENOMINATOR IS STORED IN FIRST IQ    ARAT 290
C                   LOCATIONS, THE NUMERATOR IN THE FOLLOWING IP        ARAT 300
C                   LOCATIONS.                                          ARAT 310
C                   COEFFICIENTS ARE ORDERED FROM LOW TO HIGH.          ARAT 320
C           IP    - DIMENSION OF THE NUMERATOR   (INPUT VALUE)          ARAT 330
C           IQ    - DIMENSION OF THE DENOMINATOR (INPUT VALUE)          ARAT 340
C           IER   - RESULTANT ERROR PARAMETER                           ARAT 350
C                     IER =-1 MEANS FORMAL ERRORS                       ARAT 360
C                     IER = 0 MEANS NO ERRORS                           ARAT 370
C                     IER = 1,2 MEANS POOR CONVERGENCE OF ITERATION     ARAT 380
C                     IER IS ALSO USED AS INPUT VALUE                   ARAT 390
C                     A NONZERO INPUT VALUE INDICATES AVAILABILITY OF AN ARAT 400
C                     INITIAL APPROXIMATION STORED IN P                 ARAT 410
C                                                                       ARAT 420
C        REMARKS                                                        ARAT 430
C           THE COEFFICIENT VECTORS OF THE DENOMINATOR AND NUMERATOR    ARAT 440
C           OF THE RATIONAL APPROXIMATION ARE BOTH STORED IN P          ARAT 450
C           STARTING WITH LOW POWERS (DENOMINATOR FIRST).               ARAT 460
C           IP+IQ MUST NOT EXCEED N, ALL THREE VALUES MUST BE POSITIVE. ARAT 470
C           SINCE CHEBYSHEV POLYNOMIALS ARE USED AS FUNDAMENTAL         ARAT 480
C           FUNCTIONS, THE ARGUMENTS SHOULD BE REDUCED TO THE INTERVAL  ARAT 490
C           (-1,1). THIS CAN ALWAYS BE ACCOMPLISHED BY MEANS OF A LINEARARAT 500
C           TRANSFORMATION OF THE ORIGINALLY GIVEN ARGUMENTS.           ARAT 510
C           IF A FIT IN OTHER FUNCTIONS IS REQUIRED, CNP AND CNPS MUST  ARAT 520
C           BE REPLACED BY SUBROUTINES WHICH ARE OF ANALOGOUS DESIGN.   ARAT 530
C                                                                       ARAT 540
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ARAT 550
C           APLL, APFS, FRAT, CNPS, CNP                                 ARAT 560
C           CNP IS REQUIRED WITHIN FRAT                                 ARAT 570
C                                                                       ARAT 580
C        METHOD                                                         ARAT 590
C           THE ITERATIVE SCHEME USED FOR CALCULATION OF THE            ARAT 600
C           APPROXIMATION IS REPEATED SOLUTION OF THE NORMAL EQUATIONS  ARAT 610
C           WHICH ARE OBTAINED BY LINEARIZATION.                        ARAT 620
C           A REFINED TECHNIQUE OF THIS LINEAR LEAST SQUARES APPROACH   ARAT 630
C           IS USED WHICH GUARANTEES THAT THE DENOMINATOR IS FREE OF    ARAT 640
C           ZEROES WITHIN THE APPROXIMATION INTERVAL.                   ARAT 650
C           FOR REFERENCE SEE                                           ARAT 660
C           D.BRAESS, UEBER DAEMPFUNG BEI MINIMALISIERUNGSVERFAHREN,    ARAT 670
C           COMPUTING(1966), VOL.1, ED.3, PP.264-272.                   ARAT 680
C           D.W.MARQUARDT, AN ALGORITHM FOR LEAST-SQUARES ESTIMATION    ARAT 690
C           OF NONLINEAR PARAMETERS,                                    ARAT 700
C           JSIAM(1963), VOL.11, ED.2, PP.431-441.                      ARAT 710
C                                                                       ARAT 720
C     ..................................................................ARAT 730
C                                                                       ARAT 740
      SUBROUTINE ARAT(DATI,N,WORK,P,IP,IQ,IER)                          ARAT 750
C                                                                       ARAT 760
C                                                                       ARAT 770
      EXTERNAL FRAT                                                     ARAT 780
C                                                                       ARAT 790
C        DIMENSIONED LOCAL VARIABLE                                     ARAT 800
      DIMENSION IERV(3)                                                 ARAT 810
C                                                                       ARAT 820
C        DIMENSIONED DUMMY VARIABLES                                    ARAT 830
      DIMENSION DATI(1),WORK(1),P(1)                                    ARAT 840
C                                                                       ARAT 850
C        INITIALIZE TESTVALUES                                          ARAT 860
      LIMIT=20                                                          ARAT 870
      ETA =1.E-11                                                       ARAT 880
      EPS=1.E-5                                                         ARAT 890
C                                                                       ARAT 900
C        CHECK FOR FORMAL ERRORS                                        ARAT 910
      IF(N)4,4,1                                                        ARAT 920
    1 IF(IP)4,4,2                                                       ARAT 930
    2 IF(IQ)4,4,3                                                       ARAT 940
    3 IPQ=IP+IQ                                                         ARAT 950
      IF(N-IPQ)4,5,5                                                    ARAT 960
C                                                                       ARAT 970
C        ERROR RETURN IN CASE OF FORMAL ERRORS                          ARAT 980
    4 IER=-1                                                            ARAT 990
      RETURN                                                            ARAT1000
C                                                                       ARAT1010
C        INITIALIZE ITERATION PROCESS                                   ARAT1020
    5 KOUNT=0                                                           ARAT1030
      IERV(2)=IP                                                        ARAT1040
      IERV(3)=IQ                                                        ARAT1050
      NDP=N+N+1                                                         ARAT1060
      NNE=NDP+NDP                                                       ARAT1070
      IX=IPQ-1                                                          ARAT1080
      IQP1=IQ+1                                                         ARAT1090
      IRHS=NNE+IPQ*IX/2                                                 ARAT1100
      IEND=IRHS+IX                                                      ARAT1110
C                                                                       ARAT1120
C        TEST FOR AVAILABILITY OF AN INITIAL APPROXIMATION              ARAT1130
      IF(IER)8,6,8                                                      ARAT1140
C                                                                       ARAT1150
C        INITIALIZE NUMERATOR AND DENOMINATOR                           ARAT1160
    6 DO 7 I=2,IPQ                                                      ARAT1170
    7 P(I)=0.                                                           ARAT1180
      P(1)=1.                                                           ARAT1190
C                                                                       ARAT1200
C        CALCULATE VALUES OF NUMERATOR AND DENOMINATOR FOR INITIAL      ARAT1210
C        APPROXIMATION                                                  ARAT1220
    8 DO 9 J=1,N                                                        ARAT1230
      T=DATI(J)                                                         ARAT1240
      I=J+N                                                             ARAT1250
      CALL CNPS(WORK(I),T,P(IQP1),IP)                                   ARAT1260
      K=I+N                                                             ARAT1270
    9 CALL CNPS(WORK(K),T,P,IQ)                                         ARAT1280
C                                                                       ARAT1290
C        SET UP NORMAL EQUATIONS (MAIN LOOP OF ITERATION)               ARAT1300
   10 CALL APLL(FRAT,N,IX,WORK,WORK(IEND+1),DATI,IERV)                  ARAT1310
C                                                                       ARAT1320
C        CHECK FOR ZERO DENOMINATOR                                     ARAT1330
      IF(IERV(1))4,11,4                                                 ARAT1340
   11 INCR=0                                                            ARAT1350
      RELAX=2.                                                          ARAT1360
C                                                                       ARAT1370
C        RESTORE MATRIX IN WORKING STORAGE                              ARAT1380
   12 J=IEND                                                            ARAT1390
      DO 13 I=NNE,IEND                                                  ARAT1400
      J=J+1                                                             ARAT1410
   13 WORK(I)=WORK(J)                                                   ARAT1420
      IF(KOUNT)14,14,15                                                 ARAT1430
C                                                                       ARAT1440
C        SAVE SQUARE SUM OF ERRORS                                      ARAT1450
   14 OSUM=WORK(IEND)                                                   ARAT1460
      DIAG=OSUM*EPS                                                     ARAT1470
      K=IQ                                                              ARAT1480
C                                                                       ARAT1490
C        ADD CONSTANT TO DIAGONAL                                       ARAT1500
      IF(WORK(NNE))17,17,19                                             ARAT1510
   15 IF(INCR)19,19,16                                                  ARAT1520
   16 K=IPQ                                                             ARAT1530
   17 J=NNE-1                                                           ARAT1540
      DO 18 I=1,K                                                       ARAT1550
      WORK(J)=WORK(J)+DIAG                                              ARAT1560
   18 J=J+I                                                             ARAT1570
C                                                                       ARAT1580
C        SOLVE NORMAL EQUATIONS                                         ARAT1590
   19 CALL APFS(WORK(NNE),IX,IPES,1,EPS,ETA,IER)                        ARAT1600
C                                                                       ARAT1610
C        CHECK FOR FAILURE OF EQUATION SOLVER                           ARAT1620
```

```
      IF(IPES)4,4,20                                                    AFATI630
C                                                                       ARATI640
C        TEST FOR DEFECTIVE NORMALEQUATIONS                             ARATI650
   20 IF(IPES-IX)21,24,24                                               ARATI660
   21 IF(INCR)22,22,23                                                  ARATI670
   22 DIAG=DIAG*0.125                                                   ARATI680
   23 DIAG=DIAG+DIAG                                                    ARATI690
      INCR=INCR+1                                                       ARATI700
C                                                                       ARATI710
C        START WITH OVER RELAXATION                                     ARATI720
      RELAX=8.                                                          ARATI730
      IF(INCR-LIMIT)12,45,45                                            ARATI740
C                                                                       ARATI750
C        CALCULATE VALUES OF CHANGE OF NUMERATOR AND DENOMINATOR        ARATI760
   24 L=NDP                                                             ARATI770
      J=NNE+IRES*(IRES-1)/2-1                                           ARATI780
      K=J+IQ                                                            ARATI790
      WORK(J)=0.                                                        ARATI800
      IFQ=IQ                                                            ARATI810
      IRP=IRES-IQ+1                                                     ARATI820
      IF(IRP)25,26,26                                                   ARATI830
   25 IFQ=IPES+1                                                        ARATI840
   26 DO 29 I=1,N                                                       ARATI850
      T=DATI(I)                                                         AFATI860
      WORK(I)=0.                                                        ARATI870
      CALL CNPS(WORK(I),T,WORK(K),IRP)                                  ARATI880
      M=L+N                                                             ARATI890
      CALL CNPS(WORK(M),T,WORK(J),IRQ)                                  ARATI900
      IF(WORK(M)*WORK(L))27,29,29                                       ARATI910
   27 SUM=WORK(L)/WORK(M)                                               AFATI920
      IF(RELAX+SUM)29,29,28                                             ARATI930
   28 RELAX=-SUM                                                        ARATI940
   29 L=L+1                                                             ARATI950
C                                                                       AFATI960
C        MODIFY RELAXATION FACTOR IF NECESSARY                          ARATI970
      SSOE=OSUM                                                         AFATI980
      ITER=LIMIT                                                        ARATI990
   30 SUM=0.                                                            ARAT2000
      RELAX=RELAX*0.5                                                   AFAT2010
      DO 32 I=1,N                                                       ARAT2020
      M=I+N                                                             ARAT2030
      K=M+N                                                             AFAT2040
      L=K+N                                                             APAT2050
      SAVE=DATI(M)-(WORK(M)+RELAX*WORK(I))/(WORK(K)+RELAX*WORK(L))      ARAT2060
      SAVE=SAVE*SAVE                                                    AFAT2070
      IF(DATI(NDP))32,32,31                                             ARAT2080
   31 SAVE=SAVE*DATI(K)                                                 ARAT2090
   32 SUM=SUM+SAVE                                                      APAT2100
      IF(ITER)45,33,33                                                  ARAT2110
   33 ITER=ITER-1                                                       ARAT2120
      IF(SUM-OSUM)34,37,35                                              AFAT2130
   34 OSUM=SUM                                                          ARAT2140
      GOTO 30                                                           ARAT2150
C                                                                       ARAT2160
C        TEST FOR IMPROVEMENT                                           ARAT2170
   35 IF(OSUM-SSOE)36,30,30                                             ARAT2180
   36 RELAX=RELAX+RELAX                                                 ARAT2190
   37 T=0.                                                              ARAT2200
      SAVE=0.                                                           ARAT2210
      K=IPES+1                                                          ARAT2220
      DO 38 I=2,K                                                       ARAT2230
      J=J+1                                                             ARAT2240
      T=T+ABS(P(I))                                                     ARAT2250
      P(I)=P(I)+RELAX*WORK(J)                                           ARAT2260
   38 SAVE=SAVE+ABS(P(I))                                               ARAT2270
C                                                                       ARAT2280
C        UPDATE CURRENT VALUES OF NUMERATOR AND DENOMINATOR             ARAT2290
      DO 39 I=1,N                                                       ARAT2300
      J=I+N                                                             ARAT2310
      K=J+N                                                             ARAT2320
      L=K+N                                                             ARAT2330
      WORK(J)=WORK(J)+RELAX*WORK(I)                                     ARAT2340
   39 WORK(K)=WORK(K)+RELAX*WORK(L)                                     ARAT2350
C                                                                       ARAT2360
C        TEST FOR CONVERGENCE                                           ARAT2370
      IF(INCR)40,40,42                                                  ARAT2380
   40 IF(SSOE-OSUM-RELAX*EPS*OSUM)46,46,41                              ARAT2390
   41 IF(ABS(T-SAVE)-RELAX*EPS*SAVE)46,46,42                            ARAT2400
   42 IF(OSUM-ETA*SAVE)46,46,43                                         ARAT2410
   43 KOUNT=KOUNT+1                                                     AFAT2420
      IF(KOUNT-LIMIT)10,44,44                                           ARAT2430
C                                                                       ARAT2440
C        ERROR RETURN IN CASE OF POOR CONVERGENCE                       AFAT2450
   44 IER=2                                                             ARAT2460
      RETURN                                                            ARAT2470
   45 IER=1                                                             AFAT2480
      RETURN                                                            ARAT2490
C                                                                       ARAT2500
C        NORMAL RETURN                                                  AFAT2510
   46 IER=0                                                             ARAT2520
      RETURN                                                            ARAT2530
      END                                                               ARAT2540
```

```
C                                                                       FRAT  10
C     ..................................................................FRAT  20
C                                                                       FRAT  30
C        SUBROUTINE FRAT                                                FRAT  40
C                                                                       FRAT  50
C        PURPOSE                                                        FRAT  60
C           FRAT IS USED FOR HANDLING OF DATA AND FUNDAMENTAL FUNCTIONS FRAT  70
C           WITH RATIONAL APPROXIMATION. IT IS A SUBSTANTIAL PART OF    FRAT  80
C           RATIONAL APPROXIMATION AND HAS NO MEANING INDEPENDENTLY     FRAT  90
C                                                                       FRAT 100
C        USAGE                                                          FRAT 110
C           CALL FRAT(I,N,M,P,DATI,WGT,IER)                             FRAT 120
C                                                                       FRAT 130
C        DESCRIPTION OF PARAMETERS                                      FRAT 140
C           I      - SUBSCRIPT OF CURRENT DATA POINT                    FRAT 150
C           N      - NUMBER OF ALL DATA POINTS                          FRAT 160
C           M      - NUMBER OF FUNDAMENTAL FUNCTIONS USED               FRAT 170
C           P      - ARRAY OF DIMENSION M+1 AT LEAST, WHICH CONTAINS    FRAT 180
C                    ON RETURN THE VALUES OF THE M FUNDAMENTAL          FRAT 190
C                    FUNCTIONS, FOLLOWED BY CURRENT FUNCTION VALUE      FRAT 200
C           DATI   - ARRAY CONTAINING GIVEN N ARGUMENTS, FOLLOWED       FRAT 210
C                    BY N FUNCTION VALUES AND FINALLY BY I RESPECTIVELY FRAT 220
C                    N WEIGHT VALUES                                    FRAT 230
C           WGT    - RESULTANT WEIGHT FACTOR USED FOR I-TH TERM         FRAT 240
C           IER    - RESULTANT ERROR PARAMETER, COMBINED WITH INPUT     FRAT 250
C                    VALUES FOR CONTROL                                 FRAT 260
C                    IER(2) MEANS DIMENSION OF NUMERATOR                FRAT 270
C                    IER(3) MEANS DIMENSION OF DENOMINATOR              FRAT 280
C                    IER(1) IS USED AS RESULTANT ERROR PARAMETER,       FRAT 290
C                    IER(1) = 0 IN CASE OF NO ERRORS                    FRAT 300
C                    IER(1) = 1 OTHERWISE (ZERO DENOMINATOR)            FRAT 310
C                                                                       FRAT 320
C        REMARKS                                                        FRAT 330
C           VECTOR IEP IS USED FOR COMMUNICATION BETWEEN FRAT AND FRAT  FRAT 340
C                                                                       FRAT 350
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FRAT 360
C           CNP                                                         FRAT 370
C                                                                       FRAT 380
C        METHOD                                                         FRAT 390
C           CF. MATHEMATICAL DESCRIPTION OF SUBROUTINE ARAT             FRAT 400
C                                                                       FRAT 410
C     ..................................................................FRAT 420
C                                                                       FRAT 430
      SUBROUTINE FRAT(I,N,M,P,DATI,WGT,IER)                             FRAT 440
C                                                                       FRAT 450
C                                                                       FRAT 460
C        DIMENSIONED DUMMY VARIABLES                                    FRAT 470
      DIMENSION P(1),DATI(1),IER(1)                                     FRAT 480
C                                                                       FRAT 490
C        INITIALIZATION                                                 FRAT 500
      IP=IER(2)                                                         FRAT 510
      IQ=IER(3)                                                         FRAT 520
      IQM1=IQ-1                                                         FRAT 530
      IPQ=IP+IQ                                                         FRAT 540
C                                                                       FRAT 550
C        LOOK UP ARGUMENT, FUNCTION VALUE AND WEIGHT                    FRAT 560
C        LOOK UP NUMERATOR AND DENOMINATOR                              FRAT 570
      T=DATI(I)                                                         FRAT 580
      J=I+N                                                             FRAT 590
      F=DATI(J)                                                         FRAT 600
      FNUM=P(J)                                                         FRAT 610
      J=J+N                                                             FRAT 620
      WGT=1.                                                            FRAT 630
      IF(DATI(2*N+1))2,2,1                                              FRAT 640
    1 WGT=DATI(J)                                                       FRAT 650
    2 FDEN=P(J)                                                         FRAT 660
C                                                                       FRAT 670
C        CALCULATE FUNCTION VALUE USED                                  FRAT 680
      F=F*FDEN-FNUM                                                     FRAT 690
C                                                                       FRAT 700
C        CHECK FOR ZERO DENOMINATOR                                     FRAT 710
      IF(FDEN)4,3,4                                                     FRAT 720
C                                                                       FRAT 730
C        ERROR RETURN IN CASE OF ZERO DENOMINATOR                       FRAT 740
    3 IER(1)=1                                                          FRAT 750
      RETURN                                                            FRAT 760
C                                                                       FRAT 770
C        CALCULATE WEIGHT FACTORS USED                                  FRAT 780
    4 WGT=WGT/(FDEN*FDEN)                                               FRAT 790
      FNUM=-FNUM/FDEN                                                   FRAT 800
C                                                                       FRAT 810
C        CALCULATE FUNDAMENTAL FUNCTIONS                                FRAT 820
      J=IQM1                                                            FRAT 830
      IF(IP-IQ)6,6,5                                                    FRAT 840
    5 J=IP-1                                                            FRAT 850
    6 CALL CNP(P(IQ),T,J)                                               FRAT 860
C                                                                       FRAT 870
C        STORE VALUES OF DENOMINATOR FUNDAMENTAL FUNCTIONS              FRAT 880
    7 IF(IQM1)10,10,8                                                   FRAT 890
    8 DO 9 II=1,IQM1                                                    FRAT 900
      J=II+IQ                                                           FRAT 910
    9 P(II)=P(J)*FNUM                                                   FRAT 920
C                                                                       FRAT 930
C        STORE FUNCTION VALUE                                           FRAT 940
   10 P(IPQ)=F                                                          FRAT 950
C                                                                       FRAT 960
C        NORMAL RETURN                                                  FRAT 970
      IER(1)=0                                                          FRAT 980
      RETURN                                                            FRAT 990
      END                                                               FRAT1000
```

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C                                                                       DARA  10
C     ******************************************************************DARA  20
C                                                                       DARA  30
      SUBROUTINE DARAT                                                  DARA  40
C                                                                       DARA  50
      PURPOSE                                                           DARA  60
         CALCULATE BEST RATIONAL APPROXIMATION OF A DISCRETE            DARA  70
         FUNCTION IN THE LEAST SQUARES SENSE                            DARA  80
C                                                                       DARA  90
      USAGE                                                             DARA 100
         CALL DARAT(DATI,N,WORK,P,IP,IQ,IER)                            DARA 110
C                                                                       DARA 120
      DESCRIPTION OF PARAMETERS                                         DARA 130
         DATI  - TWODIMENSIONAL ARRAY WITH 3 COLUMNS AND N ROWS         DARA 140
                 THE FIRST COLUMN MUST CONTAIN THE GIVEN ARGUMENTS,     DARA 150
                 THE SECOND COLUMN THE GIVEN FUNCTION VALUES AND        DARA 160
                 THE THIRD COLUMN THE GIVEN WEIGHTS IF ANY.             DARA 170
                 IF NO WEIGHTS ARE TO BE USED THEN THE THIRD            DARA 180
                 COLUMN MAY BE DROPPED , EXCEPT THE FIRST ELEMENT       DARA 190
                 WHICH MUST CONTAIN A NONPOSITIVE VALUE                 DARA 200
                 DATI MUST BE OF DOUBLE PRECISION                       DARA 210
         N     - NUMBER OF NODES OF THE GIVEN DISCRETE FUNCTION         DARA 220
         WORK  - WORKING STORAGE WHICH IS OF DIMENSION                  DARA 230
                 (IP+IQ)*(IP+IQ+1)+4*N+1 AT LEAST.                      DARA 240
                 ON RETURN THE VALUES OF THE NUMERATOR ARE CONTAINED    DARA 250
                 IN WORK(N+1) UP TO WORK(2*N), WHILE THE VALUES OF      DARA 260
                 THE DENOMINATOR ARE STORED IN WORK(2*N+1) UP TO        DARA 270
                 WORK(3*N)                                              DARA 280
                 WORK MUST BE OF DOUBLE PRECISION                       DARA 290
         P     - RESULTANT COEFFICIENT VECTOR OF DENOMINATOR AND        DARA 300
                 NUMERATOR. THE DENOMINATOR IS STORED IN FIRST IQ       DARA 310
                 LOCATIONS, THE NUMERATOR IN THE FOLLOWING IP           DARA 320
                 LOCATIONS.                                             DARA 330
                 COEFFICIENTS ARE ORDERED FROM LOW TO HIGH.             DARA 340
                 P MUST BE OF DOUBLE PRECISION                          DARA 350
         IP    - DIMENSION OF THE NUMERATOR   (INPUT VALUE)            DARA 360
         IQ    - DIMENSION OF THE DENOMINATOR (INPUT VALUE)            DARA 370
         IER   - RESULTANT ERROR PARAMETER                              DARA 380
                 IER =-1 MEANS FORMAL ERRORS                            DARA 390
                 IER = 0 MEANS NO ERRORS                                DARA 400
                 IER = 1,2 MEANS POOR CONVERGENCE OF ITERATION          DARA 410
                 IER IS ALSO USED AS INPUT VALUE                        DARA 420
                 A NONZERO INPUT VALUE INDICATES AVAILABILITY OF AN     DARA 430
                 INITIAL APPROXIMATION STORED IN P                      DARA 440
C                                                                       DARA 450
      REMARKS                                                           DARA 460
         THE COEFFICIENT VECTORS OF THE DENOMINATOR AND NUMERATOR       DARA 470
         OF THE RATIONAL APPROXIMATION ARE BOTH STORED IN P             DARA 480
         STARTING WITH LOW POWERS (DENOMINATOR FIRST).                  DARA 490
         IP+IQ MUST NOT EXCEED N, ALL THREE VALUES MUST BE POSITIVE.    DARA 500
         SINCE CHEBYSHEV POLYNOMIALS ARE USED AS FUNDAMENTAL            DARA 510
         FUNCTIONS, THE ARGUMENTS SHOULD BE REDUCED TO THE INTERVAL     DARA 520
         (-1,1). THIS CAN ALWAYS BE ACCOMPLISHED BY MEANS OF A LINEAR   DARA 530
         TRANSFORMATION OF THE ORIGINALLY GIVEN ARGUMENTS.              DARA 540
         IF A FIT IN OTHER FUNCTIONS IS REQUIRED, DCNP AND DCNPS MUST   DARA 550
         BE REPLACED BY SUBROUTINES WHICH ARE OF ANALOGOUS DESIGN.      DARA 560
C                                                                       DARA 570
      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DARA 580
         DAPLL, DAPFS, DFRAT, DCNPS, DCNP                               DARA 590
         DCNP IS REQUIRED WITHIN DFRAT                                  DARA 600
C                                                                       DARA 610
      METHOD                                                            DARA 620
         THE ITERATIVE SCHEME USED FOR CALCULATION OF THE               DARA 630
         APPROXIMATION IS REPEATED SOLUTION OF THE NORMAL EQUATIONS     DARA 640
         WHICH ARE OBTAINED BY LINEARIZATION.                           DARA 650
         A REFINED TECHNIQUE OF THIS LINEAR LEAST SQUARES APPROACH      DARA 660
         IS USED WHICH GUARANTEES THAT THE DENOMINATOR IS FREE OF       DARA 670
         ZEROES WITHIN THE APPROXIMATION INTERVAL.                      DARA 680
         FOR REFERENCE SEE                                              DARA 690
         D.BRAESS, UEBER DAEMPFUNG BEI MINIMALISIERUNGSVERFAHREN,       DARA 700
         COMPUTING(1966), VOL.1, ED.3, PP.264-272.                      DARA 710
         D.W.MARQUARDT, AN ALGORITHM FOR LEAST-SQUARES ESTIMATION       DARA 720
         OF NONLINEAR PARAMETERS,                                       DARA 730
         JSIAM(1963), VOL.11, ED.2, PP.431-441.                         DARA 740
C                                                                       DARA 750
C     ******************************************************************DARA 760
C                                                                       DARA 770
      SUBROUTINE DARAT(DATI,N,WORK,P,IP,IQ,IER)                         DARA 780
C                                                                       DARA 790
C                                                                       DARA 800
      EXTERNAL DFRAT                                                    DARA 810
C                                                                       DARA 820
C        DIMENSIONED LOCAL VARIABLE                                     DARA 830
      DIMENSION IERV(3)                                                 DARA 840
C                                                                       DARA 850
C        DIMENSIONED DUMMY VARIABLES                                    DARA 860
      DIMENSION DATI(1),WORK(1),P(1)                                    DARA 870
      DOUBLE PRECISION DATI,WORK,P,T,OSUM,DIAG,RELAX,SUM,SSOE,SAVE      DARA 880
C                                                                       DARA 890
C        INITIALIZE TESTVALUES                                          DARA 900
      LIMIT=20                                                          DARA 910
      ETA=1.E-29                                                        DARA 920
      EPS=1.E-14                                                        DARA 930
C                                                                       DARA 940
C        CHECK FOR FORMAL ERRORS                                        DARA 950
      IF(N)4,4,1                                                        DARA 960
    1 IF(IP)4,4,2                                                       DARA 970
    2 IF(IQ)4,4,3                                                       DARA 980
    3 IPQ=IP+IQ                                                         DARA 990
      IF(N-IPQ)4,5,5                                                    DARA1000
C                                                                       DARA1010
C        ERROR RETURN IN CASE OF FORMAL ERRORS                          DARA1020
    4 IER=-1                                                            DARA1030
      RETURN                                                            DARA1040
C                                                                       DARA1050
C        INITIALIZE ITERATION PROCESS                                   DARA1060
    5 KOUNT=0                                                           DARA1070
      IERV(2)=IP                                                        DARA1080
      IERV(3)=IQ                                                        DARA1090
      NDP=N+N+1                                                         DARA1100
      NNE=NDP+NDP                                                       DARA1110
      IX=IPQ-1                                                          DARA1120
      IQP1=IQ+1                                                         DARA1130
      IRHS=NNE+IPQ*IX/2                                                 DARA1140
      IEND=IRHS+IX                                                      DARA1150
C                                                                       DARA1160
C        TEST FOR AVAILABILITY OF AN INITIAL APPROXIMATION              DARA1170
      IF(IER)8,6,8                                                      DARA1180
C                                                                       DARA1190
C        INITIALIZE NUMERATOR AND DENOMINATOR                           DARA1200
    6 DO 7 I=2,IPQ                                                      DARA1210
    7 P(I)=0.D0                                                         DARA1220
      P(1)=1.D0                                                         DARA1230
C                                                                       DARA1240
C        CALCULATE VALUES OF NUMERATOR AND DENOMINATOR FOR INITIAL      DARA1250
C        APPROXIMATION                                                  DARA1260
    8 DO 9 J=1,N                                                        DARA1270
      T=DATI(J)                                                         DARA1280
      I=J+N                                                             DARA1290
      CALL DCNPS(WORK(I),T,P(IQP1),IP)                                  DARA1300
      K=I+N                                                             DARA1310
    9 CALL DCNPS(WORK(K),T,P,IQ)                                        DARA1320
C                                                                       DARA1330
C        SET UP NORMAL EQUATIONS (MAIN LOOP OF ITERATION)               DARA1340
   10 CALL DAPLL(DFRAT,N,IX,WORK,WORK(IEND+1),DATI,IERV)                DARA1350
C                                                                       DARA1360
C        CHECK FOR ZERO DENOMINATOR                                     DARA1370
      IF(IERV(1))4,11,4                                                 DARA1380
   11 INCR=0                                                            DARA1390
      RELAX=2.D0                                                        DARA1400
C                                                                       DARA1410
C        RESTORE MATRIX IN WORKING STORAGE                              DARA1420
   12 J=IEND                                                            DARA1430
      DO 13 I=NNE,IEND                                                  DARA1440
      J=J+1                                                             DARA1450
   13 WORK(I)=WORK(J)                                                   DARA1460
      IF(KOUNT)14,14,15                                                 DARA1470
C                                                                       DARA1480
C        SAVE SQUARE SUM OF ERRORS                                      DARA1490
   14 OSUM=WORK(IEND)                                                   DARA1500
      DIAG=OSUM*EPS                                                     DARA1510
      K=IQ                                                              DARA1520
C                                                                       DARA1530
C        ADD CONSTANT TO DIAGONAL                                       DARA1540
      IF(WORK(NNE))17,17,19                                             DARA1550
   15 IF(INCR)19,19,16                                                  DARA1560
   16 K=IPQ                                                             DARA1570
   17 J=NNE-1                                                           DARA1580
      DO 18 I=1,K                                                       DARA1590
      WORK(J)=WORK(J)+DIAG                                              DARA1600
   18 J=J+I                                                             DARA1610
C                                                                       DARA1620
C        SOLVE NORMAL EQUATIONS                                         DARA1630
   19 CALL DAPFS(WORK(NNE),IX,IRES,1,EPS,ETA,IER)                       DARA1640
C                                                                       DARA1650
C        CHECK FOR FAILURE OF EQUATION SOLVER                           DARA1660
      IF(IRES)4,4,20                                                    DARA1670
C                                                                       DARA1680
C        TEST FOR DEFECTIVE NORMALEQUATIONS                             DARA1690
   20 IF(IRES-IX)21,24,24                                               DARA1700
   21 IF(INCR)22,22,23                                                  DARA1710
   22 DIAG=DIAG*0.125D0                                                 DARA1720
   23 DIAG=DIAG+DIAG                                                    DARA1730
      INCR=INCR+1                                                       DARA1740
C                                                                       DARA1750
C        START WITH OVER RELAXATION                                     DARA1760
      RELAX=8.D0                                                        DARA1770
      IF(INCR-LIMIT)12,45,45                                            DARA1780
C                                                                       DARA1790
C        CALCULATE VALUES OF CHANGE OF NUMERATOR AND DENOMINATOR        DARA1800
   24 L=NDP                                                             DARA1810
      J=NNE+IRES*(IRES-1)/2-1                                           DARA1820
      K=J+IQ                                                            DARA1830
      WORK(J)=0.D0                                                      DARA1840
      IRQ=IQ                                                            DARA1850
      IRP=IRES-IQ+1                                                     DARA1860
      IF(IRP)25,26,26                                                   DARA1870
   25 IRQ=IRES+1                                                        DARA1880
   26 DO 29 I=1,N                                                       DARA1890
      T=DATI(I)                                                         DARA1900
      WORK(I)=0.D0                                                      DARA1910
      CALL DCNPS(WORK(I),T,WORK(K),IRP)                                 DARA1920
      M=L+N                                                             DARA1930
      CALL DCNPS(WORK(M),T,WORK(J),IRQ)                                 DARA1940
      IF(WORK(M)*WORK(L))27,29,29                                       DARA1950
   27 SUM=WORK(L)/WORK(M)                                               DARA1960
      IF(RELAX+SUM)29,29,28                                             DARA1970
   28 RELAX=-SUM                                                        DARA1980
   29 L=L+1                                                             DARA1990
C                                                                       DARA2000
C        MODIFY RELAXATION FACTOR IF NECESSARY                          DARA2010
      SSOE=OSUM                                                         DARA2020
      ITER=LIMIT                                                        DARA2030
   30 SUM=0.D0                                                          DARA2040
      RELAX=RELAX*0.500                                                 DARA2050
      DO 32 I=1,N                                                       DARA2060
      M=I+N                                                             DARA2070
      K=M+N                                                             DARA2080
      L=K+N                                                             DARA2090
      SAVE=DATI(M)-(WORK(M)+RELAX*WORK(I))/(WORK(K)+RELAX*WORK(L))      DARA2100
      SAVE=SAVE*SAVE                                                    DARA2110
      IF(DATI(NDP))32,32,31                                             DARA2120
   31 SAVE=SAVE*DATI(K)                                                 DARA2130
   32 SUM=SUM+SAVE                                                      DARA2140
      IF(ITER)45,33,33                                                  DARA2150
   33 ITER=ITER-1                                                       DARA2160
      IF(SUM-OSUM)34,37,35                                              DARA2170
   34 OSUM=SUM                                                          DARA2180
      GOTO 30                                                           DARA2190
C                                                                       DARA2200
C        TEST FOR IMPROVEMENT                                           DARA2210
   35 IF(OSUM-SSOE)36,30,30                                             DARA2220
   36 RELAX=RELAX+RELAX                                                 DARA2230
   37 T=0.                                                              DARA2240
      SAVE=0.D0                                                         DARA2250
      K=IRES+1                                                          DARA2260
      DO 38 I=2,K                                                       DARA2270
      J=J+1                                                             DARA2280
      T=T+DABS(P(I))                                                    DARA2290
      P(I)=P(I)+RELAX*WORK(J)                                           DARA2300
   38 SAVE=SAVE+DABS(P(I))                                              DARA2310
C                                                                       DARA2320
C        UPDATE CURRENT VALUES OF NUMERATOR AND DENOMINATOR             DARA2330
      DO 39 I=1,N                                                       DARA2340
      J=I+N                                                             DARA2350
      K=J+N                                                             DARA2360
      L=K+N                                                             DARA2370
      WORK(J)=WORK(J)+RELAX*WORK(I)                                     DARA2380
   39 WORK(K)=WORK(K)+RELAX*WORK(L)                                     DARA2390
C                                                                       DARA2400
C        TEST FOR CONVERGENCE                                           DARA2410
      IF(INCR)40,40,42                                                  DARA2420
   40 IF(SSOE-OSUM-RELAX*OSUM*DBLE(EPS))46,46,41                        DARA2430
   41 IF(DABS(T-SAVE)-RELAX*SAVE*DBLE(EPS))46,46,42                     DARA2440
   42 IF(OSUM-SAVE*DBLE(ETA))46,46,43                                   DARA2450
   43 KOUNT=KOUNT+1                                                     DARA2460
      IF(KOUNT-LIMIT)10,44,44                                           DARA2470
C                                                                       DARA2480
C        ERROR RETURN IN CASE OF POOR CONVERGENCE                       DARA2490
   44 IER=2                                                             DARA2500
      RETURN                                                            DARA2510
   45 IER=1                                                             DARA2520
      RETURN                                                            DARA2530
C                                                                       DARA2540
C        NORMAL RETURN                                                  DARA2550
   46 IER=0                                                             DARA2560
      RETURN                                                            DARA2570
      END                                                               DARA2580
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C                                                                       DFRA  10
C     ..................................................................DFRA  20
C                                                                       DFRA  30
C        SUBROUTINE DFRAT                                               DFRA  40
C                                                                       DFRA  50
C        PURPOSE                                                        DFRA  60
C           DFRAT IS USED FOR HANDLING OF DATA AND FUNDAMENTAL FUNCTIONSDFRA  70
C           WITH RATIONAL APPROXIMATION. IT IS A SUBSTANTIAL PART OF    DFRA  80
C           RATIONAL APPROXIMATION AND HAS NO MEANING INDEPENDENTLY     DFRA  90
C                                                                       DFRA 100
C        USAGE                                                          DFRA 110
C           CALL DFRAT(I,N,M,P,DATI,WGT,IER)                            DFRA 120
C                                                                       DFRA 130
C        DESCRIPTION OF PARAMETERS                                      DFRA 140
C           I      - SUBSCRIPT OF CURRENT DATA POINT                    DFRA 150
C           N      - NUMBER OF ALL DATA POINTS                          DFRA 160
C           M      - NUMBER OF FUNDAMENTAL FUNCTIONS USED               DFRA 170
C           P      - ARRAY OF DIMENSION M+1 AT LEAST, WHICH CONTAINS    DFRA 180
C                    ON RETURN THE VALUES OF THE M FUNDAMENTAL          DFRA 190
C                    FUNCTIONS, FOLLOWED BY CURRENT FUNCTION VALUE      DFRA 200
C                    P MUST BE OF DOUBLE PRECISION                      DFRA 210
C           DATI   - ARRAY CONTAINING GIVEN N ARGUMENTS, FOLLOWED       DFRA 220
C                    BY N FUNCTION VALUES AND FINALLY BY N RESPECTIVELY DFRA 230
C                    N WEIGHT VALUES                                    DFRA 240
C                    DATI MUST BE OF DOUBLE PRECISION                   DFRA 250
C           WGT    - RESULTANT WEIGHT FACTOR USED FOR I-TH TERM         DFRA 260
C                    WGT MUST BE OF DOUBLE PRECISION                    DFRA 270
C           IER    - RESULTANT ERROR PARAMETER, COMBINED WITH INPUT     DFRA 280
C                    VALUES FOR CONTROL                                 DFRA 290
C                    IER(2) MEANS DIMENSION OF NUMERATOR                DFRA 300
C                    IER(3) MEANS DIMENSION OF DENOMINATOR              DFRA 310
C                    IER(1) IS USED AS RESULTANT ERROR PARAMETER,       DFRA 320
C                    IER(1) = 0 IN CASE OF NO ERRORS                    DFRA 330
C                    IER(1) = 1 OTHERWISE (ZERO DENOMINATOR)            DFRA 340
C                                                                       DFRA 350
C        REMARKS                                                        DFRA 360
C           VECTOR IER IS USED FOR COMMUNICATION BETWEEN DFRAT AND DFRATDFRA 370
C                                                                       DFRA 380
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DFRA 390
C           DCNP                                                        DFRA 400
C                                                                       DFRA 410
C        METHOD                                                         DFRA 420
C           CF. MATHEMATICAL DESCRIPTION OF SUBROUTINE ARAT             DFRA 430
C                                                                       DFRA 440
C     ..................................................................DFRA 450
C                                                                       DFRA 460
      SUBROUTINE DFRAT(I,N,M,P,DATI,WGT,IER)                            DFRA 470
C                                                                       DFRA 480
C                                                                       DFRA 490
C        DIMENSIONED DUMMY VARIABLES                                    DFRA 500
      DIMENSION P(1),DATI(1),IER(1)                                     DFRA 510
      DOUBLE PRECISION P,DATI,WGT,T,F,FNUM,FDEN                         DFRA 520
C                                                                       DFRA 530
C        INITIALIZATION                                                 DFRA 540
      IP=IER(2)                                                         DFRA 550
      IQ=IER(3)                                                         DFRA 560
      IQM1=IQ-1                                                         DFRA 570
      IPQ=IP+IQ                                                         DFRA 580
C                                                                       DFRA 590
C        LOOK UP ARGUMENT, FUNCTION VALUE AND WEIGHT                    DFRA 600
C        LOOK UP NUMERATOR AND DENOMINATOR                              DFRA 610
      T=DATI(I)                                                         DFRA 620
      J=I+N                                                             DFRA 630
      F=DATI(J)                                                         DFRA 640
      FNUM=P(J)                                                         DFRA 650
      J=J+N                                                             DFRA 660
      WGT=1.D0                                                          DFRA 670
      IF(DATI(2*N+1))2,2,1                                              DFRA 680
    1 WGT=DATI(J)                                                       DFRA 690
    2 FDEN=P(J)                                                         DFRA 700
C                                                                       DFRA 710
C        CALCULATE FUNCTION VALUE USED                                  DFRA 720
      F=F*FDEN-FNUM                                                     DFRA 730
C                                                                       DFRA 740
C        CHECK FOR ZERO DENOMINATOR                                     DFRA 750
      IF(FDEN)4,3,4                                                     DFRA 760
C                                                                       DFRA 770
C        ERROR RETURN IN CASE OF ZERO DENOMINATOR                       DFRA 780
    3 IER(1)=1                                                          DFRA 790
      RETURN                                                            DFRA 800
C                                                                       DFRA 810
C        CALCULATE WEIGHT FACTORS USED                                  DFRA 820
    4 WGT=WGT/(FDEN*FDEN)                                               DFRA 830
      FNUM=-FNUM/FDEN                                                   DFRA 840
C                                                                       DFRA 850
C        CALCULATE FUNDAMENTAL FUNCTIONS                                DFRA 860
      J=IQM1                                                            DFRA 870
      IF(IP-IQ)6,6,5                                                    DFRA 880
    5 J=IP-1                                                            DFRA 890
    6 CALL DCNP(P(IQ),T,J)                                              DFRA 900
C                                                                       DFRA 910
C        STORE VALUES OF DENOMINATOR FUNDAMENTAL FUNCTIONS              DFRA 920
    7 IF(IQM1)10,10,8                                                   DFRA 930
    8 DO 9 II=1,IQM1                                                    DFRA 940
      J=II+IQ                                                           DFRA 950
    9 P(II)=P(J)*FNUM                                                   DFRA 960
C                                                                       DFRA 970
C        STORE FUNCTION VALUE                                           DFRA 980
   10 P(IPQ)=F                                                          DFRA 990
C                                                                       DFRA1000
C        NORMAL RETURN                                                  DFRA1010
      IER(1)=0                                                          DFRA1020
      RETURN                                                            DFRA1030
      END                                                               DFRA1040
```

Subroutines APLL and DAPLL

These subroutines set up the normal equations for a linear least-squares fit to a given discrete function. APLL is a preparatory step for the calculation of the least-squares fit. Normally it is followed by subroutine APFS.

A user-coded external subroutine must be supplied to compute the values of the fundamental functions.

1. Mathematical background

Let $f(x)$, $g_i(x)$, $i = 1, 2, \ldots, m$, and $w(x) > 0$ be functions defined for $x = x_1, x_2, \ldots, x_n$ (the x_i may be vectors as well as scalars). The problem is to determine the coefficients c_i of the linear combination

$$p(x) = \sum_{i=1}^{m} c_i g_i(x)$$

such that

$$\sum_{k=1}^{n} w(x_k)\,(f(x_k) - p(x_k))^2 = \text{minimum}$$

This problem leads to a system of linear equations $AC = R$, where C is the vector of unknown coefficients, A is the m by m symmetric positive definite matrix with elements

$$a_{jk} = \sum_{i=1}^{n} w(x_i)\, g_j(x_i)\, g_k(x_i)$$

and R is an m-dimensional vector with elements

$$r_j = \sum_{i=1}^{n} w(x_i)\, f(x_i)\, g_j(x_i)$$

(See APFS for details.)

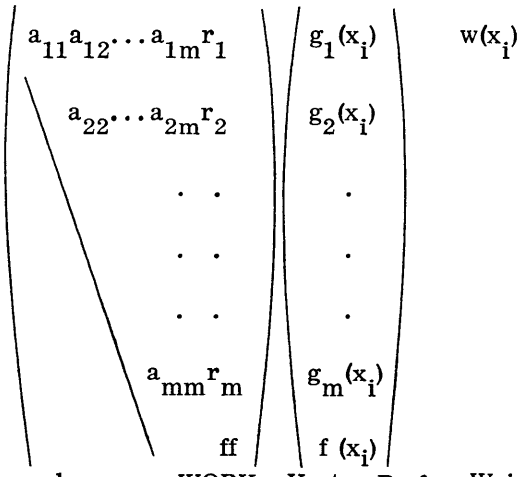
Some remarks regarding polynomial approximation are in order. Use of monomials $g_i(x) = x^{i-1}$ as fundamental functions results in a badly ill-conditioned coefficient matrix A. If Chebyshev or Legendre polynomials are used instead, the condition of the normal equations is improved remarkably, provided the arguments have a sensible distribution (for example, are equidistant in the interval -1 to +1).

2. Programming considerations

To allow for full flexibility in data handling, the user must provide an external subroutine that returns the values $g_1(x_i)$, $g_2(x_i)$,..., $g_m(x_i)$, $f(x_i)$ stored in a vector P together with the weight value $w(x_i)$. Input values to this subroutine are the current subscript value i, a number of points n, and -- for ease of communication between main line and external -- a dummy array named DATI.

Coefficient matrix A and right-hand side R are allocated adjacently. A is stored columnwise in compressed form, and R is augmented by one element ff in which the weighted square sum of function values is returned. The coefficient matrix A, right-hand side R, and square sum of function values ff are generated in a loop over i from 1 to n. Initially they are set to zero.

Storage allocation scheme:



Triangular array WORK of dimension m+1 by m+1 | Vector P of dimension m+1 | Weight WGT

For updating of the j^{th} column of the triangular array WORK, the j^{th} element of vector P is multiplied by the weight WGT, giving AUX and then P(i). AUX is added to the i^{th} element in the j^{th} column of WORK for i equal 1 up to j.

In this way the coefficient matrix A, the right-hand side R, and the square sum of function values are generated quite naturally by one and the same scheme.

a. External subroutine for data handling

The error parameter IER may be declared as scalar (that is, vector with one element) or vector in the user's main line. Within APLL it is treated as a vector with one element.

IER(1) is used for control purposes. If IER(1) is set to a nonzero value within the external subroutine, APLL returns to the calling program (main line), with an unchanged value of IER(1).

APLL sets the error parameter IER(1) to zero at the beginning. An error return with IER(1) = -1 is activated if n and m are not both positive or if n is less than m.

The user has full flexibility for handling of the data x_i, $f(x_i)$, $w(x_i)$, $g_1(x_i)$,..., $g_m(x_i)$.

(1) If he wishes to allocate x_i, $f(x_i)$, $w(x_i)$, $g_1(x_i)$,..., $g_m(x_i)$ in main storage, he may use an array the name of which replaces the dummy DATI.

Integer values needed for addressing may be inserted as additional components in the vector IER.

(2) Use of COMMON is another possibility for data exchange between the main line and the data handling external subroutine.

(3) Calculation of some or all of the required quantities as functions of the subscript or as functions of the argument x_i is another convenient choice.

(4) The needed data may be read in sequentially from one or more external devices, for example, x_i, $f(x_i)$, $w(x_i)$ from card unit, and/or $g_1(x_i)$,..., $g_m(x_i)$ from tape unit.

The four cases listed above may occur in any sensible combination.

```
C                                                                       APLL  10
C     .................................................................APLL  20
C                                                                       APLL  30
C        SUBROUTINE APLL                                                APLL  40
C                                                                       APLL  50
C        PURPOSE                                                        APLL  60
C           SET UP NORMAL EQUATIONS FOR A LINEAR LEAST SQUARES FIT      APLL  70
C           TO A GIVEN DISCRETE FUNCTION                                APLL  80
C                                                                       APLL  90
C        USAGE                                                          APLL 100
C           CALL APLL(FFCT,N,IP,P,WORK,DATI,IER)                        APLL 110
C           SUBROUTINE FFCT REQUIRES AN EXTERNAL STATEMENT              APLL 120
C                                                                       APLL 130
C        DESCRIPTION OF PARAMETERS                                      APLL 140
C           FFCT  - USER CODED SUBROUTINE WHICH MUST BE DECLARED        APLL 150
C                   EXTERNAL IN THE MAIN PROGRAM. IT IS CALLED          APLL 160
C                   CALL FFCT(I,N,IP,P,DATI,WGT,IER) AND RETURNS        APLL 170
C                   THE VALUES OF THE FUNDAMENTAL FUNCTIONS FOR         APLL 180
C                   THE I-TH ARGUMENT IN P(1) UP TO P(IP)               APLL 190
C                   FOLLOWED BY THE I-TH FUNCTION VALUE IN P(IP+1)      APLL 200
C                   N IS THE NUMBER OF ALL POINTS                       APLL 210
C                   DATI IS A DUMMY PARAMETER WHICH IS USED AS ARRAY    APLL 220
C                   NAME. THE GIVEN DATA SET MAY BE ALLOCATED IN DATI   APLL 230
C                   WGT IS THE WEIGHT FACTOR FOR THE I-TH POINT         APLL 240
C                   IER IS USED AS RESULTANT ERROR PARAMETER IN FFCT    APLL 250
C           N     - NUMBER OF GIVEN POINTS                              APLL 260
C           IP    - NUMBER OF FUNDAMENTAL FUNCTIONS USED FOR LEAST      APLL 270
C                   SQUARES FIT                                         APLL 280
C                   IP SHOULD NOT EXCEED N                              APLL 290
C           P     - WORKING STORAGE OF DIMENSION IP+1, WHICH            APLL 300
C                   IS USED AS INTERFACE BETWEEN APLL AND THE USER      APLL 310
C                   CODED SUBROUTINE FFCT                               APLL 320
C           WORK  - WORKING STORAGE OF DIMENSION (IP+1)*(IP+2)/2.       APLL 330
C                   ON RETURN WORK CONTAINS THE SYMMETRIC COEFFICIENT    APLL 340
C                   MATRIX OF THE NORMAL EQUATIONS IN COMPRESSED FORM,  APLL 350
C                   I.E. UPPER TRINGULAR PART ONLY STORED COLUMNWISE.    APLL 360
C                   THE FOLLOWING IP POSITIONS CONTAIN THE RIGHT        APLL 370
C                   HAND SIDE AND WORK((IP+1)*(IP+2)/2) CONTAINS        APLL 380
C                   THE WEIGHTED SQUARE SUM OF THE FUNCTION VALUES      APLL 390
C           DATI  - DUMMY ENTRY TO COMMUNICATE AN ARRAY NAME BETWEEN    APLL 400
C                   MAIN LINE AND SUBROUTINE FFCT.                      APLL 410
C           IER   - RESULTING ERROR PARAMETER                           APLL 420
C                   IER =-1 MEANS FORMAL ERRORS IN SPECIFIED DIMENSIONS APLL 430
C                   IER = 0 MEANS NO ERRORS                             APLL 440
C                   IER = 1 MEANS ERROR IN EXTERNAL SUBROUTINE FFCT     APLL 450
C                                                                       APLL 460
C        REMARKS                                                        APLL 470
C           TO ALLOW FOR EASY COMMUNICATION OF INTEGER VALUES           APLL 480
C           BETWEEN MAINLINE AND EXTERNAL SUBROUTINE FFCT, THE ERROR    APLL 490
C           PARAMETER IER IS TREATED AS A VECTOR OF DIMENSION 1 WITHIN  APLL 500
C           SUBROUTINE APLL. ADDITIONAL COMPONENTS OF IER MAY BE        APLL 510
C           INTRODUCED BY THE USER FOR COMMUNICATION BACK AND FORTH.    APLL 520
C           IN THIS CASE, HOWEVER, THE USER MUST SPECIFY IER AS A       APLL 530
C           VECTOR IN HIS MAINLINE.                                     APLL 540
C           EXECUTION OF SUBROUTINE APLL IS A PREPARATORY STEP FOR      APLL 550
C           CALCULATION OF THE LINEAR LEAST SQUARES FIT.                APLL 560
C           NORMALLY IT IS FOLLOWED BY EXECUTION OF SUBROUTINE APFS     APLL 570
C                                                                       APLL 580
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  APLL 590
C           THE EXTERNAL SUBROUTINE FFCT MUST BE FURNISHED BY THE USER  APLL 600
C                                                                       APLL 610
C        METHOD                                                         APLL 620
C           HANDLING OF THE GIVEN DATA SET (ARGUMENTS,FUNCTION VALUES   APLL 630
```

```
C           AND WEIGHTS) IS COMPLETELY LEFT TO THE USER                    APLL 640
C           ESSENTIALLY HE HAS THREE CHOICES                               APLL 650
C           (1) THE I-TH VALUES OF ARGUMENT, FUNCTION VALUE AND WEIGHT     APLL 660
C               ARE CALCULATED WITHIN SUBROUTINE FFCT FOR GIVEN I.         APLL 670
C           (2) THE I-TH VALUES OF ARGUMENT, FUNCTION VALUE AND WEIGHT     APLL 680
C               ARE DETERMINED BY TABLE LOOK UP. THE STORAGE LOCATIONS     APLL 690
C               REQUIRED ARE ALLOCATED WITHIN THE DUMMY ARRAY DATI         APLL 700
C               (POSSIBLY IN P TOO, IN EXCESS OF THE SPECIFIED IP + 1      APLL 710
C               LOCATIONS).                                                APLL 720
C               ANOTHER POSSIBILITY WOULD BE TO USE COMMON AS INTERFACE    APLL 730
C               BETWEEN MAIN LINE AND SUBROUTINE FFCT AND TO ALLOCATE      APLL 740
C               STORAGE FOR THE DATA SET IN COMMON.                        APLL 750
C           (3) THE I-TH VALUES OF ARGUMENT, FUNCTION VALUE AND WEIGHT     APLL 760
C               ARE READ IN FROM AN EXTERNAL DEVICE. THIS MAY BE EASILY    APLL 770
C               ACCOMPLISHED SINCE I IS USED STRICTLY INCREASING FROM      APLL 780
C               ONE UP TO N WITHIN APLL                                    APLL 790
C                                                                          APLL 800
C   ********************************************************************** APLL 810
C                                                                          APLL 820
      SUBROUTINE APLL(FFCT,N,IP,P,WORK,DATI,IER)                           APLL 830
C                                                                          APLL 840
C                                                                          APLL 850
C        DIMENSIONED DUMMY VARIABLES                                       APLL 860
      DIMENSION P(1),WORK(1),DATI(1),IER(1)                                APLL 870
C                                                                          APLL 880
C        CHECK FOR FORMAL ERRORS IN SPECIFIED DIMENSIONS                   APLL 890
      IF(N)1C,10,1                                                         APLL 900
    1 IF(IP)10,10,2                                                        APLL 910
    2 IF(N-IP)10,3,3                                                       APLL 920
C                                                                          APLL 930
C        SET WORKING STORAGE AND RIGHT HAND SIDE TO ZERO                   APLL 940
    3 IPP1=IP+1                                                            APLL 950
      M=IPP1*(IP+2)/2                                                      APLL 960
      IER(1)=0                                                             APLL 970
      DO 4 I=1,M                                                           APLL 980
    4 WORK(I)=0.                                                           APLL 990
C                                                                          APLL1000
C        START GREAT LOOP OVER ALL GIVEN POINTS                            APLL1010
      DO 8 I=1,N                                                           APLL1020
      CALL FFCT(I,N,IP,P,DATI,WGT,IER)                                     APLL1030
      IF(IER(1))9,5,9                                                      APLL1040
    5 J=0                                                                  APLL1050
      DO 7 K=1,IPP1                                                        APLL1060
      AUX=P(K)*WGT                                                         APLL1070
      DO 6 L=1,K                                                           APLL1080
      J=J+1                                                                APLL1090
    6 WORK(J)=WORK(J)+P(L)*AUX                                             APLL1100
    7 CONTINUE                                                             APLL1110
    8 CONTINUE                                                             APLL1120
C                                                                          APLL1130
C        NORMAL RETURN                                                     APLL1140
      RETURN                                                               APLL1150
    9 RETURN                                                               APLL1160
C                                                                          APLL1170
C        ERROR RETURN IN CASE OF FORMAL ERRORS                             APLL1180
   10 IER(1)=-1                                                            APLL1190
      RETURN                                                               APLL1200
      END
```

```
C                                                                          DAPL 640
C                                                                          DAPL 650
C       METHOD                                                             DAPL 660
C          HANDLING OF THE GIVEN DATA SET (ARGUMENTS,FUNCTION VALUES       DAPL 670
C          AND WEIGHTS) IS COMPLETELY LEFT TO THE USER                     DAPL 680
C          ESSENTIALLY HE HAS THREE CHOICES                                DAPL 690
C          (1) THE I-TH VALUES OF ARGUMENT, FUNCTION VALUE AND WEIGHT      DAPL 700
C              ARE CALCULATED WITHIN SUBROUTINE FFCT FOR GIVEN I.          DAPL 710
C          (2) THE I-TH VALUES OF ARGUMENT, FUNCTION VALUE AND WEIGHT      DAPL 720
C              ARE DETERMINED BY TABLE LOOK UP. THE STORAGE LOCATIONS      DAPL 730
C              REQUIRED ARE ALLOCATED WITHIN THE DUMMY ARRAY DATI          DAPL 740
C              (POSSIBLY IN P TOO, IN EXCESS OF THE SPECIFIED IP + 1       DAPL 750
C              LOCATIONS).                                                 DAPL 760
C              ANOTHER POSSIBILITY WOULD BE TO USE COMMON AS INTERFACE     DAPL 770
C              BETWEEN MAIN LINE AND SUBROUTINE FFCT AND TO ALLOCATE       DAPL 780
C              STORAGE FOR THE DATA SET IN COMMON.                         DAPL 790
C          (3) THE I-TH VALUES OF ARGUMENT, FUNCTION VALUE AND WEIGHT      DAPL 800
C              ARE READ IN FROM AN EXTERNAL DEVICE. THIS MAY BE EASILY     DAPL 810
C              ACCOMPLISHED SINCE I IS USED STRICTLY INCREASING FROM       DAPL 820
C              ONE UP TO N WITHIN APLL                                     DAPL 830
C   ********************************************************************** DAPL 840
C                                                                          DAPL 850
      SUBROUTINE DAPLL(FFCT,N,IP,P,WORK,DATI,IER)                          DAPL 860
C                                                                          DAPL 870
C                                                                          DAPL 880
C        DIMENSIONED DUMMY VARIABLES                                       DAPL 890
      DIMENSION P(1),WORK(1),DATI(1),IER(1)                                DAPL 900
      DOUBLE PRECISION P,WORK,DATI,WGT,AUX                                 DAPL 910
C                                                                          DAPL 920
C        CHECK FOR FORMAL ERRORS IN SPECIFIED DIMENSIONS                   DAPL 930
      IF(N)10,10,1                                                         DAPL 940
    1 IF(IP)10,10,2                                                        DAPL 950
    2 IF(N-IP)10,3,3                                                       DAPL 960
C                                                                          DAPL 970
C        SET WORKING STORAGE AND RIGHT HAND SIDE TO ZERO                   DAPL 980
    3 IPP1=IP+1                                                            DAPL 990
      M=IPP1*(IP+2)/2                                                      DAPL1000
      IER(1)=0                                                             DAPL1010
      DO 4 I=1,M                                                           DAPL1020
    4 WORK(I)=0.D0                                                         DAPL1030
C                                                                          DAPL1040
C        START GREAT LOOP OVER ALL GIVEN POINTS                            DAPL1050
      DO 8 I=1,N                                                           DAPL1060
      CALL FFCT(I,N,IP,P,DATI,WGT,IER)                                     DAPL1070
      IF(IER(1))9,5,9                                                      DAPL1080
    5 J=0                                                                  DAPL1090
      DO 7 K=1,IPP1                                                        DAPL1100
      AUX=P(K)*WGT                                                         DAPL1110
      DO 6 L=1,K                                                           DAPL1120
      J=J+1                                                                DAPL1130
    6 WORK(J)=WORK(J)+P(L)*AUX                                             DAPL1140
    7 CONTINUE                                                             DAPL1150
    8 CONTINUE                                                             DAPL1160
C                                                                          DAPL1170
C        NORMAL RETURN                                                     DAPL1180
    9 RETURN                                                               DAPL1190
C                                                                          DAPL1200
C        ERROR RETURN IN CASE OF FORMAL ERRORS                             DAPL1210
   10 IER(1)=-1                                                            DAPL1220
      RETURN                                                               DAPL1230
      END                                                                  DAPL1240
```

```
C                                                                          DAPL  10
C   ********************************************************************** DAPL  20
C                                                                          DAPL  30
C       SUBROUTINE DAPLL                                                   DAPL  40
C       PURPOSE                                                            DAPL  50
C          SET UP NORMAL EQUATIONS FOR A LINEAR LEAST SQUARES FIT          DAPL  60
C          TO A GIVEN DISCRETE FUNCTION                                    DAPL  70
C                                                                          DAPL  80
C       USAGE                                                              DAPL  90
C          CALL DAPLL(FFCT,N,IP,P,WORK,DATI,IER)                           DAPL 100
C          SUBROUTINE FFCT REQUIRES AN EXTERNAL STATEMENT                  DAPL 110
C                                                                          DAPL 120
C       DESCRIPTION OF PARAMETERS                                          DAPL 130
C          FFCT  - USER CODED SUBROUTINE WHICH MUST BE DECLARED            DAPL 140
C                  EXTERNAL IN THE MAIN PROGRAM. IT IS CALLED              DAPL 150
C                  CALL FFCT(I,N,IP,P,DATI,WGT,IER) AND RETURNS            DAPL 160
C                  THE VALUES OF THE FUNDAMENTAL FUNCTIONS FOR             DAPL 170
C                  THE I-TH ARGUMENT IN P(1) UP TO P(IP)                   DAPL 180
C                  FOLLOWED BY THE I-TH FUNCTION VALUE IN P(IP+1)          DAPL 190
C                  N IS THE NUMBER OF ALL POINTS                           DAPL 200
C                  P,DATI,WGT MUST BE OF DOUBLE PRECISION.                 DAPL 210
C                  DATI IS A DUMMY PARAMETER WHICH IS USED AS ARRAY        DAPL 220
C                  NAME. THE GIVEN DATA SET MAY BE ALLOCATED IN DATI       DAPL 230
C                  WGT IS THE WEIGHT FACTOR FOR THE I-TH POINT             DAPL 240
C                  IER IS USED AS RESULTANT ERROR PARAMETER IN FFCT        DAPL 250
C          N     - NUMBER OF GIVEN POINTS                                  DAPL 260
C          IP    - NUMBER OF FUNDAMENTAL FUNCTIONS USED FOR LEAST          DAPL 270
C                  SQUARES FIT                                             DAPL 280
C                  IP SHOULD NOT EXCEED N                                  DAPL 290
C          P     - WORKING STORAGE OF DIMENSION IP+1, WHICH                DAPL 300
C                  IS USED AS INTERFACE BETWEEN APLL AND THE USER          DAPL 310
C                  CODED SUBROUTINE FFCT                                   DAPL 320
C                  P MUST BE OF DOUBLE PRECISION.                          DAPL 330
C          WORK  - WORKING STORAGE OF DIMENSION (IP+1)*(IP+2)/2.           DAPL 340
C                  ON RETURN WORK CONTAINS THE SYMMETRIC COEFFICIENT        DAPL 350
C                  MATRIX OF THE NORMAL EQUATIONS IN COMPRESSED FORM,      DAPL 360
C                  I.E. UPPER TRINGULAR PART ONLY STORED COLUMNWISE.       DAPL 370
C                  THE FOLLOWING IP POSITIONS CONTAIN THE RIGHT            DAPL 380
C                  HAND SIDE AND WORK(((IP+1)*(IP+2)/2) CONTAINS           DAPL 390
C                  THE WEIGHTED SQUARE SUM OF THE FUNCTION VALUES          DAPL 400
C                  WORK MUST BE OF DOUBLE PRECISION.                       DAPL 410
C          DATI  - DUMMY ENTRY TO COMMUNICATE AN ARRAY NAME BETWEEN        DAPL 420
C                  MAIN LINE AND SUBROUTINE FFCT.                          DAPL 430
C                  DATI MUST BE OF DOUBLE PRECISION.                       DAPL 440
C          IER   - RESULTING ERROR PARAMETER                               DAPL 450
C                  IER =-1 MEANS FORMAL ERRORS IN SPECIFIED DIMENSIONS     DAPL 460
C                  IER = 0 MEANS NO ERRORS                                 DAPL 470
C                  IER = 1 MEANS ERROR IN EXTERNAL SUBROUTINE FFCT         DAPL 480
C                                                                          DAPL 490
C       REMARKS                                                            DAPL 500
C          TO ALLOW FOR EASY COMMUNICATION OF INTEGER VALUES               DAPL 510
C          BETWEEN MAINLINE AND EXTERNAL SUBROUTINE FFCT, THE ERROR        DAPL 520
C          PARAMETER IER IS TREATED AS A VECTOR OF DIMENSION 1 WITHIN      DAPL 530
C          SUBROUTINE DAPLL. ADDITIONAL COMPONENTS OF IER MAY BE           DAPL 540
C          INTRODUCED BY THE USER FOR COMMUNICATION BACK AND FORTH.        DAPL 550
C          IN THIS CASE, HOWEVER, THE USER MUST SPECIFY IER AS A           DAPL 560
C          VECTOR IN HIS MAINLINE.                                         DAPL 570
C          EXECUTION OF SUBROUTINE DAPLL IS A PREPARATORY STEP FOR         DAPL 580
C          CALCULATION OF THE LINEAR LEAST SQUARES FIT.                    DAPL 590
C          NORMALLY IT IS FOLLOWED BY EXECUTION OF SUBROUTINE DAPFS        DAPL 600
C                                                                          DAPL 610
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                      DAPL 620
C          THE EXTERNAL SUBROUTINE FFCT MUST BE FURNISHED BY THE USER      DAPL 630
```

Subroutine FORIF

This subroutine produces the Fourier coefficients for a given periodic function.

Given:

1. A function f(x) for values of x between 0 and 2π
2. N - the spacing desired such that the interval is $2\pi/(2N + 1)$
3. M - the desired order of the Fourier coefficients, $0 \leq M \leq N$

the coefficients of the Fourier series that approximate the given function are calculated as follows:

$$C_1 = \cos\left(\frac{2\pi}{2N+1}\right) \quad (1)$$

$$S_1 = \sin\left(\frac{2\pi}{2N+1}\right) \quad (2)$$

$$U_2 = 0$$

$$U_1 = 0$$

$$C = 1$$

$$S = 0$$

$$J = 1$$

The following recursive sequence is used to compute U_0, U_1, and U_2:

$$U_0 = f\left(\frac{2m\pi}{2N+1}\right) + 2\,C\,U_1 - U_2 \quad (3)$$

$$U_2 = U_1$$

$$U_1 = U_0$$

for values of m = 2N, 2N-1, ..., 1

The coefficients are then:

$$A_J = \frac{2}{2N+1}\left(f(0) + C\,U_1 - U_2\right) \quad (4)$$

$$B_J = \frac{2}{2N+1}\,S\,U_1 \quad (5)$$

The values of C and S are updated to:

$$Q = C_1\,C - S_1\,S$$

$$S = C_1\,S + S_1\,C$$

$$C = Q$$

J is stepped by 1 and the sequence starting at equation (3) is now repeated until M+1 pairs of coefficients have been computed.

```
C                                                                       FRIF  10
C     ...................................................................FRIF  20
C                                                                       FRIF  30
C       SUBROUTINE FORIF                                                FRIF  40
C                                                                       FRIF  50
C       PURPOSE                                                         FRIF  60
C          FOURIER ANALYSIS OF A GIVEN PERIODIC FUNCTION IN THE         FRIF  70
C          RANGE 0-2PI                                                  FRIF  80
C          COMPUTES THE COEFFICIENTS OF THE DESIRED NUMBER OF TERMS     FRIF  90
C          IN THE FOURIER SERIES F(X)=A(0)+SUM(A(K)COS KX+B(K)SIN KX)   FRIF 100
C          WHERE K=1,2,...,M TO APPROXIMATE THE COMPUTED VALUES OF A    FRIF 110
C          GIVEN FUNCTION.SUBPROGRAM                                    FRIF 120
C                                                                       FRIF 130
C       USAGE                                                           FRIF 140
C          CALL FORIF(FUN,N,M,A,B,IER)                                  FRIF 150
C                                                                       FRIF 160
C       DESCRIPTION OF PARAMETERS                                       FRIF 170
C          FUN-NAME OF FUNCTION SUBPROGRAM TO BE USED FOR COMPUTING     FRIF 180
C              DATA POINTS                                              FRIF 190
C          N  -DEFINES THE INTERVAL SUCH THAT 2N+1 POINTS ARE TAKEN     FRIF 200
C              OVER THE INTERVAL (0,2PI). THE SPACING IS THUS 2PI/2N+1  FRIF 210
C          M  -THE MAXIMUM ORDER OF THE HARMONICS TO BE FITTED          FRIF 220
C          A  -RESULTANT VECTOR OF FOURIER COSINE COEFFICIENTS OF       FRIF 230
C              LENGTH M+1                                               FRIF 240
C              A SUB 0, A SUB 1,..., A SUB M                            FRIF 250
C          B  -RESULTANT VECTOR OF FOURIER SINE COEFFICIENTS OF         FRIF 260
C              LENGTH M+1                                               FRIF 270
C              B SUB 0, B SUB 1,..., B SUB M                            FRIF 280
C          IER-RESULTANT ERROR CODE WHERE                               FRIF 290
C              IER=0  NO ERROR                                          FRIF 300
C              IER=1  N NOT GREATER OR EQUAL TO M                       FRIF 310
C              IER=2  M LESS THAN 0                                     FRIF 320
C                                                                       FRIF 330
C       REMARKS                                                         FRIF 340
C          M MUST BE GREATER THAN OR EQUAL TO ZERO                      FRIF 350
C          N MUST BE GREATER THAN OR EQUAL TO M                         FRIF 360
C          THE FIRST ELEMENT IN VECTOR B IS ZERO IN ALL CASES           FRIF 370
C                                                                       FRIF 380
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   FRIF 390
C          FUN-NAME OF USER FUNCTION SUBPROGRAM USED FOR COMPUTING      FRIF 400
C              DATA POINTS                                              FRIF 410
C          CALLING PROGRAM MUST HAVE FORTRAN EXTERNAL STATEMENT         FRIF 420
C          CONTAINING NAMES OF FUNCTION SUBPROGRAMS LISTED IN CALL TO   FRIF 430
C          FORIF                                                        FRIF 440
C                                                                       FRIF 450
C       METHOD                                                          FRIF 460
C          USES RECURSIVE TECHNIQUE DESCRIBED IN A. RALSTON, H. WILF,   FRIF 470
C          'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS', JOHN WILEY     FRIF 480
C          AND SONS, NEW YORK, 1960, CHAPTER 24. THE METHOD OF          FRIF 490
C          INDEXING THROUGH THE PROCEDURE HAS BEEN MODIFIED TO          FRIF 500
C          SIMPLIFY THE COMPUTATION.                                    FRIF 510
C                                                                       FRIF 520
C     ...................................................................FRIF 530
      SUBROUTINE FORIF(FUN,N,M,A,B,IER)                                 FRIF 540
      DIMENSION A(1),B(1)                                               FRIF 550
C                                                                       FRIF 560
C        CHECK FOR PARAMETER ERRORS                                     FRIF 570
C                                                                       FRIF 580
      IER=0                                                             FRIF 590
   20 IF(M) 30,40,40                                                    FRIF 600
   30 IER=2                                                             FRIF 610
      RETURN                                                            FRIF 620
   40 IF(M-N) 60,60,50                                                  FRIF 630
   50 IER=1                                                             FRIF 640
      RETURN                                                            FRIF 650
C                                                                       FRIF 660
C        COMPUTE AND PRESET CONSTANTS                                   FRIF 670
C                                                                       FRIF 680
   60 AN=N                                                              FRIF 690
      COEF=2.0/(2.0*AN+1.0)                                             FRIF 700
      CONST=3.141593*COEF                                               FRIF 710
      SI=SIN(CONST)                                                     FRIF 720
      CI=COS(CONST)                                                     FRIF 730
      C=1.0                                                             FRIF 740
      S=0.0                                                             FRIF 750
      J=1                                                               FRIF 760
      FUNZ=FUN(0.0)                                                     FRIF 770
   70 U2=0.0                                                            FRIF 780
      U1=0.0                                                            FRIF 790
      AI=2*N                                                            FRIF 800
C                                                                       FRIF 810
C        FORM FOURIER COEFFICIENTS RECURSIVELY                          FRIF 820
C                                                                       FRIF 830
   75 X=AI*CONST                                                        FRIF 840
      U0=FUN(X)+2.0*C*U1-U2                                             FRIF 850
      U2=U1                                                             FRIF 860
      U1=U0                                                             FRIF 870
      AI=AI-1.0                                                         FRIF 880
      IF(AI) 80,80,75                                                   FRIF 890
   80 A(J)=COEF*(FUNZ+C*U1-U2)                                          FRIF 900
      B(J)=COEF*S*U1                                                    FRIF 910
      IF(J-(M+1)) 90,100,100                                            FRIF 920
   90 Q=CI*C-SI*S                                                       FRIF 930
      S=CI*S+SI*C                                                       FRIF 940
      C=Q                                                               FRIF 950
      J=J+1                                                             FRIF 960
      GO TO 70                                                          FRIF 970
  100 A(1)=A(1)*0.5                                                     FRIF 980
      RETURN                                                            FRIF 990
      END                                                               FRIF1000
                                                                        FRIF1010
```

Subroutine FORIT

This subroutine produces the Fourier coefficients of a tabulated function.

Given:

1. Tabulated values of a function f(x) for x between 0 and 2π in steps of $2\pi/(2N+1)$

2. N such that there are 2N+1 tabulated data points: $2K\pi/(2N+1)$, K = 0, 1, 2, ..., 2N

3. M - the desired order of the Fourier coefficients where $0 \leq M \leq N$

the coefficients of the Fourier series which approximate the given function are calculated as follows:

$$C_1 = \cos\left(\frac{2\pi}{2N+1}\right) \quad (1)$$

$$S_1 = \sin\left(\frac{2\pi}{2N+1}\right) \quad (2)$$

$$U_2 = 0$$

$$U_1 = 0$$

$$C = 1$$

$$S = 0$$

$$J = 1$$

The following recursive sequence is used to compute U_0, U_1, and U_2

$$U_0 = f\left(\frac{2m\pi}{2N+1}\right) + 2 C U_1 - U_2 \quad (3)$$

$$U_2 = U_1$$

$$U_1 = U_0$$

for values of m = 2N, 2N-1, ..., 1

The coefficients are then:

$$A_J = \frac{2}{2N+1}\left(f(0) + C U_1 - U_2\right) \quad (4)$$

$$B_J = \frac{2}{2N+1} S U_1 \quad (5)$$

The values of C and S are updated to:

$$Q = C_1 C - S_1 S$$

$$S = C_1 S + S_1 C$$

$$C = Q$$

j is stepped by 1 and the sequence starting at equation (3) is now repeated until M+1 pairs of coefficients have been computed.

```
C                                                                       FRIT  10
C     ...............................................................   FRIT  20
C                                                                       FRIT  30
C        SUBROUTINE FORIT                                               FRIT  40
C                                                                       FRIT  50
C        PURPOSE                                                        FRIT  60
C           FOURIER ANALYSIS OF A PERIODICALLY TABULATED FUNCTION.      FRIT  70
C           COMPUTES THE COEFFICIENTS OF THE DESIRED NUMBER OF TERMS    FRIT  80
C           IN THE FOURIER SERIES F(X)=A(0)+SUM(A(K)COS KX+B(K)SIN KX)  FRIT  90
C           WHERE K=1,2,...,M TO APPROXIMATE A GIVEN SET OF             FRIT 100
C           PERIODICALLY TABULATED VALUES OF A FUNCTION.                FRIT 110
C                                                                       FRIT 120
C        USAGE                                                          FRIT 130
C           CALL FORIT(FNT,N,M,A,B,IER)                                 FRIT 140
C                                                                       FRIT 150
C        DESCRIPTION OF PARAMETERS                                      FRIT 160
C           FNT-VECTOR OF TABULATED FUNCTION VALUES OF LENGTH 2N+1      FRIT 170
C           N  -DEFINES THE INTERVAL SUCH THAT 2N+1 POINTS ARE TAKEN    FRIT 180
C               OVER THE INTERVAL (0,2PI). THE SPACING IS THUS 2PI/2N+1 FRIT 190
C           M  -MAXIMUM ORDER OF HARMONICS TO BE FITTED                 FRIT 200
C           A  -RESULTANT VECTOR OF FOURIER COSINE COEFFICIENTS OF      FRIT 210
C               LENGTH M+1                                              FRIT 220
C               A SUB 0, A SUB 1,..., A SUB M                           FRIT 230
C           B  -RESULTANT VECTOR OF FOURIER SINE COEFFICIENTS OF        FRIT 240
C               LENGTH M+1                                              FRIT 250
C               B SUB 0, B SUB 1,..., B SUB M                           FRIT 260
C           IER-RESULTANT ERROR CODE WHERE                              FRIT 270
C               IER=0  NO ERROR                                         FRIT 280
C               IER=1  N NOT GREATER OR EQUAL TO M                      FRIT 290
C               IER=2  M LESS THAN 0                                    FRIT 300
C                                                                       FRIT 310
C        REMARKS                                                        FRIT 320
C           M MUST BE GREATER THAN OR EQUAL TO ZERO                     FRIT 330
C           N MUST BE GREATER THAN OR EQUAL TO M                        FRIT 340
C           THE FIRST ELEMENT OF VECTOR B IS ZERO IN ALL CASES          FRIT 350
C                                                                       FRIT 360
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FRIT 370
C           NONE                                                        FRIT 380
C                                                                       FRIT 390
C        METHOD                                                         FRIT 400
C           USES RECURSIVE TECHNIQUE DESCRIBED IN A. RALSTON, H. WILF,  FRIT 410
C           'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS', JOHN WILEY    FRIT 420
C           AND SONS, NEW YORK, 1960, CHAPTER 24. THE METHOD OF INDEXINGFRIT 430
C           THROUGH THE PROCEDURE HAS BEEN MODIFIED TO SIMPLIFY THE     FRIT 440
C           COMPUTATION.                                                FRIT 450
C                                                                       FRIT 460
C     ...............................................................   FRIT 470
C                                                                       FRIT 480
      SUBROUTINE FORIT(FNT,N,M,A,B,IER)                                 FRIT 490
      DIMENSION A(1),B(1),FNT(1)                                        FRIT 500
C                                                                       FRIT 510
C        CHECK FOR PARAMETER ERRORS                                     FRIT 520
C                                                                       FRIT 530
      IER=0                                                             FRIT 540
   20 IF(M) 30,40,40                                                    FRIT 550
   30 IER=2                                                             FRIT 560
      RETURN                                                            FRIT 570
   40 IF(M-N) 60,60,50                                                  FRIT 580
   50 IER=1                                                             FRIT 590
      RETURN                                                            FRIT 600
C                                                                       FRIT 610
C        COMPUTE AND PRESET CONSTANTS                                   FRIT 620
C                                                                       FRIT 630
   60 AN=N                                                              FRIT 640
      COEF=2.0/(2.0*AN+1.0)                                             FRIT 650
      CONST=3.141593*COEF                                               FRIT 660
      S1=SIN(CONST)                                                     FRIT 670
      C1=COS(CONST)                                                     FRIT 680
      C=1.0                                                             FRIT 690
      S=0.0                                                             FRIT 700
      J=1                                                               FRIT 710
      FNTZ=FNT(1)                                                       FRIT 720
   70 U2=0.0                                                            FRIT 730
      U1=0.0                                                            FRIT 740
      I=2*N+1                                                           FRIT 750
C                                                                       FRIT 760
C        FORM FOURIER COEFFICIENTS RECURSIVELY                          FRIT 770
C                                                                       FRIT 780
   75 U0=FNT(I)+2.0*C*U1-U2                                             FRIT 790
      U2=U1                                                             FRIT 800
      U1=U0                                                             FRIT 810
      I=I-1                                                             FRIT 820
      IF(I-1) 80,80,75                                                  FRIT 830
   80 A(J)=COEF*(FNTZ+C*U1-U2)                                          FRIT 840
      B(J)=COEF*S*U1                                                    FRIT 850
      IF(J-(M+1)) 90,100,100                                            FRIT 860
   90 Q=C1*C-S1*S                                                       FRIT 870
      S=C1*S+S1*C                                                       FRIT 880
      C=Q                                                               FRIT 890
      J=J+1                                                             FRIT 900
      GO TO 70                                                          FRIT 910
  100 A(1)=A(1)*0.5                                                     FRIT 920
      RETURN                                                            FRIT 930
      END                                                               FRIT 940
```

Subroutines HARM and DHARM

Given three integers $M_\nu, \nu = 1, 2, 3$ and a three-dimensional array of complex numbers $A(k_1, k_2, k_3)$ where $k_\nu = 0, 1, \ldots, N_\nu - 1$ and $N_\nu = 2^{M_\nu}$, this subroutine computes the three-dimensional, complex Fourier series:

$$X(j_1, j_2, j_3) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} \sum_{k_3=0}^{N_3-1} A(k_1, k_2, k_3) \; e^{2\pi i \left(\frac{j_1 \cdot k_1}{N_1} + \frac{j_2 \cdot k_2}{N_2} + \frac{j_3 \cdot k_3}{N_3} \right)} \quad (1)$$

where

$$j_\nu = 0, 1, \ldots, N_\nu - 1 \text{ and } \nu = 1, 2, 3.$$

The inverse series may also be computed:

$$A(k_1, k_2, k_3) = \frac{1}{N_1 * N_2 * N_3} \sum_{j_1=0}^{N_1-1} \sum_{j_2=0}^{N_2-1} \sum_{j_3=0}^{N_3-1} X(j_1, j_2, j_3) \; e^{-2\pi i \left(\frac{j_1 \cdot k_1}{N_1} + \frac{j_2 \cdot k_2}{N_2} + \frac{j_3 \cdot k_3}{N_3} \right)} \quad (2)$$

For one dimension, the algorithm for the complex Fourier transform of complex numbers A (k) is:

$$X(j) = \sum_{k=0}^{N-1} A(k) \, w^{jk} \quad (3)$$

where $w = e^{\frac{2\pi i}{N}}$, $N = 2^M$, $j = 0, 1, 2, \ldots, N - 1$ expresses X(j) as a function of the M arguments $j_{M-1}, j_{M-2}, \ldots, j_1, j_0$ of the binary representation of j:

$$j = j_{M-1} \cdot 2^{M-1} + \ldots + j_1 2 + j_0, \; j_\nu = 0 \text{ or } 1$$

Then (3) can be written:

$$X(j_{M-1}, \ldots, j_1, j_0) = \sum_{k_0=0}^{1} \sum_{k_1=0}^{1} \cdots \sum_{k_{M-1}=0}^{1} A(k_{M-1}, \ldots, k_0) w^{j \cdot k_{M-1} \cdot 2^{M-1} + \ldots + j \cdot k_0 \cdot 2^0} \quad (4)$$

Then $w^{jk_{M-1}2^{M-1}} = w^{j \cdot k_{M-1} 2^{M-1}}$ since $e^{2\pi i} = 1$, and the innermost sum in (4) yields an array:

$$A_1(j_0, k_{M-2}, \ldots, k_0) = \sum_{k_{M-1}=0}^{1} A(k_{M-1}, \ldots, k_0) w^{j_0 \cdot k_{M-1} \cdot 2^{M-1}} \quad (5)$$

Successive arrays $A_2, \ldots, A_M$ obtained by summing over $k_{M-2}, \ldots, k_0$ respectively are computed. The general formula is:

$$A_L(j_0, \ldots, j_{L-1}, k_{M-L-1}, \ldots, k_0) = \sum_{k_{M-L}=0}^{1} A_{L-1}(j_0, \ldots, j_{L-2}, k_{M-L}, \ldots, k_0) w^{(j_{L-1} \cdot 2^{L-1} + \ldots + j_0) \, k_{M-L} 2^{M-L}} \quad (6)$$

The final array will be the desired X. The storage indexing convention used is to let the M arguments of $A_L(j_0, \ldots, k_0)$ be the binary representation of the index of the storage location for $A_L(j_0, \ldots, k_0)$. In this way, each step of the algorithm involves fetching from two storage locations and returning results in the same two locations, thereby saving storage. However, the elements of the final array:

$$X(j_{M-1}, \ldots, j_1, j_0) = A_M(j_0, k_1, \ldots, j_{M-1})$$

are in the wrong order. The program reverses the order of bits in bit representations to compensate.

A modification of the above algorithm is made for three dimensions, and another modification is made in the L-loop to save computations.

```
C                                                                       HARM  10
C     ..................................................................HARM  20
C                                                                       HARM  30
C        SUBROUTINE HARM                                                HARM  40
C                                                                       HARM  50
C        PURPOSE                                                        HARM  60
C           PERFORMS DISCRETE COMPLEX FOURIER TRANSFORMS ON A COMPLEX    HARM  70
C           THREE DIMENSIONAL ARRAY                                     HARM  80
C                                                                       HARM  90
C        USAGE                                                          HARM 100
C           CALL HARM (A,P,INV,S,IFSET,IFERR)                           HARM 110
C                                                                       HARM 120
C        DESCRIPTION OF PARAMETERS                                      HARM 130
C           A     - AS INPUT, A CONTAINS THE COMPLEX, 3-DIMENSIONAL     HARM 140
C                   ARRAY TO BE TRANSFORMED.  THE REAL PART OF          HARM 150
C                   A(I1,I2,I3) IS STORED IN VECTOR FASHION IN A CELL   HARM 160
C                   WITH INDEX 2*(I3*N1*N2 + I2*N1 + I1) + 1 WHERE      HARM 170
C                   N1 = 2**P(1), I=1,2,3 AND I1 = 0,1,...,N1-1 ETC.    HARM 180
C                   THE IMAGINARY PART IS IN THE CELL IMMEDIATELY       HARM 190
C                   FOLLOWING.  NOTE THAT THE SUBSCRIPT I1 INCREASES    HARM 200
C                   MOST RAPIDLY AND I3 INCREASES LEAST RAPIDLY.        HARM 210
C                   AS OUTPUT, A CONTAINS THE COMPLEX FOURIER           HARM 220
C                   TRANSFORM.  THE NUMBER OF CORE LOCATIONS OF         HARM 230
C                   ARRAY A IS 2*(N1*N2*N3)                             HARM 240
C           P     - A THREE CELL VECTOR WHICH DETERMINES THE SIZES      HARM 250
C                   OF THE 3 DIMENSIONS OF THE ARRAY A.   THE SIZE,     HARM 260
C                   N1, OF THE I DIMENSION OF A IS 2**P(I), I = 1,2,3   HARM 270
C           INV   - A VECTOR WORK AREA FOR BIT AND INDEX MANIPULATION   HARM 280
C                   OF DIMENSION ONE FOURTH OF THE QUANTITY             HARM 290
C                   MAX(N1,N2,N3)                                       HARM 300
C                   LOCATIONS OF A, VIZ., (1/8)*2*N1*N2*N3              HARM 300
C           S     - A VECTOR WORK AREA FOR SINE TABLES WITH DIMENSION   HARM 310
C                   THE SAME AS INV                                     HARM 320
C           IFSET - AN OPTION PARAMETER WITH THE FOLLOWING SETTINGS     HARM 330
C                     0    SET UP SINE AND INV TABLES ONLY             HARM 340
C                     1    SET UP SINE AND INV TABLES ONLY AND         HARM 350
C                          CALCULATE FOURIER TRANSFORM                 HARM 360
C                    -1    SET UP SINE AND INV TABLES ONLY AND         HARM 370
C                          CALCULATE INVERSE FOURIER TRANSFORM (FOR    HARM 380
C                          THE MEANING OF INVERSE SEE THE EQUATIONS    HARM 390
C                          UNDER METHOD BELOW)                         HARM 400
C                     2    CALCULATE FOURIER TRANSFORM ONLY (ASSUME    HARM 410
C                          SINE AND INV TABLES EXIST)                  HARM 420
C                    -2    CALCULATE INVERSE FOURIER TRANSFORM ONLY     HARM 430
C                          (ASSUME SINE AND INV TABLES EXIST)          HARM 440
C           IFERR - ERROR INDICATOR.   WHEN IFSET IS 0,+1,-1,           HARM 450
C                   IFERR = 1 MEANS THE MAXIMUM P(I) IS GREATER THAN    HARM 460
C                   20 , I=1,2,3   WHEN IFSET IS 2,-2 , IFERR = 1       HARM 470
C                   MEANS THAT THE SINE AND INV TABLES ARE NOT LARGE    HARM 480
C                   ENOUGH OR HAVE NOT BEEN COMPUTED .                  HARM 490
C                                                          E ABOVE      HARM 500
C                                                                       HARM 510
C                                                                       HARM 520
C        REMARKS                                                        HARM 530
C           THIS SUBROUTINE IS TO BE USED FOR COMPLEX, 3-DIMENSIONAL    HARM 540
C           ARRAYS IN WHICH EACH DIMENSION IS A POWER OF 2.  THE        HARM 550
C           MAXIMUM P(I) MUST NOT BE LESS THAN 3 OR GREATER THAN 20,    HARM 560
C           I = 1,2,3                                                   HARM 570
C                                                                       HARM 580
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  HARM 590
C           NONE                                                        HARM 600
C                                                                       HARM 610
C        METHOD                                                         HARM 620
C           FOR IFSET = +1, OR +2, THE FOURIER TRANSFORM OF COMPLEX     HARM 630
C           ARRAY A IS OBTAINED.                                        HARM 640
C                                                                       HARM 650
C                    N1-1   N2-1   N3-1                 L1   L2   L3    HARM 660
C     X(J1,J2,J3)=SUM     SUM     SUM     A(K1,K2,K3)*W1  **K2  **W3   HARM 670
C                    K1=0   K2=0   K3=0                                 HARM 680
C                                                                       HARM 690
C                    WHERE W1 IS THE N(1) ROOT OF UNITY AND L1=K1*J1,    HARM 700
C                          L2=K2*J2, L3=K3*J3                           HARM 710
C                                                                       HARM 720
C                                                                       HARM 730
C           FOR IFSET = -1, OR -2, THE INVERSE FOURIER TRANSFORM A OF   HARM 740
C           COMPLEX ARRAY X IS OBTAINED.                                HARM 750
C                                                                       HARM 760
C     A(K1,K2,K3)=                                                      HARM 770
C                 1       N1-1   N2-1   N3-1                  -L1  -L2  -L3 HARM 780
C           -------- *SUM     SUM     SUM     X(J1,J2,J3)*W1  **K2  **W3  HARM 790
C           N1*N2*N3   J1=0   J2=0   J3=0                               HARM 800
C                                                                       HARM 810
C                                                                       HARM 820
C           SEE J.W. COOLEY AND J.W. TUKEY, 'AN ALGORITHM FOR THE       HARM 830
C           MACHINE CALCULATION OF COMPLEX FOURIER SERIES',             HARM 840
C           MATHEMATICS OF COMPUTATION, VOL. 19 (APR. 1965), P. 297.    HARM 850
C                                                                       HARM 860
C     ..................................................................HARM 870
C                                                                       HARM 880
      SUBROUTINE HARM(A,P,INV,S,IFSET, IFERR)                           HARM 890
      DIMENSION A(1),INV(1),S(1),N(3),P(3),AP(3),W(2),W2(2),W3(2)       HARM 900
      EQUIVALENCE (N1,N(1)),(N2,N(2)),(N3,N(3))                         HARM 910
   10 IF( IABS(IFSET) - 1) 50,50,12                                     HARM 920
   12 PTT=MAX0(P(1),P(2),P(3)) -2                                       HARM 930
      RCOT2 = SQRT(2.)                                                  HARM 940
      IF (PTT-PT ) 14,14,13                                             HARM 950
   13 IFERR=1                                                           HARM 960
      RETURN                                                            HARM 970
   14 IFERR=0                                                           HARM 980
      P1=P(1)                                                           HARM 990
      P2=P(2)                                                           HARM1000
      P3=P(3)                                                           HARM1010
      N1=2**P1                                                          HARM1020
      N2=2**P2                                                          HARM1030
      N3=2**P3                                                          HARM1040
   16 IF(IFSET) 18,18,20                                                HARM1050
   18 NX= N1*N2*N3                                                      HARM1060
      FN = NX                                                           HARM1070
      DO 19 I = 1,NX                                                    HARM1080
      A(2*I-1) = A(2*I-1)/FN                                            HARM1090
   19 A(2*I) = -A(2*I)/FN                                               HARM1100
   20 NP(1)=N1*2                                                        HARM1110
      NP(2)= NP(1)*N2                                                   HARM1120
      NP(3)=NP(2)*N3                                                    HARM1130
      DO 25C IC=1,3                                                     HARM1140
      IL = NP(IC)                                                       HARM1150
      IL1 = IL*1                                                        HARM1160
      P1 = P(IC)                                                        HARM1170
      IF (P1)25C,25C,3C                                                 HARM1180
   3C IGIF=NP(IC)                                                       HARM1190
      KEIT=NP(IC)                                                       HARM1200
      PEV = 2*(P1/2)                                                    HARM1210
      IF (P1 - PEV )6C,6C,4C                                            HARM1220
C                                                                       HARM1230
C     P IS ODD, DO L=1 CASE                                             HARM1240
   4C KEIT=KEIT/2                                                       HARM1250
      KL=KEIT-2                                                         HARM1260
      DO 5C I=1,IL1,IGIF                                                HARM1270
      KLAST=KL+1                                                        HARM1280
      DO 5C K=1,KLAST,2                                                 HARM1290
      KL=K+KEIT                                                         HARM1300
C                                                                       HARM1310
C     DO ONE STEP WITH L=1,J=0                                          HARM1320
C     A(K)=A(K)+A(KC)                                                   HARM1330
C     A(KC)=A(K)-A(KC)                                                  HARM1340
C                                                                       HARM1350
      T=A(KC)                                                           HARM1360
      A(KC)=A(K)-T                                                      HARM1370
      A(K)=A(K)+T                                                       HARM1380
      T=A(KC+1)                                                         HARM1390
      A(KC+1)=A(K+1)-T                                                  HARM1400
   5C A(K+1)=A(K+1)+T                                                   HARM1410
      IF (P1 - 1)25C,25C,52                                             HARM1420
   52 LFINST =3                                                         HARM1430
C                                                                       HARM1440
C     DEF = JLAST = 2**(L-2) -1                                         HARM1450
      JLAST=1                                                           HARM1460
      DO 7C 7C                                                          HARM1470
C                                                                       HARM1480
C     P IS EVEN                                                         HARM1490
   6C LFINST = 2                                                        HARM1500
      JLAST=0                                                           HARM1510
   7C DO 24C L=LFINST,P1,2                                              HARM1520
      JJGIF=KEIT                                                        HARM1530
      KEIT=KEIT/                                                        HARM1540
      KL=KEIT-2                                                         HARM1550
C                                                                       HARM1560
C     DO FOR J=0                                                        HARM1570
      DO 8C I=1,IL1,IGIF                                                HARM1580
      KLAST=I+KL                                                        HARM1590
      DO 8C K=I,KLAST,2                                                 HARM1600
      K1=K+KEIT                                                         HARM1610
      K2=K1+KEIT                                                        HARM1620
      K3=K2+KEIT                                                        HARM1630
C                                                                       HARM1640
C     DO THE STEPS WITH J=0                                             HARM1650
C     A(K)=A(K)+A(K2)                                                   HARM1660
C     A(K2)=A(K)-A(K2)                                                  HARM1670
C     A(K1)=A(K1)+A(K3)                                                 HARM1680
C     A(K3)=A(K1)-A(K3)                                                 HARM1690
C                                                                       HARM1700
C     A(K)=A(K)+A(K1)                                                   HARM1710
C     A(K1)=A(K)-A(K1)                                                  HARM1720
C     A(K2)=A(K2)+A(K3)*I                                               HARM1730
C     A(K3)=A(K2)-A(K3)*I                                               HARM1740
C                                                                       HARM1750
      T=A(K2)                                                           HARM1760
      A(K2)=A(K)-T                                                      HARM1770
      A(K)=A(K)+T                                                       HARM1780
      T=A(K2+1)                                                         HARM1790
      A(K2+1)=A(K+1)-T                                                  HARM1800
      A(K+1)=A(K+1)+T                                                   HARM1810
C                                                                       HARM1820
      T=A(K3)                                                           HARM1830
      A(K3)=A(K1)-T                                                     HARM1840
      A(K1)=A(K1)+T                                                     HARM1850
      T=A(K3+1)                                                         HARM1860
      A(K3+1)=A(K1+1)-T                                                 HARM1870
      A(K1+1)=A(K1+1)+T                                                 HARM1880
C                                                                       HARM1890
      T=A(K1)                                                           HARM1900
      A(K1)=A(K)-T                                                      HARM1910
      A(K)=A(K)+T                                                       HARM1920
      T=A(K1+1)                                                         HARM1930
      A(K1+1)=A(K+1)-T                                                  HARM1940
      A(K+1)=A(K+1)+T                                                   HARM1950
C                                                                       HARM1960
      R=-A(K3+1)                                                        HARM1970
      T = A(K3)                                                         HARM1980
      A(K3)=A(K2)-R                                                     HARM1990
      A(K2)=A(K2)+R                                                     HARM2000
      A(K3+1)=A(K2+1)-T                                                 HARM2010
   8C A(K2+1)=A(K2+1)+T                                                 HARM2020
      IF (JLAST) 235,235,82                                             HARM2030
   82 JJ=JJGIF   +1                                                     HARM2040
C                                                                       HARM2050
C     DO FOR J=1                                                        HARM2060
      ILAST= IL +JJ                                                     HARM2070
      DO 85 I = JJ,ILAST,IGIF                                           HARM2080
      KLAST = KL+I                                                      HARM2090
      DO 85 K=I,KLAST,2                                                 HARM2100
      K1 = K+KEIT                                                       HARM2110
      K2 = K1+KEIT                                                      HARM2120
      K3 = K2+KEIT                                                      HARM2130
C                                                                       HARM2140
C     LETTING W=(1+I)/RCOT2,W3=(-1+I)/RCOT2,W2=I.                       HARM2150
C     A(K)=A(K)+A(K2)*I                                                 HARM2160
C     A(K2)=A(K)-A(K2)*I                                                HARM2170
C     A(K1)=A(K1)*W+A(K3)*W3                                            HARM2180
C     A(K3)=A(K1)*W-A(K3)*W3                                            HARM2190
C                                                                       HARM2200
C     A(K)=A(K)+A(K1)                                                   HARM2210
C     A(K1)=A(K)-A(K1)                                                  HARM2220
C     A(K2)=A(K2)+A(K3)*I                                               HARM2230
C     A(K3)=A(K2)-A(K3)*I                                               HARM2240
C                                                                       HARM2250
      R =-A(K2+1)                                                       HARM2260
      T = A(K2)                                                         HARM2270
      A(K2) = A(K)-R                                                    HARM2280
      A(K) = A(K)+R                                                     HARM2290
      A(K2+1)=A(K+1)-T                                                  HARM2300
      A(K+1)=A(K+1)+T                                                   HARM2310
C                                                                       HARM2320
      AWR=A(K1)-A(K1+1)                                                 HARM2330
      AWI = A(K1+1)+A(K1)                                               HARM2340
      R=-A(K3)-A(K3+1)                                                  HARM2350
      T=A(K3)-A(K3+1)                                                   HARM2360
      A(K3)=(AWR-AI)/RCOT2                                              HARM2370
      A(K3+1)=(AWI-T)/RCOT2                                             HARM2380
      A(K1)=(AWR+AI)/RCOT2                                              HARM2390
      A(K1+1)=(AWI+T)/RCOT2                                             HARM2400
      T= A(K1)                                                          HARM2410
      A(K1)=A(K)-T                                                      HARM2420
      A(K)=A(K)+T                                                       HARM2430
      T=A(K1+1)                                                         HARM2440
      A(K1+1)=A(K+1)-T                                                  HARM2450
      A(K+1)=A(K+1)+T                                                   HARM2460
      R=-A(K3+1)                                                        HARM2470
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      T=A(K3)                                                          HARM2480
      A(K3)=A(K2)-R                                                    HARM2490
      A(K2)=A(K2)+R                                                    HARM2500
      A(K3+1)=A(K2+1)-T                                                HARM2510
   85 A(K2+1)=A(K2+1)+T                                                HARM2520
      IF(JLAST-1) 235,235,90                                           HARM2530
   90 JJ= JJ + JJCIF                                                   HARM2540
C                                                                      HARM2550
C     NOW DO THE REMAINING J'S                                         HARM2560
      DO 230 J=2,JLAST                                                 HARM2570
C                                                                      HARM2580
C     FETCH W'S                                                        HARM2590
C     DEF- W=W**INV(J), W2=W**2, W3=W**3                               HARM2600
   95 I=INV(J+1)                                                       HARM2610
   98 IC=NT-I                                                          HARM2620
      W(1)=S(IC)                                                       HARM2630
      W(2)=S(I)                                                        HARM2640
      I2=2*I                                                           HARM2650
      I2C=NT-I2                                                        HARM2660
      IF(I2C)120,110,100                                               HARM2670
C                                                                      HARM2680
C     2*I IS IN FIRST QUADRANT                                         HARM2690
  100 W2(1)=S(I2C)                                                     HARM2700
      W2(2)=S(I2)                                                      HARM2710
      GO TO 130                                                        HARM2720
  110 W2(1)=0.                                                         HARM2730
      W2(2)=1.                                                         HARM2740
      GO TO 130                                                        HARM2750
C                                                                      HARM2760
C     2*I IS IN SECOND QUADRANT                                        HARM2770
  120 I2CC = I2C+NT                                                    HARM2780
      I2C=-I2C                                                         HARM2790
      W2(1)=-S(I2C)                                                    HARM2800
      W2(2)=S(I2CC)                                                    HARM2810
  130 I3=I+I2                                                          HARM2820
      I3C=NT-I3                                                        HARM2830
      IF(I3C)140,150,140                                               HARM2840
C                                                                      HARM2850
C     I3 IN FIRST QUADRANT                                             HARM2860
  140 W3(1)=S(I3C)                                                     HARM2870
      W3(2)=S(I3)                                                      HARM2880
      GO TO 200                                                        HARM2890
  150 W3(1)=0.                                                         HARM2900
      W3(2)=1.                                                         HARM2910
      GO TO 200                                                        HARM2920
C                                                                      HARM2930
  160 I3CC=I2C+NT                                                      HARM2940
      IF(I3CC)150,180,170                                              HARM2950
C                                                                      HARM2960
C     I3 IN SECOND QUADRANT                                            HARM2970
  170 I3C=-I3C                                                         HARM2980
      W3(1)=-S(I3C)                                                    HARM2990
      W3(2)=S(I3CC)                                                    HARM3000
      GO TO 200                                                        HARM3010
  180 W3(1)=-1.                                                        HARM3020
      W3(2)=0.                                                         HARM3030
      GO TO 200                                                        HARM3040
C                                                                      HARM3050
C     3*I IN THIRD QUADRANT                                            HARM3060
  190 I3CCC=NT+I3CC                                                    HARM3070
      I3CC = -I3CC                                                     HARM3080
      W3(1)=-S(I3CCC)                                                  HARM3090
      W3(2)=-S(I3CC)                                                   HARM3100
  200 ILAST=IL+JJ                                                      HARM3110
      DO 220 I=JJ,IL    ,JCIF                                          HARM3120
      KLAST=KL+I                                                       HARM3130
      DO 220 K=I,KLAST,2                                               HARM3140
      K1=K+KEIT                                                        HARM3150
      K2=K1+KEIT                                                       HARM3160
      K3=K2+KEIT                                                       HARM3170
C                                                                      HARM3180
C     DO THE STEPS WITH J NOT 0                                        HARM3190
C     A(K)=A(K)+A(K2)*W2                                               HARM3200
C     A(K2)=A(K)-A(K2)*W2                                              HARM3210
C     A(K1)=A(K1)*W+A(K3)*W3                                           HARM3220
C     A(K3)=A(K1)*W-A(K3)*W3                                           HARM3230
C                                                                      HARM3240
C     A(K)=A(K)+A(K1)                                                  HARM3250
C     A(K1)=A(K)-A(K1)                                                 HARM3260
C     A(K2)=A(K2)+A(K3)*I                                              HARM3270
C     A(K3)=A(K2)-A(K3)*I                                              HARM3280
C                                                                      HARM3290
      R=A(K2)*W2(1)-A(K2+1)*W2(2)                                      HARM3300
      T=A(K2)*W2(2)+A(K2+1)*W2(1)                                      HARM3310
      A(K2)=A(K)-R                                                     HARM3320
      A(K)=A(K)+R                                                      HARM3330
      A(K2+1)=A(K+1)-T                                                 HARM3340
      A(K+1)=A(K+1)+T                                                  HARM3350
C                                                                      HARM3360
      R=A(K3)*W3(1)-A(K3+1)*W3(2)                                      HARM3370
      T=A(K3)*W3(2)+A(K3+1)*W3(1)                                      HARM3380
      ABR=A(K1)*W(1)-A(K1+1)*W(2)                                      HARM3390
      ABI=A(K1)*W(2)+A(K1+1)*W(1)                                      HARM3400
      A(K3)=ABR-R                                                      HARM3410
      A(K3+1)=ABI-T                                                    HARM3420
      A(K1)=ABR+R                                                      HARM3430
      A(K1+1)=ABI+T                                                    HARM3440
      T=A(K1)                                                          HARM3450
      A(K1)=A(K)-T                                                     HARM3460
      A(K)=A(K)+T                                                      HARM3470
      T=A(K1+1)                                                        HARM3480
      A(K1+1)=A(K+1)-T                                                 HARM3490
      A(K+1)=A(K+1)+T                                                  HARM3500
      R=-A(K2+1)                                                       HARM3510
      T=A(K2)                                                          HARM3520
      A(K3)=A(K2)-R                                                    HARM3530
      A(K2)=A(K2)+R                                                    HARM3540
      A(K3+1)=A(K2+1)-T                                                HARM3550
  220 A(K2+1)=A(K2+1)+T                                                HARM3560
C     END OF I AND K LOOPS                                             HARM3570
C                                                                      HARM3580
  230 JJ=JJCIF+JJ                                                      HARM3590
C     END OF J-LOOP                                                    HARM3600
C                                                                      HARM3610
  235 JLAST=4*JLAST+3                                                  HARM3620
  240 CONTINUE                                                         HARM3630
C     END OF   L  LOOP                                                 HARM3640
C                                                                      HARM3650
  250 CONTINUE                                                         HARM3660
C     END OF   IC  LOOP                                                HARM3670
C                                                                      HARM3680
C     WE NOW HAVE THE COMPLEX FOURIER SUMS BUT THEIR ACCESSES ARE      HARM3690
C     BIT-REVERSED.  THE FOLLOWING ROUTINE PUTS THEM IN ORDER          HARM3700
      NTSC=NT*NT                                                       HARM3710
      P3PT=P3-PT                                                       HARM3720
  255 IF(P3PT) 270,340,260                                             HARM3730
C                                                                      HARM3740
C     P3 GR. OR EQ. PT                                                 HARM3750
  260 IGC3=1                                                           HARM3760
      N3VAT=N3/NT                                                      HARM3770
      P1NA3=N1                                                         HARM3780
      GO TO 340                                                        HARM3790
C                                                                      HARM3800
C     P3 LESS THAN PT                                                  HARM3810
  270 IGC3=2                                                           HARM3820
      N3VAT=1                                                          HARM3830
      NTVA3=NT/N3                                                      HARM3840
      P1NA3=N2                                                         HARM3850
  340 JJC3 = NTSC/N3                                                   HARM3860
      P2PT=P2-PT                                                       HARM3870
  450 IF (P2PT)470,460,460                                             HARM3880
C                                                                      HARM3890
C     P2 GR. OR EQ. PT                                                 HARM3900
  460 IGC2=1                                                           HARM3910
      N2VAT=N2/NT                                                      HARM3920
      P1NA2=NT                                                         HARM3930
      GO TO 480                                                        HARM3940
C                                                                      HARM3950
C     P2 LESS THAN PT                                                  HARM3960
  470 IGC2 = 2                                                         HARM3970
      N2VAT=1                                                          HARM3980
      NTVA2=NT/N2                                                      HARM3990
      P1NA2=N2                                                         HARM4000
  480 JJC2=NTSC/N2                                                     HARM4010
      P1PT=P1-PT                                                       HARM4020
  550 IF(P1PT)570,560,560                                              HARM4030
C                                                                      HARM4040
C     P1 GR. OR EQ. PT                                                 HARM4050
  560 IGC1=1                                                           HARM4060
      N1VAT=N1/NT                                                      HARM4070
      P1NA1=N1                                                         HARM4080
      GO TO 580                                                        HARM4090
C                                                                      HARM4100
C     P1 LESS THAN PT                                                  HARM4110
  570 IGC1=2                                                           HARM4120
      N1VAT=1                                                          HARM4130
      NTVA1=NT/N1                                                      HARM4140
      P1NA1=N1                                                         HARM4150
  580 JJC1=NTSC/N1                                                     HARM4160
  600 JJ3=1                                                            HARM4170
      J=1                                                              HARM4180
      GO TO 800 JF3=1,N3VAT                                            HARM4190
      IPF3=INV(JJ3)                                                    HARM4200
      GO TO 630 JF3=1,P1NA3                                            HARM4210
      GO TO (610,620),IGC3                                             HARM4220
  610 IF3=INV(JF3)*N3VAT                                               HARM4230
      GO TO 630                                                        HARM4240
  620 IF3=(INV(JF3)/NTVA3                                              HARM4250
  630 I3=(IPF3+IP3)*N2                                                 HARM4260
  700 JJ2=1                                                            HARM4270
      GO TO 670 JF2=1,N2VAT                                            HARM4280
      IPF2=INV(JJ2)+I3                                                 HARM4290
      GO TO 800 JF2=1,P1NA2                                            HARM4300
      GO TO (710,720),IGC2                                             HARM4310
  710 IF2=INV(JF2)*N2VAT                                               HARM4320
      GO TO 730                                                        HARM4330
  720 IF2=INV(JF2)/NTVA2                                               HARM4340
  730 I2=(IPF2+IP2)*N1                                                 HARM4350
  800 JJ1=1                                                            HARM4360
      GO TO 860 JF1=1,N1VAT                                            HARM4370
      IPF1=INV(JJ1)+I2                                                 HARM4380
      GO TO 850 JF1=1,P1NA1                                            HARM4390
      GO TO (810,820),IGC1                                             HARM4400
  810 IF1=INV(JF1)*N1VAT                                               HARM4410
      GO TO 830                                                        HARM4420
  820 IF1=INV(JF1)/NTVA1                                               HARM4430
  830 I=2*(IPF1+IF1)+1                                                 HARM4440
      IF (J-I) 840,850,850                                             HARM4450
  840 T=A(I)                                                           HARM4460
      A(I)=A(J)                                                        HARM4470
      A(J)=T                                                           HARM4480
      T=A(I+1)                                                         HARM4490
      A(I+1)=A(J+1)                                                    HARM4500
      A(J+1)=T                                                         HARM4510
  850 J=J+2                                                            HARM4520
  860 JJ1=JJ1+JJC1                                                     HARM4530
C     END OF JF1 AND JF2                                               HARM4540
C                                                                      HARM4550
  870 JJ2=JJ2+JJC2                                                     HARM4560
C     END OF JF2 AND JF3 LOOPS                                         HARM4570
C                                                                      HARM4580
  880 JJ3 = JJ3+JJC3                                                   HARM4590
C     END OF JF3 LOOP                                                  HARM4600
C                                                                      HARM4610
  890 IF(ISET)ES1,895,895                                              HARM4620
  891 DO 892 I = 1,NX                                                  HARM4630
  892 A(2*I) = -A(2*I)                                                 HARM4640
  895 RETURN                                                           HARM4650
C                                                                      HARM4660
C     THE FOLLOWING PROGRAM COMPUTES THE SIN AND INV TABLES.           HARM4670
C                                                                      HARM4680
  900 PI=PARC(P(1),P(2),P(3)) -2                                       HARM4690
      PT = PARC(2,PI)                                                  HARM4700
  904 IF (PI-1E) 906,906,13                                            HARM4710
  906 IFERR=0                                                          HARM4720
      NT=2*PT                                                          HARM4730
      NTV2=NT/2                                                        HARM4740
C                                                                      HARM4750
C     SET UP SIN TABLE                                                 HARM4760
C     THETA=PIE/2**(L+1) FOR L=1                                       HARM4770
  910 THETA=.7853981634                                                HARM4780
C                                                                      HARM4790
C     JSTEP=2**(PT-L+1) FOR L=1                                        HARM4800
      JSTEP=NT                                                         HARM4810
C                                                                      HARM4820
C     JCIF=2**(PT-L) FOR L=1                                           HARM4830
      JCIF=NTV2                                                        HARM4840
      S(JCIF)=SIN(THETA)                                               HARM4850
      DO 950 L=2,PT                                                    HARM4860
      THETA=THETA/2.                                                   HARM4870
      JSTEP2=JSTEP                                                     HARM4880
      JSTEP=JCIF                                                       HARM4890
      JCIF=JSTEP/2                                                     HARM4900
      S(JCIF)=SIN(THETA)                                               HARM4910
      JC1=NT-JCIF                                                      HARM4920
      S(JC1)=COS(THETA)                                                HARM4930
      JLAST=NT-JSTEP2                                                  HARM4940
      IF(JLAST - JSTEP) 950,920,920                                    HARM4950
  920 DO 940 J=JSTEP,JLAST,JSTEP                                       HARM4960
      JC=NT-J                                                          HARM4970
      JC=J+JCIF                                                        HARM4980
  940 S(JC)=S(J)*S(JC1)+S(JCIF)*S(JC)                                  HARM4990
  950 CONTINUE                                                         HARM5000
C                                                                      HARM5010
C     SET UP INV(J) TABLE                                              HARM5020
C                                                                      HARM5030
  960 PTLESP=NTV2                                                      HARM5040
C                                                                      HARM5050
C     PTLESP=2**(PT-L). FOR L=1                                        HARM5060
      LPIESP=1                                                         HARM5070
      P1NA1=N1                                                         HARM5080
      P1NA2=N2                                                         HARM5090
      P1NA3=N3                                                         HARM5100
      GO TO 1000                                                       HARM5110
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C                                                                       HARM5120
C     LPIEXP=200*(L-1), FOR L=1                                         HARM5130
      INV(1)=C                                                          HARM5140
      CC 46C L=1,PT                                                     HARM5150
      INV(LPIEXP+1) = PTLEXP                                            HARM5160
      CC 47C J=2,LPIEXP                                                 HARM5170
      JJ=J+LPIEXP                                                       HARM5180
  47C INV(JJ)=INV(J)+PTLEXP                                             HARM5190
      PTLEXP=PTLEXP/2                                                   HARM5200
  48C LPIEXP=LPIEXP*2                                                   HARM5210
  46C IF(IFSET)112,655,12                                               HARM5220
      END                                                               HARM5230
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C                                                                       DHAR  10
C     ..................................................................DHAR  20
C                                                                       DHAR  30
C        SUBROUTINE CHARM                                               DHAR  40
C                                                                       DHAR  50
C        PURPOSE                                                        DHAR  60
C           PERFORMS DISCRETE COMPLEX FOURIER TRANSFORMS ON A COMPLEX    DHAR  70
C           DOUBLE PRECISION,THREE DIMENSIONAL ARRAY                    DHAR  80
C                                                                       DHAR  90
C        USAGE                                                          DHAR 100
C           CALL CHARM(A,P,INV,S,IFSET,IFERR)                           DHAR 110
C                                                                       DHAR 120
C        DESCRIPTION OF PARAMETERS                                      DHAR 130
C           A     - A DOUBLE PRECISION VECTOR                           DHAR 140
C                   AS INPUT, A CONTAINS THE COMPLEX, 3-DIMENSIONAL     DHAR 150
C                   ARRAY TO BE TRANSFORMED.  THE REAL PART OF          DHAR 160
C                   A(I1,I2,I3) IS STORED IN VECTOR FASHION IN A CELL   DHAR 170
C                   WITH INDEX 2*(I3*N1*N2 + I2*N1 + I1) + 1 WHERE      DHAR 180
C                   NI = 2**P(I), I=1,2,3 AND I1 = 0,1,...,N1-1 ETC.    DHAR 190
C                   THE IMAGINARY PART IS IN THE CELL IMMEDIATELY       DHAR 200
C                   FOLLOWING.  NOTE THAT THE SUBSCRIPT I1 INCREASES    DHAR 210
C                   MOST RAPIDLY AND I3 INCREASES LEAST RAPIDLY.        DHAR 220
C                   AS OUTPUT, A CONTAINS THE COMPLEX FOURIER           DHAR 230
C                   TRANSFORM.  THE NUMBER OF CORE LOCATIONS OF         DHAR 240
C                   ARRAY A IS 2*(N1*N2*N3)                             DHAR 250
C           P     - A THREE CELL VECTOR WHICH DETERMINES THE SIZES      DHAR 260
C                   OF THE 3 DIMENSIONS OF THE ARRAY A.   THE SIZE,     DHAR 270
C                   NI, OF THE I DIMENSION OF A IS 2**M(I), I = 1,2,3   DHAR 280
C           INV   - A VECTOR WORK AREA FOR BIT AND INDEX MANIPULATION    DHAR 290
C                   OF DIMENSION ONE FOURTH OF THE QUANTITY             DHAR 300
C                   MAX(N1,N2,N3)                                       DHAR 310
C                   LOCATIONS OF A, WILL BE (1/8)*2*N1*N2*N3            DHAR 310
C           S     - A DOUBLE PRECISION VECTOR WORK AREA FOR SINE TABLES DHAR 320
C                   WITH DIMENSION THE SAME AS INV                      DHAR 330
C           IFSET - AN OPTION PARAMETER WITH THE FOLLOWING SETTINGS     DHAR 340
C                     0    SET UP SINE AND INV TABLES ONLY             DHAR 350
C                     1    SET UP SINE AND INV TABLES ONLY AND         DHAR 360
C                          CALCULATE FOURIER TRANSFORM                 DHAR 370
C                    -1    SET UP SINE AND INV TABLES ONLY AND         DHAR 380
C                          CALCULATE INVERSE FOURIER TRANSFORM (FOR     DHAR 390
C                          THE MEANING OF INVERSE SEE THE EQUATIONS     DHAR 400
C                          UNDER METHOD BELOW)                          DHAR 410
C                     2    CALCULATE FOURIER TRANSFORM ONLY (ASSUME     DHAR 420
C                          SINE AND INV TABLES EXIST)                   DHAR 430
C                    -2    CALCULATE INVERSE FOURIER TRANSFORM ONLY      DHAR 440
C                          (ASSUME SINE AND INV TABLES EXIST)           DHAR 450
C           IFERR - ERROR INDICATOR.   WHEN IFSET IS 0,+1,-1,           DHAR 460
C                   IFERR = 1 MEANS THE MAXIMUM P(I) IS GREATER THAN    DHAR 470
C                   20, I=1,2,3   WHEN IFSET IS 2,-2 , IFERR = 1        DHAR 480
C                   MEANS THAT THE SINE AND INV TABLES ARE NOT LARGE     DHAR 490
C                   ENOUGH OR HAVE NOT BEEN COMPUTED .                  DHAR 500
C                   IF ON RETURN IFERR = 0 THEN NONE OF THE ABOVE       DHAR 510
C                   CONDITIONS ARE PRESENT                              DHAR 520
C                                                                       DHAR 530
C        REMARKS                                                        DHAR 540
C           THIS SUBROUTINE IS TO BE USED FOR COMPLEX, DOUBLE PRECISION,DHAR 550
C           3-DIMENSIONAL ARRAYS IN WHICH EACH DIMENSION IS A POWER OF  DHAR 560
C           2. THE MAXIMUM P(I) MUST NOT BE LESS THAN 3 OR GREATER THAN DHAR 570
C           20, I = 1,2,3.                                              DHAR 580
C                                                                       DHAR 590
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DHAR 600
C           NONE                                                        DHAR 610
C                                                                       DHAR 620
C        METHOD                                                         DHAR 630
C           FOR IFSET = +1, OR +2, THE FOURIER TRANSFORM OF COMPLEX     DHAR 640
C           ARRAY A IS OBTAINED.                                        DHAR 650
C                                                                       DHAR 660
C                    N1-1   N2-1   N3-1                 L1   L2   L3   DHAR 670
C     X(J1,J2,J3)=SUM   SUM   SUM     A(K1,K2,K3)*W1  **J2  **J3      DHAR 680
C                 K1=0   K2=0   K3=0                                    DHAR 690
C                                                                       DHAR 700
C                    WHERE W1 IS THE N(I) ROOT OF UNITY AND L1=K1*J1,    DHAR 710
C                          L2=K2*J2, L3=K3*J3                           DHAR 720
C                                                                       DHAR 730
C                                                                       DHAR 740
C           FOR IFSET = -1, OR -2, THE INVERSE FOURIER TRANSFORM A OF   DHAR 750
C           COMPLEX ARRAY X IS OBTAINED.                                DHAR 760
C                                                                       DHAR 770
C     A(K1,K2,K3)=                                                      DHAR 780
C            1      N1-1   N2-1   N3-1                  -L1  -L2  -L3   DHAR 790
C        -------- *SUM    SUM    SUM     X(J1,J2,J3)*W1  **J2  **J3    DHAR 800
C        N1*N2*N3   J1=0   J2=0   J3=0                                  DHAR 810
C                                                                       DHAR 820
C                                                                       DHAR 830
C           SEE J.W. COOLEY AND J.W. TUKEY, 'AN ALGORITHM FOR THE       DHAR 840
C           MACHINE CALCULATION OF COMPLEX FOURIER SERIES',             DHAR 850
C           MATHEMATICS OF COMPUTATIONS, VOL. 19 (APR. 1965), P. 297.   DHAR 860
C                                                                       DHAR 870
C     ..................................................................DHAR 880
C                                                                       DHAR 890
      SUBROUTINE CHARM(A,P,INV,S,IFSET,IFERR)                           DHAR 900
      DIMENSION A(1),INV(1),S(1),M(3),NP(3),N(2),W2(2),W3(2)            DHAR 910
      DOUBLE PRECISION A,W,W3,W2,THETA,RCCT2,S,T,W,R2,FA,AKR            DHAR 920
      EQUIVALENCE (N1,N(1)),(N2,N(2)),(N3,N(3))                         DHAR 930
   1C IF( IABS(IFSET) - 1) 5CC,3CC,12                                   DHAR 940
   12 PTT=P**2+P(1)+P(2)+P(3) -2                                        DHAR 950
      RCCT2=0.5**(PTT/2.CCC)                                            DHAR 960
      IF (PTT-PT ) 14,14,13                                             DHAR 970
   13 IFERR=1                                                           DHAR 980
      RETURN                                                            DHAR 990
   14 IFERR=C                                                           DHAR1000
      M1=M(1)                                                           DHAR1010
      M2=M(2)                                                           DHAR1020
      M3=M(3)                                                           DHAR1030
      N1=2**M1                                                          DHAR1040
      N2=2**M2                                                          DHAR1050
      N3=2**M3                                                          DHAR1060
      IE IF(IFSET) 1E,1E,2C                                             DHAR1070
   1E N=N1*N2*N3                                                        DHAR1080
      FA = NN                                                           DHAR1090
      CC 15 I = 1,NN                                                    DHAR1100
      A(2*I-1) = A(2*I-1)/FA                                            DHAR1110
   15 A(2*I) = -A(2*I)/FA                                               DHAR1120
   2C NP(1)=N1C2                                                        DHAR1130
      NP(2)= NP(1)*N2                                                   DHAR1140
      NP(3)=NP(2)*N3                                                    DHAR1150
      CC 25C IC=1,3                                                     DHAR1160
      IL = NP(3)-NP(IC)                                                 DHAR1170
      IL1 = IL+1                                                        DHAR1180
      M1 = M(IC)                                                        DHAR1190
      IF (M1)25C,25C,3C                                                 DHAR1200
   3C ICIF=NP(IC)                                                       DHAR1210
      KEIT=NP(IC)                                                       DHAR1220
      MEV = 2*(M1/2)                                                    DHAR1230
      IF (M1 - MEV) 36C,4C,4C                                           DHAR1240
C                                                                       DHAR1250
C     P IS CCC, CC L=1 CASE                                             DHAR1260
   4C KEIT=KEIT/2                                                       DHAR1270
      KL=KEIT-2                                                         DHAR1280
      CC 5C I=1,IL1,ICIF                                                DHAR1290
      KLAST=KL+I                                                        DHAR1300
      CC 5C K=I,KLAST,2                                                 DHAR1310
      KC=K+KEIT                                                         DHAR1320
C                                                                       DHAR1330
C     CC ONE STEP WITH L=1,J=C                                          DHAR1340
C     A(K)=A(K)+A(KC)                                                   DHAR1350
C     A(KC)=A(K)-A(KC)                                                  DHAR1360
C                                                                       DHAR1370
      T=A(KC)                                                           DHAR1380
      A(KC)=A(K)-T                                                      DHAR1390
      A(K)=A(K)+T                                                       DHAR1400
      T=A(KC+1)                                                         DHAR1410
      A(KC+1)=A(K+1)-T                                                  DHAR1420
   5C A(K+1)=A(K+1)+T                                                   DHAR1430
      IF (M1 - 1)25C,25C,52                                             DHAR1440
   52 LFIRST =2                                                         DHAR1450
C                                                                       DHAR1460
C     CEF = JLAST = 2**(L-2) -1                                         DHAR1470
      JLAST=1                                                           DHAR1480
      CC TC 7C                                                          DHAR1490
C                                                                       DHAR1500
C     P IS EVEN                                                         DHAR1510
   6C LFIRST = 2                                                        DHAR1520
      JLAST=C                                                           DHAR1530
   7C CC 24C L=LFIRST,M1,2                                              DHAR1540
      JJCIF=KEIT                                                        DHAR1550
      KEIT=KEIT/4                                                       DHAR1560
      KL=KEIT-2                                                         DHAR1570
C                                                                       DHAR1580
C     CC FCR J=C                                                        DHAR1590
      CC 8C I=1,IL1,ICIF                                                DHAR1600
      KLAST=I+KL                                                        DHAR1610
      CC 8C K=I,KLAST,2                                                 DHAR1620
      K1=K+KEIT                                                         DHAR1630
      K2=K1+KEIT                                                        DHAR1640
      K3=K2+KEIT                                                        DHAR1650
C                                                                       DHAR1660
C     CC TWC STEPS WITH J=C                                             DHAR1670
C     A(K)=A(K)+A(K2)                                                   DHAR1680
C     A(K2)=A(K)-A(K2)                                                  DHAR1690
C     A(K1)=A(K1)+A(K3)                                                 DHAR1700
C     A(K3)=A(K1)-A(K3)                                                 DHAR1710
C                                                                       DHAR1720
C     A(K)=A(K)+A(K1)                                                   DHAR1730
C     A(K1)=A(K)-A(K1)                                                  DHAR1740
C     A(K2)=A(K2)+A(K3)*I                                               DHAR1750
C     A(K3)=A(K2)-A(K3)*I                                               DHAR1760
C                                                                       DHAR1770
      T=A(K2)                                                           DHAR1780
      A(K2)=A(K)-T                                                      DHAR1790
      A(K)=A(K)+T                                                       DHAR1800
      T=A(K2+1)                                                         DHAR1810
      A(K2+1)=A(K+1)-T                                                  DHAR1820
      A(K+1)=A(K+1)+T                                                   DHAR1830
C                                                                       DHAR1840
      T=A(K3)                                                           DHAR1850
      A(K3)=A(K1)-T                                                     DHAR1860
      A(K1)=A(K1)+T                                                     DHAR1870
      T=A(K3+1)                                                         DHAR1880
      A(K3+1)=A(K1+1)-T                                                 DHAR1890
      A(K1+1)=A(K1+1)+T                                                 DHAR1900
C                                                                       DHAR1910
      T=A(K1)                                                           DHAR1920
      A(K1)=A(K)-T                                                      DHAR1930
      A(K)=A(K)+T                                                       DHAR1940
      T=A(K1+1)                                                         DHAR1950
      A(K1+1)=A(K+1)-T                                                  DHAR1960
      A(K+1)=A(K+1)+T                                                   DHAR1970
C                                                                       DHAR1980
      R=-A(K3+1)                                                        DHAR1990
      T = A(K3)                                                         DHAR2000
      A(K3)=A(K2)-R                                                     DHAR2010
      A(K2)=A(K2)+R                                                     DHAR2020
      A(K3+1)=A(K2+1)-T                                                 DHAR2030
   8C A(K2+1)=A(K2+1)+T                                                 DHAR2040
      IF (JLAST) 235,235,82                                             DHAR2050
   82 JJ=JJCIF   +1                                                     DHAR2060
C                                                                       DHAR2070
C     CC FCR J=1                                                        DHAR2080
      ILAST= IL +JJ                                                     DHAR2090
      CC 85 I = JJ,ILAST,ICIF                                           DHAR2100
      KLAST = KL+I                                                      DHAR2110
      CC 85 K=I,KLAST,2                                                 DHAR2120
      K1 = K+KEIT                                                       DHAR2130
      K2 = K1+KEIT                                                      DHAR2140
      K3 = K2+KEIT                                                      DHAR2150
C                                                                       DHAR2160
C     LETTING W=(I+1)/RCCT2,W3=(-1+I)/RCCT2,W2=I,                       DHAR2170
C     A(K)=A(K)+A(K2)*I                                                 DHAR2180
C     A(K2)=A(K)-A(K2)*I                                                DHAR2190
C     A(K1)=A(K1)*W+A(K3)*W3                                            DHAR2200
C     A(K3)=A(K1)*W-A(K3)*W3                                            DHAR2210
C                                                                       DHAR2220
C     A(K)=A(K)+A(K1)                                                   DHAR2230
C     A(K1)=A(K)-A(K1)                                                  DHAR2240
C     A(K2)=A(K2)+A(K3)*I                                               DHAR2250
C     A(K3)=A(K2)-A(K3)*I                                               DHAR2260
C                                                                       DHAR2270
      R =-A(K2+1)                                                       DHAR2280
      T = A(K2)                                                         DHAR2290
      A(K2) = A(K)-R                                                    DHAR2300
      A(K) = A(K)+R                                                     DHAR2310
      A(K2+1)=A(K+1)-T                                                  DHAR2320
      A(K+1)=A(K+1)+T                                                   DHAR2330
C                                                                       DHAR2340
      AKR=A(K1)-A(K1+1)                                                 DHAR2350
```

```
      AK1 = A(K1+1)*A(K1)
      A=-A(K2)-A(K2+1)
      T=A(K2)-A(K2+1)
      A(K2)=(AKM-AK1/RCCT2
      A(K2+1)=(AM+AK1-T)/RCCT2
      A(K1)=(AM+AK1/RCCT2
      A(K1+1)=(AA[+T]/RCCT2
      T= A(K1)
      A(K1)=A(K)-T
      A(K)=A(K)+T
      T=A(K1+1)
      A(K1+1)=A(K+1)-T
      A(K+1)=A(K+1)+T
      A=-A(K2+1)
      T=A(K2)
      A(K2)=A(K2)-A
      A(K2)=A(K2)+A
      A(K2+1)=A(K2+1)-T
   85 A(K2+1)=A(K2+1)+T
      IF(JLAST-1) 225,225,90
   90 ... JJ + JJDIF
C
C     NOW DO THE REMAINING J'S
      DO 220 J=2,JLAST
C
C     FETCH W'S
C     DEF- W=W**2,W2=W**2, W3=W**3
   96 I=INV(J+1)
      96 IC=NT-I
      W(1)=S(IC)
      W(2)=S(I)
      I2=2*I
      I2C=NT-I2
      IF(I2C)12C,11C,1CC
C
C     2*I IS IN FIRST QUADRANT
  1CC W2(1)=S(I2C)
      W2(2)=S(I2)
      GO TO 13C
  11C W2(1)=C.
      W2(2)=1.
      GO TO 13C
C
C     2*I IS IN SECOND QUADRANT
  12C I2CC = I2C+NT
      I2C=-I2C
      W2(1)=-S(I2C)
      W2(2)=S(I2CC)
  13C I3=I+I2
      I3C=NT-I3
      IF(I3C)14C,15C,14C
C
C     I3 IN FIRST QUADRANT
  14C W3(1)=S(I3C)
      W3(2)=S(I3)
      GO TO 2CC
  15C W3(1)=C.
      W3(2)=1.
      GO TO 2CC
C
  16C I3CC=I3C+NT
      IF(I3CC)15C,18C,17C
C
C     I3 IN SECOND QUADRANT
  17C I3C=-I3C
      W3(1)=-S(I3C)
      W3(2)=S(I3CC)
      GO TO 2CC
  18C W3(1)=-1.
      W3(2)=C.
      GO TO 2CC
C
C     2*I IN THIRD QUADRANT
  19C I3CCC=NT+I3CC
      I3CC = -I3CC
      W3(1)=-S(I3CCC)
      W3(2)=-S(I3CC)
 2CC ILAST=IL+JJ
      DO 22C I=JJ,ILAST,JDIF
      KLAST=KL+1
      DO 22C K=I,KLAST,2
      K1=K+KDIF
      K2=K1+KDIF
      K3=K2+KDIF
C
C     DO THE STEPS WITH J NOT C
C     A(K)=A(K)+A(K2)*W2
C     A(K2)=A(K)-A(K2)*W2
C     A(K1)=A(K1)*W**2+A(K3)*W3
C     A(K3)=A(K1)*W-A(K3)*W3
C
C     A(K)=A(K)+A(K1)
C     A(K1)=A(K)-A(K1)
C     A(K2)=A(K2)+A(K3)*I
C     A(K3)=A(K2)-A(K3)*I
C
      A=A(K2)*W2(1)-A(K2+1)*W2(2)
      T=A(K2)*W2(2)+A(K2+1)*W2(1)
      A(K2)=A(K)-A
      A(K)=A(K)+A
      A(K2+1)=A(K+1)-T
      A(K+1)=A(K+1)+T
C
      A=A(K3)*W3(1)-A(K3+1)*W3(2)
      T=A(K3)*W3(2)+A(K3+1)*W3(1)
      AWR=A(K1)*W(1)-A(K1+1)*W(2)
      AW[=A(K1)*W(2)+A(K1+1)*W(1)
      A(K3)=AWR-A
      A(K3+1)=AW[-T
      A(K1)=AWR+A
      A(K1+1)=AW[+T
      T=A(K1)
      A(K1)=A(K)-T
      A(K)=A(K)+T
      T=A(K1+1)
      A(K1+1)=A(K+1)-T
      A(K+1)=A(K+1)+T
      A=-A(K3+1)
      T=A(K3)
      A(K3)=A(K2)-A
      A(K2)=A(K2)+A
      A(K3+1)=A(K2+1)-T
  22C A(K2+1)=A(K2+1)+T
C     END OF I AND K LOOPS
C
  23C JJ=JJDIF+JJ
C     END OF J-LOOP
C
  225 JLAST=4*JLAST+3
  24C CONTINUE
C     END OF L  LOOP
C
  25C CONTINUE
C     END OF  IC  LOOP
C
C     WE NOW HAVE THE COMPLEX FOURIER SUMS BUT THEIR ADDRESSES ARE
C     BIT-REVERSED.  THE FOLLOWING ROUTINE PUTS THEM IN ORDER
      NTSC=NT+NT
      M3PT=M3-MT
  35C IF(M3PT) 37C,3EC,3EC
C
C     M3 GR. OR EQ. MT
  3EC IGC3=1
      N3VNT=N3/NT
      MINN3=NT
      GO TO 3EC
C
C     M3 LESS THAN MT
  37C IGC3=2
      N3VNT=1
      NTVN3=NT/N3
      MINN3=N3
  3EC JJC3 = NTSC/N3
      M2MT=M2-MT
  45C IF (M2MT)47C,46C,46C
C
C     M2 GR. OR EQ. MT
  46C IGC2=1
      N2VNT=N2/NT
      MINN2=MT
      GO TO 48C
C
C     M2 LESS THAN MT
  47C IGC2 = 2
      N2VNT=1
      NTVN2=NT/N2
      MINN2=N2
  48C JJC2=NTSC/N2
      M1M1=M1-MT
  55C IF(M1MT)57C,56C,56C
C
C     M1 GR. OR EQ. MT
  56C IGC1=1
      N1VNT=N1/NT
      MINN1=NT
      GO TO 56C
C
C     M1 LESS THAN MT
  57C IGC1=2
      N1VNT=1
      NTVN1=NT/N1
      MINN1=N1
  58C JJC1=NTSC/N1
  6CC JJ3=1
      J=1
      DO 88C JP3=1,N3VNT
      IP3=INV(JJ3)
      DO 67C JP3=1,MINN3
      GO TO (61C,62C),IGC3
  61C IP3=INV(JP3)*N3VNT
      GO TO 63C
  62C IP3=INV(JP3)/NTVN3
  63C I3=(IP3+IP3)*N2
  7CC JJ2=1
      DO 87C JP2=1,N2VNT
      IP2=INV(JJ2)+I3
      DO 86C JP2=1,MINN2
      GO TO (71C,72C),IGC2
  71C IP2=INV(JP2)*N2VNT
      GO TO 73C
  72C IP2=INV(JP2)/NTVN2
  73C I2=(IP2+IP2)*N1
  8CC JJ1=1
      DO 86C JP1=1,N1VNT
      IP1=INV(JJ1)+I2
      DO 85C JP1=1,MINN1
      GO TO (81C,82C),IGC1
  81C IP1=INV(JP1)*N1VNT
      GO TO 83C
  82C IP1=INV(JP1)/NTVN1
  83C I=2*(IP1+IP1)+1
      IF (J-I) 84C,85C,85C
  84C T=A(I)
      A(I)=A(J)
      A(J)=T
      T=A(I+1)
      A(I+1)=A(J+1)
      A(J+1)=T
  85C J=J+2
  86C JJ1=JJ1+JJD1
C
  87C JJ2=JJ2+JJD2
C     END OF JP2 AND JP3 LOOPS
C
  88C JJ3 = JJ3+JJC3
C     END OF JP3 LOOP
C
  89C IF(IFSET)891,895,895
  891 DO 892 I = 1,NX
  892 A(2*I) = -A(2*I)
  895 RETURN
C
C     THE FOLLOWING PROGRAM COMPUTES THE SIN AND INV TABLES.
C
  9CC PI=PARC(P(1),M(2),M(3)) -2
      MT = PARC(2,MT)
  SC4 IF (NT-1E) SC6,SC6,13
  SC6 IFERR=C
      NT=2**MT
      NTV2=NT/2
C
C     SET UP SIN TABLE
C     THETA=PIE/200(L+1) FOR L=1
  91C THETA=.7853981633974483
C
C     JSTEP=200(MT-L+1) FOR L=1
      JSTEP=NT
C
C     JDIF=200(MT-L) FOR L=1
      JDIF=NTV2
      S(JDIF)=CSIN(THETA)
      DO 950 L=2,MT
      THETA=THETA/2.0D0
      JSTEP2=JSTEP
      JSTEP=JDIF
      JDIF=JSTEP/2
      S(JDIF)=CSIN(THETA)
```

```
      JC1=NT-JCIF                                                       DHAR4970
      S(JC1)=CCCS(THETA)                                                DHAR4980
      JLAST=NT-JSTEP2                                                   DHAR4990
      IF(JLAST - JSTEP) 95C,92C,92C                                     DHAR5000
  920 CC 94C J=JSTEP,JLAST,JSTEP                                        DHAR5010
      JC=NT-J                                                           DHAR5020
      JC=J+JCIF                                                         DHAR5030
  94C S(JC)=S(J)+S(JC1)+S(JCIF)*S(JC)                                   DHAR5040
  95C CONTINUE                                                          DHAR5050
C                                                                       DHAR5060
C     SET UP INV(J) TABLE                                               DHAR5070
C                                                                       DHAR5080
  96C RTLEXP=NTV2                                                       DHAR5090
C                                                                       DHAR5100
C     PTLEXP=2**(NT-L). FOR L=1                                         DHAR5110
      LMIEXP=1                                                          DHAR5120
C                                                                       DHAR5130
C     LMIEXP=2**(L-1). FOR L=1                                          DHAR5140
      INV(1)=0                                                          DHAR5150
      CC 980 L=1,NT                                                     DHAR5160
      INV(LMIEXP+1) = RTLEXP                                            DHAR5170
      CO 970 J=2,LMIEXP                                                 DHAR5180
      JJ=J+LMIEXP                                                       DHAR5190
  970 INV(JJ)=INV(J)+RTLEXP                                             DHAR5200
      RTLEXP=RTLEXP/2                                                   DHAR5210
  980 LMIEXP=LMIEXP*2                                                   DHAR5220
  982 IF(IFSET)12,995,12                                                DHAR5230
      END                                                               DHAR5240
```

Subroutines RHARM and DRHARM

Given 2N real numbers $X_0, X_1, \ldots, X_{2N-1}$, the subroutine computes Fourier coefficients $a_0, a_1, b_1, a_2, b_2, \ldots, a_{N-1}, b_{N-1}, a_N$ in the equation:

$$X_j = \frac{1}{2}a_0 + \sum_{k=1}^{N-1} \left(a_k \cos\left(\frac{\pi \cdot j \cdot k}{N}\right) + b_k \sin\left(\frac{\pi \cdot j \cdot k}{N}\right)\right) + \frac{1}{2}a_N (-1)^j$$

where

$$j = 0,\ 1, \ldots,\ 2N-1$$

The subroutine HARM is called to compute the complex coefficients:

$$A_k = \frac{1}{N} \sum_{j=0}^{N-1} (X_{2j} - iX_{2j+1})\, e^{\frac{2\pi i}{N} \cdot j \cdot k},$$

$$k = 0, 1, 2, \ldots, N-1$$

Then for $k = 1, 2, \ldots, \frac{N}{2} - 1, \frac{N}{2}$ (the bar is conjugation):

$$A'_k = \frac{1}{2}(\bar{A}_k + A_{N-k})$$

$$A''_k = \frac{1}{2}(\bar{A}_{N-k} - A_k)$$

and:

$$C_k = \frac{1}{2}(A'_k + \bar{A}''_k\, e^{(\frac{\pi}{2} - \frac{\pi}{N}k)i})$$

$$\text{for } k = 1, 2, \ldots, \frac{N}{2} - 1, \frac{N}{2}$$

$$C_{N-k} = \frac{1}{2}(\bar{A}'_k - A''_k\, e^{(\frac{\pi}{N-k} - \frac{\pi}{2})i})$$

$$\text{for } k = 1, 2, \ldots, \frac{N}{2} - 1$$

Let:

$$C_o = \frac{1}{2}(\text{Re } A_o - \text{Im } A_o)$$

$$C_N = \frac{1}{2}(\text{Re } A_o + \text{Im } A_o)$$

Finally:

$$a_o = 2 \text{ Re } (C_o)$$

$$a_k = 2 \text{ Re } (C_k)$$

$$b_k = -2 \text{ Im } (C_k)$$

$$a_N = 2 \text{ Re } (C_N)$$

```
      AP2RE=A(K6)*CO+A(K6+1)*SI                                          RHAR1000
      AP2IM=-A(K6)*SI+A(K6+1)*CO                                         RHAR1010
      CIRE=.5*(A(2*I-1)+AP2RE)                                           RHAR1020
      CIIM=.5*(A(2*I)+AP2IM)                                             RHAR1030
      CNIRE=.5*(A(2*I-1)-AP2RE)                                          RHAR1040
      CNIIM=.5*(A(2*I)-AP2IM)                                            RHAR1050
      A(2*I-1)=CIRE                                                      RHAR1060
      A(2*I)=CIIM                                                        RHAR1070
      A(K6)=CNIRE                                                        RHAR1080
      A(K6+1)=-CNIIM                                                     RHAR1090
      SIS=SI                                                             RHAR1100
      SI=SI*SC+CO*SS                                                     RHAR1110
  116 CO=CO*SC-SIS*SS                                                    RHAR1120
C                                                                        RHAR1130
C     SHIFT C(J)S FOR J=N/2+1 TO J=N UP ONE SLOT                         RHAR1140
      DO 117 I=1,NTOT,2                                                  RHAR1150
      K8=NTOT+4+I                                                        RHAR1160
      A(K8-2)=A(K8)                                                      RHAR1170
  117 A(K8-1)=A(K8+1)                                                    RHAR1180
      DO 500 I=3,NTOT2,2                                                 RHAR1190
      A(I) = 2. * A(I)                                                   RHAR1200
  500 A(I + 1) = -2. * A(I + 1)                                          RHAR1210
      RETURN                                                             RHAR1220
      END                                                                RHAR1230
```

```
C                                                                        RHAR  10
C     ..................................................................RHAR  20
C                                                                        RHAR  30
C        SUBROUTINE RHARM                                                RHAR  40
C                                                                        RHAR  50
C        PURPOSE                                                         RHAR  60
C           FINDS THE FOURIER COEFFICIENTS OF ONE DIMENSIONAL REAL DATA  RHAR  70
C                                                                        RHAR  80
C        USAGE                                                           RHAR  90
C           CALL RHARM (A,M,INV,S,IFERR)                                 RHAR 100
C                                                                        RHAR 110
C        DESCRIPTION OF PARAMETERS                                       RHAR 120
C           A      - AS INPUT, CONTAINS ONE DIMENSIONAL REAL DATA. A IS  RHAR 130
C                    2*N+4 CORE LOCATIONS, WHERE N = 2**M. 2*N REAL      RHAR 140
C                    NUMBERS ARE PUT INTO THE FIRST 2*N CORE LOCATIONS   RHAR 150
C                    OF A                                                RHAR 160
C                    AS OUTPUT, A CONTAINS THE FOURIER COEFFICIENTS      RHAR 170
C                    A0/2,B0=0,A1,B1,A2,B2,...,AN/2,BN=0 RESPECTIVELY IN RHAR 180
C                    THE FIRST 2N+2 CORE LOCATIONS OF A                  RHAR 190
C           M      - AN INTEGER WHICH DETERMINES THE SIZE OF THE VECTOR  RHAR 200
C                    A. THE SIZE OF A IS 2*(2**M) + 4                    RHAR 210
C           INV    - A VECTOR WORK AREA FOR BIT AND INDEX MANIPULATION OFRHAR 220
C                    DIMENSION ONE EIGHTH THE NUMBER OF REAL INPUT, VIZ..RHAR 230
C                    (1/8)*2*(2**M)                                      RHAR 240
C           S      - A VECTOR WORK AREA FOR SINE TABLES WITH DIMENSION  RHAR 250
C                    THE SAME AS INV                                     RHAR 260
C           IFERR  - A RETURNED VALUE OF 1 MEANS THAT M IS LESS THAN 3 ORRHAR 270
C                    GREATER THAN 20. OTHERWISE IFERR IS SET = 0         RHAR 280
C                                                                        RHAR 290
C        REMARKS                                                         RHAR 300
C           THIS SUBROUTINE GIVES THE FOURIER COEFFICIENTS OF 2*(2**M)   RHAR 310
C           REAL POINTS. SEE SUBROUTINE HARM FOR THREE DIMENSIONAL,      RHAR 320
C           COMPLEX FOURIER TRANSFORMS                                   RHAR 330
C                                                                        RHAR 340
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   RHAR 350
C           HARM                                                         RHAR 360
C                                                                        RHAR 370
C        METHOD                                                          RHAR 380
C           THE FOURIER COEFFICIENTS A0,B0=0,A1,B1,...,AN,BN=0 ARE       RHAR 390
C           OBTAINED FOR INPUT XJ, J=0,1,2,...,2N-1 FOR THE FOLLOWING    RHAR 400
C           EQUATION (PI = 3.14159...)                                   RHAR 410
C                                                                        RHAR 420
C                    N-1                                              J  RHAR 430
C        XJ=(1/2)A0+SUM (AK*COS(PI*J*K/N)+BK*SIN(PI*J*K/N))+(1/2)AN(-1)  RHAR 440
C                    K=1                                                 RHAR 450
C                                                                        RHAR 460
C           SEE REFERENCE UNDER SUBROUTINE HARM                          RHAR 470
C                                                                        RHAR 480
C     ..................................................................RHAR 490
      SUBROUTINE RHARM(A,M,INV,S,IFERR)                                  RHAR 500
      DIMENSION A(1),L(3),INV(1),S(1)                                    RHAR 510
      IFSET=1                                                            RHAR 520
      L(1)=M                                                             RHAR 530
      L(2)=0                                                             RHAR 540
      L(3)=0                                                             RHAR 550
      NTOT=2**M                                                          RHAR 560
      NTOT2 = 2*NTOT                                                     RHAR 570
      FN = NTOT                                                          RHAR 580
      DO   3 I = 2,NTOT2,2                                               RHAR 590
    3 A(I) = -A(I)                                                       RHAR 600
      DO   6 I = 1,NTOT2                                                 RHAR 610
    6 A(I) = A(I)/FN                                                     RHAR 620
      CALL HARM(A,L,INV,S ,IFSET,IFERR)                                  RHAR 630
C                                                                        RHAR 640
C     MOVE LAST HALF OF A(J)S DOWN ONE SLOT AND ADD A(N) AT BOTTOM TO    RHAR 650
C     GIVE ARRAY FOR A1PRIME AND A2PRIME CALCULATION                     RHAR 660
C                                                                        RHAR 670
      DO  52 I=1,NTOT,2                                                  RHAR 680
      JC=NTOT2+2-I                                                       RHAR 690
      A(JO)=A(JO-2)                                                      RHAR 700
   52 A(JO+1)=A(JO-1)                                                    RHAR 710
      A(NTOT2+3)=A(1)                                                    RHAR 720
      A(NTOT2+4)=A(2)                                                    RHAR 730
C                                                                        RHAR 740
C     CALCULATE A1PRIMES AND STORE IN FIRST N SLOTS                      RHAR 750
C     CALCULATE A2PRIMES AND STORE IN SECOND N SLOTS IN REVERSE ORDER    RHAR 760
      KO=NTOT+1                                                          RHAR 770
      DO 104 I=1,KO,2                                                    RHAR 780
      K1=NTOT2-I+4                                                       RHAR 790
      AP1RE=.5*(A(I)+A(K1))                                              RHAR 800
      AP2RE=-.5*(A(I+1)+A(K1+1))                                         RHAR 810
      AP1IM=.5*(-A(I+1)+A(K1+1))                                         RHAR 820
      AP2IM=-.5*(A(I)-A(K1))                                             RHAR 830
      A(I)=AP1RE                                                         RHAR 840
      A(I+1)=AP1IM                                                       RHAR 850
      A(K1)=AP2RE                                                        RHAR 860
  104 A(K1+1)=AP2IM                                                      RHAR 870
      NTO = NTOT/2                                                       RHAR 880
  110 NT=NTO+1                                                           RHAR 890
      DEL=3.1415927/FLOAT(NTOT)                                          RHAR 900
      SS=SIN(DEL)                                                        RHAR 910
      SC=COS(DEL)                                                        RHAR 920
      SI=0.0                                                             RHAR 930
      CO=1.0                                                             RHAR 940
C                                                                        RHAR 950
C     COMPUTE C(J)S FOR J=0 THRU J=N                                     RHAR 960
  114 DO 116 I=1,NT                                                      RHAR 970
      K6=NTOT2-2*I+5                                                     RHAR 980
                                                                         RHAR 990
```

```
C                                                                        DRAR  10
C     ..................................................................DRAR  20
C                                                                        DRAR  30
C        SUBROUTINE DRHARM                                               DRAR  40
C                                                                        DRAR  50
C        PURPOSE                                                         DRAR  60
C           FINDS THE FOURIER COEFFICIENTS OF ONE DIMENSIONAL DOUBLE     DRAR  70
C           PRECISION REAL DATA                                          DRAR  80
C                                                                        DRAR  90
C        USAGE                                                           DRAR 100
C           CALL DRHARM(A,M,INV,S,IFERR)                                 DRAR 110
C                                                                        DRAR 120
C        DESCRIPTION OF PARAMETERS                                       DRAR 130
C           A      - A DOUBLE PRECISION VECTOR                           DRAR 140
C                    AS INPUT, CONTAINS ONE DIMENSIONAL REAL DATA. A IS  DRAR 150
C                    2*N+4 CORE LOCATIONS, WHERE N = 2**M. 2*N REAL      DRAR 160
C                    NUMBERS ARE PUT INTO THE FIRST 2*N CORE LOCATIONS   DRAR 170
C                    OF A                                                DRAR 180
C                    AS OUTPUT, A CONTAINS THE FOURIER COEFFICIENTS      DRAR 190
C                    A0/2,B0=0,A1,B1,A2,B2,...,AN/2,BN=0 RESPECTIVELY IN DRAR 200
C                    THE FIRST 2N+2 CORE LOCATIONS OF A                  DRAR 210
C           M      - AN INTEGER WHICH DETERMINES THE SIZE OF THE VECTOR  DRAR 220
C                    A. THE SIZE OF A IS 2*(2**M) + 4                    DRAR 230
C           INV    - A VECTOR WORK AREA FOR BIT AND INDEX MANIPULATION OFDRAR 240
C                    DIMENSION ONE EIGHTH THE NUMBER OF REAL INPUT, VIZ..DRAR 250
C                    (1/8)*2*(2**M)                                      DRAR 260
C           S      - A DOUBLE PRECISION VECTOR WORK AREA FOR SINE TABLES DRAR 270
C                    WITH DIMENSION THE SAME AS INV                      DRAR 280
C           IFERR  - A RETURNED VALUE OF 1 MEANS THAT M IS LESS THAN 3 ORDRAR 290
C                    GREATER THAN 20. OTHERWISE IFERR IS SET = 0         DRAR 300
C                                                                        DRAR 310
C        REMARKS                                                         DRAR 320
C           THIS SUBROUTINE GIVES THE FOURIER COEFFICIENTS OF 2*(2**M)   DRAR 330
C           REAL POINTS. SEE SUBROUTINE DHARM FOR THREE DIMENSIONAL,     DRAR 340
C           DOUBLE PRECISION, COMPLEX FOURIER TRANSFORMS.                DRAR 350
C                                                                        DRAR 360
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DRAR 370
C           DHARM                                                        DRAR 380
C                                                                        DRAR 390
C        METHOD                                                          DRAR 400
C           THE FOURIER COEFFICIENTS A0,B0=0,A1,B1,...,AN,BN=0 ARE       DRAR 410
C           OBTAINED FOR INPUT XJ, J=0,1,2,...,2N-1 FOR THE FOLLOWING    DRAR 420
C           EQUATION (PI = 3.14159...)                                   DRAR 430
C                                                                        DRAR 440
C                    N-1                                              J  DRAR 450
C        XJ=(1/2)A0+SUM (AK*COS(PI*J*K/N)+BK*SIN(PI*J*K/N))+(1/2)AN(-1)  DRAR 460
C                    K=1                                                 DRAR 470
C                                                                        DRAR 480
C           SEE REFERENCE UNDER SUBROUTINE DHARM                         DRAR 490
C                                                                        DRAR 500
C     ..................................................................DRAR 510
      SUBROUTINE DRHARM(A,M,INV,S,IFERR)                                 DRAR 520
      DIMENSION A(1),L(3),INV(1),S(1)                                    DRAR 530
      DOUBLE PRECISION A,SI,AP1IM,FN,CO,CIRE,AP2IM,S,SS,DEL,CIIM,AP1RE,  DRAR 540
     1 CNIRE,SC,SIS,AP2RE,CNIIM                                          DRAR 550
      IFSET=1                                                            DRAR 560
      L(1)=M                                                             DRAR 570
      L(2)=0                                                             DRAR 580
      L(3)=0                                                             DRAR 590
      NTOT=2**M                                                          DRAR 600
      NTOT2 = 2*NTOT                                                     DRAR 610
      FN = NTOT                                                          DRAR 620
      DO   3 I = 2,NTOT2,2                                               DRAR 630
    3 A(I) = -A(I)                                                       DRAR 640
      DO   6 I = 1,NTOT2                                                 DRAR 650
    6 A(I) = A(I)/FN                                                     DRAR 660
      CALL DHARM(A,L,INV,S,IFSET,IFERR)                                  DRAR 670
C                                                                        DRAR 680
C     MOVE LAST HALF OF A(J)S DOWN ONE SLOT AND ADD A(N) AT BOTTOM TO    DRAR 690
C     GIVE ARRAY FOR A1PRIME AND A2PRIME CALCULATION                     DRAR 700
C                                                                        DRAR 710
      DO  52 I=1,NTOT,2                                                  DRAR 720
      JC=NTOT2+2-I                                                       DRAR 730
      A(JC)=A(JO-2)                                                      DRAR 740
   52 A(JO+1)=A(JC-1)                                                    DRAR 750
      A(NTOT2+3)=A(1)                                                    DRAR 760
      A(NTOT2+4)=A(2)                                                    DRAR 770
C                                                                        DRAR 780
C     CALCULATE A1PRIMES AND STORE IN FIRST N SLOTS                      DRAR 790
C     CALCULATE A2PRIMES AND STORE IN SECOND N SLOTS IN REVERSE ORDER    DRAR 800
      KO=NTOT+1                                                          DRAR 810
      DO 104 I=1,KO,2                                                    DRAR 820
      KI=NTOT2-I+4                                                       DRAR 830
      AP1RE=.5*(A(I)+A(K1))                                              DRAR 840
      AP2RE=-.5*(A(I+1)+A(K1+1))                                         DRAR 850
      AP1IM=.5*(-A(I+1)+A(K1+1))                                         DRAR 860
      AP2IM=-.5*(A(I)-A(K1))                                             DRAR 870
      A(I)=AP1RE                                                         DRAR 880
      A(I+1)=AP1IM                                                       DRAR 890
      A(K1)=AP2RE                                                        DRAR 900
  104 A(K1+1)=AP2IM                                                      DRAR 910
      NTO = NTOT/2                                                       DRAR 920
  110 NT=NTO+1                                                           DRAR 930
      DEL=3.14159265358979 3/DFLOAT(NTOT)                                DRAR 940
      SS=DSIN(DEL)                                                       DRAR 950
      SC=DCOS(DEL)                                                       DRAR 960
      SI=0.0                                                             DRAR 970
      CO=1.0                                                             DRAR 980
                                                                         DRAR 990
```

```
C
C     COMPUTE C(J)S FOR J=0 THRU J=N
  114 DO 116 I=1,NT
      K6=NTOT2-2*I+5
      AP2RE=A(K6)*CO+A(K6+1)*SI
      AP2IM=-A(K6)*SI+A(K6+1)*CO
      CIRE=.5*(A(2*I-1)+AP2RE)
      CIIM=.5*(A(2*I)+AP2IM)
      CNIRE=.5*(A(2*I-1)-AP2RE)
      CNIIM=.5*(A(2*I)-AP2IM)
      A(2*I-1)=CIRE
      A(2*I)=CIIM
      A(K6)=CNIRE
      A(K6+1)=-CNIIM
      SIS=SI
      SI=SI*SC+CO*SS
  116 CO=CO*SC-SIS*SS
C
C     SHIFT C(J)S FOR J=N/2+1 TO J=N UP ONE SLOT
      DO 117 I=1,NTOT,2
      K8=NTOT+4+I
      A(K8-2)=A(K8)
  117 A(K8-1)=A(K8+1)
      DO 500 I=3,NTOT2,2
      A(I) = 2. * A(I)
  500 A(I + 1) = -2. * A(I + 1)
      RETURN
      END
```

DRAR1000
DRAR1010
DRAR1020
DRAR1030
DRAR1040
DRAR1050
DRAR1060
DRAR1070
DRAR1080
DRAR1090
DRAR1100
DRAR1110
DRAR1120
DRAR1130
DRAR1140
DRAR1150
DRAR1160
DRAR1170
DRAR1180
DRAR1190
DRAR1200
DRAR1210
DRAR1220
DRAR1230
DRAR1240
DRAR1250
DRAR1260
DRAR1270

Subroutines APMM and DAPMM

These subroutines determine a linear combination of M linearly independent given continuous real functions, which constitute the Chebyshev approximation of a given real function over a discrete range.

1. Mathematical background

Let us consider a set of discrete data $\{x_k, f_k = f(x_k)\}$, $k = 1, \ldots, N$, which defines a real valued function f(x) over a discrete range, and M real continuous given functions $\{\varphi_i(x)\}$, $i = 1, \ldots, M$, on an interval containing $[x_1, x_N]$.

The problem is to determine a set of M real coefficients $\{a_i\}$ that minimizes

$$w = \operatorname*{Max}_{1 \le k \le N} \left| \varphi(x_k) - f_k \right|, \text{ where } \varphi(x) = \sum_{i=1}^{M} a_i \varphi_i(x)$$

This problem can be expressed in terms of linear programming. At first, let us shift the unknowns so that the resulting ones are nonnegative:

$$b_i = a_i + b_{M+1}, \quad i = 1, \ldots, M,$$

where

$$b_{M+1} = - \operatorname{Min} [0, a_1, \ldots, a_M]$$

At each point, the error of approximation is given by

$$e_k = \varphi(x_k) - f_k$$

or

$$e_k = \sum_{i=1}^{M+1} b_i \varphi_i(x_k) - f_k$$

where

$$\varphi_{M+1}(x) = -\sum_{i=1}^{M} \varphi_i(x)$$

By definition

$$w = \operatorname*{Max}_{1 \le k \le N} \left| e_k \right|$$

If we put $\varphi_{ik} = \varphi_i(x_k)$, the original problem can be expressed as: Minimize w, subject to:

$$w + \sum_{i=1}^{M+1} \varphi_{ik} b_i \geq f_k$$

$$w - \sum_{i=1}^{M+1} \varphi_{ik} b_i \geq f_k$$

$$b_i \geq 0 \text{ for } i = 1, \ldots, M+1$$

$$w \geq 0$$

In practice, it is more convenient to solve the following dual problem in the nonnegative variables $\{s_k, t_k\}$, $k = 1, \ldots, N$:

$$\text{Maximize } \sum_{k=1}^{N} f_k (s_k - t_k), \text{ subject to:}$$

$$\sum_{k=1}^{N} (s_k + t_k) \leq 1$$

$$\sum_{k=1}^{N} \varphi_{ik} (s_k - t_k) \leq 0, \quad i = 1, \ldots, M+1$$

$$s_k \geq 0, \; t_k \geq 0, \text{ for } k = 1, \ldots, N$$

Using the variables of the dual problem as slacks, these n + 2 constraints can be written as equalities:

$$w + \sum_{k=1}^{N} (s_k + t_k) = 1$$

$$b_i + \sum_{k=1}^{N} \varphi_{ik} (s_k - t_k) = 0$$

The dual problem is solved by means of a revised simplex method (inverse matrix algorithm) using the following initial simplex tableau where w, b_1, $\ldots, b_{M+1}$, are basic variables:

Note that the entries in the transformed top row under w, $b_1, \ldots, b_{M+1}$ will be the optimal solution to the primal, that is, w and the b_i's.

A condensed tableau is used for calculation. The correspondence between the subscripts of the full tableau and these of the condensed one is given by means of the index vector IHE.

When the procedure has reached the optimum, the top row contains on return:

w	Maximum error of approximation
b_i, $i = 1, \ldots, M+1$	Coefficients from which we can get the unknowns by $a_i = b_i - b_{M+1}$ for $i = 1, \ldots, M$
s_k, $k = 1, \ldots, N$	The error at the given points, according to $e_k = s_k - w$

	Variables	$s_1 \ldots s_N$	$t_1 \ldots t_N$	w	b_1	b_2	$\ldots$	b_{M+1}
Top Row	Maximize	$f_1 \ldots f_N$	$-f_1 \ldots -f_N$	0	0	0	$\ldots$	0
	1	$= 1 \ldots 1$	$1 \ldots 1$	1	0	0	$\ldots$	0
	0	$= \varphi_{11} \ldots \varphi_{1N}$	$-\varphi_{11} \ldots -\varphi_{1N}$	0	1	0	$\ldots$	0
	0	$= \varphi_{21} \ldots \varphi_{2N}$	$-\varphi_{21} \ldots -\varphi_{2N}$	0	0	1	$\ldots$	0
	0	$= \varphi_{M+1,1} \; \varphi_{M+1,N}$	$-\varphi_{M+1,1} \; -\varphi_{M+1,N}$		0	0	$\ldots$	1

2. Programming considerations

For economy of storage requirements, the full simplex tableau is not stored, but only the top row at any iteration step. Therefore, we must update an inverse matrix T which allows us to generate the needed pivot column at any iteration step from the corresponding initial column. The procedure terminates for the following reasons:

a. An optimal top row is reached, indicated by the resultant error parameter IER, which is set to zero. All the relevant data are contained in this top row. The corresponding subscripts are stored in a part of the integer vector IHE.

b. No suitable pivot can be found. The resultant error parameter IER is set to -1.

c. The number of iterations ITER has reached the internal maximum N+M. The error parameter IER is set to 1 as a warning.

The subroutines APMM and DAPMM contain two tests for loss of significance:

a. The first test is made when an initial column is multiplied by the rows of matrix T. The corresponding result DSUM is set equal to zero if the following inequality is valid:

$$\left|DSUM\right| \leqq HELP * EPS$$

where HELP is the absolutely greatest intermediate sum formed during calculation of the scalar product-sum DSUM, and EPS is an internal tolerance:

$$EPS = \begin{cases} 10^{-5} & \text{in APMM} \\ 10^{-14} & \text{in DAPMM} \end{cases}$$

b. The second test is made when a new element in the top row TOP is generated. The new element $\overline{TOP_i}$ is calculated from the previous value TOP_i by the addition

$$\overline{TOP_i} = TOP_i + DSUM_i$$

The new value $\overline{TOP_i}$ is replaced by zero if

$$\left|TOP_i + DSUM_i\right| \leqq \left|DSUM_i\right| * EPS$$

where EPS is the above-mentioned internal tolerance.

Some remarks are in order:

a. In cases where the given approximating functions are polynomials, APMM and DAPMM are more efficient when used with orthogonal polynomials than with ordinary polynomials. The number of iterations required usually decreases with orthogonal functions, and the magnitude of the roundoff errors may be significantly reduced. When using an ordinary polynomial approximating function it seems that the roundoff errors are due to the wide range of values of the elements $\varphi_{i,k}$ in the initial tableau.

b. If approximation by normal Chebyshev polynomials, shifted Chebyshev polynomials, Legendre polynomials, Laguerre polynomials, or Hermite polynomials is desired, the subroutines CNP, CSP, LEP, LAP, or HEP, respectively from the SSP (Scientific Subroutine Package) can be used as the external subroutine FCT.

For reference see:

1. I. Barrodale and A. Young, "Algorithms for Best L_1 and L^∞, Linear Approximations on a Discrete Set", Numerische Mathematik, vol. 8, iss. 3 (1966), pp. 295-306.

2. S. Vajda, Mathematical Programming, Addison-Wesley Publishing Company, Inc., London, 1961.

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C                                                                       APMM  10
C     ...................................................................APMM  20
C                                                                       APMM  30
C        SUBROUTINE APMM                                                APMM  40
C                                                                       APMM  50
C        PURPOSE                                                        APMM  60
C           APPROXIMATE A FUNCTION TABULATED IN N POINTS BY ANY LINEAR  APMM  70
C           COMBINATION OF M GIVEN CONTINUOUS FUNCTIONS IN THE SENSE    APMM  80
C           OF CHEBYSHEV..                                              APMM  90
C                                                                       APMM 100
C        USAGE                                                          APMM 110
C           CALL APMM(FCT,N,M,TOP,IHE,PIV,T,ITER,IEP)                   APMM 120
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT IN THE         APMM 130
C           CALLING PROGRAM.                                            APMM 140
C                                                                       APMM 150
C        DESCRIPTION OF PARAMETERS                                      APMM 160
C           FCT    - NAME OF SUBROUTINE TO BE SUPPLIED BY THE USER.     APMM 170
C                    IT COMPUTES VALUES OF M GIVEN FUNCTIONS FOR        APMM 180
C                    ARGUMENT VALUE X.                                  APMM 190
C                    USAGE                                              APMM 200
C                       CALL FCT(Y,X,K)                                 APMM 210
C                    DESCRIPTION OF PARAMETERS                          APMM 220
C                       Y   - RESULT VECTOR OF DIMENSION K CONTAINING   APMM 230
C                             THE VALUES OF GIVEN CONTINUOUS FUNCTIONS  APMM 240
C                             FOR GIVEN ARGUMENT X                      APMM 250
C                       X   - ARGUMENT VALUE                            APMM 260
C                       K   - AN INTEGER VALUE WHICH IS EQUAL TO M-1    APMM 270
C                    REMARKS                                            APMM 280
C                       IF APPROXIMATION BY NORMAL CHEBYSHEV, SHIFTED   APMM 290
C                       CHEBYSHEV, LEGENDRE, LAGUERRE, HERMITE POLYNO-  APMM 300
C                       MIALS IS DESIRED SUBROUTINES CNP, CSP, LEP,     APMM 310
C                       LAP, HEP, RESPECTIVELY FROM SSP COULD BE USED.  APMM 320
C           N      - NUMBER OF DATA POINTS DEFINING THE FUNCTION WHICH  APMM 330
C                    IS TO BE APPROXIMATED                              APMM 340
C           M      - NUMBER OF GIVEN CONTINUOUS FUNCTIONS FROM WHICH    APMM 350
C                    THE APPROXIMATING FUNCTION IS CONSTRUCTED.         APMM 360
C           TOP    - VECTOR OF DIMENSION 3*N.                           APMM 370
C                    ON ENTRY IT MUST CONTAIN FROM TOP(1) UP TO TOP(N)  APMM 380
C                    THE GIVEN N FUNCTION VALUES AND FROM TOP(N+1) UP   APMM 390
C                    TO TOP(2*N) THE CORRESPONDING NODES                APMM 400
C                    ON RETURN TOP CONTAINS FROM TOP(1) UP TO TOP(N)    APMM 410
C                    THE ERRORS AT THOSE N NODES.                       APMM 420
C                    OTHER VALUES OF TOP ARE SCRATCH.                   APMM 430
C           IHE    - INTEGER VECTOR OF DIMENSION 3*M+4*N+6              APMM 440
C           PIV    - VECTOR OF DIMENSION 3*M+6.                         APMM 450
C                    ON RETURN PIV CONTAINS AT PIV(1) UP TO PIV(M) THE  APMM 460
C                    RESULTING COEFFICIENTS OF LINEAR APPROXIMATION.    APMM 470
C           T      - AUXILIARY VECTOR OF DIMENSION (M+2)*(M+2)          APMM 480
C           ITER   - RESULTANT INTEGER WHICH SPECIFIES THE NUMBER OF    APMM 490
C                    ITERATIONS NEEDED                                  APMM 500
C           IEP    - RESULTANT ERROR PARAMETER CODED IN THE FOLLOWING   APMM 510
C                    FORM                                               APMM 520
C                       IER=0  - NO ERROR                               APMM 530
C                       IER=1  - THE NUMBER OF ITERATIONS HAS REACHED   APMM 540
C                                THE INTERNAL MAXIMUM N+M               APMM 550
C                       IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARA- APMM 560
C                                METER M OR N OR SINCE AT SOME ITERATION APMM 570
C                                NO SUITABLE PIVOT COULD BE FOUND       APMM 580
C                                                                       APMM 590
C        REMARKS                                                        APMM 600
C           NO ACTION BESIDES ERROR MESSAGE IN CASE M LESS THAN 1 OR    APMM 610
C           N LESS THAN 2.                                              APMM 620
C                                                                       APMM 630
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  APMM 640
C           THE EXTERNAL SUBROUTINE FCT MUST BE FURNISHED BY THE USER.  APMM 650
C                                                                       APMM 660
C        METHOD                                                         APMM 670
C           THE PROBLEM OF APPROXIMATION A TABULATED FUNCTION BY ANY    APMM 680
C           LINEAR COMBINATION OF GIVEN FUNCTIONS IN THE SENSE OF       APMM 690
C           CHEBYSHEV (I.E. TO MINIMIZE THE MAXIMUM ERROR) IS TRANS-    APMM 700
C           FORMED INTO A LINEAR PROGRAMMING PROBLEM. APMM USES A       APMM 710
C           REVISED SIMPLEX METHOD TO SOLVE A CORRESPONDING DUAL        APMM 720
C           PROBLEM. FOR REFERENCE, SEE                                 APMM 730
C           I.BARRODALE/A.YOUNG, ALGORITHMS FOR BEST L-SUB-ONE AND      APMM 740
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C          L-SUB-INFINITY, LINEAR APPROXIMATIONS ON A DISCRETE SET,
C          NUMERISCHE MATHEMATIK, VOL.8, ISS.3 (1966), PP.295-306.
C
C     ------------------------------------------------------------------
      SUBROUTINE APMM(FCT,N,M,TOP,THE,PIV,T,ITER,IER)

C
C
      DIMENSION TOP(1),THE(1),PIV(1),T(1)
      DOUBLE PRECISION DSUM

C     TEST ON WRONG INPUT PARAMETERS N AND M
      IER=-1
      IF (N-1) 81,81,1
    1 IF(M) 81,81,2

C     INITIALIZE CHARACTERISTIC VECTORS FOR THE TABLEAU
    2 IER=0

C     PREPARE TOP-ROW TOP
      DO 3 I=1,N
      K=I+N
      J=K+N
      TOP(J)=TOP(K)
    3 TOP(K)=-TOP(I)

C     PREPARE INVERSE TRANSFORMATION MATRIX T
      L=M+2
      LL=L*L
      DO 4 I=1,LL
    4 T(I)=0.
      K=1
      J=L+1
      DO 5 I=1,L
      T(K)=1.
    5 K=K+J

C     PREPARE INDEX-VECTOR THE
      DO 6 I=1,L
      K=I+L
      J=K+L
      THE(I)=0
      THE(K)=I
    6 THE(J)=I-1
      NAN=N+N
      K=L+L+L
      J=K+NAN
      DO 7 I=1,NAN
      K=K+1
      THE(K)=I
      J=J+1
    7 THE(J)=I

C     SET COUNTER ITER FOR ITERATION-STEPS
      ITER=-1
    8 ITER=ITER+1

C     TEST FOR MAXIMUM ITERATION-STEPS
      IF(N*M-ITER) 9,9,10
    9 IER=1
      GO TO 69

C     DETERMINE THE COLUMN WITH THE MOST POSITIVE ELEMENT IN TOP
   10 ISE=0
      PIV=0
      K=L+L+L
      SAVE=0.

C     START TOP-LOOP
      DO 14 I=1,NAN
      IDO=K+I
      HELP=TOP(I)
      IF(HELP-SAVE) 12,12,11
   11 SAVE=HELP
      IPIV=I
   12 IF(THE(IDO)) 14,13,14
   13 ISE=1
   14 CONTINUE

C     END OF TOP-LOOP

C     IS OPTIMAL TABLEAU REACHED
      IF(IPIV) 68,69,15

C     DETERMINE THE PIVOT-ELEMENT FOR THE COLUMN CHOSEN ABOVE
   15 ILAB=1
      IND=0
      J=ISE
      IF(J) 21,21,34

C     TRANSFER K-TH COLUMN FROM T TO PIV
   16 K=(K-1)*L
      DO 17 I=1,L
      J=L+I
      K=K+1
   17 PIV(J)=T(K)

C     IS ANOTHER COLUMN NEEDED FOR SEARCH FOR PIVOT-ELEMENT
   18 IF(ISE) 22,22,19
   19 ISE=-ISE

C     TRANSFER COLUMNS IN PIV
      J=L+1
      IDO=L+L
      DO 20 I=J,IDO
      K=I+L
   20 PIV(K)=PIV(I)
   21 J=IPIV
      GO TO 34

C     SEARCH PIVOT-ELEMENT PIV(IND)
   22 SAVE=1.E38
      IDO=0
      K=L+1
      LL=L+L
      IND=0

C     START PIVOT-LOOP
      DO 29 I=K,LL
      J=I+L
      HELP=PIV(I)
      IF(HELP) 29,29,23
   23 HELP=-HELP
      IF(ISE) 26,24,26
   24 IF(THE(J)) 27,25,27
   25 IDO=I
      GO TO 29
   26 HELP=-PIV(J)/HELP
   27 IF(HELP-SAVE) 28,29,29
   28 SAVE=HELP
      IND=I
   29 CONTINUE

C     END OF PIVOT-LOOP

C     TEST FOR SUITABLE PIVOT-ELEMENT
      IF(IND) 30,30,32
   30 IF(IDO) 68,68,31
   31 IND=IDO

C     PIVOT-ELEMENT IS STORED IN PIV(IND)

C     COMPUTE THE RECIPROCAL OF THE PIVOT-ELEMENT REPI
   32 REPI=1./PIV(IND)
      IND=IND-L

C     UPDATE THE TOP-ROW TOP OF THE TABLEAU
      ILAB=0
      SAVE=-TOP(IPIV)*REPI
      TOP(IPIV)=SAVE

C     INITIALIZE J AS COUNTER FOR TOP-LOOP
      J=NAN
   33 IF(J-IPIV) 34,53,34
   34 K=0

C     SEARCH COLUMN IN TRANSFORMATION-MATRIX T
      DO 36 I=1,L
      IF(THE(I)-J) 36,35,36
   35 K=I
      IF(ILAB) 50,50,14
   36 CONTINUE

C     GENERATE COLUMN USING SUBROUTINE FCT AND TRANSFORMATION-MATRIX
      I=L+L+NAN+J
      I=THE(I)-N
      IF(I) 37,37,38
   37 I=I+N
      K=1
   38 I=I+NAN

C     CALL SUBROUTINE FCT
      CALL FCT(PIV,TOP(I),M-1)

C     PREPARE THE CALLED VECTOR PIV
      DSUM=0.D0
      IDO=M
      DO 41 I=1,M
      HELP=PIV(IDO)
      IF(K) 39,39,40
   39 HELP=-HELP
   40 DSUM=DSUM+DBLE(HELP)
      PIV(IDO+1)=HELP
   41 IDO=IDO-1
      PIV(L)=-DSUM
      PIV(1)=1.

C     TRANSFORM VECTOR PIV WITH ROWS OF MATRIX T
      IDO=IND
      IF(ILAB) 44,44,42
   42 K=1
   43 IDO=K
   44 DSUM=0.D0
      HELP=0.

C     START MULTIPLICATION-LOOP
      DO 46 I=1,L
      DSUM=DSUM+DBLE(PIV(I)*T(IDO))
      TOL=ABS(SNGL(DSUM))
      IF(TOL-HELP) 46,46,45
   45 HELP=TOL
   46 IDO=IDO+L

C     END OF MULTIPLICATION-LOOP

      TOL=1.E-5*HELP
      IF(ABS(SNGL(DSUM))-TOL) 47,47,48
   47 DSUM=0.D0
   48 IF(ILAB) 51,51,49
   49 I=K+L
      PIV(I)=DSUM

C     TEST FOR LAST COLUMN-TERM
      K=K+1
      IF(K-L) 43,43,18
   50 I=(K-1)*L+IND
      DSUM=T(I)

C     COMPUTE NEW TOP-ELEMENT
   51 DSUM=DSUM*DBLE(SAVE)
      TOL=1.E-5*ABS(SNGL(DSUM))
      TOP(J)=TOP(J)+SNGL(DSUM)
      IF(ABS(TOP(J))-TOL) 52,52,53
   52 TOP(J)=0.

C     TEST FOR LAST TOP-TERM
   53 J=J-1
      IF(J) 54,54,33

C     END OF TOP-LOOP

C     TRANSFORM PIVOT-COLUMN
   54 I=IND+L
      PIV(I)=-1.
      DO 55 I=1,L
      J=I+L
   55 PIV(I)=-PIV(J)*REPI

C     UPDATE TRANSFORMATION-MATRIX T
      J=0
      DO 57 I=1,L
      IDO=J+IND
      SAVE=T(IDO)
      T(IDO)=0.
      DO 56 K=1,L
      ISE=K+J
   56 T(ISE)=T(ISE)+SAVE*PIV(K)
   57 J=J+L

C     UPDATE INDEX-VECTOR THE
C     INITIALIZE CHARACTERISTICS
      J=0
      K=0
      ISE=0
      IDO=0

C     START QUESTION-LOOP
      DO 61 I=1,L
      LL=I+L
      ILAB=THE(LL)
      IF(THE(I)-IPIV) 59,58,59
   58 ISE=I
      J=ILAB
```

```
      59 IF(ILAB-IND) 61,60,61                                          APMM3330
      60 IDO=I                                                          APMM3340
         K=IHE(I)                                                       APMM3350
      61 CONTINUE                                                       APMM3360
C           END OF QUESTION-LOOP                                        APMM3370
C                                                                       APMM3380
C           START MODIFICATION                                          APMM3390
         IF(K) 62,62,63                                                 APMM3400
      62 IHE(IDO)=IPIV                                                  APMM3410
         IF(ISE) 67,67,65                                               APMM3420
      63 IF(IND-J) 64,66,64                                             APMM3430
      64 LL=L+L+L+NAN                                                   APMM3440
         K=K+LL                                                         APMM3450
         I=IPIV+LL                                                      APMM3460
         ILAB=IHE(K)                                                    APMM3470
         IHE(K)=IHE(I)                                                  APMM3480
         IHE(I)=ILAB                                                    APMM3490
         IF(ISE) 67,67,65                                               APMM3500
      65 IDO=IDO+L                                                      APMM3510
         I=ISE+L                                                        APMM3520
         IHE(IDO)=J                                                     APMM3530
         IHE(I)=IND                                                     APMM3540
      66 IHE(ISE)=0                                                     APMM3550
      67 LL=L+L                                                         APMM3560
         J=LL+IND                                                       APMM3570
         I=LL+L+IPIV                                                    APMM3580
         ILAB=IHE(I)                                                    APMM3590
         IHE(I)=IHE(J)                                                  APMM3600
         IHE(J)=ILAB                                                    APMM3610
C           END OF MODIFICATION                                         APMM3620
C                                                                       APMM3630
         GO TO 8                                                        APMM3640
C                                                                       APMM3650
C           SET ERROR PARAMETER IER=-1 SINCE NO SUITABLE PIVOT IS FOUND APMM3660
      68 IER=-1                                                         APMM3670
C                                                                       APMM3680
C           EVALUATE FINAL TABLEAU                                      APMM3690
C           COMPUTE SAVE AS MAXIMUM ERROR OF APPROXIMATION AND          APMM3700
C           HELP AS ADDITIVE CONSTANCE FOR RESULTING COEFFICIENTS       APMM3710
      69 SAVE=0.                                                        APMM3720
         HELP=0.                                                        APMM3730
         K=L+L+L                                                        APMM3740
         DO 73 I=1,NAN                                                  APMM3750
         IDO=K+I                                                        APMM3760
         J=IHE(IDO)                                                     APMM3770
         IF(J) 71,70,73                                                 APMM3780
      70 SAVE=-TOP(I)                                                   APMM3790
      71 IF(M+J+1) 73,72,73                                             APMM3800
      72 HELP=TOP(I)                                                    APMM3810
      73 CONTINUE                                                       APMM3820
C                                                                       APMM3830
C           PREPARE T,TOP,PIV                                           APMM3840
         T(1)=SAVE                                                      APMM3850
         IDO=NAN+1                                                      APMM3860
         J=NAN+N                                                        APMM3870
         DO 74 I=IDO,J                                                  APMM3880
      74 TOP(I)=SAVE                                                    APMM3890
         DO 75 I=1,M                                                    APMM3900
      75 PIV(I)=HELP                                                    APMM3910
C                                                                       APMM3920
C           COMPUTE COEFFICIENTS OF RESULTING POLYNOMIAL IN PIV(1) UP TO PIAPMM3930
C           AND CALCULATE ERRORS AT GIVEN NODES IN TOP(1) UP TO TOP(N)  APMM3940
         DO 79 I=1,NAN                                                  APMM3950
         IDO=K+I                                                        APMM3960
         J=IHE(IDO)                                                     APMM3970
         IF(J) 76,79,77                                                 APMM3980
      76 J=-J                                                           APMM3990
         PIV(J)=HELP-TOP(I)                                             APMM4000
         GO TO 79                                                       APMM4010
      77 IF(J-N) 78,78,79                                               APMM4020
      78 J=J+NAN                                                        APMM4030
         TOP(J)=SAVE+TOP(I)                                             APMM4040
      79 CONTINUE                                                       APMM4050
         DO 80 I=1,N                                                    APMM4060
         IDO=NAN+I                                                      APMM4070
      80 TOP(I)=TOP(IDO)                                                APMM4080
      81 RETURN                                                         APMM4090
         END                                                            APMM4100
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C                                                                       DAPM  10
C   ****************************************************************DAPM  20
C                                                                       DAPM  30
C      SUBROUTINE DAPMM                                                 DAPM  40
C                                                                       DAPM  50
C      PURPOSE                                                          DAPM  60
C         APPROXIMATE A FUNCTION TABULATED IN N POINTS BY ANY LINEAR    DAPM  70
C         COMBINATION OF M GIVEN CONTINUOUS FUNCTIONS IN THE SENSE      DAPM  80
C         OF CHEBYSHEV.                                                 DAPM  90
C                                                                       DAPM 100
C      USAGE                                                            DAPM 110
C         CALL DAPMM(FCT,N,M,TOP,IHE,PIV,T,ITER,IER)                    DAPM 120
C         PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT IN THE           DAPM 130
C         CALLING PROGRAM.                                              DAPM 140
C                                                                       DAPM 150
C      DESCRIPTION OF PARAMETERS                                        DAPM 160
C         FCT    - NAME OF SUBROUTINE TO BE SUPPLIED BY THE USER.       DAPM 170
C                  IT COMPUTES VALUES OF M GIVEN FUNCTIONS FOR          DAPM 180
C                  ARGUMENT VALUE X.                                    DAPM 190
C                  USAGE                                                DAPM 200
C                     CALL FCT(Y,X,K)                                   DAPM 210
C                  DESCRIPTION OF PARAMETERS                            DAPM 220
C                     Y    - DOUBLE PRECISION RESULT VECTOR OF DIMEN-   DAPM 230
C                            SION M CONTAINING THE VALUES OF GIVEN      DAPM 240
C                            CONTINUOUS FUNCTIONS FOR GIVEN ARGUMENT X  DAPM 250
C                     X    - DOUBLE PRECISON ARGUMENT VALUE             DAPM 260
C                     K    - AN INTEGER VALUE WHICH IS EQUAL TO M-1     DAPM 270
C                  REMARKS                                              DAPM 280
C                     IF APPROXIMATION BY NORMAL CHEBYSHEV, SHIFTED     DAPM 290
C                     CHEBYSHEV, LEGENDRE, LAGUERRE, HERMITE POLYNO-    DAPM 300
C                     MIALS IS DESIRED SUBROUTINES DCAP,DCSP,DLEP,      DAPM 310
C                     DLAP,DHEP, RESPECTIVELY FROM SSP COULD BE USED.   DAPM 320
C         N      - NUMBER OF DATA POINTS DEFINING THE FUNCTION WHICH    DAPM 330
C                  IS TO BE APPROXIMATED                                DAPM 340
C         M      - NUMBER OF GIVEN CONTINUOUS FUNCTIONS FROM WHICH      DAPM 350
C                  THE APPROXIMATING FUNCTION IS CONSTRUCTED.           DAPM 360
C         TOP    - DOUBLE PRECISION VECTOR OF DIMENSION 3*N.            DAPM 370
C                  ON ENTRY IT MUST CONTAIN FROM TOP(1) UP TO TOP(N)    DAPM 380
C                  THE GIVEN N FUNCTION VALUES AND FROM TOP(N+1) UP     DAPM 390
C                  TO TOP(2*N) THE CORRESPONDING NODES                  DAPM 400
C                  ON RETURN TOP CONTAINS FROM TOP(1) UP TO TOP(N)      DAPM 410
C                  THE ERRORS AT THOSE N NODES.                         DAPM 420
C                  OTHER VALUES OF TOP ARE SCRATCH.                     DAPM 430
C         IHE    - INTEGER VECTOR OF DIMENSION 3*M+4*N+6                DAPM 440
C         PIV    - DOUBLE PRECISION VECTOR OF DIMENSION 3*M+6.          DAPM 450
C                  ON RETURN PIV CONTAINS AT PIV(1) UP TO PIV(M) THE    DAPM 460
C                  RESULTING COEFFICIENTS OF LINEAR APPROXIMATION.      DAPM 470
C         T      - DOUBLE PRECISION AUXILIARY VECTOR OF DIMENSION       DAPM 480
C                  (M+2)*(M+2)                                          DAPM 490
C         ITER   - RESULTANT INTEGER WHICH SPECIFIES THE NUMBER OF      DAPM 500
C                  ITERATIONS NEEDED                                    DAPM 510
C         IER    - RESULTANT ERROR PARAMETER CODED IN THE FOLLOWING     DAPM 520
C                  FORM                                                 DAPM 530
C                     IER=0  - NO ERROR                                 DAPM 540
C                     IER=1  - THE NUMBER OF ITERATIONS HAS REACHED     DAPM 550
C                              THE INTERNAL MAXIMUM N+M                 DAPM 560
C                     IER=-1 - NO RESULT BECAUSE OF WRONG INPUT PARA-   DAPM 570
C                              METER M OR N OR SINCE AT SOME ITERATION  DAPM 580
C                              NO SUITABLE PIVOT COULD BE FOUND         DAPM 590
C                                                                       DAPM 600
C      REMARKS                                                          DAPM 610
C         NO ACTION BESIDES ERROR MESSAGE IN CASE M LESS THAN 1 OR      DAPM 620
C         N LESS THAN 2.                                                DAPM 630
C                                                                       DAPM 640
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                    DAPM 650
C         THE EXTERNAL SUBROUTINE FCT MUST BE FURNISHED BY THE USER.    DAPM 660
C                                                                       DAPM 670
C      METHOD                                                           DAPM 680
C         THE PROBLEM OF APPROXIMATION A TABULATED FUNCTION BY ANY      DAPM 690
C         LINEAR COMBINATION OF GIVEN FUNCTIONS IN THE SENSE OF         DAPM 700
C         CHEBYSHEV (I.E. TO MINIMIZE THE MAXIMUM ERROR) IS TRANS-      DAPM 710
C         FORMED INTO A LINEAR PROGRAMMING PROBLEM. DAPMM USES A        DAPM 720
C         REVISED SIMPLEX METHOD TO SOLVE A CORRESPONDING DUAL          DAPM 730
C         PROBLEM. FOR REFERENCE, SEE                                   DAPM 740
C         I.BARRODALE/A.YOUNG, ALGORITHMS FOR BEST L-SUB-ONE AND        DAPM 750
C         L-SUB-INFINITY, LINEAR APPROXIMATIONS ON A DISCRETE SET,      DAPM 760
C         NUMERISCHE MATHEMATIK, VOL.8, ISS.3 (1966), PP.295-306.       DAPM 770
C                                                                       DAPM 780
C   ****************************************************************DAPM 790
      SUBROUTINE DAPMM(FCT,N,M,TOP,IHE,PIV,T,ITER,IER)                  DAPM 800
C                                                                       DAPM 810
C                                                                       DAPM 820
      DIMENSION TOP(1),IHE(1),PIV(1),T(1)                               DAPM 830
      DOUBLE PRECISION DSUM,TOP,PIV,T,SAVE,HELP,REPI,TOL                DAPM 840
C                                                                       DAPM 850
C        TEST ON WRONG INPUT PARAMETERS N AND M                         DAPM 860
      IER=-1                                                            DAPM 870
      IF (N-1) 81,81,1                                                  DAPM 880
    1 IF(M) 81,81,2                                                     DAPM 890
C                                                                       DAPM 900
C        INITIALIZE CHARACTERISTIC VECTORS FOR THE TABLEAU              DAPM 910
    2 IER=0                                                             DAPM 920
C                                                                       DAPM 930
C        PREPARE TOP-ROW TOP                                            DAPM 940
      DO 3 I=1,N                                                        DAPM 950
      K=I+N                                                             DAPM 960
      J=K+N                                                             DAPM 970
      TOP(J)=TOP(K)                                                     DAPM 980
    3 TOP(K)=-TOP(I)                                                    DAPM 990
C                                                                       DAPM1000
C        PREPARE INVERSE TRANSFORMATION MATRIX T                        DAPM1010
      L=M+2                                                             DAPM1020
      LL=L*L                                                            DAPM1030
      DO 4 I=1,LL                                                       DAPM1040
    4 T(I)=0.D0                                                         DAPM1050
      K=1                                                               DAPM1060
      J=L+1                                                             DAPM1070
      DO 5 I=1,L                                                        DAPM1080
      T(K)=1.D0                                                         DAPM1090
    5 K=K+J                                                             DAPM1100
C                                                                       DAPM1110
C        PREPARE INDEX-VECTOR IHE                                       DAPM1120
      DO 6 I=1,L                                                        DAPM1130
      K=I+L                                                             DAPM1140
      J=K+L                                                             DAPM1150
      IHE(I)=0                                                          DAPM1160
      IHE(K)=I                                                          DAPM1170
    6 IHE(J)=1-I                                                        DAPM1180
      NAN=N+N                                                           DAPM1190
      K=L+L+L                                                           DAPM1200
      J=K+NAN                                                           DAPM1210
      DO 7 I=1,NAN                                                      DAPM1220
      K=K+1                                                             DAPM1230
      IHE(K)=I                                                          DAPM1240
      J=J+1                                                             DAPM1250
    7 IHE(J)=I                                                          DAPM1260
C                                                                       DAPM1270
C        SET COUNTER ITER FOR ITERATION-STEPS                           DAPM1280
      ITER=-1                                                           DAPM1290
    8 ITER=ITER+1                                                       DAPM1300
C                                                                       DAPM1310
C        TEST FOR MAXIMUM ITERATION-STEPS                               DAPM1320
      IF(N+M-ITER) 9,9,10                                               DAPM1330
    9 IER=1                                                             DAPM1340
      GO TO 69                                                          DAPM1350
C                                                                       DAPM1360
C        DETERMINE THE COLUMN WITH THE MOST POSITIVE ELEMENT IN TOP     DAPM1370
   10 ISE=0                                                             DAPM1380
      IPIV=0                                                            DAPM1390
      K=L+L+L                                                           DAPM1400
      SAVE=0.D0                                                         DAPM1410
C                                                                       DAPM1420
C        START TOP-LOOP                                                 DAPM1430
      DO 14 I=1,NAN                                                     DAPM1440
      IDO=K+I                                                           DAPM1450
      HELP=TOP(I)                                                       DAPM1460
      IF(HELP-SAVE) 12,12,11                                            DAPM1470
   11 SAVE=HELP                                                         DAPM1480
      IPIV=I                                                            DAPM1490
   12 IF(IHE(IDO)) 14,13,14                                             DAPM1500
   13 ISE=I                                                             DAPM1510
   14 CONTINUE                                                          DAPM1520
C        END OF TOP-LOOP                                                DAPM1530
C                                                                       DAPM1540
C        IS OPTIMAL TABLEAU REACHED                                     DAPM1550
      IF(IPIV) 69,69,15                                                 DAPM1560
C                                                                       DAPM1570
C        DETERMINE THE PIVOT-ELEMENT FOR THE COLUMN CHOSEN UPOVE        DAPM1580
   15 ILAB=1                                                            DAPM1590
      IND=0                                                             DAPM1600
      J=ISE                                                             DAPM1610
      IF(J) 21,21,34                                                    DAPM1620
C                                                                       DAPM1630
C        TRANSFER K-TH COLUMN FROM T TO PIV                             DAPM1640
   16 K=(K-1)*L                                                         DAPM1650
      DO 17 I=1,L                                                       DAPM1660
      J=L+I                                                             DAPM1670
      K=K+1                                                             DAPM1680
   17 PIV(J)=T(K)                                                       DAPM1690
C                                                                       DAPM1700
C        IS ANOTHER COLUMN NEEDED FOR SEARCH FOR PIVOT-ELEMENT          DAPM1710
   18 IF(ISE) 22,22,19                                                  DAPM1720
                                                                        DAPM1730
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   19 ISE=-ISE                                                          DAPM1740
C                                                                       DAPM1750
C        TRANSFER COLUMNS IN PIV                                        DAPM1760
      J=L+1                                                             DAPM1770
      IDO=L+L                                                           DAPM1780
      DO 20 I=J,IDO                                                     DAPM1790
      K=I+L                                                             DAPM1800
   20 PIV(K)=PIV(I)                                                     DAPM1810
   21 J=IPIV                                                            DAPM1820
      GO TO 34                                                          DAPM1830
C                                                                       DAPM1840
C        SEARCH PIVOT-ELEMENT PIV(IND)                                  DAPM1850
   22 SAVE=1.D38                                                        DAPM1960
      IDO=0                                                             DAPM1870
      K=L+1                                                             DAPM1880
      LL=L+L                                                            DAPM1890
      IND=0                                                             DAPM1900
C                                                                       DAPM1910
C        START PIVOT-LOOP                                               DAPM1920
      DO 29 I=K,LL                                                      DAPM1930
      J=I+L                                                             DAPM1940
      HELP=PIV(I)                                                       DAPM1950
      IF(HELP) 29,29,23                                                 DAPM1960
   23 HELP=-HELP                                                        DAPM1970
      IF(ISE) 26,24,26                                                  DAPM1980
   24 IF(IHE(J)) 27,25,27                                               DAPM1990
   25 IDO=I                                                             DAPM2000
      GO TO 29                                                          DAPM2010
   26 HELP=-PIV(J)/HELP                                                 DAPM2020
   27 IF(HELP-SAVE) 28,29,29                                            DAPM2030
   28 SAVE=HELP                                                         DAPM2040
      IND=I                                                             DAPM2050
   29 CONTINUE                                                          DAPM2060
C        END OF PIVOT-LOOP                                              DAPM2070
C                                                                       DAPM2080
C        TEST FOR SUITABLE PIVOT-ELEMENT                                DAPM2090
      IF(IND) 30,30,32                                                  DAPM2100
   30 IF(IDO) 68,68,31                                                  DAPM2110
   31 IND=IDO                                                           DAPM2120
C        PIVOT-ELEMENT IS STORED IN PIV(IND)                            DAPM2130
C                                                                       DAPM2140
C        COMPUTE THE RECIPROCAL OF THE PIVOT-ELEMENT REPI               DAPM2150
   32 REPI=1.D0/PIV(IND)                                                DAPM2160
      IND=IND-L                                                         DAPM2170
C                                                                       DAPM2180
C        UPDATE THE TOP-ROW TOP OF THE TABLEAU                          DAPM2190
      ILAB=0                                                            DAPM2200
      SAVE=-TOP(IPIV)*REPI                                              DAPM2210
      TOP(IPIV)=SAVE                                                    DAPM2220
C                                                                       DAPM2230
C        INITIALIZE J AS COUNTER FOR TOP-LOOP                           DAPM2240
      J=NAN                                                             DAPM2250
   33 IF(J-IPIV) 34,53,34                                               DAPM2260
   34 K=0                                                               DAPM2270
C                                                                       DAPM2280
C        SEARCH COLUMN IN TRANSFORMATION-MATRIX T                       DAPM2290
      DO 36 I=1,L                                                       DAPM2300
      IF(IHE(I)-J) 36,35,36                                             DAPM2310
   35 K=I                                                               DAPM2320
      IF(ILAB) 50,50,16                                                 DAPM2330
   36 CONTINUE                                                          DAPM2340
C                                                                       DAPM2350
C        GENERATE COLUMN USING SUBROUTINE FCT AND TRANSFORMATION-MATRIX DAPM2360
      I=L+L+L+NAN+J                                                     DAPM2370
      I=IHE(I)-N                                                        DAPM2380
      IF(I) 37,37,38                                                    DAPM2390
   37 I=I+N                                                             DAPM2400
      K=1                                                               DAPM2410
   38 I=I+NAN                                                           DAPM2420
C                                                                       DAPM2430
C        CALL SUBROUTINE FCT                                            DAPM2440
      CALL FCT(PIV,TOP(I),M-1)                                          DAPM2450
C                                                                       DAPM2460
C        PREPARE THE CALLED VECTOR PIV                                  DAPM2470
      DSUM=0.D0                                                         DAPM2480
      IDO=M                                                             DAPM2490
      DO 41 I=1,M                                                       DAPM2500
      HELP=PIV(IDO)                                                     DAPM2510
      IF(K) 39,39,40                                                    DAPM2520
   39 HELP=-HELP                                                        DAPM2530
   40 DSUM=DSUM+HELP                                                    DAPM2540
      PIV(IDO+1)=HELP                                                   DAPM2550
   41 IDO=IDO-1                                                         DAPM2560
      PIV(L)=-DSUM                                                      DAPM2570
      PIV(1)=1.D0                                                       DAPM2580
C                                                                       DAPM2590
C        TRANSFORM VECTOR PIV WITH ROWS OF MATRIX T                     DAPM2600
      IDO=IND                                                           DAPM2610
      IF(ILAB) 44,44,42                                                 DAPM2620
   42 K=1                                                               DAPM2630
   43 IDO=K                                                             DAPM2640
   44 DSUM=0.D0                                                         DAPM2650
      HELP=0.D0                                                         DAPM2660
C                                                                       DAPM2670
C        START MULTIPLICATION-LOOP                                      DAPM2680
      DO 46 I=1,L                                                       DAPM2690
      DSUM=DSUM+PIV(I)*T(IDO)                                           DAPM2700
      TOL=DABS(DSUM)                                                    DAPM2710
      IF(TOL-HELP) 46,46,45                                             DAPM2720
   45 HELP=TOL                                                          DAPM2730
   46 IDO=IDO+L                                                         DAPM2740
C        END OF MULTIPLICATION-LOOP                                     DAPM2750
C                                                                       DAPM2760
      TOL=1.D-14*HELP                                                   DAPM2770
      IF(DABS(DSUM)-TOL) 47,47,48                                       DAPM2780
   47 DSUM=0.D0                                                         DAPM2790
   48 IF(ILAB) 51,51,49                                                 DAPM2800
   49 I=K+L                                                             DAPM2810
      PIV(I)=DSUM                                                       DAPM2820
C                                                                       DAPM2830
C        TEST FOR LAST COLUMN-TERM                                      DAPM2840
      K=K+1                                                             DAPM2850
      IF(K-L) 43,43,18                                                  DAPM2860
   50 I=(K-1)*L+IND                                                     DAPM2870
      DSUM=T(I)                                                         DAPM2880
C                                                                       DAPM2890
C        COMPUTE NEW TOP-ELEMENT                                        DAPM2900
   51 DSUM=DSUM*SAVE                                                    DAPM2910
      TOL=1.D-14*DABS(DSUM)                                             DAPM2920
      TOP(J)=TOP(J)+DSUM                                                DAPM2930
      IF(DABS(TOP(J))-TOL) 52,52,53                                     DAPM2940
   52 TOP(J)=0.D0                                                       DAPM2950
C                                                                       DAPM2960
C        TEST FOR LAST TOP-TERM                                         DAPM2970
   53 J=J-1                                                             DAPM2980
      IF(J) 54,54,33                                                    DAPM2990
C        END OF TOP-LOOP                                                DAPM3000
C                                                                       DAPM3010
C        TRANSFORM PIVOT-COLUMN                                         DAPM3020
   54 I=IND+L                                                           DAPM3030
      PIV(I)=-1.D0                                                      DAPM3040
      DO 55 I=1,L                                                       DAPM3050
      J=I+L                                                             DAPM3060
   55 PIV(I)=-PIV(J)*REPI                                               DAPM3070
C                                                                       DAPM3080
C        UPDATE TRANSFORMATION-MATRIX T                                 DAPM3090
      J=0                                                               DAPM3100
      DO 57 I=1,L                                                       DAPM3110
      IDO=J+IND                                                         DAPM3120
      SAVE=T(IDO)                                                       DAPM3130
      T(IDO)=0.D0                                                       DAPM3140
      DO 56 K=1,L                                                       DAPM3150
      ISE=K+J                                                           DAPM3160
   56 T(ISE)=T(ISE)+SAVE*PIV(K)                                         DAPM3170
   57 J=J+L                                                             DAPM3180
C                                                                       DAPM3190
C        UPDATE INDEX-VECTOR IHE                                        DAPM3200
C        INITIALIZE CHARACTERISTICS                                     DAPM3210
      J=0                                                               DAPM3220
      K=0                                                               DAPM3230
      ISE=0                                                             DAPM3240
      IDO=0                                                             DAPM3250
C                                                                       DAPM3260
C        START QUESTION-LOOP                                            DAPM3270
      DO 61 I=1,L                                                       DAPM3280
      LL=I+L                                                            DAPM3290
      ILAB=IHE(LL)                                                      DAPM3300
      IF(IHE(I)-IPIV) 59,58,59                                          DAPM3310
   58 ISE=I                                                             DAPM3320
      J=ILAB                                                            DAPM3330
   59 IF(ILAB-IND) 61,60,61                                             DAPM3340
   60 IDO=I                                                             DAPM3350
      K=IHE(I)                                                          DAPM3360
   61 CONTINUE                                                          DAPM3370
C        END OF QUESTION-LOOP                                           DAPM3380
C                                                                       DAPM3390
C        START MODIFICATION                                             DAPM3400
      IF(K) 62,62,63                                                    DAPM3410
   62 IHE(IDO)=IPIV                                                     DAPM3420
      IF(ISE) 67,67,65                                                  DAPM3430
   63 IF(IND-J) 64,56,64                                                DAPM3440
   64 LL=L+L+NAN                                                        DAPM3450
      K=K+LL                                                            DAPM3460
      I=IPIV+LL                                                         DAPM3470
      ILAB=IHE(K)                                                       DAPM3480
      IHE(K)=IHE(I)                                                     DAPM3490
      IHE(I)=ILAB                                                       DAPM3500
      IF(ISE) 67,67,65                                                  DAPM3510
   65 IDO=ISE+L                                                         DAPM3520
      I=ISE+NAN                                                         DAPM3530
      IHE(IDO)=J                                                        DAPM3540
      IHE(I)=IND                                                        DAPM3550
   66 IHE(ISE)=0                                                        DAPM3560
   67 LL=L+L                                                            DAPM3570
      J=LL+IND                                                          DAPM3580
      I=LL+L+IPIV                                                       DAPM3590
      ILAB=IHE(I)                                                       DAPM3600
      IHE(I)=IHE(J)                                                     DAPM3610
      IHE(J)=ILAB                                                       DAPM3620
C        END OF MODIFICATION                                            DAPM3630
C                                                                       DAPM3640
      GO TO 8                                                           DAPM3650
C                                                                       DAPM3660
C        SET ERROR PARAMETER IER=-1 SINCE NO SUITABLE PIVOT IS FOUND    DAPM3670
   68 IER=-1                                                            DAPM3680
C                                                                       DAPM3690
C        EVALUATE FINAL TABLEAU                                         DAPM3700
C        COMPUTE SAVE AS MAXIMUM ERROR OF APPROXIMATION VALUES          DAPM3710
C        HELP AS ADDITIVE CONSTANCE FOR RESULTING COEFFICIENTS          DAPM3720
   69 SAVE=0.D0                                                         DAPM3730
      HELP=0.D0                                                         DAPM3740
      K=L+L+L                                                           DAPM3750
      DO 73 I=1,NAN                                                     DAPM3760
      IDO=K+I                                                           DAPM3770
      J=IHE(IDO)                                                        DAPM3780
      IF(J) 71,70,73                                                    DAPM3790
   70 SAVE=-TOP(I)                                                      DAPM3800
   71 IF(M+J+1) 73,72,73                                                DAPM3810
   72 HELP=TOP(I)                                                       DAPM3820
   73 CONTINUE                                                          DAPM3830
C                                                                       DAPM3840
C        PREPARE T,TOP,PIV                                              DAPM3850
      T(1)=SAVE                                                         DAPM3860
      IDO=NAN+1                                                         DAPM3870
      J=KAT+N                                                           DAPM3880
      DO 74 I=IDO,J                                                     DAPM3890
   74 TOP(I)=SAVE                                                       DAPM3900
      DO 75 I=1,M                                                       DAPM3910
   75 PIV(I)=HELP                                                       DAPM3920
C        COMPUTE COEFFICIENTS OF RESULTING POLYNOMIAL IN PIV(I) UP TO PIDAPM3930
C        AND CALCULATE ERRORS AT GIVEN NODES IN TOP(I) UP TO TOP(N)     DAPM3940
      DO 79 I=1,NAN                                                     DAPM3950
      IDO=K+I                                                           DAPM3960
      J=IHE(IDO)                                                        DAPM3970
      IF(J) 76,79,77                                                    DAPM3980
   76 J=-J                                                              DAPM3990
      PIV(J)=HELP-TOP(I)                                                DAPM4000
      GO TO 79                                                          DAPM4010
   77 IF(J-N) 78,78,79                                                  DAPM4020
   78 J=J+NAN                                                           DAPM4030
      TOP(J)=SAVE+TOP(I)                                                DAPM4040
   79 CONTINUE                                                          DAPM4050
      DO 80 I=1,N                                                       DAPM4060
      IDO=NAN+I                                                         DAPM4070
   80 TOP(I)=TOP(IDO)                                                   DAPM4080
   81 RETURN                                                            DAPM4090
      END                                                               DAPM4100
```

Numerical Quadrature

Subroutines QTFG and DQTFG

These subroutines perform the integration of a monotonically tabulated function by trapezoidal rule.

To compute the vector of integral values:

$$z_i = z(x_i) = \int_{x_1}^{x_i} y(x)\,dx \quad (i = 1,2,\ldots,n)$$

for a given table $(x_i, y_i; i = 1,2,\ldots,n)$ of monotonic arguments and their function values, the trapezoidal rule is used. It is assumed that the function to be integrated is continuous and can be differentiated at least twice. Starting with integral value $z_1 = 0$, successive integral values z_i $(i = 2,3,..,n)$ are computed, using the trapezoidal rule in the following form:

$$z_1 = z_{i-1} + \frac{x_i - x_{i-1}}{2}(y_i + y_{i-1}) \quad (i = 2,3,\ldots,n)$$

Local truncation error at each step is:

$$R_i = -\frac{1}{12}(x_i - x_{i-1})^3 \cdot y''(\xi_i) \quad (\xi_i \quad [x_{i-1}, x_i])$$

However, these truncation errors may accumulate.

For reference see F.B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 75.

```
C                                                                       QTFG  10
C     ******************************************************************QTFG  20
C                                                                       QTFG  30
C        SUBROUTINE QTFG                                                QTFG  40
C                                                                       QTFG  50
C        PURPOSE                                                        QTFG  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        QTFG  70
C           GENERAL TABLE OF ARGUMENT AND FUNCTION VALUES.              QTFG  80
C                                                                       QTFG  90
C        USAGE                                                          QTFG 100
C           CALL QTFG (X,Y,Z,NDIM)                                      QTFG 110
C                                                                       QTFG 120
C        DESCRIPTION OF PARAMETERS                                      QTFG 130
C           X      - THE INPUT VECTOR OF ARGUMENT VALUES.               QTFG 140
C           Y      - THE INPUT VECTOR OF FUNCTION VALUES.               QTFG 150
C           Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE  QTFG 160
C                    IDENTICAL WITH X OR Y.                             QTFG 170
C           NDIM   - THE DIMENSION OF VECTORS X,Y,Z.                    QTFG 180
C                                                                       QTFG 190
C        REMARKS                                                        QTFG 200
C           NO ACTION IN CASE NDIM LESS THAN 1.                         QTFG 210
C                                                                       QTFG 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QTFG 230
C           NONE                                                        QTFG 240
C                                                                       QTFG 250
C        METHOD                                                         QTFG 260
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    QTFG 270
C           MEANS OF TRAPEZOIDAL RULE (SECOND ORDER FORMULA).           QTFG 280
C           FOR REFERENCE, SEE                                          QTFG 290
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         QTFG 300
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.75.          QTFG 310
C                                                                       QTFG 320
C     ******************************************************************QTFG 330
      SUBROUTINE QTFG(X,Y,Z,NDIM)                                       QTFG 340
C                                                                       QTFG 350
C                                                                       QTFG 360
      DIMENSION X(1),Y(1),Z(1)                                          QTFG 370
C                                                                       QTFG 380
      SUM2=0.                                                           QTFG 390
      IF(NDIM-1)4,3,1                                                   QTFG 400
C                                                                       QTFG 410
C     INTEGRATION LOOP                                                  QTFG 420
    1 DO 2 I=2,NDIM                                                     QTFG 430
      SUM1=SUM2                                                         QTFG 440
      SUM2=SUM2+.5*(X(I)-X(I-1))*(Y(I)+Y(I-1))                          QTFG 450
    2 Z(I-1)=SUM1                                                       QTFG 460
    3 Z(NDIM)=SUM2                                                      QTFG 470
    4 RETURN                                                            QTFG 480
      END                                                               QTFG 490
                                                                        QTFG 500
```

```
C                                                                       DTFG  10
C     ******************************************************************DTFG  20
C                                                                       DTFG  30
C        SUBROUTINE DQTFG                                               DTFG  40
C                                                                       DTFG  50
C        PURPOSE                                                        DTFG  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DTFG  70
C           GENERAL TABLE OF ARGUMENT AND FUNCTION VALUES.              DTFG  80
C                                                                       DTFG  90
C        USAGE                                                          DTFG 100
C           CALL DQTFG (X,Y,Z,NDIM)                                     DTFG 110
C                                                                       DTFG 120
C        DESCRIPTION OF PARAMETERS                                      DTFG 130
C           X      - DOUBLE PRECISION INPUT VECTOR OF ARGUMENT VALUES.  DTFG 140
C           Y      - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES.  DTFG 150
C           Z      - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL      DTFG 160
C                    VALUES. Z MAY BE IDENTICAL WITH X OR Y.            DTFG 170
C           NDIM   - THE DIMENSION OF VECTORS X,Y,Z.                    DTFG 180
C                                                                       DTFG 190
C        REMARKS                                                        DTFG 200
C           NO ACTION IN CASE NDIM LESS THAN 1.                         DTFG 210
C                                                                       DTFG 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTFG 230
C           NONE                                                        DTFG 240
C                                                                       DTFG 250
C        METHOD                                                         DTFG 260
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DTFG 270
C           MEANS OF TRAPEZOIDAL RULE (SECOND ORDER FORMULA).           DTFG 280
C           FOR REFERENCE, SEE                                          DTFG 290
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         DTFG 300
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.75.          DTFG 310
C                                                                       DTFG 320
C     ******************************************************************DTFG 330
      SUBROUTINE DQTFG(X,Y,Z,NDIM)                                      DTFG 340
C                                                                       DTFG 350
C                                                                       DTFG 360
      DIMENSION X(1),Y(1),Z(1)                                          DTFG 370
      DOUBLE PRECISION X,Y,Z,SUM1,SUM2                                  DTFG 380
C                                                                       DTFG 390
      SUM2=0.D0                                                         DTFG 400
      IF(NDIM-1)4,3,1                                                   DTFG 410
C                                                                       DTFG 420
C     INTEGRATION LOOP                                                  DTFG 430
    1 DO 2 I=2,NDIM                                                     DTFG 440
      SUM1=SUM2                                                         DTFG 450
      SUM2=SUM2+.5D0*(X(I)-X(I-1))*(Y(I)+Y(I-1))                        DTFG 460
    2 Z(I-1)=SUM1                                                       DTFG 470
    3 Z(NDIM)=SUM2                                                      DTFG 480
    4 RETURN                                                            DTFG 490
      END                                                               DTFG 500
                                                                        DTFG 510
```

Subroutines QTFE and DQTFE

These subroutines perform the integration of an equidistantly tabulated function by trapezoidal rule.

To compute the vector of integral values:

$$\left.\begin{aligned} z_i = z(x_i) &= \int_a^{x_i} y(x)\,dx \\ \text{with } x_i &= a + (i-1)\,h \end{aligned}\right\} (i = 1,2,3,\ldots,n)$$

for a table of function values y_i $(i = 1,2,\ldots,n)$, given at equidistant points $x_i = a + (i-1)\cdot h$ $(i = 1,2,\ldots,n)$, the trapezoidal rule is used. It is assumed that the function to be integrated is continuous and can be differentiated at least twice. Starting with the integral value $z_1 = 0$, successive integral values z_i $(i = 2,3,\ldots,n)$ are computed, using the trapezoidal rule in the following form:

$$z_i = z_{i-1} + \frac{h}{2}(y_i + y_{i-1}) \qquad (i=2,3,\ldots,n)$$

with a given increment h of argument values.

As local truncation error at each step is:

$$R_i = -\frac{1}{12} h^3 \cdot y''(\xi_i) \qquad (\xi_i \in [x_{i-1}, x_i])$$

the global truncation error R in z_n appears as follows:

$$R = -\frac{1}{12}(n-1)\,h^3\,y''(\xi) \qquad (\xi \in [x_1, x_n])$$

or

$$R = -\frac{\ell}{12} \cdot h^2 \cdot y''(\xi)$$

where ℓ is the length of the whole integration interval.

For reference see F.B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 75.

```
C                                                                       QTFE  10
C     ...................................................................QTFE  20
C                                                                       QTFE  30
C        SUBROUTINE QTFE                                                QTFE  40
C                                                                       QTFE  50
C        PURPOSE                                                        QTFE  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        QTFE  70
C           EQUIDISTANT TABLE OF FUNCTION VALUES.                       QTFE  80
C                                                                       QTFE  90
C        USAGE                                                          QTFE 100
C           CALL QTFE (H,Y,Z,NDIM)                                      QTFE 110
C                                                                       QTFE 120
C        DESCRIPTION OF PARAMETERS                                      QTFE 130
C           H      - THE INCREMENT OF ARGUMENT VALUES.                  QTFE 140
C           Y      - THE INPUT VECTOR OF FUNCTION VALUES.               QTFE 150
C           Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE  QTFE 160
C                    IDENTICAL WITH Y.                                  QTFE 170
C           NDIM   - THE DIMENSION OF VECTORS Y AND Z.                  QTFE 180
C                                                                       QTFE 190
C        REMARKS                                                        QTFE 200
C           NO ACTION IN CASE NDIM LESS THAN 1.                         QTFE 210
C                                                                       QTFE 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QTFE 230
C           NONE                                                        QTFE 240
C                                                                       QTFE 250
C        METHOD                                                         QTFE 260
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    QTFE 270
C           MEANS OF TRAPEZOIDAL RULE (SECOND ORDER FORMULA).           QTFE 280
C           FOR REFERENCE, SEE                                          QTFE 290
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         QTFE 300
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.75.          QTFE 310
C                                                                       QTFE 320
C     ...................................................................QTFE 330
C                                                                       QTFE 340
      SUBROUTINE QTFE(H,Y,Z,NDIM)                                       QTFE 350
C                                                                       QTFE 360
C                                                                       QTFE 370
      DIMENSION Y(1),Z(1)                                               QTFE 380
C                                                                       QTFE 390
      SUM2=0.                                                           QTFE 400
      IF(NDIM-1)4,3,1                                                   QTFE 410
    1 HH=.5*H                                                           QTFE 420
C                                                                       QTFE 430
C     INTEGRATION LOOP                                                  QTFE 440
      DO 2 I=2,NDIM                                                     QTFE 450
      SUM1=SUM2                                                         QTFE 460
      SUM2=SUM2+HH*(Y(I)+Y(I-1))                                        QTFE 470
    2 Z(I-1)=SUM1                                                       QTFE 480
    3 Z(NDIM)=SUM2                                                      QTFE 490
    4 RETURN                                                            QTFE 500
      END                                                               QTFE 510
```

```
C                                                                       DTFE  10
C     ...................................................................DTFE  20
C                                                                       DTFE  30
C        SUBROUTINE DQTFE                                               DTFE  40
C                                                                       DTFE  50
C        PURPOSE                                                        DTFE  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DTFE  70
C           EQUIDISTANT TABLE OF FUNCTION VALUES.                       DTFE  80
C                                                                       DTFE  90
C        USAGE                                                          DTFE 100
C           CALL DQTFE (H,Y,Z,NDIM)                                     DTFE 110
C                                                                       DTFE 120
C        DESCRIPTION OF PARAMETERS                                      DTFE 130
C           H      - DOUBLE PRECISION INCREMENT OF ARGUMENT VALUES.     DTFE 140
C           Y      - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES.  DTFE 150
C           Z      - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL      DTFE 160
C                    VALUES. Z MAY BE IDENTICAL WITH Y.                 DTFE 170
C           NDIM   - THE DIMENSION OF VECTORS Y AND Z.                  DTFE 180
C                                                                       DTFE 190
C        REMARKS                                                        DTFE 200
C           NO ACTION IN CASE NDIM LESS THAN 1.                         DTFE 210
C                                                                       DTFE 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DTFE 230
C           NONE                                                        DTFE 240
C                                                                       DTFE 250
C                                                                       DTFE 260
C        METHOD                                                         DTFE 270
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DTFE 280
C           MEANS OF TRAPEZOIDAL RULE (SECOND ORDER FORMULA).           DTFE 290
C           FOR REFERENCE, SEE                                          DTFE 300
C           F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,         DTFE 310
C           MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.75.          DTFE 320
C                                                                       DTFE 330
C     ...................................................................DTFE 340
C                                                                       DTFE 350
      SUBROUTINE DQTFE(H,Y,Z,NDIM)                                      DTFE 360
C                                                                       DTFE 370
C                                                                       DTFE 380
      DIMENSION Y(1),Z(1)                                               DTFE 390
      DOUBLE PRECISION Y,Z,H,HH,SUM1,SUM2                               DTFE 400
C                                                                       DTFE 410
      SUM2=0.D0                                                         DTFE 420
      IF(NDIM-1)4,3,1                                                   DTFE 430
    1 HH=.5D0*H                                                         DTFE 440
C                                                                       DTFE 450
C     INTEGRATION LOOP                                                  DTFE 460
      DO 2 I=2,NDIM                                                     DTFE 470
      SUM1=SUM2                                                         DTFE 480
      SUM2=SUM2+HH*(Y(I)+Y(I-1))                                        DTFE 490
    2 Z(I-1)=SUM1                                                       DTFE 500
    3 Z(NDIM)=SUM2                                                      DTFE 510
    4 RETURN                                                            DTFE 520
      END
```

Subroutines QSF and DQSF

These subroutines perform the integration of an equidistantly tabulated function by Simpson's rule. To compute the vector of integral values:

$$z_i = z(x_i) = \int_a^{x_i} y(x)\,dx \quad \text{with } x_i = a + (i-1)\,h \qquad (i=1,2,\ldots,n)$$

for a table of function values $y_i\,(i=1,2,\ldots,n)$, given at equidistant points $x_i = a+(i-1)\,h\ (i=1,2,\ldots,n)$, Simpson's rule together with Newton's 3/8 rule or a combination of these two rules is used. Local truncation error is of the order h^5 in all cases with more than three points in the given table. Only z_2 has a truncation error of the order h^4 if there are only three points in the given table. No action takes place if the table consists of less than three sample points.

The function to be integrated is assumed to be continuous and differentiable (three or four times, depending on the rule used).

Formulas used in this subroutine (z_j are integral values, y_j function values) are:

$$z_j = z_{j-1} + \frac{h}{3}(1.25\,y_{j-1} + 2y_j - 0.25\,y_{j+1}) \qquad (1)$$

$$z_j = z_{j-2} + \frac{h}{3}(y_{j-2} + 4y_{j-1} + y_j) \quad \text{(Simpson's rule)} \qquad (2)$$

$$z_j = z_{j-3} + \frac{3}{8}h\,(y_{j-3} + 3y_{j-2} + 3y_{j-1} + y_j) \qquad (3)$$

(Newton's 3/8 rule)

$$z_j = z_{j-5} + \frac{h}{3}(y_{j-5} + 3.875\,y_{j-4} + 2.625\,y_{j-3} + 2.625\,y_{j-2} + 3.875\,y_{j-1} + y_j) \qquad (4)$$

[combination of (2) and (3)]

Sometimes formula (2) is used in the following form:

$$z_j = z_{j+2} - \frac{h}{3}(y_j + 4\,y_{j+1} + y_{j+2}) \qquad (5)$$

Local truncation errors of formulas (1) . . . (4) are, respectively:

$$R_1 = \frac{1}{24}h^4\,y'''\ (\xi_1) \quad (\xi_1 \in [x_{j-1},\ x_{j+1}])$$

$$R_2 = -\frac{1}{90}h^5\,y''''\ (\xi_2) \quad (\xi_2 \in [x_{j-2},\ x_j])$$

$$R_3 = -\frac{3}{80}h^5\,y''''\ (\xi_3) \quad (\xi_3 \in [x_{j-3},\ x_j])$$

$$R_4 = -\frac{1}{144}h^5\,y''''\ (\xi_4) \quad (\xi_4 \in [x_{j-5},\ x_j])$$

However, these truncation errors may accumulate.

For reference see:

(1) F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 71-76.

(2) R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 214-221.


```
C                                                                       QSF  10
C  ...................................................................QSF  20
C                                                                       QSF  30
C     SUBROUTINE QSF                                                    QSF  40
C                                                                       QSF  50
C     PURPOSE                                                           QSF  60
C        TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN           QSF  70
C        EQUIDISTANT TABLE OF FUNCTION VALUES.                          QSF  80
C                                                                       QSF  90
C     USAGE                                                             QSF 100
C        CALL QSF (H,Y,Z,NDIM)                                          QSF 110
C                                                                       QSF 120
C     DESCRIPTION OF PARAMETERS                                         QSF 130
C        H      - THE INCREMENT OF ARGUMENT VALUES.                     QSF 140
C        Y      - THE INPUT VECTOR OF FUNCTION VALUES.                  QSF 150
C        Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE     QSF 160
C                 IDENTICAL WITH Y.                                     QSF 170
C        NDIM   - THE DIMENSION OF VECTORS Y AND Z.                     QSF 180
C                                                                       QSF 190
C     REMARKS                                                           QSF 200
C        NO ACTION IN CASE NDIM LESS THAN 3.                            QSF 210
C                                                                       QSF 220
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     QSF 230
C        NONE                                                           QSF 240
C                                                                       QSF 250
C     METHOD                                                            QSF 260
C        BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY       QSF 270
C        MEANS OF SIMPSONS RULE (TOGETHER WITH NEWTONS 3/8 RULE FOR A   QSF 280
C        COMBINATION OF THESE TWO RULES). TRUNCATION ERROR IS OF        QSF 290
C        ORDER H**5 (I.E. FOURTH ORDER METHOD). ONLY IN CASE NDIM=3     QSF 300
C        TRUNCATION ERROR OF Z(2) IS OF ORDER H**4.                     QSF 310
C        FOR REFERENCE, SEE                                             QSF 320
C        (1) F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,        QSF 330
C            MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.71-76.      QSF 340
C        (2) R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND      QSF 350
C            PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963,    QSF 360
C            PP.214-221.                                                QSF 370
C                                                                       QSF 380
C  ...................................................................QSF 390
C                                                                       QSF 400
      SUBROUTINE QSF(H,Y,Z,NDIM)                                        QSF 410
C                                                                       QSF 420
C                                                                       QSF 430
      DIMENSION Y(1),Z(1)                                               QSF 440
C                                                                       QSF 450
      HT=.33333334*H                                                    QSF 460
      IF(NDIM-5)17,6,1                                                  QSF 470
C                                                                       QSF 480
C     NDIM IS GREATER THAN 5. PREPARATIONS FOR INTEGRATION LOOP         QSF 490
    1 SUM1=Y(2)+Y(2)                                                    QSF 500
      SUM1=SUM1+SUM1                                                    QSF 510
      SUM1=HT*(Y(1)+SUM1+Y(3))                                          QSF 520
      ALX1=Y(4)+Y(4)                                                    QSF 530
      ALX1=ALX1+ALX1                                                    QSF 540
      ALX1=SUM1+HT*(Y(3)+ALX1+Y(5))                                     QSF 550
      ALX2=HT*(Y(1)+3.875*(Y(2)+Y(5))+2.625*(Y(3)+Y(4))+Y(6))           QSF 560
      SUM2=Y(5)+Y(5)                                                    QSF 570
      SUM2=SUM2+SUM2                                                    QSF 580
      SUM2=ALX2-HT*(Y(4)+SUM2+Y(6))                                     QSF 590
      Z(1)=0.                                                           QSF 600
      ALX=Y(3)+Y(3)                                                     QSF 610
      ALX=ALX+ALX                                                       QSF 620
      Z(2)=SUM2-HT*(Y(2)+ALX+Y(4))                                      QSF 630
      Z(3)=SUM1                                                         QSF 640
      Z(4)=SUM2                                                         QSF 650
      IF(NDIM-6)15,5,2                                                  QSF 660
C                                                                       QSF 670
C     INTEGRATION LOOP                                                  QSF 680
    2 DO 4 I=7,NDIM,2                                                   QSF 690
      SUM1=ALX1                                                         QSF 700
      SUM2=ALX2                                                         QSF 710
      ALX1=Y(I-1)+Y(I-1)                                                QSF 720
      ALX1=ALX1+ALX1                                                    QSF 730
      ALX1=SUM1+HT*(Y(I-2)+ALX1+Y(I))                                   QSF 740
      Z(I-2)=SUM1                                                       QSF 750
      IF(I-NDIM)3,4,4                                                   QSF 760
    3 ALX2=Y(I)+Y(I)                                                    QSF 770
      ALX2=ALX2+ALX2                                                    QSF 780
      ALX2=SUM2+HT*(Y(I-1)+ALX2+Y(I+1))                                 QSF 790
    4 Z(I-1)=SUM2                                                       QSF 800
    5 Z(NDIM-1)=ALX1                                                    QSF 810
      Z(NDIM)=ALX2                                                      QSF 820
      RETURN                                                            QSF 830
    6 Z(NDIM-1)=SUM2                                                    QSF 840
      Z(NDIM)=ALX1                                                      QSF 850
      RETURN                                                            QSF 860
C     END OF INTEGRATION LOOP                                           QSF 870
```

```
C                                                                       QSF  880
    7 IF(NDIM-3)12,11,8                                                 QSF  890
C                                                                       QSF  900
C     NDIM IS EQUAL TO 4 OR 5                                           QSF  910
    8 SUM2=1.12500*HT*(Y(1)+Y(2)+Y(2)+Y(2)+Y(3)+Y(3)+Y(3)+Y(4))         QSF  920
      SUM1=Y(2)+Y(2)                                                    QSF  930
      SUM1=SUM1+SUM1                                                    QSF  940
      SUM1=HT*(Y(1)+SUM1+Y(3))                                          QSF  950
      Z(1)=0.                                                           QSF  960
      AUX1=Y(3)+Y(3)                                                    QSF  970
      AUX1=AUX1+AUX1                                                    QSF  980
      Z(2)=SUM2-HT*(Y(2)+AUX1+Y(4))                                     QSF  990
      IF(NDIM-5)10,9,9                                                  QSF 1000
    9 AUX1=Y(4)+Y(4)                                                    QSF 1010
      AUX1=AUX1+AUX1                                                    QSF 1020
      Z(5)=SUM1+HT*(Y(3)+AUX1+Y(5))                                     QSF 1030
   10 Z(3)=SUM1                                                         QSF 1040
      Z(4)=SUM2                                                         QSF 1050
      RETURN                                                            QSF 1060
C                                                                       QSF 1070
C     NDIM IS EQUAL TO 3                                                QSF 1080
   11 SUM1=HT*(1.25*Y(1)+Y(2)+Y(2)-.25*Y(3))                            QSF 1090
      SUM2=Y(2)+Y(2)                                                    QSF 1100
      SUM2=SUM2+SUM2                                                    QSF 1110
      Z(3)=HT*(Y(1)+SUM2+Y(3))                                          QSF 1120
      Z(1)=0.                                                           QSF 1130
      Z(2)=SUM1                                                         QSF 1140
   12 RETURN                                                            QSF 1150
      END                                                               QSF 1160
```

```
      6 Z(NDIM-1)=SUM2                                                  DQSF 850
        Z(NDIM)=AUX1                                                    DQSF 860
        RETURN                                                          DQSF 870
C       END OF INTEGRATION LOOP                                         DQSF 880
C                                                                       DQSF 890
      7 IF(NDIM-3)12,11,8                                               DQSF 900
C                                                                       DQSF 910
C     NDIM IS EQUAL TO 4 OR 5                                           DQSF 920
      8 SUM2=1.12500*HT*(Y(1)+Y(2)+Y(2)+Y(2)+Y(3)+Y(3)+Y(3)+Y(4))       DQSF 930
        SUM1=Y(2)+Y(2)                                                  DQSF 940
        SUM1=SUM1+SUM1                                                  DQSF 950
        SUM1=HT*(Y(1)+SUM1+Y(3))                                        DQSF 960
        Z(1)=0.D0                                                       DQSF 970
        AUX1=Y(3)+Y(3)                                                  DQSF 980
        AUX1=AUX1+AUX1                                                  DQSF 990
        Z(2)=SUM2-HT*(Y(2)+AUX1+Y(4))                                   DQSF1000
        IF(NDIM-5)10,9,9                                                DQSF1010
      9 AUX1=Y(4)+Y(4)                                                  DQSF1020
        AUX1=AUX1+AUX1                                                  DQSF1030
        Z(5)=SUM1+HT*(Y(3)+AUX1+Y(5))                                   DQSF1040
     10 Z(3)=SUM1                                                       DQSF1050
        Z(4)=SUM2                                                       DQSF1060
        RETURN                                                          DQSF1070
C                                                                       DQSF1080
C     NDIM IS EQUAL TO 3                                                DQSF1090
     11 SUM1=HT*(1.2500*Y(1)+Y(2)+Y(2)-.2500*Y(3))                      DQSF1100
        SUM2=Y(2)+Y(2)                                                  DQSF1110
        SUM2=SUM2+SUM2                                                  DQSF1120
        Z(3)=HT*(Y(1)+SUM2+Y(3))                                        DQSF1130
        Z(1)=0.D0                                                       DQSF1140
        Z(2)=SUM1                                                       DQSF1150
     12 RETURN                                                          DQSF1160
        END                                                             DQSF1170
```

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C                                                                       DQSF  10
C     ..................................................................DQSF  20
C                                                                       DQSF  30
C        SUBROUTINE DQSF                                                DQSF  40
C                                                                       DQSF  50
C        PURPOSE                                                        DQSF  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DQSF  70
C           EQUIDISTANT TABLE OF FUNCTION VALUES.                       DQSF  80
C                                                                       DQSF  90
C        USAGE                                                          DQSF 100
C           CALL DQSF (H,Y,Z,NDIM)                                      DQSF 110
C                                                                       DQSF 120
C        DESCRIPTION OF PARAMETERS                                      DQSF 130
C           H       - DOUBLE PRECISION INCREMENT OF ARGUMENT VALUES.    DQSF 140
C           Y       - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES. DQSF 150
C           Z       - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL     DQSF 160
C                     VALUES. Z MAY BE IDENTICAL WITH Y.                DQSF 170
C           NDIM    - THE DIMENSION OF VECTORS Y AND Z.                 DQSF 180
C                                                                       DQSF 190
C        REMARKS                                                        DQSF 200
C           NO ACTION IN CASE NDIM LESS THAN 3.                         DQSF 210
C                                                                       DQSF 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQSF 230
C           NONE                                                        DQSF 240
C                                                                       DQSF 250
C        METHOD                                                         DQSF 260
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DQSF 270
C           MEANS OF SIMPSONS RULE TOGETHER WITH NEWTONS 3/8 RULE OR A  DQSF 280
C           COMBINATION OF THESE TWO RULES. TRUNCATION ERROR IS OF      DQSF 290
C           ORDER H**5 (I.E. FOURTH ORDER METHOD). ONLY IN CASE NDIM=3  DQSF 300
C           TRUNCATION ERROR OF Z(2) IS OF ORDER H**4.                  DQSF 310
C           FOR REFERENCE, SEE                                          DQSF 320
C           (1) F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,     DQSF 330
C               MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.71-76.   DQSF 340
C           (2) R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND   DQSF 350
C               PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963, DQSF 360
C               PP.214-221.                                             DQSF 370
C                                                                       DQSF 380
C     ..................................................................DQSF 390
C                                                                       DQSF 400
      SUBROUTINE DQSF(H,Y,Z,NDIM)                                       DQSF 410
C                                                                       DQSF 420
C                                                                       DQSF 430
      DIMENSION Y(1),Z(1)                                               DQSF 440
      DOUBLE PRECISION Y,Z,H,HT,SUM1,SUM2,AUX,AUX1,AUX2                 DQSF 450
C                                                                       DQSF 460
      HT=.33333333333333330D0*H                                         DQSF 470
      IF(NDIM-5)7,8,1                                                   DQSF 480
C                                                                       DQSF 490
C     NDIM IS GREATER THAN 5. PREPARATIONS OF INTEGRATION LOOP          DQSF 500
    1 SUM1=Y(2)+Y(2)                                                    DQSF 510
      SUM1=SUM1+SUM1                                                    DQSF 520
      SUM1=HT*(Y(1)+SUM1+Y(3))                                          DQSF 530
      AUX1=Y(4)+Y(4)                                                    DQSF 540
      AUX1=AUX1+AUX1                                                    DQSF 550
      AUX1=SUM1+HT*(Y(3)+AUX1+Y(5))                                     DQSF 560
      AUX2=HT*(Y(1)+3.875D0*(Y(2)+Y(5))+2.625D0*(Y(3)+Y(4))+Y(6))       DQSF 570
      SUM2=Y(5)+Y(5)                                                    DQSF 580
      SUM2=SUM2+SUM2                                                    DQSF 590
      SUM2=AUX2-HT*(Y(4)+SUM2+Y(6))                                     DQSF 600
      Z(1)=0.D0                                                         DQSF 610
      AUX=Y(3)+Y(3)                                                     DQSF 620
      AUX=AUX+AUX                                                       DQSF 630
      Z(2)=SUM2-HT*(Y(2)+AUX+Y(4))                                      DQSF 640
      Z(3)=SUM1                                                         DQSF 650
      Z(4)=SUM2                                                         DQSF 660
      IF(NDIM-6)5,5,2                                                   DQSF 670
C                                                                       DQSF 680
C     INTEGRATION LOOP                                                  DQSF 690
    2 DO 4 I=7,NDIM,2                                                   DQSF 700
      SUM1=AUX1                                                         DQSF 710
      SUM2=AUX2                                                         DQSF 720
      AUX1=Y(I-1)+Y(I-1)                                                DQSF 730
      AUX1=AUX1+AUX1                                                    DQSF 740
      AUX1=SUM1+HT*(Y(I-2)+AUX1+Y(I))                                   DQSF 750
      Z(I-2)=SUM1                                                       DQSF 760
      IF(I-NDIM)3,6,6                                                   DQSF 770
    3 AUX2=Y(I)+Y(I)                                                    DQSF 780
      AUX2=AUX2+AUX2                                                    DQSF 790
      AUX2=SUM2+HT*(Y(I-1)+AUX2+Y(I+1))                                 DQSF 800
    4 Z(I-1)=SUM2                                                       DQSF 810
    5 Z(NDIM-1)=AUX1                                                    DQSF 820
      Z(NDIM)=AUX2                                                      DQSF 830
      RETURN                                                            DQSF 840
```

Subroutines QHFG and DQHFG

These subroutines perform the integration of a monotonically tabulated function with first derivative by a Hermitian formula of first order. To compute the vector of integral values:

$$z_i = z(x_i) = \int_{x_1}^{x_i} y(x)\,dx \quad (i = 1, 2, \ldots, n)$$

for a given table x_i, y_i, y_i' $(i = 1, 2, \ldots, n)$ of monotonic arguments and their function and derivative values, a first-order Hermitian formula is used. It is assumed that the function to be integrated is continuous and can be differentiated at least four times. Starting with the integral value $z_1 = 0$, successive integral values z_i $(i = 2, 3, \ldots, n)$ are computed by means of the following formula:

$$z_i = z_{i-1} + \frac{x_i - z_{i-1}}{2}\left[y_{i-1} + y_i + \frac{x_i - x_{i-1}}{6}(y'_{i-1} - y'_i)\right]$$

$$(i = 2, 3, \ldots, n)$$

Local truncation error at each step is:

$$R_i = \frac{(x_i - x_{i-1})^5}{720} \cdot y^{(4)}(\xi_i) \quad (\xi_i \in [x_{i-1}, x_i])$$

However, these truncation errors may accumulate.

For reference see:

(1) F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 314-319.

(2) R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 227-230.

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C                                                                       QHFG  10
C     ..................................................................QHFG  20
C                                                                       QHFG  30
C        SUBROUTINE QHFG                                                QHFG  40
C                                                                       QHFG  50
C        PURPOSE                                                        QHFG  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        QHFG  70
C           GENERAL TABLE OF ARGUMENT, FUNCTION, AND DERIVATIVE VALUES. QHFG  80
C                                                                       QHFG  90
C        USAGE                                                          QHFG 100
C           CALL QHFG (X,Y,DERY,Z,NDIM)                                 QHFG 110
C                                                                       QHFG 120
C        DESCRIPTION OF PARAMETERS                                      QHFG 130
C           X      - THE INPUT VECTOR OF ARGUMENT VALUES.               QHFG 140
C           Y      - THE INPUT VECTOR OF FUNCTION VALUES.               QHFG 150
C           DERY   - THE INPUT VECTOR OF DERIVATIVE VALUES.             QHFG 160
C           Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE  QHFG 170
C                    IDENTICAL WITH X,Y OR DERY.                        QHFG 180
C           NDIM   - THE DIMENSION OF VECTORS X,Y,DERY,Z.               QHFG 190
C                                                                       QHFG 200
C        REMARKS                                                        QHFG 210
C           NO ACTION IN CASE NDIM LESS THAN 1.                         QHFG 220
C                                                                       QHFG 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QHFG 240
C           NONE                                                        QHFG 250
C                                                                       QHFG 260
C        METHOD                                                         QHFG 270
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    QHFG 280
C           MEANS OF HERMITEAN FOURTH ORDER INTEGRATION FORMULA.        QHFG 290
C           FOR REFERENCE, SEE                                          QHFG 300
C           (1) F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,     QHFG 310
C               MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.314-319. QHFG 320
C           (2) R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND   QHFG 330
C               PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963, QHFG 340
C               PP.227-230.                                             QHFG 350
C                                                                       QHFG 360
C     ..................................................................QHFG 370
C                                                                       QHFG 380
      SUBROUTINE QHFG(X,Y,DERY,Z,NDIM)                                  QHFG 390
C                                                                       QHFG 400
C                                                                       QHFG 410
      DIMENSION X(1),Y(1),DERY(1),Z(1)                                  QHFG 420
C                                                                       QHFG 430
      SUM2=0.                                                           QHFG 440
      IF(NDIM-1)4,3,1                                                   QHFG 450
C                                                                       QHFG 460
C     INTEGRATION LOOP                                                  QHFG 470
    1 DO 2 I=2,NDIM                                                     QHFG 480
      SUM1=SUM2                                                         QHFG 490
      SUM2=.5*(X(I)-X(I-1))                                             QHFG 500
      SUM2=SUM1+SUM2*((Y(I)+Y(I-1))+.3333333*SUM2*(DERY(I-1)-DERY(I)))  QHFG 510
    2 Z(I-1)=SUM1                                                       QHFG 520
    3 Z(NDIM)=SUM2                                                      QHFG 530
    4 RETURN                                                            QHFG 540
      END                                                               QHFG 550
```

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C                                                                       DQHG  10
C     ..................................................................DQHG  20
C                                                                       DQHG  30
C        SUBROUTINE DQHFG                                               DQHG  40
C                                                                       DQHG  50
C        PURPOSE                                                        DQHG  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DQHG  70
C           GENERAL TABLE OF ARGUMENT, FUNCTION, AND DERIVATIVE VALUES. DQHG  80
C                                                                       DQHG  90
C        USAGE                                                          DQHG 100
C           CALL DQHFG (X,Y,DERY,Z,NDIM)                                DQHG 110
C                                                                       DQHG 120
C        DESCRIPTION OF PARAMETERS                                      DQHG 130
C           X      - DOUBLE PRECISION INPUT VECTOR OF ARGUMENT VALUES.  DQHG 140
C           Y      - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES.  DQHG 150
C           DERY   - DOUBLE PRECISION INPUT VECTOR OF DERIVATIVE VALUES.DQHG 160
C           Z      - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL      DQHG 170
C                    VALUES. Z MAY BE IDENTICAL WITH X, Y OR DERY.      DQHG 180
C           NDIM   - THE DIMENSION OF VECTORS X,Y,DERY,Z.               DQHG 190
C                                                                       DQHG 200
C        REMARKS                                                        DQHG 210
C           NO ACTION IN CASE NDIM LESS THAN 1.                         DQHG 220
C                                                                       DQHG 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQHG 240
C           NONE                                                        DQHG 250
C                                                                       DQHG 260
C        METHOD                                                         DQHG 270
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DQHG 280
C           MEANS OF HERMITEAN FOURTH ORDER INTEGRATION FORMULA.        DQHG 290
C           FOR REFERENCE, SEE                                          DQHG 300
C           (1) F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,     DQHG 310
C               MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.314-319. DQHG 320
C           (2) R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND   DQHG 330
C               PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963, DQHG 340
C               PP.227-230.                                             DQHG 350
C                                                                       DQHG 360
C     ..................................................................DQHG 370
C                                                                       DQHG 380
      SUBROUTINE DQHFG(X,Y,DERY,Z,NDIM)                                 DQHG 390
C                                                                       DQHG 400
C                                                                       DQHG 410
      DIMENSION X(1),Y(1),DERY(1),Z(1)                                  DQHG 420
      DOUBLE PRECISION X,Y,DERY,Z,SUM1,SUM2                             DQHG 430
C                                                                       DQHG 440
      SUM2=0.D0                                                         DQHG 450
      IF(NDIM-1)4,3,1                                                   DQHG 460
C                                                                       DQHG 470
C     INTEGRATION LOOP                                                  DQHG 480
    1 DO 2 I=2,NDIM                                                     DQHG 490
      SUM1=SUM2                                                         DQHG 500
      SUM2=.5D0*(X(I)-X(I-1))                                           DQHG 510
      SUM2=SUM1+SUM2*((Y(I)+Y(I-1))+.3333333333333333D0*SUM2*           DQHG 520
     1(DERY(I-1)-DERY(I)))                                              DQHG 530
    2 Z(I-1)=SUM1                                                       DQHG 540
    3 Z(NDIM)=SUM2                                                      DQHG 550
    4 RETURN                                                            DQHG 560
      END                                                               DQHG 570
```

Subroutines QHFE and DQHFE

These subroutines perform the integration of an equidistantly tabulated function with first derivative by a Hermitian formula of first order. To compute the vector of integral values:

$$z_i = z(x_i) = \int_a^{x_i} y(x)\,dx \Bigg\} (i = 1, 2, \ldots, n)$$

with $x_i = a + (i-1)\,h$

for a table of function and first derivative values y_i, y_i' $(i = 1, 2, \ldots, n)$, given at equidistant points $x_i = a + (i - 1)\,h$, a first-order Hermitian formula is used. It is assumed that the function to be integrated is continuous and can be differentiated at least four times. Starting with the integral value $z_1 = 0$, successive integral values z_i $(i = 2, 3, \ldots, n)$ are computed by means of the following formula:

$$z_i = z_{i-1} + \frac{h}{2}\cdot\left[y_{i-1} + y_i + \frac{h}{6}\,(y'_{i-1} - y'_i)\right]$$

$$(i = 1, 2, \ldots, n)$$

with a given increment h of argument values.

As the local truncation error at each step is:

$$R_i = \frac{h^5}{720}\cdot y^{(4)}(\xi_i) \quad (\xi_i \in [\,x_{i-1},\, x_i\,])$$

the global truncation error R in z_n appears as follows:

$$R = \frac{1}{720}\,(n-1)\,h^5\,y^{(4)}(\xi) \quad (\xi \in [x_1,\, x_n\,])$$

or

$$R = \frac{\ell}{720}\,h^4\,y^{(4)}(\xi)$$

where ℓ is the length of the whole integration interval.

For reference see:

(1) F.B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 314-319.

(2) R. Zurmühl, Praktische Mathematik für Ingenieure and Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 227-230.

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C                                                                       QHFE  10
C     ...................................................................QHFE  20
C                                                                       QHFE  30
C        SUBROUTINE QHFE                                                QHFE  40
C                                                                       QHFE  50
C        PURPOSE                                                        QHFE  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        QHFE  70
C           EQUIDISTANT TABLE OF FUNCTION AND DERIVATIVE VALUES.        QHFE  80
C                                                                       QHFE  90
C        USAGE                                                          QHFE 100
C           CALL QHFE (H,Y,DERY,Z,NDIM)                                 QHFE 110
C                                                                       QHFE 120
C        DESCRIPTION OF PARAMETERS                                      QHFE 130
C           H      - THE INCREMENT OF ARGUMENT VALUES.                  QHFE 140
C           Y      - THE INPUT VECTOR OF FUNCTION VALUES.               QHFE 150
C           DERY   - THE INPUT VECTOR OF DERIVATIVE VALUES.             QHFE 160
C           Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE  QHFE 170
C                    IDENTICAL WITH Y OR DERY.                          QHFE 180
C           NDIM   - THE DIMENSION OF VECTORS Y,DERY,Z.                 QHFE 190
C                                                                       QHFE 200
C        REMARKS                                                        QHFE 210
C           NO ACTION IN CASE NDIM LESS THAN 1.                         QHFE 220
C                                                                       QHFE 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QHFE 240
C           NONE                                                        QHFE 250
C                                                                       QHFE 260
C        METHOD                                                         QHFE 270
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    QHFE 280
C           MEANS OF HERMITEAN FOURTH ORDER INTEGRATION FORMULA.        QHFE 290
C           FOR REFERENCE, SEE                                          QHFE 300
C           (1) F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,     QHFE 310
C               MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.314-319. QHFE 320
C           (2) R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND   QHFE 330
C               PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963, QHFE 340
C               PP.227-230.                                             QHFE 350
C                                                                       QHFE 360
C     ...................................................................QHFE 370
C                                                                       QHFE 380
      SUBROUTINE QHFE(H,Y,DERY,Z,NDIM)                                  QHFE 390
C                                                                       QHFE 400
C                                                                       QHFE 410
      DIMENSION Y(1),DERY(1),Z(1)                                       QHFE 420
C                                                                       QHFE 430
      SUM2=0.                                                           QHFE 440
      IF(NDIM-1)4,3,1                                                   QHFE 450
    1 HH=.5*H                                                           QHFE 460
      HS=.1666667*H                                                     QHFE 470
C                                                                       QHFE 480
C     INTEGRATION LOOP                                                  QHFE 490
      DO 2 I=2,NDIM                                                     QHFE 500
      SUM1=SUM2                                                         QHFE 510
      SUM2=SUM2+HH*((Y(I)+Y(I-1))+HS*(DERY(I-1)-DERY(I)))               QHFE 520
    2 Z(I-1)=SUM1                                                       QHFE 530
    3 Z(NDIM)=SUM2                                                      QHFE 540
    4 RETURN                                                            QHFE 550
      END                                                               QHFE 560
```

```
C                                                                       DQHE  10
C     ...................................................................DQHE  20
C                                                                       DQHE  30
C        SUBROUTINE DQHFE                                               DQHE  40
C                                                                       DQHE  50
C        PURPOSE                                                        DQHE  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DQHE  70
C           EQUIDISTANT TABLE OF FUNCTION AND DERIVATIVE VALUES.        DQHE  80
C                                                                       DQHE  90
C        USAGE                                                          DQHE 100
C           CALL DQHFE (H,Y,DERY,Z,NDIM)                                DQHE 110
C                                                                       DQHE 120
C        DESCRIPTION OF PARAMETERS                                      DQHE 130
C           H      - DOUBLE PRECISION INCREMENT OF ARGUMENT VALUES.     DQHE 140
C           Y      - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES.  DQHE 150
C           DERY   - DOUBLE PRECISION INPUT VECTOR OF DERIVATIVE VALUES.DQHE 160
C           Z      - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL      DQHE 170
C                    VALUES. Z MAY BE IDENTICAL WITH Y OR DERY.         DQHE 180
C           NDIM   - THE DIMENSION OF VECTORS Y,DERY,Z.                 DQHE 190
C                                                                       DQHE 200
C        REMARKS                                                        DQHE 210
C           NO ACTION IN CASE NDIM LESS THAN 1.                         DQHE 220
C                                                                       DQHE 230
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQHE 240
C           NONE                                                        DQHE 250
C                                                                       DQHE 260
C        METHOD                                                         DQHE 270
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DQHE 280
C           MEANS OF HERMITEAN FOURTH ORDER INTEGRATION FORMULA.        DQHE 290
C           FOR REFERENCE, SEE                                          DQHE 300
C           (1) F.B.HILDEBRAND, INTRODUCTION TO NUMERICAL ANALYSIS,     DQHE 310
C               MCGRAW-HILL, NEW YORK/TORONTO/LONDON, 1956, PP.314-319. DQHE 320
C           (2) R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND   DQHE 330
C               PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963, DQHE 340
C               PP.227-230.                                             DQHE 350
C                                                                       DQHE 360
C     ...................................................................DQHE 370
C                                                                       DQHE 380
      SUBROUTINE DQHFE(H,Y,DERY,Z,NDIM)                                 DQHE 390
C                                                                       DQHE 400
C                                                                       DQHE 410
      DIMENSION Y(1),DERY(1),Z(1)                                       DQHE 420
      DOUBLE PRECISION Y,DERY,Z,H,HH,HS,SUM1,SUM2                       DQHE 430
C                                                                       DQHE 440
      SUM2=0.D0                                                         DQHE 450
      IF(NDIM-1)4,3,1                                                   DQHE 460
    1 HH=.5D0*H                                                         DQHE 470
      HS=.16666666666666700*H                                           DQHE 480
C                                                                       DQHE 490
C     INTEGRATION LOOP                                                  DQHE 500
      DO 2 I=2,NDIM                                                     DQHE 510
      SUM1=SUM2                                                         DQHE 520
      SUM2=SUM2+HH*((Y(I)+Y(I-1))+HS*(DERY(I-1)-DERY(I)))               DQHE 530
    2 Z(I-1)=SUM1                                                       DQHE 540
    3 Z(NDIM)=SUM2                                                      DQHE 550
    4 RETURN                                                            DQHE 560
      END                                                               DQHE 570
```

Subroutines QHSG and DQHSG

These subroutines perform the integration of a monotonically tabulated function with first and second derivatives by a Hermitian formula of second order. To compute the vector of integral values:

$$z_i = z(x_i) = \int_{x_1}^{x_i} y(x)\,dx \quad (i = 1,2,\ldots,n)$$

for a given table x_i, y_i, y_i', y_i'' $(i=1,2,\ldots,n)$ of monotonic arguments and their function and first and second derivative values, a second-order Hermitian formula is used. It is assumed that the function to be integrated is continuous and can be differentiated at least six times. Starting with the integral value $z_1 = 0$, successive integral values z_i $(i = 2,3,\ldots,n)$ are computed by means of the following formula:

$$z_i = z_{i-1} + \frac{x_i - x_{i-1}}{2}\left\{y_{i-1} + y_i + \frac{x_i - x_{i-1}}{5}\left[y'_{i-1} - y'_i + \frac{x_i - x_{i-1}}{12}\,(y''_{i-1} + y''_i)\right]\right\} \quad (i=2,3,\ldots,n)$$

Local truncation error at each step is:

$$R_i = -\frac{(x_i - x_{i-1})^7}{100\ 800}\,y^{(6)}(\xi_i) \quad (\xi_i \in [x_{i-1}\ \ x_i])$$

However, these truncation errors may accumulate.

For reference see R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 227-230.

```
C                                                                       QHSG  10
C     ...................................................................QHSG  20
C                                                                       QHSG  30
C        SUBROUTINE QHSG                                                QHSG  40
C                                                                       QHSG  50
C        PURPOSE                                                        QHSG  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        QHSG  70
C           GENERAL TABLE OF ARGUMENT, FUNCTION, FIRST DERIVATIVE,      QHSG  80
C           AND SECOND DERIVATIVE VALUES.                               QHSG  90
C                                                                       QHSG 100
C        USAGE                                                          QHSG 110
C           CALL QHSG (X,Y,FDY,SDY,Z,NDIM)                              QHSG 120
C                                                                       QHSG 130
C        DESCRIPTION OF PARAMETERS                                      QHSG 140
C           X      - THE INPUT VECTOR OF ARGUMENT VALUES.               QHSG 150
C           Y      - THE INPUT VECTOR OF FUNCTION VALUES.               QHSG 160
C           FDY    - THE INPUT VECTOR OF FIRST DERIVATIVE.              QHSG 170
C           SDY    - THE INPUT VECTOR OF SECOND DERIVATIVE.             QHSG 180
C           Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE  QHSG 190
C                    IDENTICAL WITH X,Y,FDY OR SDY.                     QHSG 200
C           NDIM   - THE DIMENSION OF VECTORS X,Y,FDY,SDY,Z.            QHSG 210
C                                                                       QHSG 220
C        REMARKS                                                        QHSG 230
C           NO ACTION IN CASE NDIM LESS THAN 1.                         QHSG 240
C                                                                       QHSG 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QHSG 260
C           NONE                                                        QHSG 270
C                                                                       QHSG 280
C        METHOD                                                         QHSG 290
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    QHSG 300
C           MEANS OF HERMITEAN SIXTH ORDER INTEGRATION FORMULA.         QHSG 310
C           FOR REFERENCE, SEE                                          QHSG 320
C           R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND       QHSG 330
C           PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963,     QHSG 340
C           PP.227-230.                                                 QHSG 350
C                                                                       QHSG 360
C     ...................................................................QHSG 370
C                                                                       QHSG 380
      SUBROUTINE QHSG(X,Y,FDY,SDY,Z,NDIM)                               QHSG 390
C                                                                       QHSG 400
C                                                                       QHSG 410
      DIMENSION X(1),Y(1),FDY(1),SDY(1),Z(1)                            QHSG 420
C                                                                       QHSG 430
      SUM2=0.                                                           QHSG 440
      IF(NDIM-1)4,3,1                                                   QHSG 450
C                                                                       QHSG 460
C     INTEGRATION LOOP                                                  QHSG 470
    1 DO 2 I=2,NDIM                                                     QHSG 480
      SUM1=SUM2                                                         QHSG 490
      SUM2=.5*(X(I)-X(I-1))                                             QHSG 500
     OSUM2=SUM1+SUM2*((Y(I-1)+Y(I))+.4*SUM2*((FDY(I-1)-FDY(I))+         QHSG 510
     1     .166666 7*SUM2*(SDY(I-1)+SDY(I))))                           QHSG 520
    2 Z(I-1)=SUM1                                                       QHSG 530
    3 Z(NDIM)=SUM2                                                      QHSG 540
    4 RETURN                                                            QHSG 550
      END                                                               QHSG 560
```

```
C                                                                       DHSG  10
C     ...................................................................DHSG  20
C                                                                       DHSG  30
C        SUBROUTINE DQHSG                                               DHSG  40
C                                                                       DHSG  50
C        PURPOSE                                                        DHSG  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DHSG  70
C           GENERAL TABLE OF ARGUMENT, FUNCTION, FIRST DERIVATIVE,      DHSG  80
C           AND SECOND DERIVATIVE VALUES.                               DHSG  90
C                                                                       DHSG 100
C        USAGE                                                          DHSG 110
C           CALL DQHSG (X,Y,FDY,SDY,Z,NDIM)                             DHSG 120
C                                                                       DHSG 130
C        DESCRIPTION OF PARAMETERS                                      DHSG 140
C           X      - DOUBLE PRECISION INPUT VECTOR OF ARGUMENT VALUES.  DHSG 150
C           Y      - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES.  DHSG 160
C           FDY    - DOUBLE PRECISION INPUT VECTOR OF FIRST DERIVATIVE. DHSG 170
C           SDY    - DOUBLE PRECISION INPUT VECTOR OF SECOND DERIVATIVE.DHSG 180
C           Z      - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL      DHSG 190
C                    VALUES. Z MAY BE IDENTICAL WITH X, Y, FDY OR SDY.  DHSG 200
C           NDIM   - THE DIMENSION OF VECTORS X,Y,FDY,SDY,Z.            DHSG 210
C                                                                       DHSG 220
C        REMARKS                                                        DHSG 230
C           NO ACTION IN CASE NDIM LESS THAN 1.                         DHSG 240
C                                                                       DHSG 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DHSG 260
C           NONE                                                        DHSG 270
C                                                                       DHSG 280
C        METHOD                                                         DHSG 290
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DHSG 300
C           MEANS OF HERMITEAN SIXTH ORDER INTEGRATION FORMULA.         DHSG 310
C           FOR REFERENCE, SEE                                          DHSG 320
C           R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND       DHSG 330
C           PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963,     DHSG 340
C           PP.227-230.                                                 DHSG 350
C                                                                       DHSG 360
C     ...................................................................DHSG 370
C                                                                       DHSG 380
      SUBROUTINE DQHSG(X,Y,FDY,SDY,Z,NDIM)                              DHSG 390
C                                                                       DHSG 400
C                                                                       DHSG 410
      DIMENSION X(1),Y(1),FDY(1),SDY(1),Z(1)                            DHSG 420
      DOUBLE PRECISION X,Y,FDY,SDY,Z,SUM1,SUM2                          DHSG 430
C                                                                       DHSG 440
      SUM2=0.D0                                                         DHSG 450
      IF(NDIM-1)4,3,1                                                   DHSG 460
C                                                                       DHSG 470
C     INTEGRATION LOOP                                                  DHSG 480
    1 DO 2 I=2,NDIM                                                     DHSG 490
      SUM1=SUM2                                                         DHSG 500
      SUM2=.5D0*(X(I)-X(I-1))                                           DHSG 510
     OSUM2=SUM1+SUM2*((Y(I-1)+Y(I))+.4D0*SUM2*((FDY(I-1)-FDY(I))+       DHSG 520
     1     .16666666666666667D0*SUM2*(SDY(I-1)+SDY(I))))                DHSG 530
    2 Z(I-1)=SUM1                                                       DHSG 540
    3 Z(NDIM)=SUM2                                                      DHSG 550
    4 RETURN                                                            DHSG 560
      END                                                               DHSG 570
```

Subroutines QHSE and DQHSE

These subroutines perform the integration of an equidistantly tabulated function with first and second derivatives by a Hermitian formula of second order.

To compute the vector of integral values:

$$\left.\begin{aligned} z_i = z(x_i) &= \int_a^{x_i} y(x)\,dx \\ \text{with } x_i &= a + (i-1)\,h \end{aligned}\right\} (i = 1,2,\ldots,n)$$

for a table of function and first and second derivative values y_i, y'_i, y''_i $(i = 1,2,\ldots,n)$, given at equidistant points $x_i = a + (i-1)\,h$, a second-order Hermitian formula is used. It is assumed that the function to be integrated is continuous and can be differentiated at least six times. Starting with the integral value $z_1 = 0$, successive integral values z_i $(i = 2,3,\ldots,n)$ are computed by means of the following formula:

$$z_i = z_{i-1} + \frac{h}{2}\left\{y_{i-1} + y_i + \frac{h}{5}\left[y'_{i-1} - y'_i + \frac{h}{12}\left(y''_{i-1} + y''_i\right)\right]\right\} \quad (i=2,3,\ldots,n)$$

with a given increment h of argument values.

As the local truncation error at each step is:

$$R_i = -\frac{h^7}{100\,800}\,y^{(6)}(\xi_i) \quad (\xi_i \in [x_{i-1}, x_i]),$$

the global truncation error R in z_n appears as follows:

$$R = -\frac{1}{100\,800}\,(n-1)\,h^7\,y^{(6)}(\xi) \quad (\xi \in [x_1, xn])$$

or

$$R = -\frac{\ell}{100\,800}\,h^6\,y^{(6)}(\xi)$$

where ℓ is the length of the whole integration interval.

For reference see R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker. Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 227-230.

```
C                                                                       QHSE  10
C     ...................................................................QHSE  20
C                                                                       QHSE  30
C        SUBROUTINE QHSE                                                QHSE  40
C                                                                       QHSE  50
C        PURPOSE                                                        QHSE  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        QHSE  70
C           EQUIDISTANT TABLE OF FUNCTION, FIRST DERIVATIVE,            QHSE  80
C           AND SECOND DERIVATIVE VALUES.                               QHSE  90
C                                                                       QHSE 100
C        USAGE                                                          QHSE 110
C           CALL QHSE (H,Y,FDY,SDY,Z,NDIM)                              QHSE 120
C                                                                       QHSE 130
C        DESCRIPTION OF PARAMETERS                                      QHSE 140
C           H      - THE INCREMENT OF ARGUMENT VALUES.                  QHSE 150
C           Y      - THE INPUT VECTOR OF FUNCTION VALUES.               QHSE 160
C           FDY    - THE INPUT VECTOR OF FIRST DERIVATIVE.              QHSE 170
C           SDY    - THE INPUT VECTOR OF SECOND DERIVATIVE.             QHSE 180
C           Z      - THE RESULTING VECTOR OF INTEGRAL VALUES. Z MAY BE  QHSE 190
C                    IDENTICAL WITH Y,FDY OR SDY.                       QHSE 200
C           NDIM   - THE DIMENSION OF VECTORS Y,FDY,SDY,Z.              QHSE 210
C                                                                       QHSE 220
C        REMARKS                                                        QHSE 230
C           NO ACTION IN CASE NDIM LESS THAN 1.                         QHSE 240
C                                                                       QHSE 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QHSE 260
C           NONE                                                        QHSE 270
C                                                                       QHSE 280
C        METHOD                                                         QHSE 290
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    QHSE 300
C           MEANS OF HERMITEAN SIXTH ORDER INTEGRATION FORMULA.         QHSE 310
C           FOR REFERENCE, SEE                                          QHSE 320
C           R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND       QHSE 330
C           PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963,     QHSE 340
C           PP.227-230.                                                 QHSE 350
C                                                                       QHSE 360
C     ...................................................................QHSE 370
C                                                                       QHSE 380
      SUBROUTINE QHSE(H,Y,FDY,SDY,Z,NDIM)                               QHSE 390
C                                                                       QHSE 400
C                                                                       QHSE 410
      DIMENSION Y(1),FDY(1),SDY(1),Z(1)                                 QHSE 420
C                                                                       QHSE 430
      SUM2=0.                                                           QHSE 440
      IF(NDIM-1)4,3,1                                                   QHSE 450
    1 HH=.5*H                                                           QHSE 460
      HF=.2*H                                                           QHSE 470
      HT=.08333333*H                                                    QHSE 480
C                                                                       QHSE 490
C     INTEGRATION LOOP                                                  QHSE 500
      DO 2 I=2,NDIM                                                     QHSE 510
      SUM1=SUM2                                                         QHSE 520
      SUM2=SUM2+HH*((Y(I-1)+Y(I))+HF*((FDY(I-1)-FDY(I))+                QHSE 530
     1            HT*(SDY(I-1)+SDY(I))))                                QHSE 540
    2 Z(I-1)=SUM1                                                       QHSE 550
    3 Z(NDIM)=SUM2                                                      QHSE 560
    4 RETURN                                                            QHSE 570
      END                                                               QHSE 580
```

```
C                                                                       DQHS  10
C     ...................................................................DQHS  20
C                                                                       DQHS  30
C        SUBROUTINE DQHSE                                               DQHS  40
C                                                                       DQHS  50
C        PURPOSE                                                        DQHS  60
C           TO COMPUTE THE VECTOR OF INTEGRAL VALUES FOR A GIVEN        DQHS  70
C           EQUIDISTANT TABLE OF FUNCTION, FIRST DERIVATIVE,            DQHS  80
C           AND SECOND DERIVATIVE VALUES.                               DQHS  90
C                                                                       DQHS 100
C        USAGE                                                          DQHS 110
C           CALL DQHSE (H,Y,FDY,SDY,Z,NDIM)                             DQHS 120
C                                                                       DQHS 130
C        DESCRIPTION OF PARAMETERS                                      DQHS 140
C           H      - DOUBLE PRECISION INCREMENT OF ARGUMENT VALUES.     DQHS 150
C           Y      - DOUBLE PRECISION INPUT VECTOR OF FUNCTION VALUES.  DQHS 160
C           FDY    - DOUBLE PRECISION INPUT VECTOR OF FIRST DERIVATIVE. DQHS 170
C           SDY    - DOUBLE PRECISION INPUT VECTOR OF SECOND DERIVATIVE.DQHS 180
C           Z      - RESULTING DOUBLE PRECISION VECTOR OF INTEGRAL      DQHS 190
C                    VALUES. Z MAY BE IDENTICAL WITH Y, FDY OR SDY.     DQHS 200
C           NDIM   - THE DIMENSION OF VECTORS Y,FDY,SDY,Z.              DQHS 210
C                                                                       DQHS 220
C        REMARKS                                                        DQHS 230
C           NO ACTION IN CASE NDIM LESS THAN 1.                         DQHS 240
C                                                                       DQHS 250
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQHS 260
C           NONE                                                        DQHS 270
C                                                                       DQHS 280
C        METHOD                                                         DQHS 290
C           BEGINNING WITH Z(1)=0, EVALUATION OF VECTOR Z IS DONE BY    DQHS 300
C           MEANS OF HERMITEAN SIXTH ORDER INTEGRATION FORMULA.         DQHS 310
C           FOR REFERENCE, SEE                                          DQHS 320
C           R.ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND       DQHS 330
C           PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963,     DQHS 340
C           PP.227-230.                                                 DQHS 350
C                                                                       DQHS 360
C     ...................................................................DQHS 370
C                                                                       DQHS 380
      SUBROUTINE DQHSE(H,Y,FDY,SDY,Z,NDIM)                              DQHS 390
C                                                                       DQHS 400
C                                                                       DQHS 410
      DIMENSION Y(1),FDY(1),SDY(1),Z(1)                                 DQHS 420
      DOUBLE PRECISION Y,FDY,SDY,Z,H,HH,HF,HT,SUM1,SUM2                 DQHS 430
C                                                                       DQHS 440
      SUM2=0.D0                                                         DQHS 450
      IF(NDIM-1)4,3,1                                                   DQHS 460
    1 HH=.500*H                                                         DQHS 470
      HF=.200*H                                                         DQHS 480
      HT=.08333333333333333D0*H                                         DQHS 490
C                                                                       DQHS 500
C     INTEGRATION LOOP                                                  DQHS 510
      DO 2 I=2,NDIM                                                     DQHS 520
      SUM1=SUM2                                                         DQHS 530
      SUM2=SUM2+HH*((Y(I-1)+Y(I))+HF*((FDY(I-1)-FDY(I))+                DQHS 540
     1            HT*(SDY(I-1)+SDY(I))))                                DQHS 550
    2 Z(I-1)=SUM1                                                       DQHS 560
    3 Z(NDIM)=SUM2                                                      DQHS 570
    4 RETURN                                                            DQHS 580
      END                                                               DQHS 590
```

Subroutines QATR and DQATR

These subroutines perform the integration of a given function by the trapezoidal rule together with Romberg's extrapolation method in order to compute an approximation for:

$$y = \int_a^b f(x)\,dx \qquad (1)$$

Successively dividing the interval $[a,b]$ into 2^i equidistant subintervals ($i = 0,1,2,\ldots$) and using the following notations:

$$h_i = \frac{b-a}{2^i}\ ;\ x_{i,k} = a + k \cdot h_i,\ f_{i,k} = f(x_{i,k})$$

$$(k = 0,1,2,\ldots,2^i)$$

the trapezoidal rule gives approximations $T_{o,i}$ to the integral value y:

$$T_{o,i} = h_i\left\{\sum_{k=0}^{2^i} f_{i,k} - \frac{1}{2}(f(a) + f(b))\right\} \qquad (2)$$

Then the following can be written:

$$T_{o,i} = y + \sum_{r=1}^{\infty} C_{o,2r} \cdot h_i^{2r}$$

with unknown coefficients $C_{o,2r}$ which do not depend on i. Thus there is a truncation error of the order h_i^2.

Knowing two successive approximations, $T_{o,i}$ and $T_{o,i+1}$, an extrapolated value can be generated:

$$T_{1,i} = T_{o,\,i+1} + \frac{T_{o,i+1} - T_{o,i}}{2^2 - 1} \qquad (3)$$

This is a better approximation to y because:

$$T_{1,i} = y + \frac{1}{2^2-1}\sum_{r=1}^{\infty} C_{o,2r}\,(2^2 h_{i+1}^{2r} - h_i^{2r})$$

Noting that $2^2 h_{i+1}^2 - h_i^2 = 0$ and setting:

$$C_{1,2r} = \frac{1}{2^2-1}\,(2^2 - 2^{2r}) \cdot C_{o,2r}$$

$T_{1,i}$ becomes:

$$T_{1,i} = y + \sum_{r=2}^{\infty} C_{1,2r}\, h_{i+1}^{2r}$$

This gives a truncation error of the order h_{i+1}^4.

Knowing $T_{o,\,i+2}$ also, $T_{1,\,i+1}$ can be generated (formula 3), and:

$$T_{2,i} = T_{1,\,i+1} + \frac{T_{1,i+1} - T_{1,i}}{2^4 - 1} \qquad (4)$$

Thus:

$$T_{2,i} = y + \sum_{r=3}^{\infty} C_{2,2r} \cdot h_{i+2}^{2r}$$

with $C_{2,2r} = \frac{1}{2^4-1}\,(2^4 - 2^{2r})\,C_{1,2r}$

with a truncation error of the order h_{i+2}^6. Observe that the order of truncation error increases by 2 at each new extrapolation step.

The subroutine uses the scheme shown in Figure 25 for computation of T-values and generates the upward diagonal in the one-dimensional storage array AUX, using the general formula:

$$T_{k,j} = T_{k-1,j+1} + \frac{T_{k-1,j+1} - T_{k-1,j}}{2^{2k}-1} \quad (k+j=i,$$

$$j = i-1, i-2, \ldots, 2, 1, 0) \qquad (5)$$

and storing:

$T_{o,i}$ into AUX (i+1)

$T_{1,i-1}$ into AUX (i)

....

$T_{k,0}$ into AUX (1)

Truncation error		$O(h_i^2)$	$O(h_i^4)$	$O(h_i^6)$	$O(h_i^8)\ldots$
step length h_i	i \ j	0	1	2	3 ...
b-a	0	$T_{o,0}$	$T_{1,0}$	$T_{2,0}$	$T_{3,0}$ ...
$\frac{b-a}{2}$	1	$T_{o,1}$	$T_{1,1}$	$T_{2,1}$	⋮
$\frac{b-a}{4}$	2	$T_{o,2}$	$T_{1,2}$	⋮	
$\frac{b-a}{8}$	3	$T_{o,3}$	⋮		
⋮	⋮	⋮			

Figure 25. Computation of T-values (QATR)

The procedure stops if the difference between two successive values of AUX (1) is less than a given tolerance, or if the values of AUX (1) start oscillating, thus showing the influence of rounding errors.

For reference see S. Filippi, "Das Verfahren von Romberg-Stiefel-Bauer als Spezialfall des allgemeinen Prinzips von Richardson", Mathematik-Technik-Wirtschaft, vol. 11, iss. 2 (1964), pp. 49 - 54.

```
C                                                                       QATR  10
C     ..................................................................QATR  20
C                                                                       QATR  30
C        SUBROUTINE QATR                                                QATR  40
C                                                                       QATR  50
C        PURPOSE                                                        QATR  60
C           TO COMPUTE AN APPROXIMATION FOR INTEGRAL(FCT(X), SUMMED     QATR  70
C           OVER X FROM XL TO XU).                                      QATR  80
C                                                                       QATR  90
C        USAGE                                                          QATR 100
C           CALL QATR (XL,XU,EPS,NDIM,FCT,Y,IER,AUX)                    QATR 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               QATR 120
C                                                                       QATR 130
C        DESCRIPTION OF PARAMETERS                                      QATR 140
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QATR 150
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QATR 160
C           EPS     - THE UPPER BOUND OF THE ABSOLUTE ERROR.            QATR 170
C           NDIM    - THE DIMENSION OF THE AUXILIARY STORAGE ARRAY AUX. QATR 180
C                     NDIM-1 IS THE MAXIMAL NUMBER OF BISECTIONS OF     QATR 190
C                     THE INTERVAL (XL,XU).                             QATR 200
C           FCT     - THE NAME OF THE EXTERNAL FUNCTION SUBPROGRAM USED. QATR 210
C           Y       - THE RESULTING APPROXIMATION FOR THE INTEGRAL VALUE.QATR 220
C           IER     - A RESULTING ERROR PARAMETER.                      QATR 230
C           AUX     - AN AUXILIARY STORAGE ARRAY WITH DIMENSION NDIM.   QATR 240
C                                                                       QATR 250
C        REMARKS                                                        QATR 260
C           ERROR PARAMETER IER IS CODED IN THE FOLLOWING FORM          QATR 270
C           IER=0  - IT WAS POSSIBLE TO REACH THE REQUIRED ACCURACY.    QATR 280
C                    NO ERROR.                                          QATR 290
C           IER=1  - IT IS IMPOSSIBLE TO REACH THE REQUIRED ACCURACY    QATR 300
C                    BECAUSE OF ROUNDING ERRORS.                        QATR 310
C           IER=2  - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE NDIM   QATR 320
C                    IS LESS THAN 5, OR THE REQUIRED ACCURACY COULD NOT QATR 330
C                    BE REACHED WITHIN NDIM-1 STEPS. NDIM SHOULD BE     QATR 340
C                    INCREASED.                                         QATR 350
C                                                                       QATR 360
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QATR 370
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE CODED BY    QATR 380
C           THE USER. ITS ARGUMENT X SHOULD NOT BE DESTROYED.           QATR 390
C                                                                       QATR 400
C        METHOD                                                         QATR 410
C           EVALUATION OF Y IS DONE BY MEANS OF TRAPEZOIDAL RULE IN     QATR 420
C           CONNECTION WITH ROMBERGS PRINCIPLE. ON RETURN Y CONTAINS    QATR 430
C           THE BEST POSSIBLE APPROXIMATION OF THE INTEGRAL VALUE AND   QATR 440
C           VECTOR AUX THE UPWARD DIAGONAL OF ROMBERG SCHEME.           QATR 450
C           COMPONENTS AUX(I) (I=1,2,...,IEND, WITH IEND LESS THAN OR   QATR 460
C           EQUAL TO NDIM) BECOME APPROXIMATIONS TO INTEGRAL VALUE WITH QATR 470
C           DECREASING ACCURACY BY MULTIPLICATION WITH (XU-XL).         QATR 480
C           FOR REFERENCE, SEE                                          QATR 490
C           (1) FILIPPI, DAS VERFAHREN VON ROMBERG-STIEFEL-BAUER ALS    QATR 500
C               SPEZIALFALL DES ALLGEMEINEN PRINZIPS VON RICHARDSON,    QATR 510
C               MATHEMATIK-TECHNIK-WIRTSCHAFT, VOL.11, ISS.2 (1964),    QATR 520
C               PP.49-54.                                               QATR 530
C           (2) BAUER, ALGORITHM 60, CACM, VOL.4, ISS.6 (1961), PP.255. QATR 540
C                                                                       QATR 550
C     ..................................................................QATR 560
C                                                                       QATR 570
      SUBROUTINE QATR(XL,XU,EPS,NDIM,FCT,Y,IER,AUX)                     QATR 580
C                                                                       QATR 590
C                                                                       QATR 600
      DIMENSION AUX(1)                                                  QATR 610
C                                                                       QATR 620
C     PREPARATIONS OF ROMBERG-LOOP                                      QATR 630
      AUX(1)=.5*(FCT(XL)+FCT(XU))                                       QATR 640
      H=XU-XL                                                           QATR 650
      IF(NDIM-1)8,8,1                                                   QATR 660
    1 IF(H)2,10,2                                                       QATR 670
C                                                                       QATR 680
C     NDIM IS GREATER THAN 1 AND H IS NOT EQUAL TO 0.                   QATR 690
    2 HH=H                                                              QATR 700
      E=EPS/ABS(H)                                                      QATR 710
      DELT2=0.                                                          QATR 720
      P=1.                                                              QATR 730
      JJ=1                                                              QATR 740
      DO 7 I=2,NDIM                                                     QATR 750
      Y=AUX(1)                                                          QATR 760
      DELT1=DELT2                                                       QATR 770
      HD=HH                                                             QATR 780
      HH=.5*HH                                                          QATR 790
      P=.5*P                                                            QATR 800
      X=XL+HH                                                           QATR 810
      SM=0.                                                             QATR 820
      DO 3 J=1,JJ                                                       QATR 830
      SM=SM+FCT(X)                                                      QATR 840
    3 X=X+HD                                                            QATR 850
      AUX(I)=.5*AUX(I-1)+P*SM                                           QATR 860
C     A NEW APPROXIMATION OF INTEGRAL VALUE IS COMPUTED BY MEANS OF     QATR 870
C     TRAPEZOIDAL RULE.                                                 QATR 880
C                                                                       QATR 890
C     START OF ROMBERGS EXTRAPOLATION METHOD.                           QATR 900
      Q=1.                                                              QATR 910
      JI=I-1                                                            QATR 920
      DO 4 J=1,JI                                                       QATR 930
      II=I-J                                                            QATR 940
      Q=Q+Q                                                             QATR 950
      Q=Q+Q                                                             QATR 960
    4 AUX(II)=AUX(II+1)+(AUX(II+1)-AUX(II))/(Q-1.)                      QATR 970
C     END OF ROMBERG-STEP                                               QATR 980
C                                                                       QATR 990
      DELT2=ABS(Y-AUX(1))                                               QATR1000
      IF(I-5)7,5,5                                                      QATR1010
    5 IF(DELT2-E)10,10,6                                                QATR1020
    6 IF(DELT2-DELT1)7,11,11                                            QATR1030
    7 JJ=JJ+JJ                                                          QATR1040
    8 IER=2                                                             QATR1050
    9 Y=H*AUX(1)                                                        QATR1060
      RETURN                                                            QATR1070
   10 IER=0                                                             QATR1080
      GO TO 9                                                           QATR1090
   11 IER=1                                                             QATR1100
      Y=H*Y                                                             QATR1110
      RETURN                                                            QATR1120
      END                                                               QATR1130
```

```
C                                                                       DQAT  10
C     ..................................................................DQAT  20
C                                                                       DQAT  30
C        SUBROUTINE DQATR                                               DQAT  40
C                                                                       DQAT  50
C                                                                       DQAT  60
C        PURPOSE                                                        DQAT  70
C           TO COMPUTE AN APPROXIMATION FOR INTEGRAL(FCT(X), SUMMED     DQAT  80
C           OVER X FROM XL TO XU).                                      DQAT  90
C                                                                       DQAT 100
C        USAGE                                                          DQAT 110
C           CALL DQATR (XL,XU,EPS,NDIM,FCT,Y,IER,AUX)                   DQAT 120
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT.               DQAT 130
C                                                                       DQAT 140
C        DESCRIPTION OF PARAMETERS                                      DQAT 150
C           XL      - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.     DQAT 160
C           XU      - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.     DQAT 170
C           EPS     - SINGLE PRECISION UPPER BOUND OF THE ABSOLUTE ERROR.DQAT 180
C           NDIM    - THE DIMENSION OF THE AUXILIARY STORAGE ARRAY AUX. DQAT 190
C                     NDIM-1 IS THE MAXIMAL NUMBER OF BISECTIONS OF     DQAT 200
C                     THE INTERVAL (XL,XU).                             DQAT 210
C           FCT     - THE NAME OF THE EXTERNAL DOUBLE PRECISION FUNCTION DQAT 220
C                     SUBPROGRAM USED.                                  DQAT 230
C           Y       - RESULTING DOUBLE PRECISION APPROXIMATION FOR THE  DQAT 240
C                     INTEGRAL VALUE.                                   DQAT 250
C           IER     - A RESULTING ERROR PARAMETER.                      DQAT 260
C           AUX     - AUXILIARY DOUBLE PRECISION STORAGE ARRAY WITH     DQAT 270
C                     DIMENSION NDIM.                                   DQAT 280
C                                                                       DQAT 290
C        REMARKS                                                        DQAT 300
C           ERROR PARAMETER IER IS CODED IN THE FOLLOWING FORM          DQAT 310
C           IER=0  - IT WAS POSSIBLE TO REACH THE REQUIRED ACCURACY.    DQAT 320
C                    NO ERROR.                                          DQAT 330
C           IER=1  - IT IS IMPOSSIBLE TO REACH THE REQUIRED ACCURACY    DQAT 340
C                    BECAUSE OF ROUNDING ERRORS.                        DQAT 350
C           IER=2  - IT WAS IMPOSSIBLE TO CHECK ACCURACY BECAUSE NDIM   DQAT 360
C                    IS LESS THAN 5, OR THE REQUIRED ACCURACY COULD NOT DQAT 370
C                    BE REACHED WITHIN NDIM-1 STEPS. NDIM SHOULD BE     DQAT 380
C                    INCREASED.                                         DQAT 390
C                                                                       DQAT 400
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQAT 410
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DQAT 420
C           MUST BE CODED BY THE USER. ITS DOUBLE PRECISION ARGUMENT X  DQAT 430
C           SHOULD NOT BE DESTROYED.                                    DQAT 440
C                                                                       DQAT 450
C        METHOD                                                         DQAT 460
C           EVALUATION OF Y IS DONE BY MEANS OF TRAPEZOIDAL RULE IN     DQAT 470
C           CONNECTION WITH ROMBERGS PRINCIPLE. ON RETURN Y CONTAINS    DQAT 480
C           THE BEST POSSIBLE APPROXIMATION OF THE INTEGRAL VALUE AND   DQAT 490
C           VECTOR AUX THE UPWARD DIAGONAL OF ROMBERG SCHEME.           DQAT 500
C           COMPONENTS AUX(I) (I=1,2,...,IEND, WITH IEND LESS THAN OR   DQAT 510
C           EQUAL TO NDIM) BECOME APPROXIMATIONS TO INTEGRAL VALUE WITH DQAT 520
C           DECREASING ACCURACY BY MULTIPLICATION WITH (XU-XL).         DQAT 530
C           FOR REFERENCE, SEE                                          DQAT 540
C           (1) FILIPPI, DAS VERFAHREN VON ROMBERG-STIEFEL-BAUER ALS    DQAT 550
C               SPEZIALFALL DES ALLGEMEINEN PRINZIPS VON RICHARDSON,    DQAT 560
C               MATHEMATIK-TECHNIK-WIRTSCHAFT, VOL.11, ISS.2 (1964),    DQAT 570
C               PP.49-54.                                               DQAT 580
C           (2) BAUER, ALGORITHM 60, CACM, VOL.4, ISS.6 (1961), PP.255. DQAT 590
C                                                                       DQAT 600
C     ..................................................................DQAT 610
C                                                                       DQAT 620
      SUBROUTINE DQATR(XL,XU,EPS,NDIM,FCT,Y,IER,AUX)                    DQAT 630
C                                                                       DQAT 640
C                                                                       DQAT 650
      DIMENSION AUX(1)                                                  DQAT 660
      DOUBLE PRECISION AUX,XL,XU,X,Y,H,HH,HD,P,Q,SM,FCT                 DQAT 670
C                                                                       DQAT 680
C     PREPARATIONS OF ROMBERG-LOOP                                      DQAT 690
      AUX(1)=.500*(FCT(XL)+FCT(XU))                                     DQAT 700
      H=XU-XL                                                           DQAT 710
      IF(NDIM-1)8,8,1                                                   DQAT 720
    1 IF(H)2,10,2                                                       DQAT 730
C                                                                       DQAT 740
C     NDIM IS GREATER THAN 1 AND H IS NOT EQUAL TO 0.                   DQAT 750
    2 HH=H                                                              DQAT 760
      E=EPS/DABS(H)                                                     DQAT 770
      DELT2=0.                                                          DQAT 780
      P=1.D0                                                            DQAT 790
      JJ=1                                                              DQAT 800
      DO 7 I=2,NDIM                                                     DQAT 810
      Y=AUX(1)                                                          DQAT 820
      DELT1=DELT2                                                       DQAT 830
      HD=HH                                                             DQAT 840
      HH=.500*HH                                                        DQAT 850
      P=.500*P                                                          DQAT 860
      X=XL+HH                                                           DQAT 870
      SM=0.D0                                                           DQAT 880
      DO 3 J=1,JJ                                                       DQAT 890
      SM=SM+FCT(X)                                                      DQAT 900
    3 X=X+HD                                                            DQAT 910
      AUX(I)=.500*AUX(I-1)+P*SM                                         DQAT 920
C     A NEW APPROXIMATION OF INTEGRAL VALUE IS COMPUTED BY MEANS OF     DQAT 930
C     TRAPEZOIDAL RULE.                                                 DQAT 940
C                                                                       DQAT 950
C     START OF ROMBERGS EXTRAPOLATION METHOD.                           DQAT 960
      Q=1.D0                                                            DQAT 970
      JI=I-1                                                            DQAT 980
      DO 4 J=1,JI                                                       DQAT 990
      II=I-J                                                            DQAT1000
      Q=Q+Q                                                             DQAT1010
      Q=Q+Q                                                             DQAT1020
    4 AUX(II)=AUX(II+1)+(AUX(II+1)-AUX(II))/(Q-1.D0)                    DQAT1030
C     END OF ROMBERG-STEP                                               DQAT1040
C                                                                       DQAT1050
      DELT2=DABS(Y-AUX(1))                                              DQAT1060
      IF(I-5)7,5,5                                                      DQAT1070
    5 IF(DELT2-E)10,10,6                                                DQAT1080
    6 IF(DELT2-DELT1)7,11,11                                            DQAT1090
    7 JJ=JJ+JJ                                                          DQAT1100
    8 IER=2                                                             DQAT1110
    9 Y=H*AUX(1)                                                        DQAT1120
      RETURN                                                            DQAT1130
   10 IER=0                                                             DQAT1140
      GO TO 9                                                           DQAT1150
   11 IER=1                                                             DQAT1160
      Y=H*Y                                                             DQAT1170
      RETURN                                                            DQAT1180
      END                                                               DQAT1190
```

Subroutines QG2, QG3,..., QG10, DQG4, DQG8, DQG12, DQG16, DQG24, DQG32

These subroutines perform the integration of a given function by Gaussian quadrature formulas.

To compute:

$$y = \int_a^b f(x)\,dx$$

Gaussian quadrature formulas with n = 2,3,..., 10 (or n = 4,8,12,16,24,32) points are used. Transforming the range x = a...b into t = -1...1 by:

$$t = \frac{2x - (a+b)}{b - a}, \quad x = \frac{b-a}{2}t + \frac{b+a}{2}$$

the result is:

$$y = \frac{b-a}{2} \cdot \int_{-1}^{1} \varphi(t)\,dt \text{ with } \varphi(t) = f\left(\frac{b-a}{2} \cdot + \frac{b+a}{2}\right)$$

Using:

$$\int_{-1}^{1} \varphi(t)\,dt = \sum_{k=1}^{n} \left[A_k^{(n)} \varphi(t_k^{(n)})\right] (n = 2,3,\ldots)$$

with coefficients $A_k^{(n)}$ and nodes $t_k^{(n)}$ (note that $t_k^{(n)}$ are the roots of Legendre polynomials of degree n), the result is the approximations:

$$y_n = (b-a) \cdot \sum_{k=1}^{n} \left\{ \frac{A_k^{(n)}}{2} \cdot f\left[(b-a) \cdot \frac{t_k^{(n)}}{2} + \frac{b+a}{2}\right]\right\} (n = 2,3,\ldots), \quad (1)$$

which are exact whenever f(x) is a polynomial up to the degree 2n-1.

The $A_k^{(n)}$ and $t_k^{(n)}$ are symmetric with respect to t = 0:

$$A_k^{(n)} = A_{n-k+1}^{(n)}, \quad t_k^{(n)} = -t_{n-k+1}^{(n)}$$

For reference see: V.J. Krylov, Approximate Calculation of Integrals. Macmillan, New York/London, 1962, pp. 100-111 and 337-340.

```
C                                                                       QG2   10
C ......................................................................QG2   20
C                                                                       QG2   30
C     SUBROUTINE QG2                                                    QG2   40
C                                                                       QG2   50
C     PURPOSE                                                           QG2   60
C        TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)       QG2   70
C                                                                       QG2   80
C     USAGE                                                             QG2   90
C        CALL QG2 (XL,XU,FCT,Y)                                         QG2  100
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   QG2  110
C                                                                       QG2  120
C     DESCRIPTION OF PARAMETERS                                         QG2  130
C        XL      - THE LOWER BOUND OF THE INTERVAL.                     QG2  140
C        XU      - THE UPPER BOUND OF THE INTERVAL.                     QG2  150
C        FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.    QG2  160
C        Y       - THE RESULTING INTEGRAL VALUE.                        QG2  170
C                                                                       QG2  180
C     REMARKS                                                           QG2  190
C        NONE                                                           QG2  200
C                                                                       QG2  210
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     QG2  220
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED      QG2  230
C        BY THE USER.                                                   QG2  240
C                                                                       QG2  250
C     METHOD                                                            QG2  260
C        EVALUATION IS DONE BY MEANS OF 2-POINT GAUSS QUADRATURE        QG2  270
C        FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 3           QG2  280
C        EXACTLY.                                                       QG2  290
C        FOR REFERENCE, SEE                                             QG2  300
C        V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,              QG2  310
C        MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.      QG2  320
C                                                                       QG2  330
C ......................................................................QG2  340
C                                                                       QG2  350
      SUBROUTINE QG2(XL,XU,FCT,Y)                                       QG2  360
C                                                                       QG2  370
C                                                                       QG2  380
      A=.5*(XU+XL)                                                      QG2  390
      B=XU-XL                                                           QG2  400
      Y=.2886751*B                                                      QG2  410
      Y=.5*B*(FCT(A+Y)+FCT(A-Y))                                        QG2  420
      RETURN                                                            QG2  430
      END                                                               QG2  440
```

```
C                                                                       QG3   10
C ......................................................................QG3   20
C                                                                       QG3   30
C     SUBROUTINE QG3                                                    QG3   40
C                                                                       QG3   50
C     PURPOSE                                                           QG3   60
C        TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)       QG3   70
C                                                                       QG3   80
C     USAGE                                                             QG3   90
C        CALL QG3 (XL,XU,FCT,Y)                                         QG3  100
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   QG3  110
C                                                                       QG3  120
C     DESCRIPTION OF PARAMETERS                                         QG3  130
C        XL      - THE LOWER BOUND OF THE INTERVAL.                     QG3  140
C        XU      - THE UPPER BOUND OF THE INTERVAL.                     QG3  150
C        FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.    QG3  160
C        Y       - THE RESULTING INTEGRAL VALUE.                        QG3  170
C                                                                       QG3  180
C     REMARKS                                                           QG3  190
C        NONE                                                           QG3  200
C                                                                       QG3  210
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     QG3  220
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED      QG3  230
C        BY THE USER.                                                   QG3  240
C                                                                       QG3  250
C     METHOD                                                            QG3  260
C        EVALUATION IS DONE BY MEANS OF 3-POINT GAUSS QUADRATURE        QG3  270
C        FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 5           QG3  280
C        EXACTLY.                                                       QG3  290
C        FOR REFERENCE, SEE                                             QG3  300
C        V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,              QG3  310
C        MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.      QG3  320
C                                                                       QG3  330
C ......................................................................QG3  340
C                                                                       QG3  350
      SUBROUTINE QG3(XL,XU,FCT,Y)                                       QG3  360
C                                                                       QG3  370
C                                                                       QG3  380
      A=.5*(XU+XL)                                                      QG3  390
      B=XU-XL                                                           QG3  400
      Y=.3872983*B                                                      QG3  410
      Y=.2777778*(FCT(A+Y)+FCT(A-Y))                                    QG3  420
      Y=B*(Y+.4444444*FCT(A))                                           QG3  430
      RETURN                                                            QG3  440
      END                                                               QG3  450
```

```
C                                                                       QG4   10
C     ...................................................................QG4   20
C                                                                       QG4   30
C        SUBROUTINE QG4                                                 QG4   40
C                                                                       QG4   50
C        PURPOSE                                                        QG4   60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    QG4   70
C                                                                       QG4   80
C        USAGE                                                          QG4   90
C           CALL QG4 (XL,XU,FCT,Y)                                      QG4  100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QG4  110
C                                                                       QG4  120
C        DESCRIPTION OF PARAMETERS                                      QG4  130
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QG4  140
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QG4  150
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QG4  160
C           Y       - THE RESULTING INTEGRAL VALUE.                     QG4  170
C                                                                       QG4  180
C        REMARKS                                                        QG4  190
C           NONE                                                        QG4  200
C                                                                       QG4  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QG4  220
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QG4  230
C           BY THE USER.                                                QG4  240
C                                                                       QG4  250
C        METHOD                                                         QG4  260
C           EVALUATION IS DONE BY MEANS OF 4-POINT GAUSS QUADRATURE     QG4  270
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 7        QG4  280
C           EXACTLY.                                                    QG4  290
C           FOR REFERENCE, SEE                                          QG4  300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QG4  310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.   QG4  320
C                                                                       QG4  330
C     ...................................................................QG4  340
C                                                                       QG4  350
      SUBROUTINE QG4(XL,XU,FCT,Y)                                       QG4  360
C                                                                       QG4  370
C                                                                       QG4  380
      A=.5*(XU+XL)                                                      QG4  390
      B=XU-XL                                                           QG4  400
      C=.4305682*B                                                      QG4  410
      Y=.1739274*(FCT(A+C)+FCT(A-C))                                    QG4  420
      C=.1699905*B                                                      QG4  430
      Y=B*(Y+.3260726*(FCT(A+C)+FCT(A-C)))                              QG4  440
      RETURN                                                            QG4  450
      END                                                               QG4  460
```

```
C                                                                       QG5   10
C     ...................................................................QG5   20
C                                                                       QG5   30
C        SUBROUTINE QG5                                                 QG5   40
C                                                                       QG5   50
C        PURPOSE                                                        QG5   60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    QG5   70
C                                                                       QG5   80
C        USAGE                                                          QG5   90
C           CALL QG5 (XL,XU,FCT,Y)                                      QG5  100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QG5  110
C                                                                       QG5  120
C        DESCRIPTION OF PARAMETERS                                      QG5  130
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QG5  140
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QG5  150
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QG5  160
C           Y       - THE RESULTING INTEGRAL VALUE.                     QG5  170
C                                                                       QG5  180
C        REMARKS                                                        QG5  190
C           NONE                                                        QG5  200
C                                                                       QG5  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QG5  220
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QG5  230
C           BY THE USER.                                                QG5  240
C                                                                       QG5  250
C        METHOD                                                         QG5  260
C           EVALUATION IS DONE BY MEANS OF 5-POINT GAUSS QUADRATURE     QG5  270
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 9        QG5  280
C           EXACTLY.                                                    QG5  290
C           FOR REFERENCE, SEE                                          QG5  300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QG5  310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.   QG5  320
C                                                                       QG5  330
C     ...................................................................QG5  340
C                                                                       QG5  350
      SUBROUTINE QG5(XL,XU,FCT,Y)                                       QG5  360
C                                                                       QG5  370
C                                                                       QG5  380
      A=.5*(XU+XL)                                                      QG5  390
      B=XU-XL                                                           QG5  400
      C=.4530899*B                                                      QG5  410
      Y=.1184634*(FCT(A+C)+FCT(A-C))                                    QG5  420
      C=.2692347*B                                                      QG5  430
      Y=Y+.2393143*(FCT(A+C)+FCT(A-C))                                  QG5  440
      Y=B*(Y+.2844444*FCT(A))                                           QG5  450
      RETURN                                                            QG5  460
      END                                                               QG5  470
```

```
C                                                                       DQG4  10
C     ...................................................................DQG4  20
C                                                                       DQG4  30
C        SUBROUTINE DQG4                                                DQG4  40
C                                                                       DQG4  50
C        PURPOSE                                                        DQG4  60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    DQG4  70
C                                                                       DQG4  80
C        USAGE                                                          DQG4  90
C           CALL DQG4 (XL,XU,FCT,Y)                                     DQG4 100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DQG4 110
C                                                                       DQG4 120
C        DESCRIPTION OF PARAMETERS                                      DQG4 130
C           XL      - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.     DQG4 140
C           XU      - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.     DQG4 150
C           FCT     - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DQG4 160
C                     SUBPROGRAM USED.                                  DQG4 170
C           Y       - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DQG4 180
C                                                                       DQG4 190
C        REMARKS                                                        DQG4 200
C           NONE                                                        DQG4 210
C                                                                       DQG4 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQG4 230
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DQG4 240
C           MUST BE FURNISHED BY THE USER.                              DQG4 250
C                                                                       DQG4 260
C        METHOD                                                         DQG4 270
C           EVALUATION IS DONE BY MEANS OF 4-POINT GAUSS QUADRATURE     DQG4 280
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 7        DQG4 290
C           EXACTLY. FOR REFERENCE, SEE                                 DQG4 300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           DQG4 310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-340.   DQG4 320
C                                                                       DQG4 330
C     ...................................................................DQG4 340
C                                                                       DQG4 350
      SUBROUTINE DQG4(XL,XU,FCT,Y)                                      DQG4 360
C                                                                       DQG4 370
C                                                                       DQG4 380
      DOUBLE PRECISION XL,XU,Y,A,B,C,FCT                                DQG4 390
C                                                                       DQG4 400
      A=.500*(XU+XL)                                                    DQG4 410
      B=XU-XL                                                           DQG4 420
      C=.43056815579702629D0*B                                          DQG4 430
      Y=.17392742256872693D0*(FCT(A+C)+FCT(A-C))                        DQG4 440
      C=.16999052179242813D0*B                                          DQG4 450
      Y=B*(Y+.32607257743127307D0*(FCT(A+C)+FCT(A-C)))                  DQG4 460
      RETURN                                                            DQG4 470
      END                                                               DQG4 480
```

```
C                                                                       QG6   10
C     ...................................................................QG6   20
C                                                                       QG6   30
C        SUBROUTINE QG6                                                 QG6   40
C                                                                       QG6   50
C        PURPOSE                                                        QG6   60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    QG6   70
C                                                                       QG6   80
C        USAGE                                                          QG6   90
C           CALL QG6 (XL,XU,FCT,Y)                                      QG6  100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QG6  110
C                                                                       QG6  120
C        DESCRIPTION OF PARAMETERS                                      QG6  130
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QG6  140
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QG6  150
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QG6  160
C           Y       - THE RESULTING INTEGRAL VALUE.                     QG6  170
C                                                                       QG6  180
C        REMARKS                                                        QG6  190
C           NONE                                                        QG6  200
C                                                                       QG6  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QG6  220
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QG6  230
C           BY THE USER.                                                QG6  240
C                                                                       QG6  250
C        METHOD                                                         QG6  260
C           EVALUATION IS DONE BY MEANS OF 6-POINT GAUSS QUADRATURE     QG6  270
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 11       QG6  280
C           EXACTLY.                                                    QG6  290
C           FOR REFERENCE, SEE                                          QG6  300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QG6  310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.   QG6  320
C                                                                       QG6  330
C     ...................................................................QG6  340
C                                                                       QG6  350
      SUBROUTINE QG6(XL,XU,FCT,Y)                                       QG6  360
C                                                                       QG6  370
C                                                                       QG6  380
      A=.5*(XU+XL)                                                      QG6  390
      B=XU-XL                                                           QG6  400
      C=.4662348*B                                                      QG6  410
      Y=.38566225*(FCT(A+C)+FCT(A-C))                                   QG6  420
      C=.3306047*B                                                      QG6  430
      Y=Y+.1803808*(FCT(A+C)+FCT(A-C))                                  QG6  440
      C=.1193096*B                                                      QG6  450
      Y=B*(Y+.2339570*(FCT(A+C)+FCT(A-C)))                              QG6  460
      RETURN                                                            QG6  470
      END                                                               QG6  480
```

```
C                                                                       QG7   10
C     ******************************************************************QG7   20
C                                                                       QG7   30
C        SUBROUTINE QG7                                                 QG7   40
C                                                                       QG7   50
C        PURPOSE                                                        QG7   60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    QG7   70
C                                                                       QG7   80
C        USAGE                                                          QG7   90
C           CALL QG7 (XL,XU,FCT,Y)                                      QG7  100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QG7  110
C                                                                       QG7  120
C        DESCRIPTION OF PARAMETERS                                      QG7  130
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QG7  140
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QG7  150
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QG7  160
C           Y       - THE RESULTING INTEGRAL VALUE.                     QG7  170
C                                                                       QG7  180
C        REMARKS                                                        QG7  190
C           NONE                                                        QG7  200
C                                                                       QG7  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QG7  220
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QG7  230
C           BY THE USER.                                                QG7  240
C                                                                       QG7  250
C        METHOD                                                         QG7  260
C           EVALUATION IS DONE BY MEANS OF 7-POINT GAUSS QUADRATURE     QG7  270
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 13       QG7  280
C           EXACTLY.                                                    QG7  290
C           FOR REFERENCE, SEE                                          QG7  300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QG7  310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.   QG7  320
C                                                                       QG7  330
C     ******************************************************************QG7  340
      SUBROUTINE QG7(XL,XU,FCT,Y)                                       QG7  350
C                                                                       QG7  360
C                                                                       QG7  370
      A=.5*(XU+XL)                                                      QG7  380
      B=XU-XL                                                           QG7  390
      C=.4745540*B                                                      QG7  400
      Y=.06474248*(FCT(A+C)+FCT(A-C))                                   QG7  410
      C=.3707656*B                                                      QG7  420
      Y=Y+.1398527*(FCT(A+C)+FCT(A-C))                                  QG7  430
      C=.2029226*B                                                      QG7  440
      Y=Y+.1909150*(FCT(A+C)+FCT(A-C))                                  QG7  450
      Y=B*(Y+.2089796*FCT(A))                                           QG7  460
      RETURN                                                            QG7  470
      END                                                               QG7  480
```

```
C                                                                       DQG8  10
C     ******************************************************************DQG8  20
C                                                                       DQG8  30
C        SUBROUTINE DQG8                                                DQG8  40
C                                                                       DQG8  50
C        PURPOSE                                                        DQG8  60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    DQG8  70
C                                                                       DQG8  80
C        USAGE                                                          DQG8  90
C           CALL DQG8 (XL,XU,FCT,Y)                                     DQG8 100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DQG8 110
C                                                                       DQG8 120
C        DESCRIPTION OF PARAMETERS                                      DQG8 130
C           XL      - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.     DQG8 140
C           XU      - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.     DQG8 150
C           FCT     - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DQG8 160
C                     SUBPROGRAM USED.                                  DQG8 170
C           Y       - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DQG8 180
C                                                                       DQG8 190
C        REMARKS                                                        DQG8 200
C           NONE                                                        DQG8 210
C                                                                       DQG8 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQG8 230
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DQG8 240
C           MUST BE FURNISHED BY THE USER.                              DQG8 250
C                                                                       DQG8 260
C        METHOD                                                         DQG8 270
C           EVALUATION IS DONE BY MEANS OF 8-POINT GAUSS QUADRATURE     DQG8 280
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 15       DQG8 290
C           EXACTLY. FOR REFERENCE, SEE                                 DQG8 300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           DQG8 310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-340.   DQG8 320
C                                                                       DQG8 330
C     ******************************************************************DQG8 340
      SUBROUTINE DQG8(XL,XU,FCT,Y)                                      DQG8 350
C                                                                       DQG8 360
C                                                                       DQG8 370
      DOUBLE PRECISION XL,XU,Y,A,B,C,FCT                                DQG8 380
C                                                                       DQG8 390
      A=.500*(XU+XL)                                                    DQG8 400
      B=XU-XL                                                           DQG8 410
      C=.48014492824876812D0*B                                          DQG8 420
      Y=.50614268145188130D-1*(FCT(A+C)+FCT(A-C))                       DQG8 430
      C=.39833323870681337D0*B                                          DQG8 440
      Y=Y+.11119051722668724D0*(FCT(A+C)+FCT(A-C))                      DQG8 450
      C=.26276620495816449D0*B                                          DQG8 460
      Y=Y+.15685332293894364D0*(FCT(A+C)+FCT(A-C))                      DQG8 470
      C=.91717321247824902D-1*B                                         DQG8 480
      Y=B*(Y+.18134189168918099D0*(FCT(A+C)+FCT(A-C)))                  DQG8 490
      RETURN                                                            DQG8 500
      END                                                               DQG8 510
```

```
C                                                                       QG8   10
C     ******************************************************************QG8   20
C                                                                       QG8   30
C        SUBROUTINE QG8                                                 QG8   40
C                                                                       QG8   50
C        PURPOSE                                                        QG8   60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    QG8   70
C                                                                       QG8   80
C        USAGE                                                          QG8   90
C           CALL QG8 (XL,XU,FCT,Y)                                      QG8  100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QG8  110
C                                                                       QG8  120
C        DESCRIPTION OF PARAMETERS                                      QG8  130
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QG8  140
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QG8  150
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QG8  160
C           Y       - THE RESULTING INTEGRAL VALUE.                     QG8  170
C                                                                       QG8  180
C        REMARKS                                                        QG8  190
C           NONE                                                        QG8  200
C                                                                       QG8  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QG8  220
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QG8  230
C           BY THE USER.                                                QG8  240
C                                                                       QG8  250
C        METHOD                                                         QG8  260
C           EVALUATION IS DONE BY MEANS OF 8-POINT GAUSS QUADRATURE     QG8  270
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 15       QG8  280
C           EXACTLY.                                                    QG8  290
C           FOR REFERENCE, SEE                                          QG8  300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QG8  310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.   QG8  320
C                                                                       QG8  330
C     ******************************************************************QG8  340
      SUBROUTINE QG8(XL,XU,FCT,Y)                                       QG8  350
C                                                                       QG8  360
C                                                                       QG8  370
      A=.5*(XU+XL)                                                      QG8  380
      B=XU-XL                                                           QG8  390
      C=.4801449*B                                                      QG8  400
      Y=.05061427*(FCT(A+C)+FCT(A-C))                                   QG8  410
      C=.3983332*B                                                      QG8  420
      Y=Y+.1111905*(FCT(A+C)+FCT(A-C))                                  QG8  430
      C=.2627662*B                                                      QG8  440
      Y=Y+.1568533*(FCT(A+C)+FCT(A-C))                                  QG8  450
      C=.09171732*B                                                     QG8  460
      Y=B*(Y+.1813419*(FCT(A+C)+FCT(A-C)))                              QG8  470
      RETURN                                                            QG8  480
      END                                                               QG8  490
```

```
C                                                                       QG9   10
C     ******************************************************************QG9   20
C                                                                       QG9   30
C        SUBROUTINE QG9                                                 QG9   40
C                                                                       QG9   50
C        PURPOSE                                                        QG9   60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    QG9   70
C                                                                       QG9   80
C        USAGE                                                          QG9   90
C           CALL QG9 (XL,XU,FCT,Y)                                      QG9  100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QG9  110
C                                                                       QG9  120
C        DESCRIPTION OF PARAMETERS                                      QG9  130
C           XL      - THE LOWER BOUND OF THE INTERVAL.                  QG9  140
C           XU      - THE UPPER BOUND OF THE INTERVAL.                  QG9  150
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QG9  160
C           Y       - THE RESULTING INTEGRAL VALUE.                     QG9  170
C                                                                       QG9  180
C        REMARKS                                                        QG9  190
C           NONE                                                        QG9  200
C                                                                       QG9  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QG9  220
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QG9  230
C           BY THE USER.                                                QG9  240
C                                                                       QG9  250
C        METHOD                                                         QG9  260
C           EVALUATION IS DONE BY MEANS OF 9-POINT GAUSS QUADRATURE     QG9  270
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 17       QG9  280
C           EXACTLY.                                                    QG9  290
C           FOR REFERENCE, SEE                                          QG9  300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QG9  310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.   QG9  320
C                                                                       QG9  330
C     ******************************************************************QG9  340
      SUBROUTINE QG9(XL,XU,FCT,Y)                                       QG9  350
C                                                                       QG9  360
C                                                                       QG9  370
      A=.5*(XU+XL)                                                      QG9  380
      B=XU-XL                                                           QG9  390
      C=.4840801*B                                                      QG9  400
      Y=.04063719*(FCT(A+C)+FCT(A-C))                                   QG9  410
      C=.4180156*B                                                      QG9  420
      Y=Y+.09032408*(FCT(A+C)+FCT(A-C))                                 QG9  430
      C=.3066857*B                                                      QG9  440
      Y=Y+.1303053*(FCT(A+C)+FCT(A-C))                                  QG9  450
      C=.1621267*B                                                      QG9  460
      Y=Y+.1561735*(FCT(A+C)+FCT(A-C))                                  QG9  470
      Y=B*(Y+.1651197*FCT(A))                                           QG9  480
      RETURN                                                            QG9  490
      END                                                               QG9  500
```

```
C
C     ..................................................................
C
C        SUBROUTINE QG10
C
C        PURPOSE
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)
C
C        USAGE
C           CALL QG10(XL,XU,FCT,Y)
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT
C
C        DESCRIPTION OF PARAMETERS
C           XL     - THE LOWER BOUND OF THE INTERVAL.
C           XU     - THE UPPER BOUND OF THE INTERVAL.
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.
C           Y      - THE RESULTING INTEGRAL VALUE.
C
C        REMARKS
C           NONE
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED
C           BY THE USER.
C
C        METHOD
C           EVALUATION IS DONE BY MEANS OF 10-POINT GAUSS QUADRATURE
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 19
C           EXACTLY.
C           FOR REFERENCE, SEE
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-338.
C
C     ..................................................................
C
      SUBROUTINE QG10(XL,XU,FCT,Y)
C
C
      A=.5*(XU+XL)
      B=XU-XL
      C=.4869533*B
      Y=.03333567*(FCT(A+C)+FCT(A-C))
      C=.4325317*B
      Y=Y+.07472567*(FCT(A+C)+FCT(A-C))
      C=.3397048*B
      Y=Y+.1095432*(FCT(A+C)+FCT(A-C))
      C=.2166977*B
      Y=Y+.1346334*(FCT(A+C)+FCT(A-C))
      C=.07443717*B
      Y=B*(Y+.1477621*(FCT(A+C)+FCT(A-C)))
      RETURN
      END
```

```
C
C     ..................................................................
C
C        SUBROUTINE DQG12
C
C        PURPOSE
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)
C
C        USAGF
C           CALL DQG12 (XL,XU,FCT,Y)
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT
C
C        DESCRIPTION OF PARAMETERS
C           XL     - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.
C           XU     - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION
C                    SUBPROGRAM USED.
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.
C
C        REMARKS
C           NONE
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)
C           MUST BE FURNISHED BY THE USER.
C
C        METHOD
C           EVALUATION IS DONE BY MEANS OF 12-POINT GAUSS QUADRATURE
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 23
C           EXACTLY. FOR REFERENCE, SEE
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-340.
C
C     ..................................................................
C
      SUBROUTINE DQG12(XL,XU,FCT,Y)
C
C
      DOUBLE PRECISION XL,XU,Y,A,B,C,FCT
C
      A=.5D0*(XU+XL)
      B=XU-XL
      C=.49078031712335963D0*B
      Y=.23587668193255914D-1*(FCT(A+C)+FCT(A-C))
      C=.45205862818523743D0*B
      Y=Y+.53469662997659215D-1*(FCT(A+C)+FCT(A-C))
      C=.38495133709715234D0*B
      Y=Y+.80039164271673111D-1*(FCT(A+C)+FCT(A-C))
      C=.29365897714330872D0*B
      Y=Y+.10158371336153296D0*(FCT(A+C)+FCT(A-C))
      C=.18391574949909010D0*B
      Y=Y+.11674626826917740D0*(FCT(A+C)+FCT(A-C))
      C=.62616704255734458D-1*B
      Y=B*(Y+.12457352290670139D0*(FCT(A+C)+FCT(A-C)))
      RETURN
      END
```

```
C
C     ..................................................................
C
C        SUBROUTINE DQG16
C
C        PURPOSE
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)
C
C        USAGE
C           CALL DQG16 (XL,XU,FCT,Y)
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT
C
C        DESCRIPTION OF PARAMETERS
C           XL     - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.
C           XU     - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION
C                    SUBPROGRAM USED.
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.
C
C        REMARKS
C           NONE
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)
C           MUST BE FURNISHED BY THE USER.
C
C        METHOD
C           EVALUATION IS DONE BY MEANS OF 16-POINT GAUSS QUADRATURE
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 31
C           EXACTLY. FOR REFERENCE, SEE
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-340.
C
C     ..................................................................
C
      SUBROUTINE DQG16(XL,XU,FCT,Y)
C
C
      DOUBLE PRECISION XL,XU,Y,A,B,C,FCT
C
      A=.5D0*(XU+XL)
      B=XU-XL
      C=.49470046749582497D0*B
      Y=.13576229705877047D-1*(FCT(A+C)+FCT(A-C))
      C=.47228751153661629D0*B
      Y=Y+.31126761969323946D-1*(FCT(A+C)+FCT(A-C))
      C=.43281560119391587D0*B
      Y=Y+.47579255841246392D-1*(FCT(A+C)+FCT(A-C))
      C=.37770220417750152D0*B
      Y=Y+.62314485627766936D-1*(FCT(A+C)+FCT(A-C))
      C=.30893812220132187D0*B
      Y=Y+.74797994408288370D-1*(FCT(A+C)+FCT(A-C))
      C=.22900838882861369D0*B
      Y=Y+.84578259697501270D-1*(FCT(A+C)+FCT(A-C))
      C=.14080177538962946D0*B
      Y=Y+.91301707522461790D-1*(FCT(A+C)+FCT(A-C))
      C=.47506254918818720D-1*B
      Y=B*(Y+.94725305227534250D-1*(FCT(A+C)+FCT(A-C)))
      RETURN
      END
```

```
C
C     ..................................................................
C
C        SUBROUTINE DQG24
C
C        PURPOSE
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)
C
C        USAGE
C           CALL DQG24 (XL,XU,FCT,Y)
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT
C
C        DESCRIPTION OF PARAMETERS
C           XL     - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.
C           XU     - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION
C                    SUBPROGRAM USED.
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.
C
C        REMARKS
C           NONE
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)
C           MUST BE FURNISHED BY THE USER.
C
C        METHOD
C           EVALUATION IS DONE BY MEANS OF 24-POINT GAUSS QUADRATURE
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 47
C           EXACTLY. FOR REFERENCE, SEE
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-340.
C
C     ..................................................................
C
      SUBROUTINE DQG24(XL,XU,FCT,Y)
C
C
      DOUBLE PRECISION XL,XU,Y,A,B,C,FCT
C
      A=.5D0*(XU+XL)
      B=XU-XL
      C=.49759360999851068D0*B
      Y=.61706148999935998D-2*(FCT(A+C)+FCT(A-C))
      C=.48736427798565475D0*B
      Y=Y+.14265694314466832D-1*(FCT(A+C)+FCT(A-C))
      C=.46913727600136638D0*B
      Y=Y+.22138719408709903D-1*(FCT(A+C)+FCT(A-C))
      C=.44320776350220052D0*B
      Y=Y+.29649292457718390D-1*(FCT(A+C)+FCT(A-C))
      C=.41000099298695146D0*B
      Y=Y+.36673240705540153D-1*(FCT(A+C)+FCT(A-C))
      C=.37006209578927718D0*B
      Y=Y+.43095080765976638D-1*(FCT(A+C)+FCT(A-C))
      C=.32404682596848778D0*B
      Y=Y+.48809326052056944D-1*(FCT(A+C)+FCT(A-C))
      C=.27271073569441977D0*B
      Y=Y+.53722135057982817D-1*(FCT(A+C)+FCT(A-C))
      C=.21689675381302257D0*B
      Y=Y+.57752834026862801D-1*(FCT(A+C)+FCT(A-C))
      C=.15752133984808169D0*B
      Y=Y+.60835236463901696D-1*(FCT(A+C)+FCT(A-C))
      C=.95559433736808150D-1*B
      Y=Y+.62918728173414148D-1*(FCT(A+C)+FCT(A-C))
      C=.32028446431302813D-1*B
      Y=B*(Y+.63969097673376078D-1*(FCT(A+C)+FCT(A-C)))
      RETURN
      END
```

```
C                                                                       DG32  10
C     ..................................................................DG32  20
C                                                                       DG32  30
C        SUBROUTINE DQG32                                               DG32  40
C                                                                       DG32  50
C        PURPOSE                                                        DG32  60
C           TO COMPUTE INTEGRAL(FCT(X), SUMMED OVER X FROM XL TO XU)    DG32  70
C                                                                       DG32  80
C        USAGE                                                          DG32  90
C           CALL DQG32 (XL,XU,FCT,Y)                                    DG32 100
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DG32 110
C                                                                       DG32 120
C        DESCRIPTION OF PARAMETERS                                      DG32 130
C           XL      - DOUBLE PRECISION LOWER BOUND OF THE INTERVAL.     DG32 140
C           XU      - DOUBLE PRECISION UPPER BOUND OF THE INTERVAL.     DG32 150
C           FCT     - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DG32 160
C                     SUBPROGRAM USED.                                  DG32 170
C           Y       - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DG32 180
C                                                                       DG32 190
C        REMARKS                                                        DG32 200
C           NONE                                                        DG32 210
C                                                                       DG32 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DG32 230
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DG32 240
C           MUST BE FURNISHED BY THE USER.                              DG32 250
C                                                                       DG32 260
C        METHOD                                                         DG32 270
C           EVALUATION IS DONE BY MEANS OF 32-POINT GAUSS QUADRATURE    DG32 280
C           FORMULA, WHICH INTEGRATES POLYNOMIALS UP TO DEGREE 63       DG32 290
C           EXACTLY. FOR REFERENCE, SEE                                 DG32 300
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           DG32 310
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.100-111 AND 337-340.   DG32 320
C                                                                       DG32 330
C     ..................................................................DG32 340
C                                                                       DG32 350
      SUBROUTINE DQG32(XL,XU,FCT,Y)                                     DG32 360
C                                                                       DG32 370
C                                                                       DG32 380
      DOUBLE PRECISION XL,XU,Y,A,B,C,FCT                                DG32 390
C                                                                       DG32 400
      A=.500*(XU+XL)                                                    DG32 410
      B=XU-XL                                                           DG32 420
      C=.49863193092474078D0*B                                          DG32 430
      Y=.35093050047350483D-2*(FCT(A+C)+FCT(A-C))                       DG32 440
      C=.49280575577263417D0*B                                          DG32 450
      Y=Y+.81371973654528350-2*(FCT(A+C)+FCT(A-C))                      DG32 460
      C=.48238112779375322D0*B                                          DG32 470
      Y=Y+.12696032654631030D-1*(FCT(A+C)+FCT(A-C))                     DG32 480
      C=.46745303796886984D0*B                                          DG32 490
      Y=Y+.17136931456510717D-1*(FCT(A+C)+FCT(A-C))                     DG32 500
      C=.44816057788302606D0*B                                          DG32 510
      Y=Y+.21417949011113340D-1*(FCT(A+C)+FCT(A-C))                     DG32 520
      C=.42468380686628499D0*B                                          DG32 530
      Y=Y+.25499029631188088D-1*(FCT(A+C)+FCT(A-C))                     DG32 540
      C=.39724189798397120D0*B                                          DG32 550
      Y=Y+.29342046739267774D-1*(FCT(A+C)+FCT(A-C))                     DG32 560
      C=.36609105937014484D0*B                                          DG32 570
      Y=Y+.32911111388180923D-1*(FCT(A+C)+FCT(A-C))                     DG32 580
      C=.33152213346510760D0*B                                          DG32 590
      Y=Y+.36172897054424253D-1*(FCT(A+C)+FCT(A-C))                     DG32 600
      C=.29385787862038116D0*B                                          DG32 610
      Y=Y+.39096947893535153D-1*(FCT(A+C)+FCT(A-C))                     DG32 620
      C=.25344995446611470D0*B                                          DG32 630
      Y=Y+.41655962113473378D-1*(FCT(A+C)+FCT(A-C))                     DG32 640
      C=.21067563806531767D0*B                                          DG32 650
      Y=Y+.43826046502201906D-1*(FCT(A+C)+FCT(A-C))                     DG32 660
      C=.16593430114106382D0*B                                          DG32 670
      Y=Y+.45586939347881942D-1*(FCT(A+C)+FCT(A-C))                     DG32 680
      C=.11964368112606854D0*B                                          DG32 690
      Y=Y+.46922199540402283D-1*(FCT(A+C)+FCT(A-C))                     DG32 700
      C=.72235980791398250-1*B                                          DG32 710
      Y=Y+.47819360039637430D-1*(FCT(A+C)+FCT(A-C))                     DG32 720
      C=.24153832843869158D-1*B                                         DG32 730
      Y=B*(Y+.48270044257363900D-1*(FCT(A+C)+FCT(A-C)))                 DG32 740
      RETURN                                                            DG32 750
      END                                                               DG32 760
```

Subroutines QL2, QL3, ..., QL10; DQL4, DQL8, DQL12, DQL16, DQL24, DQL32

These subroutines perform the integration of a given function by Gaussian-Laguerre quadrature formulas:

To compute:

$$y = \int_0^\infty e^{-x} f(x)\,dx$$

Gaussian-Laguerre quadrature formulas with $n = 2,3,\ldots, 10$ (or $n = 4,8,12,16,24,32$) points are used to get the approximations:

$$y_n = \sum_{k=1}^{n} \left[A_k^{(n)} \cdot f\left(x_k^{(n)}\right) \right] \quad (n = 2,3,\ldots) \qquad (1)$$

which are exact whenever f(x) is a polynomial up to the degree 2n-1. Note that nodes $x_k^{(n)}$ are the roots of the Laguerre polynomials $L_n(x)$ of degree n.

For reference see:

(1) H.E. Salzer/R. Zucker, "Table of Zeros and Weight Factors of the First Fifteen Laguerre Polynomials". Bul. Amer. Math. Soc., vol 55 (1949), pp 1004-1012.

(2) V.I. Krylov, Approximate Calculation of Integrals. Macmillan, New York/London, 1962, pp. 130-132 and 347-352.

(3) Shao/Chen/Frank, "Tables of Zeros and Gaussian Weights of Certain Associated Laguerre Polynomials and the Related Generalized Hermite Polynomials", IBM Technical Report TR 00.1100 (March, 1964) pp. 24-25.

```
C                                                                       QL2   10
C     ..................................................................QL2   20
C                                                                       QL2   30
C        SUBROUTINE QL2                                                 QL2   40
C                                                                       QL2   50
C        PURPOSE                                                        QL2   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL2   70
C                              TO INFINITY).                            QL2   80
C                                                                       QL2   90
C        USAGE                                                          QL2  100
C           CALL QL2 (FCT,Y)                                            QL2  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL2  120
C                                                                       QL2  130
C        DESCRIPTION OF PARAMETERS                                      QL2  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL2  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL2  160
C                                                                       QL2  170
C        REMARKS                                                        QL2  180
C           NONE                                                        QL2  190
C                                                                       QL2  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL2  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL2  220
C           BY THE USER.                                                QL2  230
C                                                                       QL2  240
C        METHOD                                                         QL2  250
C           EVALUATION IS DONE BY MEANS OF 2-POINT GAUSSIAN-LAGUERRE    QL2  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL2  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 3.                      QL2  280
C           FOR REFERENCE, SEE                                          QL2  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL2  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL2  310
C                                                                       QL2  320
C     ..................................................................QL2  330
      SUBROUTINE QL2(FCT,Y)                                             QL2  340
C                                                                       QL2  350
C                                                                       QL2  360
      X=3.414214                                                        QL2  370
      Y=.1464466*FCT(X)                                                 QL2  380
      X=.5857864                                                        QL2  390
      Y=Y+.8535534*FCT(X)                                               QL2  400
      RETURN                                                            QL2  410
      END                                                               QL2  420
```

```
C                                                                       QL3   10
C     ...................................................................QL3   20
C                                                                       QL3   30
C        SUBROUTINE QL3                                                 QL3   40
C                                                                       QL3   50
C        PURPOSE                                                        QL3   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL3   70
C                              TO INFINITY).                            QL3   80
C                                                                       QL3   90
C        USAGE                                                          QL3  100
C           CALL QL3 (FCT,Y)                                            QL3  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL3  120
C                                                                       QL3  130
C        DESCRIPTION OF PARAMETERS                                      QL3  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL3  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL3  160
C                                                                       QL3  170
C        REMARKS                                                        QL3  180
C           NONE                                                        QL3  190
C                                                                       QL3  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL3  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL3  220
C           BY THE USER.                                                QL3  230
C                                                                       QL3  240
C        METHOD                                                         QL3  250
C           EVALUATION IS DONE BY MEANS OF 3-POINT GAUSSIAN-LAGUERRE    QL3  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL3  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 5.                      QL3  280
C           FOR REFERENCE, SEE                                          QL3  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL3  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL3  310
C                                                                       QL3  320
C     ...................................................................QL3  330
C                                                                       QL3  340
      SUBROUTINE QL3(FCT,Y)                                             QL3  350
C                                                                       QL3  360
C                                                                       QL3  370
      X=6.289945                                                        QL3  380
      Y=.01038926*FCT(X)                                                QL3  390
      X=2.294280                                                        QL3  400
      Y=Y+.2785177*FCT(X)                                               QL3  410
      X=.4157746                                                        QL3  420
      Y=Y+.7110930*FCT(X)                                               QL3  430
      RETURN                                                            QL3  440
      END                                                               QL3  450
```

```
C                                                                       DQL4  10
C     ...................................................................DQL4  20
C                                                                       DQL4  30
C        SUBROUTINE DQL4                                                DQL4  40
C                                                                       DQL4  50
C        PURPOSE                                                        DQL4  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X           DQL4  70
C                              FROM 0 TO INFINITY).                     DQL4  80
C                                                                       DQL4  90
C        USAGE                                                          DQL4 100
C           CALL DQL4 (FCT,Y)                                           DQL4 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DQL4 120
C                                                                       DQL4 130
C        DESCRIPTION OF PARAMETERS                                      DQL4 140
C           FCT     - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DQL4 150
C                     SUBPROGRAM USED.                                  DQL4 160
C           Y       - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DQL4 170
C                                                                       DQL4 180
C        REMARKS                                                        DQL4 190
C           NONE                                                        DQL4 200
C                                                                       DQL4 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQL4 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DQL4 230
C           MUST BE FURNISHED BY THE USER.                              DQL4 240
C                                                                       DQL4 250
C        METHOD                                                         DQL4 260
C           EVALUATION IS DONE BY MEANS OF 4-POINT GAUSSIAN-LAGUERRE    DQL4 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,               DQL4 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 7.             DQL4 290
C           FOR REFERENCE, SEE                                          DQL4 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DQL4 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DQL4 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DQL4 330
C           TR00.1100 (MARCH 1964), PP.24-25.                           DQL4 340
C                                                                       DQL4 350
C     ...................................................................DQL4 360
C                                                                       DQL4 370
      SUBROUTINE DQL4(FCT,Y)                                            DQL4 380
C                                                                       DQL4 390
C                                                                       DQL4 400
      DOUBLE PRECISION X,Y,FCT                                          DQL4 410
C                                                                       DQL4 420
      X=.93950709123011330I                                             DQL4 430
      Y=.5392947055613274S0-3*FCT(X)                                    DQL4 440
      X=.4536620296921128001                                            DQL4 450
      Y=Y+.3888790851500538D0-1*FCT(X)                                  DQL4 460
      X=.1745761101158346601                                            DQL4 470
      Y=Y+.3574186924377996900*FCT(X)                                   DQL4 480
      X=.3225476896193923100                                            DQL4 490
      Y=Y+.6031541043416336000*FCT(X)                                   DQL4 500
      RETURN                                                            DQL4 510
      END                                                               DQL4 520
```

```
C                                                                       QL4   10
C     ...................................................................QL4   20
C                                                                       QL4   30
C        SUBROUTINE QL4                                                 QL4   40
C                                                                       QL4   50
C        PURPOSE                                                        QL4   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL4   70
C                              TO INFINITY).                            QL4   80
C                                                                       QL4   90
C        USAGE                                                          QL4  100
C           CALL QL4 (FCT,Y)                                            QL4  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL4  120
C                                                                       QL4  130
C        DESCRIPTION OF PARAMETERS                                      QL4  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL4  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL4  160
C                                                                       QL4  170
C        REMARKS                                                        QL4  180
C           NONE                                                        QL4  190
C                                                                       QL4  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL4  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL4  220
C           BY THE USER.                                                QL4  230
C                                                                       QL4  240
C        METHOD                                                         QL4  250
C           EVALUATION IS DONE BY MEANS OF 4-POINT GAUSSIAN-LAGUERRE    QL4  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL4  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 7.                      QL4  280
C           FOR REFERENCE, SEE                                          QL4  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL4  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL4  310
C                                                                       QL4  320
C     ...................................................................QL4  330
C                                                                       QL4  340
      SUBROUTINE QL4(FCT,Y)                                             QL4  350
C                                                                       QL4  360
C                                                                       QL4  370
      X=9.395071                                                        QL4  380
      Y=.5392947E-3*FCT(X)                                              QL4  390
      X=4.536620                                                        QL4  400
      Y=Y+.0388879I*FCT(X)                                              QL4  410
      X=1.745761                                                        QL4  420
      Y=Y+.3574187*FCT(X)                                               QL4  430
      X=.3225477                                                        QL4  440
      Y=Y+.6031541*FCT(X)                                               QL4  450
      RETURN                                                            QL4  460
      END                                                               QL4  470
```

```
C                                                                       QL5   10
C     ...................................................................QL5   20
C                                                                       QL5   30
C        SUBROUTINE QL5                                                 QL5   40
C                                                                       QL5   50
C        PURPOSE                                                        QL5   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL5   70
C                              TO INFINITY).                            QL5   80
C                                                                       QL5   90
C        USAGE                                                          QL5  100
C           CALL QL5 (FCT,Y)                                            QL5  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL5  120
C                                                                       QL5  130
C        DESCRIPTION OF PARAMETERS                                      QL5  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL5  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL5  160
C                                                                       QL5  170
C        REMARKS                                                        QL5  180
C           NONE                                                        QL5  190
C                                                                       QL5  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL5  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL5  220
C           BY THE USER.                                                QL5  230
C                                                                       QL5  240
C        METHOD                                                         QL5  250
C           EVALUATION IS DONE BY MEANS OF 5-POINT GAUSSIAN-LAGUERRE    QL5  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL5  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 9.                      QL5  280
C           FOR REFERENCE, SEE                                          QL5  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL5  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL5  310
C                                                                       QL5  320
C     ...................................................................QL5  330
C                                                                       QL5  340
      SUBROUTINE QL5(FCT,Y)                                             QL5  350
C                                                                       QL5  360
C                                                                       QL5  370
      X=12.64080                                                        QL5  380
      Y=.2336997E-4*FCT(X)                                              QL5  390
      X=7.085810                                                        QL5  400
      Y=Y+.3611759E-2*FCT(X)                                            QL5  410
      X=3.596426                                                        QL5  420
      Y=Y+.07594245*FCT(X)                                              QL5  430
      X=1.413403                                                        QL5  440
      Y=Y+.3986668*FCT(X)                                               QL5  450
      X=.2635603                                                        QL5  460
      Y=Y+.5217556*FCT(X)                                               QL5  470
      RETURN                                                            QL5  480
      END                                                               QL5  490
```

```
C                                                                       QL6   10
C     ***************************************************************QL6   20
C                                                                       QL6   30
C        SUBROUTINE QL6                                                 QL6   40
C                                                                       QL6   50
C        PURPOSE                                                        QL6   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL6   70
C                              TO INFINITY).                            QL6   80
C                                                                       QL6   90
C        USAGE                                                          QL6  100
C           CALL QL6 (FCT,Y)                                            QL6  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL6  120
C                                                                       QL6  130
C        DESCRIPTION OF PARAMETERS                                      QL6  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL6  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL6  160
C                                                                       QL6  170
C        REMARKS                                                        QL6  180
C           NONE                                                        QL6  190
C                                                                       QL6  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL6  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL6  220
C           BY THE USER.                                                QL6  230
C                                                                       QL6  240
C        METHOD                                                         QL6  250
C           EVALUATION IS DONE BY MEANS OF 6-POINT GAUSSIAN-LAGUERRE    QL6  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL6  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 11.                     QL6  280
C           FOR REFERENCE, SEE                                          QL6  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL6  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL6  310
C                                                                       QL6  320
C     ***************************************************************QL6   330
C                                                                       QL6   340
      SUBROUTINE QL6(FCT,Y)                                             QL6   350
C                                                                       QL6   360
C                                                                       QL6   370
      X=15.98287                                                        QL6   380
      Y=.8985479E-6*FCT(X)                                              QL6   390
      X=9.837467                                                        QL6   400
      Y=Y+.2610172E-3*FCT(X)                                            QL6   410
      X=5.775144                                                        QL6   420
      Y=Y+.0103990*FCT(X)                                               QL6   430
      X=2.992736                                                        QL6   440
      Y=Y+.1133734*FCT(X)                                               QL6   450
      X=1.188932                                                        QL6   460
      Y=Y+.4170908*FCT(X)                                               QL6   470
      X=.2228466                                                        QL6   480
      Y=Y+.4589647*FCT(X)                                               QL6   490
      RETURN                                                            QL6   500
      END                                                               QL6   510
```

```
C                                                                       QL8   10
C     ***************************************************************QL8   20
C                                                                       QL8   30
C        SUBROUTINE QL8                                                 QL8   40
C                                                                       QL8   50
C        PURPOSE                                                        QL8   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL8   70
C                              TO INFINITY).                            QL8   80
C                                                                       QL8   90
C        USAGE                                                          QL8  100
C           CALL QL8 (FCT,Y)                                            QL8  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL8  120
C                                                                       QL8  130
C        DESCRIPTION OF PARAMETERS                                      QL8  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL8  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL8  160
C                                                                       QL8  170
C        REMARKS                                                        QL8  180
C           NONE                                                        QL8  190
C                                                                       QL8  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL8  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL8  220
C           BY THE USER.                                                QL8  230
C                                                                       QL8  240
C        METHOD                                                         QL8  250
C           EVALUATION IS DONE BY MEANS OF 8-POINT GAUSSIAN-LAGUERRE    QL8  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL8  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 15.                     QL8  280
C           FOR REFERENCE, SEE                                          QL8  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL8  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL8  310
C                                                                       QL8  320
C     ***************************************************************QL8   330
C                                                                       QL8   340
      SUBROUTINE QL8(FCT,Y)                                             QL8   350
C                                                                       QL8   360
C                                                                       QL8   370
      X=22.86313                                                        QL8   380
      Y=.1049001E-8*FCT(X)                                              QL8   390
      X=15.74068                                                        QL8   400
      Y=Y+.8485747E-6*FCT(X)                                            QL8   410
      X=10.75852                                                        QL8   420
      Y=Y+.9076509E-4*FCT(X)                                            QL8   430
      X=7.045905                                                        QL8   440
      Y=Y+.2794536E-2*FCT(X)                                            QL8   450
      X=4.266700                                                        QL8   460
      Y=Y+.0333439*FCT(X)                                               QL8   470
      X=2.251087                                                        QL8   480
      Y=Y+.1757950*FCT(X)                                               QL8   490
      X=.9037018                                                        QL8   500
      Y=Y+.4187868*FCT(X)                                               QL8   510
      X=.1702796                                                        QL8   520
      Y=Y+.3691886*FCT(X)                                               QL8   530
      RETURN                                                            QL8   540
      END                                                               QL8   550
```

```
C                                                                       QL7   10
C     ***************************************************************QL7   20
C                                                                       QL7   30
C        SUBROUTINE QL7                                                 QL7   40
C                                                                       QL7   50
C        PURPOSE                                                        QL7   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL7   70
C                              TO INFINITY).                            QL7   80
C                                                                       QL7   90
C        USAGE                                                          QL7  100
C           CALL QL7 (FCT,Y)                                            QL7  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL7  120
C                                                                       QL7  130
C        DESCRIPTION OF PARAMETERS                                      QL7  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QL7  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QL7  160
C                                                                       QL7  170
C        REMARKS                                                        QL7  180
C           NONE                                                        QL7  190
C                                                                       QL7  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL7  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL7  220
C           BY THE USER.                                                QL7  230
C                                                                       QL7  240
C        METHOD                                                         QL7  250
C           EVALUATION IS DONE BY MEANS OF 7-POINT GAUSSIAN-LAGUERRE    QL7  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL7  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 13.                     QL7  280
C           FOR REFERENCE, SEE                                          QL7  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL7  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL7  310
C                                                                       QL7  320
C     ***************************************************************QL7   330
C                                                                       QL7   340
      SUBROUTINE QL7(FCT,Y)                                             QL7   350
C                                                                       QL7   360
C                                                                       QL7   370
      X=19.39573                                                        QL7   380
      Y=.3170315E-7*FCT(X)                                              QL7   390
      X=12.73418                                                        QL7   400
      Y=Y+.1586546E-4*FCT(X)                                            QL7   410
      X=8.182153                                                        QL7   420
      Y=Y+.1074010E-2*FCT(X)                                            QL7   430
      X=4.900353                                                        QL7   440
      Y=Y+.0206335I*FCT(X)                                              QL7   450
      X=2.567877                                                        QL7   460
      Y=Y+.1471263*FCT(X)                                               QL7   470
      X=1.026665                                                        QL7   480
      Y=Y+.4218313*FCT(X)                                               QL7   490
      X=.1930437                                                        QL7   500
      Y=Y+.4093190*FCT(X)                                               QL7   510
      RETURN                                                            QL7   520
      END                                                               QL7   530
```

```
C                                                                       DQL8  10
C     ***************************************************************DQL8  20
C                                                                       DQL8  30
C        SUBROUTINE DQL8                                                DQL8  40
C                                                                       DQL8  50
C        PURPOSE                                                        DQL8  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X           DQL8  70
C                              FROM 0 TO INFINITY).                     DQL8  80
C                                                                       DQL8  90
C        USAGE                                                          DQL8 100
C           CALL DQL8 (FCT,Y)                                           DQL8 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DQL8 120
C                                                                       DQL8 130
C        DESCRIPTION OF PARAMETERS                                      DQL8 140
C           FCT     - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DQL8 150
C                     SUBPROGRAM USED.                                  DQL8 160
C           Y       - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DQL8 170
C                                                                       DQL8 180
C        REMARKS                                                        DQL8 190
C           NONE                                                        DQL8 200
C                                                                       DQL8 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQL8 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DQL8 230
C           MUST BE FURNISHED BY THE USER.                              DQL8 240
C                                                                       DQL8 250
C        METHOD                                                         DQL8 260
C           EVALUATION IS DONE BY MEANS OF 8-POINT GAUSSIAN-LAGUERRE    DQL8 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,               DQL8 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 15.            DQL8 290
C           FOR REFERENCE, SEE                                          DQL8 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DQL8 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DQL8 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DQL8 330
C           TR00.1100 (MARCH 1964), PP.24-25.                           DQL8 340
C                                                                       DQL8 350
C     ***************************************************************DQL8 360
C                                                                       DQL8 370
      SUBROUTINE DQL8(FCT,Y)                                            DQL8 380
C                                                                       DQL8 390
C                                                                       DQL8 400
      DOUBLE PRECISION X,Y,FCT                                          DQL8 410
C                                                                       DQL8 420
      X=.2286313173688926402                                            DQL8 430
      Y=.1049001174871510402-8*FCT(X)                                   DQL8 440
      X=.1574678641278005D2                                             DQL8 450
      Y=Y+.8485746716272532D-6*FCT(X)                                   DQL8 460
      X=.1075851601018099502                                            DQL8 470
      Y=Y+.9076508773358213D-4*FCT(X)                                   DQL8 480
      X=.7045905402393465701                                            DQL8 490
      Y=Y+.2794536235225672D-2*FCT(X)                                   DQL8 500
      X=.4266700170287658801                                            DQL8 510
      Y=Y+.3334349226121565D-1*FCT(X)                                   DQL8 520
      X=.2251086629866130701                                            DQL8 530
      Y=Y+.1757949866371718100*FCT(X)                                   DQL8 540
      X=.9037017767993799D0                                             DQL8 550
      Y=Y+.4187867808143429600*FCT(X)                                   DQL8 560
      X=.1702796323051010000                                            DQL8 570
      Y=Y+.3691885893416375300*FCT(X)                                   DQL8 580
      RETURN                                                            DQL8 590
      END                                                               DQL8 600
```

```
C                                                                       QL9   10
C     ..................................................................QL9   20
C                                                                       QL9   30
C        SUBROUTINE QL9                                                 QL9   40
C                                                                       QL9   50
C        PURPOSE                                                        QL9   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL9   70
C                              TO INFINITY).                            QL9   80
C                                                                       QL9   90
C        USAGE                                                          QL9  100
C           CALL QL9 (FCT,Y)                                            QL9  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL9  120
C                                                                       QL9  130
C        DESCRIPTION OF PARAMETERS                                      QL9  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QL9  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QL9  160
C                                                                       QL9  170
C        REMARKS                                                        QL9  180
C           NONE                                                        QL9  190
C                                                                       QL9  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL9  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL9  220
C           BY THE USER.                                                QL9  230
C                                                                       QL9  240
C        METHOD                                                         QL9  250
C           EVALUATION IS DONE BY MEANS OF 9-POINT GAUSSIAN-LAGUERRE    QL9  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL9  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 17.                     QL9  280
C           FOR REFERENCE, SEE                                          QL9  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL9  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL9  310
C                                                                       QL9  320
C     ..................................................................QL9  330
C                                                                       QL9  340
      SUBROUTINE QL9(FCT,Y)                                             QL9  350
C                                                                       QL9  360
C                                                                       QL9  370
      X=26.37407                                                        QL9  380
      Y=.3290874E-10*FCT(X)                                             QL9  390
      X=18.83360                                                        QL9  400
      Y=Y+.4110769E-7*FCT(X)                                            QL9  410
      X=13.46624                                                        QL9  420
      Y=Y+.6592123E-5*FCT(X)                                            QL9  430
      X=9.372985                                                        QL9  440
      Y=Y+.3052498E-3*FCT(X)                                            QL9  450
      X=6.204957                                                        QL9  460
      Y=Y+.005599627*FCT(X)                                             QL9  470
      X=3.783474                                                        QL9  480
      Y=Y+.04746056*FCT(X)                                              QL9  490
      X=2.005135                                                        QL9  500
      Y=Y+.1992875*FCT(X)                                               QL9  510
      X=.8072200                                                        QL9  520
      Y=Y+.4112140*FCT(X)                                               QL9  530
      X=.1523222                                                        QL9  540
      Y=Y+.3361264*FCT(X)                                               QL9  550
      RETURN                                                            QL9  560
      END                                                               QL9  570
```

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C                                                                       QL10  10
C     ..................................................................QL10  20
C                                                                       QL10  30
C        SUBROUTINE QL10                                                QL10  40
C                                                                       QL10  50
C        PURPOSE                                                        QL10  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X FROM 0    QL10  70
C                              TO INFINITY).                            QL10  80
C                                                                       QL10  90
C        USAGE                                                          QL10 100
C           CALL QL10(FCT,Y)                                            QL10 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QL10 120
C                                                                       QL10 130
C        DESCRIPTION OF PARAMETERS                                      QL10 140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QL10 150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QL10 160
C                                                                       QL10 170
C        REMARKS                                                        QL10 180
C           NONE                                                        QL10 190
C                                                                       QL10 200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QL10 210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QL10 220
C           BY THE USER.                                                QL10 230
C                                                                       QL10 240
C        METHOD                                                         QL10 250
C           EVALUATION IS DONE BY MEANS OF 10-POINT GAUSSIAN-LAGUERRE   QL10 260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QL10 270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 19.                     QL10 280
C           FOR REFERENCE, SEE                                          QL10 290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QL10 300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.130-132 AND 347-352.   QL10 310
C                                                                       QL10 320
C     ..................................................................QL10 330
C                                                                       QL10 340
      SUBROUTINE QL10(FCT,Y)                                            QL10 350
C                                                                       QL10 360
C                                                                       QL10 370
      X=29.92070                                                        QL10 380
      Y=.9911827E-12*FCT(X)                                             QL10 390
      X=21.99659                                                        QL10 400
      Y=Y+.1839565E-8*FCT(X)                                            QL10 410
      X=16.27926                                                        QL10 420
      Y=Y+.4249314E-6*FCT(X)                                            QL10 430
      X=11.84379                                                        QL10 440
      Y=Y+.2825923E-4*FCT(X)                                            QL10 450
      X=8.330153                                                        QL10 460
      Y=Y+.7530084E-3*FCT(X)                                            QL10 470
      X=5.552496                                                        QL10 480
      Y=Y+.009501517*FCT(X)                                             QL10 490
      X=3.401434                                                        QL10 500
      Y=Y+.06208746*FCT(X)                                              QL10 510
      X=1.808343                                                        QL10 520
      Y=Y+.2180683*FCT(X)                                               QL10 530
      X=.7294545                                                        QL10 540
      Y=Y+.4011199*FCT(X)                                               QL10 550
      X=.1377935                                                        QL10 560
      Y=Y+.3084411*FCT(X)                                               QL10 570
      RETURN                                                            QL10 580
      END                                                               QL10 590
```

```
C                                                                       DL12  10
C     ..................................................................DL12  20
C                                                                       DL12  30
C        SUBROUTINE DQL12                                               DL12  40
C                                                                       DL12  50
C        PURPOSE                                                        DL12  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X           DL12  70
C                              FROM 0 TO INFINITY).                     DL12  80
C                                                                       DL12  90
C        USAGE                                                          DL12 100
C           CALL DQL12 (FCT,Y)                                          DL12 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DL12 120
C                                                                       DL12 130
C        DESCRIPTION OF PARAMETERS                                      DL12 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DL12 150
C                    SUBPROGRAM USED.                                   DL12 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DL12 170
C                                                                       DL12 180
C        REMARKS                                                        DL12 190
C           NONE                                                        DL12 200
C                                                                       DL12 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DL12 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DL12 230
C           MUST BE FURNISHED BY THE USER.                              DL12 240
C                                                                       DL12 250
C        METHOD                                                         DL12 260
C           EVALUATION IS DONE BY MEANS OF 12-POINT GAUSSIAN-LAGUERRE   DL12 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,               DL12 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 23.            DL12 290
C           FOR REFERENCE, SEE                                          DL12 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DL12 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DL12 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DL12 330
C           TR00.1100 (MARCH 1964), PP.24-25.                           DL12 340
C                                                                       DL12 350
C     ..................................................................DL12 360
C                                                                       DL12 370
      SUBROUTINE DQL12(FCT,Y)                                           DL12 380
C                                                                       DL12 390
C                                                                       DL12 400
      DOUBLE PRECISION X,Y,FCT                                          DL12 410
C                                                                       DL12 420
      X=.370991210446692D02                                             DL12 430
      Y=.814907746742624D-15*FCT(X)                                     DL12 440
      X=.284879672509840D02                                             DL12 450
      Y=Y+.306160163503502D0-11*FCT(X)                                  DL12 460
      X=.221510903793970D02                                             DL12 470
      Y=Y+.134239103051504ID-8*FCT(X)                                   DL12 480
      X=.171168551874622560D2                                           DL12 490
      Y=Y+.166849387654091D30-6*FCT(X)                                  DL12 500
      X=.130060549933063482D2                                           DL12 510
      Y=Y+.836505585681979D0-5*FCT(X)                                   DL12 520
      X=.962131684245686701                                             DL12 530
      Y=Y+.203231592662999390-3*FCT(X)                                  DL12 540
      X=.684452545311517730I                                            DL12 550
      Y=Y+.266397354186531590-2*FCT(X)                                  DL12 560
      X=.459922763941834850I                                            DL12 570
      Y=Y+.201023811546340970-1*FCT(X)                                  DL12 580
      X=.283375133774350720I                                            DL12 590
      Y=Y+.904492222116809D0-1*FCT(X)                                   DL12 600
      X=.151261026977641880I                                            DL12 610
      Y=Y+.244082011319877560D0*FCT(X)                                  DL12 620
      X=.611757484515136700                                             DL12 630
      Y=Y+.377759275873137980D0*FCT(X)                                  DL12 640
      X=.115722117358020680D0                                           DL12 650
      Y=Y+.264731371055443190D0*FCT(X)                                  DL12 660
      RETURN                                                            DL12 670
      END                                                               DL12 680
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C                                                                       DL16  10
C     ..................................................................DL16  20
C                                                                       DL16  30
C        SUBROUTINE DQL16                                               DL16  40
C                                                                       DL16  50
C        PURPOSE                                                        DL16  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X           DL16  70
C                              FROM 0 TO INFINITY).                     DL16  80
C                                                                       DL16  90
C        USAGE                                                          DL16 100
C           CALL DQL16 (FCT,Y)                                          DL16 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DL16 120
C                                                                       DL16 130
C        DESCRIPTION OF PARAMETERS                                      DL16 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DL16 150
C                    SUBPROGRAM USED.                                   DL16 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DL16 170
C                                                                       DL16 180
C        REMARKS                                                        DL16 190
C           NONE                                                        DL16 200
C                                                                       DL16 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DL16 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DL16 230
C           MUST BE FURNISHED BY THE USER.                              DL16 240
C                                                                       DL16 250
C        METHOD                                                         DL16 260
C           EVALUATION IS DONE BY MEANS OF 16-POINT GAUSSIAN-LAGUERRE   DL16 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,               DL16 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 31.            DL16 290
C           FOR REFERENCE, SEE                                          DL16 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DL16 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DL16 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DL16 330
C           TR00.1100 (MARCH 1964), PP.24-25.                           DL16 340
C                                                                       DL16 350
C     ..................................................................DL16 360
C                                                                       DL16 370
      SUBROUTINE DQL16(FCT,Y)                                           DL16 380
C                                                                       DL16 390
C                                                                       DL16 400
      DOUBLE PRECISION X,Y,FCT                                          DL16 410
C                                                                       DL16 420
      X=.5170116033954331802                                            DL16 430
      Y=-.4161462370737855520-21*FCT(X)                                 DL16 440
      X=.419404526476883330Z                                            DL16 450
      Y=Y+.505047370003551280-17*FCT(X)                                 DL16 460
      X=.345833987C2286626O2                                            DL16 470
      Y=Y+.629796702517867800-14*FCT(X)                                 DL16 480
      X=.285787297428821400Z                                            DL16 490
      Y=Y+.212707903322410300-11*FCT(X)                                 DL16 500
      X=.235159056939919C90Z                                            DL16 510
      Y=Y+.286235024297381860-9*FCT(X)                                  DL16 520
      X=.191801568567531350Z                                            DL16 530
      Y=Y+.188102484107967320-7*FCT(X)                                  DL16 540
```

```
      X=.1544152736478161702                                            DL16 550
      Y=Y+.6828319330871199 6D-6*FCT(X)                                 DL16 560
      X=.1221422336886615902                                            DL16 570
      Y=Y+.1484458687398129 90D-4*FCT(X)                                DL16 580
      X=.9438314336919390 1                                             DL16 590
      Y=Y+.2042719153082784 60D-3*FCT(X)                                DL15 600
      X=.7070338535048234 1D1                                           DL16 610
      Y=Y+.1849070943526310 90D-2*FCT(X)                                DL16 620
      X=.5078018614549767901                                            DL16 630
      Y=Y+.1129990CC80339453 0-1*FCT(X)                                 DL16 640
      X=.3437C866338932066D1                                            DL16 650
      Y=Y+.4732892869412521 90-1*FCT(X)                                 DL16 660
      X=.2129283645098380 6D1                                           DL16 670
      Y=Y+.1362969342963775 400*FCT(X)                                  DL16 680
      X=.1141057774831226901                                            DL16 690
      Y=Y+.2657957776442141 50C*FCT(X)                                  DL16 700
      X=.4626963289150808 3D0                                           DL16 710
      Y=Y+.3110578549508841 70C*FCT(X)                                  DL16 720
      X=.8764941047892784 D-1                                           DL16 730
      Y=Y+.2061517149578009 0C*FCT(X)                                   DL16 740
      RETURN                                                            DL16 750
      END                                                               DL16 760
```

```
C                                                                       DL24  10
C     ..................................................................DL24  20
C                                                                       DL24  30
C         SUBROUTINE DQL24                                              DL24  40
C                                                                       DL24  50
C         PURPOSE                                                       DL24  60
C            TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X          DL24  70
C                           FROM 0 TO INFINITY).                        DL24  80
C                                                                       DL24  90
C         USAGE                                                         DL24 100
C            CALL DQL24 (FCT,Y)                                         DL24 110
C            PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT               DL24 120
C                                                                       DL24 130
C         DESCRIPTION OF PARAMETERS                                     DL24 140
C            FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DL24 150
C                     SUBPROGRAM USED.                                  DL24 160
C            Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DL24 170
C                                                                       DL24 180
C         REMARKS                                                       DL24 190
C            NONE                                                       DL24 200
C                                                                       DL24 210
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 DL24 220
C            THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)   DL24 230
C            MUST BE FURNISHED BY THE USER.                             DL24 240
C                                                                       DL24 250
C         METHOD                                                        DL24 260
C            EVALUATION IS DONE BY MEANS OF 24-POINT GAUSSIAN-LAGUERRE  DL24 270
C            QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,              DL24 280
C            WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 47.           DL24 290
C            FOR REFERENCE, SEE                                         DL24 300
C               SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF DL24 310
C               CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED DL24 320
C               GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT   DL24 330
C               TR00.1100 (MARCH 1964), PP.24-25.                       DL24 340
C                                                                       DL24 350
C     ..................................................................DL24 360
C                                                                       DL24 370
      SUBROUTINE DQL24(FCT,Y)                                           DL24 380
C                                                                       DL24 390
C                                                                       DL24 400
      DOUBLE PRECISION X,Y,FCT                                          DL24 410
C                                                                       DL24 420
      X=.8149827923394889D2                                             DL24 430
      Y=.5575345788328356 8D-34*FCT(X)                                  DL24 440
      X=.6996224003510503 9D2                                           DL24 450
      Y=Y+.4088301593680657 8D-29*FCT(X)                                DL24 460
      X=.6105853144721876 2D2                                           DL24 470
      Y=Y+.2451818845878402 7D-25*FCT(X)                                DL24 480
      X=.5360857454469507 0D2                                           DL24 490
      Y=Y+.3605765864552959 0D-22*FCT(X)                                DL24 500
      X=.4715310644515632 3D2                                           DL24 510
      Y=Y+.2010517464555035 0D-19*FCT(X)                                DL24 520
      X=.4145172048487076 7D2                                           DL24 530
      Y=Y+.5350188813010037 6D-17*FCT(X)                                DL24 540
      X=.3635840580165162 2D2                                           DL24 550
      Y=Y+.7819800382459448 0D-15*FCT(X)                                DL24 560
      X=.3177604135237472 3D2                                           DL24 570
      Y=Y+.6894181052958085 7D-13*FCT(X)                                DL24 580
      X=.2763593717433271 7D2                                           DL24 590
      Y=Y+.3917736515058451 4D-11*FCT(X)                                DL24 600
      X=.2388732984816973 3D2                                           DL24 610
      Y=Y+.1507008226292584 9D-9*FCT(X)                                 DL24 620
      X=.2049146008261642 5D2                                           DL24 630
      Y=Y+.4072858987549999 7D-8*FCT(X)                                 DL24 640
      X=.1741799266650897 9D2                                           DL24 650
      Y=Y+.7960812959133630 D-7*FCT(X)                                  DL24 660
      X=.1466273228959667 4D2                                           DL24 670
      Y=Y+.1151315812737279 9D-5*FCT(X)                                 DL24 680
      X=.1214610271172976 6D2                                           DL24 690
      Y=Y+.1254472197799333 3D-4*FCT(X)                                 DL24 700
      X=.9912098015077706 D1                                            DL24 710
      Y=Y+.1344612146592751 8D-3*FCT(X)                                 DL24 720
      X=.7927539247172152 D1                                            DL24 730
      Y=Y+.6721625640935547 89D-3*FCT(X)                                DL24 740
      X=.6181535118736765 4D1                                           DL24 750
      Y=Y+.3369349058478310 36D-2*FCT(X)                                DL24 760
      X=.4665083703467170 8D1                                           DL24 770
      Y=Y+.1322601940512015 70-1*FCT(X)                                 DL24 780
      X=.3370774626089977 D1                                            DL24 790
      Y=Y+.4073247815140864 6D-1*FCT(X)                                 DL24 800
      X=.2292562058632190 3D1                                           DL24 810
      Y=Y+.9816627262991889 D-1*FCT(X)                                  DL24 820
      X=.1425597590803613 D1                                            DL24 830
      Y=Y+.1833226889777780 200*FCT(X)                                  DL24 840
      X=.7660969055459366 D0                                            DL24 850
      Y=Y+.2588067072727869 80D0*FCT(X)                                 DL24 860
      X=.3112391461984837 D0                                            DL24 870
      Y=Y+.2587741075174239 0D0*FCT(X)                                  DL24 880
      X=.5901985218150797 7D-1                                          DL24 890
      Y=Y+.1428119733347818 5D0*FCT(X)                                  DL24 900
      RETURN                                                            DL24 910
      END                                                               DL24 920
```

```
C                                                                       DL32  10
C     ..................................................................DL32  20
C                                                                       DL32  30
C         SUBROUTINE DQL32                                              DL32  40
C                                                                       DL32  50
C         PURPOSE                                                       DL32  60
C            TO COMPUTE INTEGRAL(EXP(-X)*FCT(X), SUMMED OVER X          DL32  70
C                           FROM 0 TO INFINITY).                        DL32  80
C                                                                       DL32  90
C         USAGE                                                         DL32 100
C            CALL DQL32 (FCT,Y)                                         DL32 110
C            PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT               DL32 120
C                                                                       DL32 130
C         DESCRIPTION OF PARAMETERS                                     DL32 140
C            FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DL32 150
C                     SUBPROGRAM USED.                                  DL32 160
C            Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.    DL32 170
C                                                                       DL32 180
C         REMARKS                                                       DL32 190
C            NONE                                                       DL32 200
C                                                                       DL32 210
C         SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 DL32 220
C            THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)   DL32 230
C            MUST BE FURNISHED BY THE USER.                             DL32 240
C                                                                       DL32 250
C         METHOD                                                        DL32 260
C            EVALUATION IS DONE BY MEANS OF 32-POINT GAUSSIAN-LAGUERRE  DL32 270
C            QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,              DL32 280
C            WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 63.           DL32 290
C            FOR REFERENCE, SEE                                         DL32 300
C               SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF DL32 310
C               CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED DL32 320
C               GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT   DL32 330
C               TR00.1100 (MARCH 1964), PP.24-25.                       DL32 340
C                                                                       DL32 350
C     ..................................................................DL32 360
C                                                                       DL32 370
      SUBROUTINE DQL32(FCT,Y)                                           DL32 380
C                                                                       DL32 390
C                                                                       DL32 400
      DOUBLE PRECISION X,Y,FCT                                          DL32 410
C                                                                       DL32 420
      X=.1117513980979377003                                            DL32 430
      Y=.4510536193898974 2D-47*FCT(X)                                  DL32 440
      X=.9882954286828397 D2                                            DL32 450
      Y=Y+.1338616942106256 3D-41*FCT(X)                                DL32 460
      X=.8873534041789240 D2                                            DL32 470
      Y=Y+.2671511219240137 0D-37*FCT(X)                                DL32 480
      X=.8018744697791352 D2                                            DL32 490
      Y=Y+.1192248760098222 4D-33*FCT(X)                                DL32 500
      X=.7268762809066271 D2                                            DL32 510
      Y=Y+.1913375494454224 3D-30*FCT(X)                                DL32 520
      X=.6597537728793505 3D2                                           DL32 530
      Y=Y+.1418560545463036 9D-27*FCT(X)                                DL32 540
      X=.5989250916213401 8D2                                           DL32 550
      Y=Y+.5661294130397359 4D-25*FCT(X)                                DL32 560
      X=.5433372133396907 D2                                            DL32 570
      Y=Y+.1346982536637395 2D-22*FCT(X)                                DL32 580
      X=.4922439498730863 9D2                                           DL32 590
      Y=Y+.2054429673788045 4D-20*FCT(X)                                DL32 600
      X=.4450926C799575493 8D2                                          DL32 610
      Y=Y+.2119792290163618 6D-18*FCT(X)                                DL32 620
      X=.4014571977153944 2D2                                           DL32 630
      Y=Y+.1542133833393823 4D-16*FCT(X)                                DL32 640
      X=.3610049480575197 4D2                                           DL32 650
      Y=Y+.8171823443420719 0D-15*FCT(X)                                DL32 660
      X=.3234662915396473 7D2                                           DL32 670
      Y=Y+.3237801655729266 5D-13*FCT(X)                                DL32 680
      X=.2886210181632347 5D2                                           DL32 690
      Y=Y+.9799379288772790 4D-12*FCT(X)                                DL32 700
      X=.2562863602245924 8D2                                           DL32 710
      Y=Y+.2305899491891336 1D-10*FCT(X)                                DL32 720
      X=.2263088901319677 4D2                                           DL32 730
      Y=Y+.4281382971040928 9D-9*FCT(X)                                 DL32 740
      X=.1985586094033605 5D2                                           DL32 750
      Y=Y+.6350602226625806 7D-8*FCT(X)                                 DL32 760
      X=.1729245433671531 5D2                                           DL32 770
      Y=Y+.7604567879120781 D-7*FCT(X)                                  DL32 780
      X=.1493113975552255 7D2                                           DL32 790
      Y=Y+.7416404578667552 D-6*FCT(X)                                  DL32 800
      X=.1276369798674272 5D2                                           DL32 810
      Y=Y+.5934541612686329 0-5*FCT(X)                                  DL32 820
      X=.1078301863253997 2D2                                           DL32 830
      Y=Y+.3920341967987947 2D-4*FCT(X)                                 DL32 840
      X=.8982940924212596 D1                                            DL32 850
      Y=Y+.2148649188013644 9D-3*FCT(X)                                 DL32 860
      X=.7358126733186241 D1                                            DL32 870
      Y=Y+.9808033066149551 D-3*FCT(X)                                  DL32 880
      X=.5903958504174243 9D1                                           DL32 890
      Y=Y+.3738816294611524 80-2*FCT(X)                                 DL32 900
      X=.4616456769749767 4D1                                           DL32 910
      Y=Y+.1191821483483857 D-1*FCT(X)                                  DL32 920
      X=.3492213273021994 5D1                                           DL32 930
      Y=Y+.3176091250917507 00-1*FCT(X)                                 DL32 940
      X=.2528336706425794 9D1                                           DL32 950
      Y=Y+.7057862386571744 2D-1*FCT(X)                                 DL32 960
      X=.1722408776446645 4D1                                           DL32 970
      Y=Y+.1299837862860717 6D00*FCT(X)                                 DL32 980
      X=.1072448753817817 6D1                                           DL32 990
      Y=Y+.1955903335972881 04D0*FCT(X)                                 DL321000
      X=.5768846293018664 3D0                                           DL321010
      Y=Y+.2352132296669848 0D0*FCT(X)                                  DL321020
      X=.2345261095196185 6D0                                           DL321030
      Y=Y+.2104431079388132 3D0*FCT(X)                                  DL321040
      X=.4448936583326701 8D-1                                          DL321050
      Y=Y+.1092183419523849 7D0*FCT(X)                                  DL321060
      RETURN                                                            DL321070
      END                                                               DL321080
```

Subroutines QH2, QH3, ..., QH10; DQH8, DQH16, DQH24, DQH32, DQH48, DQH64

These subroutines perform the integration of a given function by Gaussian-Hermite quadrature formulas.

To compute:

$$y = \int_{-\infty}^{+\infty} e^{-x^2} f(x)\, dx$$

Gaussian-Hermite quadrature formulas with n = 2,3, ..., 10 (or n = 8, 16, 24, 32, 48, 64) points are used to get the approximations:

$$y_n = \sum_{x=1}^{n} A_k^{(n)} f(x_k^{(n)}) \qquad (n = 2,3, \ldots) \qquad (1)$$

which are exact whenever f(x) is a polynomial up to the degree 2n-1. Note that the nodes $x_k^{(n)}$ are the roots of the Hermite polynomials $H_n(x)$ of degree n. As $A_k^{(n)}$ and $x_k^{(n)}$ are symmetric with respect to x=0, therefore:

$$A_k^{(n)} = A_{n-k+1}^{(n)}, \quad x_k^{(n)} = -x_{n-k+1}^{(n)}$$

Note: In case of an even function $f(x) = \phi(x^2)$, the transformation $t=x^2$ transforms the given integral into:

$$y = \int_0^{\infty} \frac{e^{-t} \varphi(t)}{\sqrt{t}}\, dt$$

which is a form suitable to subroutines QA2, QA3, ..., QA10 and DQA4, ..., DQA32. Using these subroutines saves approximately half of the computation time.

For reference see:

(1) H.E. Salzer/R. Zucker/R. Capuano, "Table of the Zeros and Weight Factors of the First Twenty Hermite Polynomials", J. Res. Nat. Bur. Standards, vol. 48 (1952), pp. 111-116.

(2) V.I. Krylov, Approximate Calculation of Integrals. Macmillan, New York/London, 1962, pp. 129-130 and 343-346.

```
C                                                                       QH2   10
C     ..................................................................QH2   20
C                                                                       QH2   30
C        SUBROUTINE QH2                                                 QH2   40
C                                                                       QH2   50
C        PURPOSE                                                        QH2   60
C           TO COMPUTE INTEGRAL(EXP(-X**2)*FCT(X), SUMMED OVER X FROM   QH2   70
C                              -INFINITY TO +INFINITY).                 QH2   80
C                                                                       QH2   90
C        USAGE                                                          QH2  100
C           CALL QH2 (FCT,Y)                                            QH2  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH2  120
C                                                                       QH2  130
C        DESCRIPTION OF PARAMETERS                                      QH2  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH2  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH2  160
C                                                                       QH2  170
C        REMARKS                                                        QH2  180
C           NONE                                                        QH2  190
C                                                                       QH2  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH2  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH2  220
C           BY THE USER.                                                QH2  230
C                                                                       QH2  240
C        METHOD                                                         QH2  250
C           EVALUATION IS DONE BY MEANS OF 2-POINT GAUSSIAN-HERMITE     QH2  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH2  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 3.                      QH2  280
C           FOR REFERENCE, SEE                                          QH2  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH2  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH2  310
C                                                                       QH2  320
C     ..................................................................QH2  330
      SUBROUTINE QH2(FCT,Y)                                             QH2  340
C                                                                       QH2  350
C                                                                       QH2  360
      X=.7071068                                                        QH2  370
      Z=-X                                                              QH2  380
      Y=.8862269*(FCT(X)+FCT(Z))                                        QH2  390
      RETURN                                                            QH2  400
      END                                                               QH2  410
                                                                        QH2  420
```

```
C                                                                       QH3   10
C     ..................................................................QH3   20
C                                                                       QH3   30
C        SUBROUTINE QH3                                                 QH3   40
C                                                                       QH3   50
C        PURPOSE                                                        QH3   60
C           TO COMPUTE INTEGRAL(EXP(-X**2)*FCT(X), SUMMED OVER X FROM   QH3   70
C                              -INFINITY TO +INFINITY).                 QH3   80
C                                                                       QH3   90
C        USAGE                                                          QH3  100
C           CALL QH3 (FCT,Y)                                            QH3  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH3  120
C                                                                       QH3  130
C        DESCRIPTION OF PARAMETERS                                      QH3  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH3  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH3  160
C                                                                       QH3  170
C        REMARKS                                                        QH3  180
C           NONE                                                        QH3  190
C                                                                       QH3  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH3  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH3  220
C           BY THE USER.                                                QH3  230
C                                                                       QH3  240
C        METHOD                                                         QH3  250
C           EVALUATION IS DONE BY MEANS OF 3-POINT GAUSSIAN-HERMITE     QH3  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH3  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 5.                      QH3  280
C           FOR REFERENCE, SEE                                          QH3  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH3  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH3  310
C                                                                       QH3  320
C     ..................................................................QH3  330
      SUBROUTINE QH3(FCT,Y)                                             QH3  340
C                                                                       QH3  350
C                                                                       QH3  360
      X=1.224745                                                        QH3  370
      Z=-X                                                              QH3  380
      Y=.2954089*(FCT(X)+FCT(Z))                                        QH3  390
      X=0.                                                              QH3  400
      Y=Y+1.1816360*FCT(X)                                              QH3  410
      RETURN                                                            QH3  420
      END                                                               QH3  430
                                                                        QH3  440
```

```
C                                                                       QH4   10
C     ...................................................................QH4   20
C                                                                       QH4   30
C        SUBROUTINE QH4                                                 QH4   40
C                                                                       QH4   50
C        PURPOSE                                                        QH4   60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH4   70
C                              -INFINITY TO +INFINITY).                 QH4   80
C                                                                       QH4   90
C        USAGE                                                          QH4  100
C           CALL QH4 (FCT,Y)                                            QH4  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH4  120
C                                                                       QH4  130
C        DESCRIPTION OF PARAMETERS                                      QH4  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH4  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH4  160
C                                                                       QH4  170
C        REMARKS                                                        QH4  180
C           NONE                                                        QH4  190
C                                                                       QH4  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH4  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH4  220
C           BY THE USER.                                                QH4  230
C                                                                       QH4  240
C        METHOD                                                         QH4  250
C           EVALUATION IS DONE BY MEANS OF 4-POINT GAUSSIAN-HERMITE     QH4  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH4  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 7.                      QH4  280
C           FOR REFERENCE, SEE                                          QH4  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH4  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH4  310
C                                                                       QH4  320
C     ...................................................................QH4  330
C                                                                       QH4  340
      SUBROUTINE QH4(FCT,Y)                                             QH4  350
C                                                                       QH4  360
C                                                                       QH4  370
      X=1.650680                                                        QH4  380
      Z=-X                                                              QH4  390
      Y=.08131284*(FCT(X)+FCT(Z))                                       QH4  400
      X=.5246476                                                        QH4  410
      Z=-X                                                              QH4  420
      Y=Y+.8049141*(FCT(X)+FCT(Z))                                      QH4  430
      RETURN                                                            QH4  440
      END                                                               QH4  450
```

```
C                                                                       QH6   10
C     ...................................................................QH6   20
C                                                                       QH6   30
C        SUBROUTINE QH6                                                 QH6   40
C                                                                       QH6   50
C        PURPOSE                                                        QH6   60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH6   70
C                              -INFINITY TO +INFINITY).                 QH6   80
C                                                                       QH6   90
C        USAGE                                                          QH6  100
C           CALL QH6 (FCT,Y)                                            QH6  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH6  120
C                                                                       QH6  130
C        DESCRIPTION OF PARAMETERS                                      QH6  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH6  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH6  160
C                                                                       QH6  170
C        REMARKS                                                        QH6  180
C           NONE                                                        QH6  190
C                                                                       QH6  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH6  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH6  220
C           BY THE USER.                                                QH6  230
C                                                                       QH6  240
C        METHOD                                                         QH6  250
C           EVALUATION IS DONE BY MEANS OF 6-POINT GAUSSIAN-HERMITE     QH6  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH6  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 11.                     QH6  280
C           FOR REFERENCE, SEE                                          QH6  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH6  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH6  310
C                                                                       QH6  320
C     ...................................................................QH6  330
C                                                                       QH6  340
      SUBROUTINE QH6(FCT,Y)                                             QH6  350
C                                                                       QH6  360
C                                                                       QH6  370
      X=2.350605                                                        QH6  380
      Z=-X                                                              QH6  390
      Y=.004530010*(FCT(X)+FCT(Z))                                      QH6  400
      X=1.335849                                                        QH6  410
      Z=-X                                                              QH6  420
      Y=Y+.1570673*(FCT(X)+FCT(Z))                                      QH6  430
      X=.4360774                                                        QH6  440
      Z=-X                                                              QH6  450
      Y=Y+.7246296*(FCT(X)+FCT(Z))                                      QH6  460
      RETURN                                                            QH6  470
      END                                                               QH6  480
```

```
C                                                                       QH5   10
C     ...................................................................QH5   20
C                                                                       QH5   30
C        SUBROUTINE QH5                                                 QH5   40
C                                                                       QH5   50
C        PURPOSE                                                        QH5   60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH5   70
C                              -INFINITY TO +INFINITY).                 QH5   80
C                                                                       QH5   90
C        USAGE                                                          QH5  100
C           CALL QH5 (FCT,Y)                                            QH5  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH5  120
C                                                                       QH5  130
C        DESCRIPTION OF PARAMETERS                                      QH5  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH5  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH5  160
C                                                                       QH5  170
C        REMARKS                                                        QH5  180
C           NONE                                                        QH5  190
C                                                                       QH5  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH5  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH5  220
C           BY THE USER.                                                QH5  230
C                                                                       QH5  240
C        METHOD                                                         QH5  250
C           EVALUATION IS DONE BY MEANS OF 5-POINT GAUSSIAN-HERMITE     QH5  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH5  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 9.                      QH5  280
C           FOR REFERENCE, SEE                                          QH5  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH5  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH5  310
C                                                                       QH5  320
C     ...................................................................QH5  330
C                                                                       QH5  340
      SUBROUTINE QH5(FCT,Y)                                             QH5  350
C                                                                       QH5  360
C                                                                       QH5  370
      X=2.020183                                                        QH5  380
      Z=-X                                                              QH5  390
      Y=.01995324*(FCT(X)+FCT(Z))                                       QH5  400
      X=.9585725                                                        QH5  410
      Z=-X                                                              QH5  420
      Y=Y+.3936193*(FCT(X)+FCT(Z))                                      QH5  430
      X=0.                                                              QH5  440
      Y=Y+.9453087*FCT(X)                                               QH5  450
      RETURN                                                            QH5  460
      END                                                               QH5  470
```

```
C                                                                       QH7   10
C     ...................................................................QH7   20
C                                                                       QH7   30
C        SUBROUTINE QH7                                                 QH7   40
C                                                                       QH7   50
C        PURPOSE                                                        QH7   60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH7   70
C                              -INFINITY TO +INFINITY).                 QH7   80
C                                                                       QH7   90
C        USAGE                                                          QH7  100
C           CALL QH7 (FCT,Y)                                            QH7  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH7  120
C                                                                       QH7  130
C        DESCRIPTION OF PARAMETERS                                      QH7  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH7  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH7  160
C                                                                       QH7  170
C        REMARKS                                                        QH7  180
C           NONE                                                        QH7  190
C                                                                       QH7  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH7  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH7  220
C           BY THE USER.                                                QH7  230
C                                                                       QH7  240
C        METHOD                                                         QH7  250
C           EVALUATION IS DONE BY MEANS OF 7-POINT GAUSSIAN-HERMITE     QH7  260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH7  270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 13.                     QH7  280
C           FOR REFERENCE, SEE                                          QH7  290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH7  300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH7  310
C                                                                       QH7  320
C     ...................................................................QH7  330
C                                                                       QH7  340
      SUBROUTINE QH7(FCT,Y)                                             QH7  350
C                                                                       QH7  360
C                                                                       QH7  370
      X=2.651961                                                        QH7  380
      Z=-X                                                              QH7  390
      Y=.0009717812*(FCT(X)+FCT(Z))                                     QH7  400
      X=1.673552                                                        QH7  410
      Z=-X                                                              QH7  420
      Y=Y+.05451558*(FCT(X)+FCT(Z))                                     QH7  430
      X=.8162879                                                        QH7  440
      Z=-X                                                              QH7  450
      Y=Y+.4256073*(FCT(X)+FCT(Z))                                      QH7  460
      X=0.                                                              QH7  470
      Y=Y+.8102646*FCT(X)                                               QH7  480
      RETURN                                                            QH7  490
      END                                                               QH7  500
```

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C                                                                       QH8  10
C     ...................................................................QH8  20
C                                                                       QH8  30
C        SUBROUTINE QH8                                                 QH8  40
C                                                                       QH8  50
C        PURPOSE                                                        QH8  60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH8  70
C                              -INFINITY TO +INFINITY).                 QH8  80
C                                                                       QH8  90
C        USAGE                                                          QH8 100
C           CALL QH8 (FCT,Y)                                            QH8 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH8 120
C                                                                       QH8 130
C        DESCRIPTION OF PARAMETERS                                      QH8 140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH8 150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH8 160
C                                                                       QH8 170
C        REMARKS                                                        QH8 180
C           NONE                                                        QH8 190
C                                                                       QH8 200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH8 210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH8 220
C           BY THE USER.                                                QH8 230
C                                                                       QH8 240
C        METHOD                                                         QH8 250
C           EVALUATION IS DONE BY MEANS OF 8-POINT GAUSSIAN-HERMITE     QH8 260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH8 270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 15.                     QH8 280
C           FOR REFERENCE, SEE                                          QH8 290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH8 300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH8 310
C                                                                       QH8 320
C     ...................................................................QH8 330
C                                                                       QH8 340
      SUBROUTINE QH8(FCT,Y)                                             QH8 350
C                                                                       QH8 360
C                                                                       QH8 370
      X=2.930637                                                        QH8 380
      Z=-X                                                              QH8 390
      Y=.0001996041*(FCT(X)+FCT(Z))                                     QH8 400
      X=1.981657                                                        QH8 410
      Z=-X                                                              QH8 420
      Y=Y+.01707798*(FCT(X)+FCT(Z))                                     QH8 430
      X=1.157194                                                        QH8 440
      Z=-X                                                              QH8 450
      Y=Y+.2078023*(FCT(X)+FCT(Z))                                      QH8 460
      X=.3811870                                                        QH8 470
      Z=-X                                                              QH8 480
      Y=Y+.6611470*(FCT(X)+FCT(Z))                                      QH8 490
      RETURN                                                            QH8 500
      END                                                               QH8 510
```

```
C                                                                       QH9  10
C     ...................................................................QH9  20
C                                                                       QH9  30
C        SUBROUTINE QH9                                                 QH9  40
C                                                                       QH9  50
C        PURPOSE                                                        QH9  60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH9  70
C                              -INFINITY TO +INFINITY).                 QH9  80
C                                                                       QH9  90
C        USAGE                                                          QH9 100
C           CALL QH9 (FCT,Y)                                            QH9 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH9 120
C                                                                       QH9 130
C        DESCRIPTION OF PARAMETERS                                      QH9 140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH9 150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH9 160
C                                                                       QH9 170
C        REMARKS                                                        QH9 180
C           NONE                                                        QH9 190
C                                                                       QH9 200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH9 210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH9 220
C           BY THE USER.                                                QH9 230
C                                                                       QH9 240
C        METHOD                                                         QH9 250
C           EVALUATION IS DONE BY MEANS OF 9-POINT GAUSSIAN-HERMITE     QH9 260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH9 270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 17.                     QH9 280
C           FOR REFERENCE, SEE                                          QH9 290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH9 300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH9 310
C                                                                       QH9 320
C     ...................................................................QH9 330
C                                                                       QH9 340
      SUBROUTINE QH9(FCT,Y)                                             QH9 350
C                                                                       QH9 360
C                                                                       QH9 370
      X=3.190993                                                        QH9 380
      Z=-X                                                              QH9 390
      Y=.3960698E-4*(FCT(X)+FCT(Z))                                     QH9 400
      X=2.266581                                                        QH9 410
      Z=-X                                                              QH9 420
      Y=Y+.004943624*(FCT(X)+FCT(Z))                                    QH9 430
      X=1.468553                                                        QH9 440
      Z=-X                                                              QH9 450
      Y=Y+.08847453*(FCT(X)+FCT(Z))                                     QH9 460
      X=.7235510                                                        QH9 470
      Z=-X                                                              QH9 480
      Y=Y+.4326516*(FCT(X)+FCT(Z))                                      QH9 490
      X=0.                                                              QH9 500
      Y=Y+.7202352*FCT(X)                                               QH9 510
      RETURN                                                            QH9 520
      END                                                               QH9 530
```

```
C                                                                       DQH8  10
C     ...................................................................DQH8  20
C                                                                       DQH8  30
C        SUBROUTINE DQH8                                                DQH8  40
C                                                                       DQH8  50
C        PURPOSE                                                        DQH8  60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    DQH8  70
C                              -INFINITY TO +INFINITY).                 DQH8  80
C                                                                       DQH8  90
C        USAGE                                                          DQH8 100
C           CALL DQH8 (FCT,Y)                                           DQH8 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DQH8 120
C                                                                       DQH8 130
C        DESCRIPTION OF PARAMETERS                                      DQH8 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DQH8 150
C                    SUBPROGRAM USED.                                   DQH8 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DQH8 170
C                                                                       DQH8 180
C        REMARKS                                                        DQH8 190
C           NONE                                                        DQH8 200
C                                                                       DQH8 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DQH8 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DQH8 230
C           MUST BE FURNISHED BY THE USER.                              DQH8 240
C                                                                       DQH8 250
C        METHOD                                                         DQH8 260
C           EVALUATION IS DONE BY MEANS OF 8-POINT GAUSSIAN-HERMITE     DQH8 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       DQH8 280
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 15.                     DQH8 290
C           FOR REFERENCE, SEE                                          DQH8 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DQH8 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DQH8 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DQH8 330
C           TR00.1100 (MARCH 1964), PP.213-214.                         DQH8 340
C                                                                       DQH8 350
C     ...................................................................DQH8 360
C                                                                       DQH8 370
      SUBROUTINE DQH8(FCT,Y)                                            DQH8 380
C                                                                       DQH8 390
C                                                                       DQH8 400
      DOUBLE PRECISION X,Y,Z,FCT                                        DQH8 410
C                                                                       DQH8 420
      X=.2930637420257244001                                            DQH8 430
      Z=-X                                                              DQH8 440
      Y=.1996040722113676?D-3*(FCT(X)+FCT(Z))                           DQH8 450
      X=.1981656756958429D1                                             DQH8 460
      Z=-X                                                              DQH8 470
      Y=Y+.1707798300741347?D-1*(FCT(X)+FCT(Z))                         DQH8 480
      X=.1157193712446780201                                            DQH8 490
      Z=-X                                                              DQH8 500
      Y=Y+.2078023258148918800*(FCT(X)+FCT(Z))                          DQH8 510
      X=.3811869902073221200                                            DQH8 520
      Z=-X                                                              DQH8 530
      Y=Y+.6611470125582412900*(FCT(X)+FCT(Z))                          DQH8 540
      RETURN                                                            DQH8 550
      END                                                               DQH8 560
```

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C                                                                       QH10  10
C     ...................................................................QH10  20
C                                                                       QH10  30
C        SUBROUTINE QH10                                                QH10  40
C                                                                       QH10  50
C        PURPOSE                                                        QH10  60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    QH10  70
C                              -INFINITY TO +INFINITY).                 QH10  80
C                                                                       QH10  90
C        USAGE                                                          QH10 100
C           CALL QH10(FCT,Y)                                            QH10 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QH10 120
C                                                                       QH10 130
C        DESCRIPTION OF PARAMETERS                                      QH10 140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QH10 150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QH10 160
C                                                                       QH10 170
C        REMARKS                                                        QH10 180
C           NONE                                                        QH10 190
C                                                                       QH10 200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QH10 210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QH10 220
C           BY THE USER.                                                QH10 230
C                                                                       QH10 240
C        METHOD                                                         QH10 250
C           EVALUATION IS DONE BY MEANS OF 10-POINT GAUSSIAN-HERMITE    QH10 260
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       QH10 270
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 19.                     QH10 280
C           FOR REFERENCE, SEE                                          QH10 290
C           V.I.KRYLOV, APPROXIMATE CALCULATION OF INTEGRALS,           QH10 300
C           MACMILLAN, NEW YORK/LONDON, 1962, PP.129-130 AND 343-346.   QH10 310
C                                                                       QH10 320
C     ...................................................................QH10 330
C                                                                       QH10 340
      SUBROUTINE QH10(FCT,Y)                                            QH10 350
C                                                                       QH10 360
C                                                                       QH10 370
      X=3.436159                                                        QH10 380
      Z=-X                                                              QH10 390
      Y=.7640433E-5*(FCT(X)+FCT(Z))                                     QH10 400
      X=2.532732                                                        QH10 410
      Z=-X                                                              QH10 420
      Y=Y+.001343646*(FCT(X)+FCT(Z))                                    QH10 430
      X=1.756684                                                        QH10 440
      Z=-X                                                              QH10 450
      Y=Y+.03387439*(FCT(X)+FCT(Z))                                     QH10 460
      X=1.036611                                                        QH10 470
      Z=-X                                                              QH10 480
      Y=Y+.2401386*(FCT(X)+FCT(Z))                                      QH10 490
      X=.3429013                                                        QH10 500
      Z=-X                                                              QH10 510
      Y=Y+.6108626*(FCT(X)+FCT(Z))                                      QH10 520
      RETURN                                                            QH10 530
      END                                                               QH10 540
```

```
C                                                                       DH16  10
C  ...................................................................DH16  20
C                                                                       DH16  30
C     SUBROUTINE DQH16                                                  DH16  40
C                                                                       DH16  50
C     PURPOSE                                                           DH16  60
C        TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM       DH16  70
C                        -INFINITY TO +INFINITY).                       DH16  80
C                                                                       DH16  90
C     USAGE                                                             DH16 100
C        CALL DQH16 (FCT,Y)                                             DH16 110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DH16 120
C                                                                       DH16 130
C     DESCRIPTION OF PARAMETERS                                         DH16 140
C        FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION     DH16 150
C                 SUBPROGRAM USED.                                      DH16 160
C        Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.        DH16 170
C                                                                       DH16 180
C     REMARKS                                                           DH16 190
C        NONE                                                           DH16 200
C                                                                       DH16 210
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DH16 220
C        THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)       DH16 230
C        MUST BE FURNISHED BY THE USER.                                 DH16 240
C                                                                       DH16 250
C     METHOD                                                            DH16 260
C        EVALUATION IS DONE BY MEANS OF 16-POINT GAUSSIAN-HERMITE       DH16 270
C        QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER          DH16 280
C        FCT(X) IS A POLYNOMIAL UP TO DEGREE 31.                        DH16 290
C        FOR REFERENCE, SEE                                             DH16 300
C        SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF       DH16 310
C        CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED        DH16 320
C        GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT          DH16 330
C        TR00.1100 (MARCH 1964), PP.213-214.                            DH16 340
C                                                                       DH16 350
C  ...................................................................DH16 360
C                                                                       DH16 370
      SUBROUTINE DQH16(FCT,Y)                                           DH16 380
C                                                                       DH16 390
C                                                                       DH16 400
      DOUBLE PRECISION X,Y,Z,FCT                                        DH16 410
C                                                                       DH16 420
      X=.4688738939305818401                                            DH16 430
      Z=-X                                                              DH16 440
      Y=.26548074740111822D-9*(FCT(X)+FCT(Z))                           DH16 450
      X=.3869447904860122701                                            DH16 460
      Z=-X                                                              DH16 470
      Y=Y+.23209808448652107D-6*(FCT(X)+FCT(Z))                         DH16 480
      X=.3176999161979956001                                            DH16 490
      Z=-X                                                              DH16 500
      Y=Y+.27118600925378815D-4*(FCT(X)+FCT(Z))                         DH16 510
      X=.2546202157847481401                                            DH16 520
      Z=-X                                                              DH16 530
      Y=Y+.93228400862418050-3*(FCT(X)+FCT(Z))                          DH16 540
      X=.1951787990916254001                                            DH16 550
      Z=-X                                                              DH16 560
      Y=Y+.12880311535509974D-1*(FCT(X)+FCT(Z))                         DH16 570
      X=.1380258539198880801                                            DH16 580
      Z=-X                                                              DH16 590
      Y=Y+.83810041398985830-1*(FCT(X)+FCT(Z))                          DH16 600
      X=.8229514491446559D0                                             DH16 610
      Z=-X                                                              DH16 620
      Y=Y+.28064745852853368D0*(FCT(X)+FCT(Z))                          DH16 630
      X=.2734810461381524500                                            DH16 640
      Z=-X                                                              DH16 650
      Y=Y+.50792947901661374D0*(FCT(X)+FCT(Z))                          DH16 660
      RETURN                                                            DH16 670
      END                                                               DH16 680
```

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C                                                                       DH24  10
C  ...................................................................DH24  20
C                                                                       DH24  30
C     SUBROUTINE DQH24                                                  DH24  40
C                                                                       DH24  50
C     PURPOSE                                                           DH24  60
C        TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM       DH24  70
C                        -INFINITY TO +INFINITY).                       DH24  80
C                                                                       DH24  90
C     USAGE                                                             DH24 100
C        CALL DQH24 (FCT,Y)                                             DH24 110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DH24 120
C                                                                       DH24 130
C     DESCRIPTION OF PARAMETERS                                         DH24 140
C        FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION     DH24 150
C                 SUBPROGRAM USED.                                      DH24 160
C        Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.        DH24 170
C                                                                       DH24 180
C     REMARKS                                                           DH24 190
C        NONE                                                           DH24 200
C                                                                       DH24 210
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DH24 220
C        THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)       DH24 230
C        MUST BE FURNISHED BY THE USER.                                 DH24 240
C                                                                       DH24 250
C     METHOD                                                            DH24 260
C        EVALUATION IS DONE BY MEANS OF 24-POINT GAUSSIAN-HERMITE       DH24 270
C        QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER          DH24 280
C        FCT(X) IS A POLYNOMIAL UP TO DEGREE 47.                        DH24 290
C        FOR REFERENCE, SEE                                             DH24 300
C        SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF       DH24 310
C        CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED        DH24 320
C        GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT          DH24 330
C        TR00.1100 (MARCH 1964), PP.213-214.                            DH24 340
C                                                                       DH24 350
C  ...................................................................DH24 360
C                                                                       DH24 370
      SUBROUTINE DQH24(FCT,Y)                                           DH24 380
C                                                                       DH24 390
C                                                                       DH24 400
      DOUBLE PRECISION X,Y,Z,FCT                                        DH24 410
C                                                                       DH24 420
      X=.601592556142573970I                                            DH24 430
      Z=-X                                                              DH24 440
      Y=.16643684964891089D-15*(FCT(X)+FCT(Z))                          DH24 450
      X=.525938292766804401                                             DH24 460
      Z=-X                                                              DH24 470
      Y=Y+.65846202430781701D-12*(FCT(X)+FCT(Z))                        DH24 480
      X=.462566275642378730I                                            DH24 490
      Z=-X                                                              DH24 500
      Y=Y+.30462542699875639D-9*(FCT(X)+FCT(Z))                         DH24 510
      X=.405366440244814950I                                            DH24 520
      Z=-X                                                              DH24 530
      Y=Y+.40189711749414297D-7*(FCT(X)+FCT(Z))                         DH24 540
      X=.352000681303452470I                                            DH24 550
      Z=-X                                                              DH24 560
      Y=Y+.21582457049023336D-5*(FCT(X)+FCT(Z))                         DH24 570
      X=.301254613756556480I                                            DH24 580
      Z=-X                                                              DH24 590
      Y=Y+.56886916364043798D-4*(FCT(X)+FCT(Z))                         DH24 600
      X=.252388101701142700I                                            DH24 610
      Z=-X                                                              DH24 620
      Y=Y+.82369248268841750-3*(FCT(X)+FCT(Z))                          DH24 630
      X=.204900357366169810I                                            DH24 640
      Z=-X                                                              DH24 650
      Y=Y+.70483558100726710D-2*(FCT(X)+FCT(Z))                         DH24 660
      X=.158425001096169410I                                            DH24 670
      Z=-X                                                              DH24 680
      Y=Y+.37445470503230746D-1*(FCT(X)+FCT(Z))                         DH24 690
      X=.112676081761124510I                                            DH24 700
      Z=-X                                                              DH24 710
      Y=Y+.12773962178455916D0*(FCT(X)+FCT(Z))                          DH24 720
      X=.674171107037212240D                                            DH24 730
      Z=-X                                                              DH24 740
      Y=Y+.28617953534644302D0*(FCT(X)+FCT(Z))                          DH24 750
      X=.224414547472515590D                                            DH24 760
      Z=-X                                                              DH24 770
      Y=Y+.42693116386869925D0*(FCT(X)+FCT(Z))                          DH24 780
      RETURN                                                            DH24 790
      END                                                               DH24 800
```

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C                                                                       DH32  10
C     ..................................................................DH32  20
C                                                                       DH32  30
C        SUBROUTINE DQH32                                               DH32  40
C                                                                       DH32  50
C        PURPOSE                                                        DH32  60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    DH32  70
C                              -INFINITY TO +INFINITY).                 DH32  80
C                                                                       DH32  90
C        USAGE                                                          DH32 100
C           CALL DQH32 (FCT,Y)                                          DH32 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DH32 120
C                                                                       DH32 130
C        DESCRIPTION OF PARAMETERS                                      DH32 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DH32 150
C                    SUBPROGRAM USED.                                   DH32 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DH32 170
C                                                                       DH32 180
C        REMARKS                                                        DH32 190
C           NONE                                                        DH32 200
C                                                                       DH32 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DH32 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DH32 230
C           MUST BE FURNISHED BY THE USER.                              DH32 240
C                                                                       DH32 250
C        METHOD                                                         DH32 260
C           EVALUATION IS DONE BY MEANS OF 32-POINT GAUSSIAN-HERMITE    DH32 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       DH32 280
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 63.                     DH32 290
C           FOR REFERENCE, SEE                                          DH32 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DH32 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DH32 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DH32 330
C           TR00.1100 (MARCH 1964), PP.213-214.                         DH32 340
C                                                                       DH32 350
C     ..................................................................DH32 360
C                                                                       DH32 370
      SUBROUTINE DQH32(FCT,Y)                                           DH32 380
C                                                                       DH32 390
C                                                                       DH32 400
      DOUBLE PRECISION X,Y,Z,FCT                                        DH32 410
C                                                                       DH32 420
      X=.71258139098307276D1                                            DH32 430
      Z=-X                                                              DH32 440
      Y=.73106764273841620-22*(FCT(X)+FCT(Z))                           DH32 450
      X=.64094981492696604D1                                            DH32 460
      Z=-X                                                              DH32 470
      Y=Y+.92317365365182920-18*(FCT(X)+FCT(Z))                         DH32 480
      X=.58122259495159138D1                                            DH32 490
      Z=-X                                                              DH32 500
      Y=Y+.11973440170928487D-14*(FCT(X)+FCT(Z))                        DH32 510
      X=.52755509865158801D1                                            DH32 520
      Z=-X                                                              DH32 530
      Y=Y+.42150102113264476D-12*(FCT(X)+FCT(Z))                        DH32 540
      X=.47771645035025964D1                                            DH32 550
      Z=-X                                                              DH32 560
      Y=Y+.59332914633966386D-10*(FCT(X)+FCT(Z))                        DH32 570
      X=.43055479533511984D1                                            DH32 580
      Z=-X                                                              DH32 590
      Y=Y+.40988321647708966D-8*(FCT(X)+FCT(Z))                         DH32 600
      X=.38537554854714466D1                                            DH32 610
      Z=-X                                                              DH32 620
      Y=Y+.15741677925455940D-6*(FCT(X)+FCT(Z))                         DH32 630
      X=.34171674928185707D1                                            DH32 640
      Z=-X                                                              DH32 650
      Y=Y+.36505851295623761D-5*(FCT(X)+FCT(Z))                         DH32 660
      X=.29924908250023742D1                                            DH32 670
      Z=-X                                                              DH32 680
      Y=Y+.54165840618199826D-4*(FCT(X)+FCT(Z))                         DH32 690
      X=.25772495377323175D1                                            DH32 700
      Z=-X                                                              DH32 710
      Y=Y+.53626836552797205D-3*(FCT(X)+FCT(Z))                         DH32 720
      X=.21694991836061122D1                                            DH32 730
      Z=-X                                                              DH32 740
      Y=Y+.36548903266544281D-2*(FCT(X)+FCT(Z))                         DH32 750
      X=.17676541094632016D1                                            DH32 760
      Z=-X                                                              DH32 770
      Y=Y+.17553428831573430D-1*(FCT(X)+FCT(Z))                         DH32 780
      X=.13703764109528718D1                                            DH32 790
      Z=-X                                                              DH32 800
      Y=Y+.60458130955912614D-1*(FCT(X)+FCT(Z))                         DH32 810
      X=.97650046358968280D0                                            DH32 820
      Z=-X                                                              DH32 830
      Y=Y+.15126973407664248D0*(FCT(X)+FCT(Z))                          DH32 840
      X=.58497876543593245D0                                            DH32 850
      Z=-X                                                              DH32 860
      Y=Y+.27745814230252990D0*(FCT(X)+FCT(Z))                          DH32 870
      X=.19484074156939933D0                                            DH32 880
      Z=-X                                                              DH32 890
      Y=Y+.37523835259280239D0*(FCT(X)+FCT(Z))                          DH32 900
      RETURN                                                            DH32 910
      END                                                               DH32 920
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C                                                                       DH48  10
C     ..................................................................DH48  20
C                                                                       DH48  30
C        SUBROUTINE DQH48                                               DH48  40
C                                                                       DH48  50
C        PURPOSE                                                        DH48  60
C           TO COMPUTE INTEGRAL(EXP(-X*X)*FCT(X), SUMMED OVER X FROM    DH48  70
C                              -INFINITY TO +INFINITY).                 DH48  80
C                                                                       DH48  90
C        USAGE                                                          DH48 100
C           CALL DQH48 (FCT,Y)                                          DH48 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DH48 120
C                                                                       DH48 130
C        DESCRIPTION OF PARAMETERS                                      DH48 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DH48 150
C                    SUBPROGRAM USED.                                   DH48 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DH48 170
C                                                                       DH48 180
C        REMARKS                                                        DH48 190
C           NONE                                                        DH48 200
C                                                                       DH48 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DH48 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DH48 230
C           MUST BE FURNISHED BY THE USER.                              DH48 240
C                                                                       DH48 250
C        METHOD                                                         DH48 260
C           EVALUATION IS DONE BY MEANS OF 48-POINT GAUSSIAN-HERMITE    DH48 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       DH48 280
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 95.                     DH48 290
C           FOR REFERENCE, SEE                                          DH48 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DH48 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DH48 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DH48 330
C           TR00.1100 (MARCH 1964), PP.213-214.                         DH48 340
C                                                                       DH48 350
C     ..................................................................DH48 360
C                                                                       DH48 370
      SUBROUTINE DQH48(FCT,Y)                                           DH48 380
C                                                                       DH48 390
C                                                                       DH48 400
      DOUBLE PRECISION X,Y,Z,FCT                                        DH48 410
C                                                                       DH48 420
      X=.89753150819316870D1                                            DH48 430
      Z=-X                                                              DH48 440
      Y=.79355514607739970-35*(FCT(X)+FCT(Z))                           DH48 450
      X=.83107521907047840D1                                            DH48 460
      Z=-X                                                              DH48 470
      Y=Y+.59846126933138784D-30*(FCT(X)+FCT(Z))                        DH48 480
      X=.77592955197657750D1                                            DH48 490
      Z=-X                                                              DH48 500
      Y=Y+.36850360801506699D-26*(FCT(X)+FCT(Z))                        DH48 510
      X=.72660465541643500D1                                            DH48 520
      Z=-X                                                              DH48 530
      Y=Y+.55645774689022848D-23*(FCT(X)+FCT(Z))                        DH48 540
      X=.68100645780741414D1                                            DH48 550
      Z=-X                                                              DH48 560
      Y=Y+.31883873235051384D-20*(FCT(X)+FCT(Z))                        DH48 570
      X=.63805640961864106D1                                            DH48 580
      Z=-X                                                              DH48 590
      Y=Y+.87301596011866770-18*(FCT(X)+FCT(Z))                         DH48 600
      X=.59710722250135454D1                                            DH48 610
      Z=-X                                                              DH48 620
      Y=Y+.13151596226584085D-15*(FCT(X)+FCT(Z))                        DH48 630
      X=.55773169812237286D1                                            DH48 640
      Z=-X                                                              DH48 650
      Y=Y+.11975898654791794D-13*(FCT(X)+FCT(Z))                        DH48 660
      X=.51962877187923645D1                                            DH48 670
      Z=-X                                                              DH48 680
      Y=Y+.70469325815458891D-12*(FCT(X)+FCT(Z))                        DH48 690
      X=.48257572281332095D1                                            DH48 700
      Z=-X                                                              DH48 710
      Y=Y+.28152965378381691D-10*(FCT(X)+FCT(Z))                        DH48 720
      X=.44640145469344589D1                                            DH48 730
      Z=-X                                                              DH48 740
      Y=Y+.79304674951653820-9*(FCT(X)+FCT(Z))                          DH48 750
      X=.41097046035605902D1                                            DH48 760
      Z=-X                                                              DH48 770
      Y=Y+.16225141358957698D-7*(FCT(X)+FCT(Z))                         DH48 780
      X=.37617264902283578D1                                            DH48 790
      Z=-X                                                              DH48 800
      Y=Y+.24686589936697505D-6*(FCT(X)+FCT(Z))                         DH48 810
      X=.34191659693638846D1                                            DH48 820
      Z=-X                                                              DH48 830
      Y=Y+.28472586917348481D-5*(FCT(X)+FCT(Z))                         DH48 840
      X=.30812489886451058D1                                            DH48 850
      Z=-X                                                              DH48 860
      Y=Y+.25285990277848890-4*(FCT(X)+FCT(Z))                          DH48 870
      X=.27473086248223832D1                                            DH48 880
      Z=-X                                                              DH48 890
      Y=Y+.17515043180117283D-3*(FCT(X)+FCT(Z))                         DH48 900
      X=.24167609048732165D1                                            DH48 910
      Z=-X                                                              DH48 920
      Y=Y+.95639231981941530-3*(FCT(X)+FCT(Z))                          DH48 930
      X=.20890866609442764D1                                            DH48 940
      Z=-X                                                              DH48 950
      Y=Y+.41530049119775525D-2*(FCT(X)+FCT(Z))                         DH48 960
      X=.17638175798953000D1                                            DH48 970
      Z=-X                                                              DH48 980
      Y=Y+.14444961574981099D-1*(FCT(X)+FCT(Z))                         DH48 990
      X=.14405252201375652D1                                            DH481000
      Z=-X                                                              DH481010
      Y=Y+.40479676984603849D-1*(FCT(X)+FCT(Z))                         DH481020
      X=.11188121524021566D1                                            DH481030
      Z=-X                                                              DH481040
      Y=Y+.91822297079285180-1*(FCT(X)+FCT(Z))                          DH481050
      X=.79830462777856220D0                                            DH481060
      Z=-X                                                              DH481070
      Y=Y+.16920447194564111D0*(FCT(X)+FCT(Z))                          DH481080
      X=.47864633759449610D0                                            DH481090
      Z=-X                                                              DH481100
      Y=Y+.25396154266475910D0*(FCT(X)+FCT(Z))                          DH481110
      X=.15949293586886247D0                                            DH481120
      Z=-X                                                              DH481130
      Y=Y+.31100103037796308D0*(FCT(X)+FCT(Z))                          DH481140
      RETURN                                                            DH481150
      END                                                               DH481160
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C                                                                       DH64  10
C     ...................................................................DH64  20
C                                                                       DH64  30
C        SUBROUTINE DQH64                                               DH64  40
C                                                                       DH64  50
C        PURPOSE                                                        DH64  60
C           TO COMPUTE INTEGRAL(EXP(-X**X)*FCT(X), SUMMED OVER X FROM   DH64  70
C                              -INFINITY TO +INFINITY).                 DH64  80
C                                                                       DH64  90
C        USAGE                                                          DH64 100
C           CALL DQH64 (FCT,Y)                                          DH64 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DH64 120
C                                                                       DH64 130
C        DESCRIPTION OF PARAMETERS                                      DH64 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DH64 150
C                    SUBPROGRAM USED.                                   DH64 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DH64 170
C                                                                       DH64 180
C        REMARKS                                                        DH64 190
C           NONE                                                        DH64 200
C                                                                       DH64 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DH64 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DH64 230
C           MUST BE FURNISHED BY THE USER.                              DH64 240
C                                                                       DH64 250
C        METHOD                                                         DH64 260
C           EVALUATION IS DONE BY MEANS OF 64-POINT GAUSSIAN-HERMITE    DH64 270
C           QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY WHENEVER       DH64 280
C           FCT(X) IS A POLYNOMIAL UP TO DEGREE 127.                    DH64 290
C           FOR REFERENCE, SEE                                          DH64 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DH64 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DH64 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DH64 330
C           TR00.1100 (MARCH 1964), PP.213-214.                         DH64 340
C                                                                       DH64 350
C     ...................................................................DH64 360
C                                                                       DH64 370
      SUBROUTINE DQH64(FCT,Y)                                           DH64 380
C                                                                       DH64 390
C                                                                       DH64 400
      DOUBLE PRECISION X,Y,Z,FCT                                        DH64 410
C                                                                       DH64 420
      X=.1052612316796054 6D2                                           DH64 430
      Z=-X                                                              DH64 440
      Y=.5535706535856942 8D-48*(FCT(X)+FCT(Z))                         DH64 450
      X=.9895287586825390 1                                             DH64 460
      Z=-X                                                              DH64 470
      Y=Y+.1679747990108159 2D-42*(FCT(X)+FCT(Z))                       DH64 480
      X=.9373159549646721 D1                                            DH64 490
      Z=-X                                                              DH64 500
      Y=Y+.3421138011255740 5D-38*(FCT(X)+FCT(Z))                       DH64 510
      X=.8907249099647700 1                                             DH64 520
      Z=-X                                                              DH64 530
      Y=Y+.1557390624629763 8D-34*(FCT(X)+FCT(Z))                       DH64 540
      X=.8477529083378630 1                                             DH64 550
      Z=-X                                                              DH64 560
      Y=Y+.2549660899112999 3D-31*(FCT(X)+FCT(Z))                       DH64 570
      X=.8073687285010225 01                                            DH64 580
      Z=-X                                                              DH64 590
      Y=Y+.1929103595946496 9D-28*(FCT(X)+FCT(Z))                       DH64 600
      X=.7689540164040497 D1                                            DH64 610
      Z=-X                                                              DH64 620
      Y=Y+.7861797788925910 D-26*(FCT(X)+FCT(Z))                        DH64 630
      X=.7321013032780949 D1                                            DH64 640
      Z=-X                                                              DH64 650
      Y=Y+.1911706883300642 8D-23*(FCT(X)+FCT(Z))                       DH64 660
      X=.6965241120551107 5D1                                           DH64 670
      Z=-X                                                              DH64 680
      Y=Y+.2982862784279851 2D-21*(FCT(X)+FCT(Z))                       DH64 690
      X=.6620112262636027 4D1                                           DH64 700
      Z=-X                                                              DH64 710
      Y=Y+.3152254566503781 4D-19*(FCT(X)+FCT(Z))                       DH64 720
      X=.6284011228774828 2D1                                           DH64 730
      Z=-X                                                              DH64 740
      Y=Y+.2351884710675819 1D-17*(FCT(X)+FCT(Z))                       DH64 750
      X=.5955666326799486 0D1                                           DH64 760
      Z=-X                                                              DH64 770
      Y=Y+.1280093391322438 0D-15*(FCT(X)+FCT(Z))                       DH64 780
      X=.5634052164349972 1D1                                           DH64 790
      Z=-X                                                              DH64 800
      Y=Y+.5218623726590847 5D-14*(FCT(X)+FCT(Z))                       DH64 810
      X=.5318325224633270 9D1                                           DH64 820
      Z=-X                                                              DH64 830
      Y=Y+.1628340730709720 4D-12*(FCT(X)+FCT(Z))                       DH64 840
      X=.5007779602198768 2D1                                           DH64 850
      Z=-X                                                              DH64 860
      Y=Y+.3959177766947723 9D-11*(FCT(X)+FCT(Z))                       DH64 870
      X=.4701815647407498 D1                                            DH64 880
      Z=-X                                                              DH64 890
      Y=Y+.7615217250145451 D-10*(FCT(X)+FCT(Z))                        DH64 900
      X=.4399917168228137 6D1                                           DH64 910
      Z=-X                                                              DH64 920
      Y=Y+.1173616742321549 3D-8*(FCT(X)+FCT(Z))                        DH64 930
      X=.4101634474566656 7D1                                           DH64 940
      Z=-X                                                              DH64 950
      Y=Y+.1465125316476109 4D-7*(FCT(X)+FCT(Z))                        DH64 960
      X=.3806571513945360 5D1                                           DH64 970
      Z=-X                                                              DH64 980
      Y=Y+.1495532936727247 1D-6*(FCT(X)+FCT(Z))                        DH64 990
      X=.3514375935740906 2D1                                           DH641000
      Z=-X                                                              DH641010
      Y=Y+.1258340251031184 6D-5*(FCT(X)+FCT(Z))                        DH641020
      X=.3224731291992035 7D1                                           DH641030
      Z=-X                                                              DH641040
      Y=Y+.8788499230850359 D-5*(FCT(X)+FCT(Z))                         DH641050
      X=.2937350823004621 8D1                                           DH641060
      Z=-X                                                              DH641070
      Y=Y+.5125929135786274 7D-4*(FCT(X)+FCT(Z))                        DH641080
      X=.2651972435430635 0D1                                           DH641090
      Z=-X                                                              DH641100
      Y=Y+.2509836985130624 9D-3*(FCT(X)+FCT(Z))                        DH641110
      X=.2368354588632401 4D1                                           DH641120
      Z=-X                                                              DH641130
      Y=Y+.1036329099507577 7D-2*(FCT(X)+FCT(Z))                        DH641140
      X=.2086272879881762 0D1                                           DH641150
      Z=-X                                                              DH641160
      Y=Y+.3622586978534458 8D-2*(FCT(X)+FCT(Z))                        DH641170
      X=.1805517171465544 9D1                                           DH641180
      Z=-X                                                              DH641190
      Y=Y+.1075604050987913 7D-1*(FCT(X)+FCT(Z))                        DH641200
      X=.1525889140209863 7D1                                           DH641210
      Z=-X                                                              DH641220
      Y=Y+.2720312895368891 8D-1*(FCT(X)+FCT(Z))                        DH641230
      X=.1247200156943117 9D1                                           DH641240
      Z=-X                                                              DH641250
      Y=Y+.5873998196409943 5D-1*(FCT(X)+FCT(Z))                        DH641260
      X=.9692694230711780 D0                                            DH641270
      Z=-X                                                              DH641280
      Y=Y+.1084983493061868 4D0*(FCT(X)+FCT(Z))                         DH641290
      X=.6919223058100445 8D0                                           DH641300
      Z=-X                                                              DH641310
      Y=Y+.1716858423490837 0D0*(FCT(X)+FCT(Z))                         DH641320
      X=.4149888241210786 8D0                                           DH641330
      Z=-X                                                              DH641340
      Y=Y+.2329947860626780 5D0*(FCT(X)+FCT(Z))                         DH641350
      X=.1383022449870972 D0                                            DH641360
      Z=-X                                                              DH641370
      Y=Y+.2713774249413039 8D0*(FCT(X)+FCT(Z))                         DH641380
      RETURN                                                            DH641390
      END                                                               DH641400
```

Subroutines QA2, QA3, ..., QA10, DQA4, DQA8, DQA12, DQA16, DQA24, DQA32

These subroutines perform the integration of a given function by associated Gaussian-Laguerre quadrature formulas:

To compute:

$$y = \int_0^\infty \frac{e^{-x} f(x)}{\sqrt{x}} \, dx$$

generalized Gaussian-Laguerre quadrature formulas with n = 2,3,..., 10 (or n = 4,8,12,16,24,32) points are used to get approximations:

$$y_n = \sum_{k=1}^{n} A_k^{(n)} f(x_k^{(n)}) \quad (n= 2,3,\ldots) \quad (1)$$

which are exact whenever f(x) is a polynomial up to the degree 2n-1. Note that the nodes $x_k^{(n)}$ are the roots of the associated Laguerre polynomials $L_n^{(-\frac{1}{2})}(x)$ of degree n.

For reference see:

(1) Concus/Cassatt/Jaehnig/Melby, "Tables for the Evaluation of $\int_0^\infty x^\beta \cdot e^{-x} \cdot f(x) \cdot dx$ by Gauss-Laguerre Quadrature", MTAC, vol. 17, No. 83 (1963), pp. 245-256.

(2) Shao/Chen/Frank, "Tables of Zeros and Gaussian Weights of Certain Associated Laguerre Polynomials and the Related Generalized Hermite Polynomials", IBM Technical Report TR 00.1100 (March 1964), pp. 15-16.

```
C                                                                       QA2   10
C     ..................................................................QA2   20
C                                                                       QA2   30
C        SUBROUTINE QA2                                                 QA2   40
C                                                                       QA2   50
C        PURPOSE                                                        QA2   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   QA2   70
C                              FROM 0 TO INFINITY).                     QA2   80
C                                                                       QA2   90
C        USAGE                                                          QA2  100
C           CALL QA2 (FCT,Y)                                            QA2  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QA2  120
C                                                                       QA2  130
C        DESCRIPTION OF PARAMETERS                                      QA2  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QA2  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QA2  160
C                                                                       QA2  170
C        REMARKS                                                        QA2  180
C           NONE                                                        QA2  190
C                                                                       QA2  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QA2  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QA2  220
C           BY THE USER.                                                QA2  230
C                                                                       QA2  240
C        METHOD                                                         QA2  250
C           EVALUATION IS DONE BY MEANS OF 2-POINT GENERALIZED GAUSSIAN-QA2  260
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,      QA2  270
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 3.             QA2  280
C           FOR REFERENCE, SEE                                          QA2  290
C           CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF  QA2  300
C           INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO      QA2  310
C           INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,       QA2  320
C           ISS.83 (1963), PP.245-256.                                  QA2  330
C                                                                       QA2  340
C     ..................................................................QA2  350
C                                                                       QA2  360
      SUBROUTINE QA2(FCT,Y)                                             QA2  370
C                                                                       QA2  380
C                                                                       QA2  390
      X=2.724745                                                        QA2  400
      Y=.1626257*FCT(X)                                                 QA2  410
      X=.2752551                                                        QA2  420
      Y=Y+1.609828*FCT(X)                                               QA2  430
      RETURN                                                            QA2  440
      END                                                               QA2  450
```

```
C                                                                       QA3   10
C     ..................................................................QA3   20
C                                                                       QA3   30
C        SUBROUTINE QA3                                                 QA3   40
C                                                                       QA3   50
C        PURPOSE                                                        QA3   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   QA3   70
C                              FROM 0 TO INFINITY).                     QA3   80
C                                                                       QA3   90
C        USAGE                                                          QA3  100
C           CALL QA3 (FCT,Y)                                            QA3  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QA3  120
C                                                                       QA3  130
C        DESCRIPTION OF PARAMETERS                                      QA3  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QA3  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QA3  160
C                                                                       QA3  170
C        REMARKS                                                        QA3  180
C           NONE                                                        QA3  190
C                                                                       QA3  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QA3  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QA3  220
C           BY THE USER.                                                QA3  230
C                                                                       QA3  240
C        METHOD                                                         QA3  250
C           EVALUATION IS DONE BY MEANS OF 3-POINT GENERALIZED GAUSSIAN-QA3  260
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,      QA3  270
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 5.             QA3  280
C           FOR REFERENCE, SEE                                          QA3  290
C           CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF  QA3  300
C           INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO      QA3  310
C           INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,       QA3  320
C           ISS.83 (1963), PP.245-256.                                  QA3  330
C                                                                       QA3  340
C     ..................................................................QA3  350
C                                                                       QA3  360
      SUBROUTINE QA3(FCT,Y)                                             QA3  370
C                                                                       QA3  380
C                                                                       QA3  390
      X=5.525344                                                        QA3  400
      Y=.0090600020*FCT(X)                                              QA3  410
      X=1.784493                                                        QA3  420
      Y=Y+.3141346*FCT(X)                                               QA3  430
      X=.1901635                                                        QA3  440
      Y=Y+1.449259*FCT(X)                                               QA3  450
      RETURN                                                            QA3  460
      END                                                               QA3  470
```

```
C                                                                       QA4   10
C     ..................................................................QA4   20
C                                                                       QA4   30
C        SUBROUTINE QA4                                                 QA4   40
C                                                                       QA4   50
C        PURPOSE                                                        QA4   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   QA4   70
C                              FROM 0 TO INFINITY).                     QA4   80
C                                                                       QA4   90
C        USAGE                                                          QA4  100
C           CALL QA4 (FCT,Y)                                            QA4  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QA4  120
C                                                                       QA4  130
C        DESCRIPTION OF PARAMETERS                                      QA4  140
C           FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.  QA4  150
C           Y      - THE RESULTING INTEGRAL VALUE.                      QA4  160
C                                                                       QA4  170
C        REMARKS                                                        QA4  180
C           NONE                                                        QA4  190
C                                                                       QA4  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QA4  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QA4  220
C           BY THE USER.                                                QA4  230
C                                                                       QA4  240
C        METHOD                                                         QA4  250
C           EVALUATION IS DONE BY MEANS OF 4-POINT GENERALIZED GAUSSIAN-QA4  260
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,      QA4  270
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 7.             QA4  280
C           FOR REFERENCE, SEE                                          QA4  290
C           CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF  QA4  300
C           INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO      QA4  310
C           INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,       QA4  320
C           ISS.83 (1963), PP.245-256.                                  QA4  330
C                                                                       QA4  340
C     ..................................................................QA4  350
C                                                                       QA4  360
      SUBROUTINE QA4(FCT,Y)                                             QA4  370
C                                                                       QA4  380
C                                                                       QA4  390
      X=8.588636                                                        QA4  400
      Y=.0003992081*FCT(X)                                              QA4  410
      X=3.926964                                                        QA4  420
      Y=Y+.03415597*FCT(X)                                              QA4  430
      X=1.339097                                                        QA4  440
      Y=Y+.4156047*FCT(X)                                               QA4  450
      X=.1453035                                                        QA4  460
      Y=Y+1.322294*FCT(X)                                               QA4  470
      RETURN                                                            QA4  480
      END                                                               QA4  490
```

```
C                                                                       DQA4  10
C  ...................................................................DQA4  20
C                                                                       DQA4  30
C     SUBROUTINE DQA4                                                   DQA4  40
C                                                                       DQA4  50
C     PURPOSE                                                           DQA4  60
C        TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X      DQA4  70
C                            FROM 0 TO INFINITY).                       DQA4  80
C                                                                       DQA4  90
C     USAGE                                                             DQA4 100
C        CALL DQA4 (FCT,Y)                                              DQA4 110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DQA4 120
C                                                                       DQA4 130
C     DESCRIPTION OF PARAMETERS                                         DQA4 140
C        FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION     DQA4 150
C                 SUBPROGRAM USED.                                      DQA4 160
C        Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.        DQA4 170
C                                                                       DQA4 180
C     REMARKS                                                           DQA4 190
C        NONE                                                           DQA4 200
C                                                                       DQA4 210
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DQA4 220
C        THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)       DQA4 230
C        MUST BE FURNISHED BY THE USER.                                 DQA4 240
C                                                                       DQA4 250
C     METHOD                                                            DQA4 260
C        EVALUATION IS DONE BY MEANS OF 4-POINT GENERALIZED GAUSS-      DQA4 270
C        LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY          DQA4 280
C        WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 7.                DQA4 290
C        FOR REFERENCE, SEE                                             DQA4 300
C        SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF       DQA4 310
C        CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED        DQA4 320
C        GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT          DQA4 330
C        TR00.1100 (MARCH 1964), PP.15-16.                              DQA4 340
C                                                                       DQA4 350
C  ...................................................................DQA4 360
C                                                                       DQA4 370
      SUBROUTINE DQA4(FCT,Y)                                            DQA4 380
C                                                                       DQA4 390
C                                                                       DQA4 400
      DOUBLE PRECISION X,Y,FCT                                          DQA4 410
C                                                                       DQA4 420
      X=.85886356890120340                                              DQA4 430
      Y=.39920814442735240-3*FCT(X)                                     DQA4 440
      X=.39269635013582872D1                                            DQA4 450
      Y=Y+.34155966014826951D-1*FCT(X)                                  DQA4 460
      X=.13390972881263614D1                                            DQA4 470
      Y=Y+.41560465162978376D0*FCT(X)                                   DQA4 480
      X=.14530352150331709D0                                            DQA4 490
      Y=Y+.13222940251164826D1*FCT(X)                                   DQA4 500
      RETURN                                                            DQA4 510
      END                                                               DQA4 520
```

```
C                                                                       QA6   10
C  ...................................................................QA6   20
C                                                                       QA6   30
C     SUBROUTINE QA6                                                    QA6   40
C                                                                       QA6   50
C     PURPOSE                                                           QA6   60
C        TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X      QA6   70
C                            FROM 0 TO INFINITY).                       QA6   80
C                                                                       QA6   90
C     USAGE                                                             QA6  100
C        CALL QA6 (FCT,Y)                                               QA6  110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   QA6  120
C                                                                       QA6  130
C     DESCRIPTION OF PARAMETERS                                         QA6  140
C        FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.     QA6  150
C        Y      - THE RESULTING INTEGRAL VALUE.                         QA6  160
C                                                                       QA6  170
C     REMARKS                                                           QA6  180
C        NONE                                                           QA6  190
C                                                                       QA6  200
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     QA6  210
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED      QA6  220
C        BY THE USER.                                                   QA6  230
C                                                                       QA6  240
C     METHOD                                                            QA6  250
C        EVALUATION IS DONE BY MEANS OF 6-POINT GENERALIZED GAUSSIAN-   QA6  260
C        LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,         QA6  270
C        WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 11.               QA6  280
C        FOR REFERENCE, SEE                                             QA6  290
C        CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF     QA6  300
C        INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO         QA6  310
C        INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,          QA6  320
C        ISS.83 (1963), PP.245-256.                                     QA6  330
C                                                                       QA6  340
C  ...................................................................QA6  350
C                                                                       QA6  360
      SUBROUTINE QA6(FCT,Y)                                             QA6  370
C                                                                       QA6  380
C                                                                       QA6  390
      X=15.12996                                                        QA6  400
      Y=.53171103E-6*FCT(X)                                             QA6  410
      X=9.124248                                                        QA6  420
      Y=Y+.00017147370*FCT(X)                                           QA6  430
      X=5.196153                                                        QA6  440
      Y=Y+.00781078l*FCT(X)                                             QA6  450
      X=2.552590                                                        QA6  460
      Y=Y+.1032160*FCT(X)                                               QA6  470
      X=.8983028                                                        QA6  480
      Y=Y+.5209846*FCT(X)                                               QA6  490
      X=.09874701                                                       QA6  500
      Y=Y+1.140270*FCT(X)                                               QA6  510
      RETURN                                                            QA6  520
      END                                                               QA6  530
```

```
C                                                                       QA5   10
C  ...................................................................QA5   20
C                                                                       QA5   30
C     SUBROUTINE QA5                                                    QA5   40
C                                                                       QA5   50
C     PURPOSE                                                           QA5   60
C        TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X      QA5   70
C                            FROM 0 TO INFINITY).                       QA5   80
C                                                                       QA5   90
C     USAGE                                                             QA5  100
C        CALL QA5 (FCT,Y)                                               QA5  110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   QA5  120
C                                                                       QA5  130
C     DESCRIPTION OF PARAMETERS                                         QA5  140
C        FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.     QA5  150
C        Y      - THE RESULTING INTEGRAL VALUE.                         QA5  160
C                                                                       QA5  170
C     REMARKS                                                           QA5  180
C        NONE                                                           QA5  190
C                                                                       QA5  200
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     QA5  210
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED      QA5  220
C        BY THE USER.                                                   QA5  230
C                                                                       QA5  240
C     METHOD                                                            QA5  250
C        EVALUATION IS DONE BY MEANS OF 5-POINT GENERALIZED GAUSSIAN-   QA5  260
C        LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,         QA5  270
C        WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 9.                QA5  280
C        FOR REFERENCE, SEE                                             QA5  290
C        CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF     QA5  300
C        INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO         QA5  310
C        INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,          QA5  320
C        ISS.83 (1963), PP.245-256.                                     QA5  330
C                                                                       QA5  340
C  ...................................................................QA5  350
C                                                                       QA5  360
      SUBROUTINE QA5(FCT,Y)                                             QA5  370
C                                                                       QA5  380
C                                                                       QA5  390
      X=11.80719                                                        QA5  400
      Y=.1528087E-4*FCT(X)                                              QA5  410
      X=6.414730                                                        QA5  420
      Y=Y+.002687291*FCT(X)                                             QA5  430
      X=3.085937                                                        QA5  440
      Y=Y+.06774879*FCT(X)                                              QA5  450
      X=1.074562                                                        QA5  460
      Y=Y+.4802772*FCT(X)                                               QA5  470
      X=-.1175813                                                       QA5  480
      Y=Y+1.221725*FCT(X)                                               QA5  490
      RETURN                                                            QA5  500
      END                                                               QA5  510
```

```
C                                                                       QA7   10
C  ...................................................................QA7   20
C                                                                       QA7   30
C     SUBROUTINE QA7                                                    QA7   40
C                                                                       QA7   50
C     PURPOSE                                                           QA7   60
C        TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X      QA7   70
C                            FROM 0 TO INFINITY).                       QA7   80
C                                                                       QA7   90
C     USAGE                                                             QA7  100
C        CALL QA7 (FCT,Y)                                               QA7  110
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   QA7  120
C                                                                       QA7  130
C     DESCRIPTION OF PARAMETERS                                         QA7  140
C        FCT    - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED.     QA7  150
C        Y      - THE RESULTING INTEGRAL VALUE.                         QA7  160
C                                                                       QA7  170
C     REMARKS                                                           QA7  180
C        NONE                                                           QA7  190
C                                                                       QA7  200
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     QA7  210
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED      QA7  220
C        BY THE USER.                                                   QA7  230
C                                                                       QA7  240
C     METHOD                                                            QA7  250
C        EVALUATION IS DONE BY MEANS OF 7-POINT GENERALIZED GAUSSIAN-   QA7  260
C        LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,         QA7  270
C        WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 13.               QA7  280
C        FOR REFERENCE, SEE                                             QA7  290
C        CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF     QA7  300
C        INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO         QA7  310
C        INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,          QA7  320
C        ISS.83 (1963), PP.245-256.                                     QA7  330
C                                                                       QA7  340
C  ...................................................................QA7  350
C                                                                       QA7  360
      SUBROUTINE QA7(FCT,Y)                                             QA7  370
C                                                                       QA7  380
C                                                                       QA7  390
      X=18.52828                                                        QA7  400
      Y=.1725718E-7*FCT(X)                                              QA7  410
      X=11.93999                                                        QA7  420
      Y=Y+.9432969E-5*FCT(X)                                            QA7  430
      X=7.554091                                                        QA7  440
      Y=Y+.0007101852*FCT(X)                                            QA7  450
      X=4.389793                                                        QA7  460
      Y=Y+.01570911*FCT(X)                                              QA7  470
      X=2.180592                                                        QA7  480
      Y=Y+.1370111*FCT(X)                                               QA7  490
      X=.7721379                                                        QA7  500
      Y=Y+.5462112*FCT(X)                                               QA7  510
      X=.08511544                                                       QA7  520
      Y=Y+1.072812*FCT(X)                                               QA7  530
      RETURN                                                            QA7  540
      END                                                               QA7  550
```

```
C                                                                       QA8   10
C     ...................................................................QA8   20
C                                                                       QA8   30
C        SUBROUTINE QA8                                                 QA8   40
C                                                                       QA8   50
C        PURPOSE                                                        QA8   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   QA8   70
C                              FROM 0 TO INFINITY).                     QA8   80
C                                                                       QA8   90
C        USAGE                                                          QA8  100
C           CALL QA8 (FCT,Y)                                            QA8  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QA8  120
C                                                                       QA8  130
C        DESCRIPTION OF PARAMETERS                                      QA8  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QA8  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QA8  160
C                                                                       QA8  170
C        REMARKS                                                        QA8  180
C           NONE                                                        QA8  190
C                                                                       QA8  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QA8  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QA8  220
C           BY THE USER.                                                QA8  230
C                                                                       QA8  240
C        METHOD                                                         QA8  250
C           EVALUATION IS DONE BY MEANS OF 8-POINT GENERALIZED GAUSSIAN-QA8  260
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,      QA8  270
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 15.            QA8  280
C           FOR REFERENCE, SEE                                          QA8  290
C           CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF  QA8  300
C           INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO      QA8  310
C           INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,       QA8  320
C           ISS.83 (1963), PP.245-256.                                  QA8  330
C                                                                       QA8  340
C     ...................................................................QA8  350
C                                                                       QA8  360
      SUBROUTINE QA8(FCT,Y)                                             QA8  370
C                                                                       QA8  380
C                                                                       QA8  390
      X=21.99427                                                        QA8  400
      Y=.5309615E-9*FCT(X)                                              QA8  410
      X=14.97262                                                        QA8  420
      Y=Y+.4641962E-6*FCT(X)                                            QA8  430
      X=10.09332                                                        QA8  440
      Y=Y+.5423720E-4*FCT(X)                                            QA8  450
      X=6.483145                                                        QA8  460
      Y=Y+.001854568*FCT(X)                                             QA8  470
      X=3.809476                                                        QA8  480
      Y=Y+.02576062*FCT(X)                                              QA8  490
      X=1.905114                                                        QA8  500
      Y=Y+.1676201*FCT(X)                                               QA8  510
      X=.6772491                                                        QA8  520
      Y=Y+.5612949*FCT(X)                                               QA8  530
      X=.07479188                                                       QA8  540
      Y=Y+1.015859*FCT(X)                                               QA8  550
      RETURN                                                            QA8  560
      END                                                               QA8  570
```

```
C                                                                       QA9   10
C     ...................................................................QA9   20
C                                                                       QA9   30
C        SUBROUTINE QA9                                                 QA9   40
C                                                                       QA9   50
C        PURPOSE                                                        QA9   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   QA9   70
C                              FROM 0 TO INFINITY).                     QA9   80
C                                                                       QA9   90
C        USAGE                                                          QA9  100
C           CALL QA9 (FCT,Y)                                            QA9  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                QA9  120
C                                                                       QA9  130
C        DESCRIPTION OF PARAMETERS                                      QA9  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QA9  150
C           Y       - THE RESULTING INTEGRAL VALUE.                     QA9  160
C                                                                       QA9  170
C        REMARKS                                                        QA9  180
C           NONE                                                        QA9  190
C                                                                       QA9  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QA9  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED   QA9  220
C           BY THE USER.                                                QA9  230
C                                                                       QA9  240
C        METHOD                                                         QA9  250
C           EVALUATION IS DONE BY MEANS OF 9-POINT GENERALIZED GAUSSIAN-QA9  260
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,      QA9  270
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 17.            QA9  280
C           FOR REFERENCE, SEE                                          QA9  290
C           CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF  QA9  300
C           INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO      QA9  310
C           INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,       QA9  320
C           ISS.83 (1963), PP.245-256.                                  QA9  330
C                                                                       QA9  340
C     ...................................................................QA9  350
C                                                                       QA9  360
      SUBROUTINE QA9(FCT,Y)                                             QA9  370
C                                                                       QA9  380
C                                                                       QA9  390
      X=25.48598                                                        QA9  400
      Y=.1565640E-10*FCT(X)                                             QA9  410
      X=18.04651                                                        QA9  420
      Y=Y+.2093441E-7*FCT(X)                                            QA9  430
      X=12.77183                                                        QA9  440
      Y=Y+.3621309E-5*FCT(X)                                            QA9  450
      X=8.769757                                                        QA9  460
      Y=Y+.0001836225*FCT(X)                                            QA9  470
      X=5.694423                                                        QA9  480
      Y=Y+.003777045*FCT(X)                                             QA9  490
      X=3.369176                                                        QA9  500
      Y=Y+.03728008*FCT(X)                                              QA9  510
      X=1.692395                                                        QA9  520
      Y=Y+.1946035*FCT(X)                                               QA9  530
      X=.6032364                                                        QA9  540
      Y=Y+.5696146*FCT(X)                                               QA9  550
      X=.06670223                                                       QA9  560
      Y=Y+.9669914*FCT(X)                                               QA9  570
      RETURN                                                            QA9  580
      END                                                               QA9  590
```

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C                                                                      DQA8   10
C     ...................................................................DQA8   20
C                                                                      DQA8   30
C        SUBROUTINE DQA8                                               DQA8   40
C                                                                      DQA8   50
C        PURPOSE                                                       DQA8   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X  DQA8   70
C                              FROM 0 TO INFINITY).                    DQA8   80
C                                                                      DQA8   90
C        USAGE                                                         DQA8  100
C           CALL DQA8 (FCT,Y)                                          DQA8  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT               DQA8  120
C                                                                      DQA8  130
C        DESCRIPTION OF PARAMETERS                                     DQA8  140
C           FCT     - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION DQA8 150
C                     SUBPROGRAM USED.                                 DQA8  160
C           Y       - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.   DQA8  170
C                                                                      DQA8  180
C        REMARKS                                                       DQA8  190
C           NONE                                                       DQA8  200
C                                                                      DQA8  210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 DQA8  220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)   DQA8  230
C           MUST BE FURNISHED BY THE USER.                             DQA8  240
C                                                                      DQA8  250
C        METHOD                                                        DQA8  260
C           EVALUATION IS DONE BY MEANS OF 8-POINT GENERALIZED GAUSS-  DQA8  270
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY      DQA8  280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 15.           DQA8  290
C           FOR REFERENCE, SEE                                         DQA8  300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF   DQA8  310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED    DQA8  320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT      DQA8  330
C           TR00.1100 (MARCH 1964), PP.15-16.                          DQA8  340
C                                                                      DQA8  350
C     ...................................................................DQA8  360
      SUBROUTINE DQA8(FCT,Y)                                           DQA8  370
C                                                                      DQA8  380
C                                                                      DQA8  390
      DOUBLE PRECISION X,Y,FCT                                         DQA8  400
C                                                                      DQA8  410
      X=.2198427284096265102                                           DQA8  420
      Y=.5309614948022364502-9*FCT(X)                                  DQA8  430
      X=.1497262708842639302                                           DQA8  440
      Y=Y+.4641961689730421302-6*FCT(X)                                DQA8  450
      X=.1009332367522134302                                           DQA8  460
      Y=Y+.5423720185075763002-4*FCT(X)                                DQA8  470
      X=.6483145428627170401                                           DQA8  480
      Y=Y+.1864568617248361102-2*FCT(X)                                DQA8  490
      X=.3809476361484907102                                           DQA8  500
      Y=Y+.2576062307101994702-1*FCT(X)                                DQA8  510
      X=.1905113635031428401                                           DQA8  520
      Y=Y+.1676200827979716600*FCT(X)                                  DQA8  530
      X=.6772490876492891500                                           DQA8  540
      Y=Y+.5612949170570673500*FCT(X)                                  DQA8  550
      X=.7479188259681827D-1                                           DQA8  560
      Y=Y+.1015858958033227501*FCT(X)                                  DQA8  570
      RETURN                                                           DQA8  580
      END                                                              DQA8  590
                                                                       DQA8  600
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C                                                                      QA10   10
C     ...................................................................QA10   20
C                                                                      QA10   30
C        SUBROUTINE QA10                                               QA10   40
C                                                                      QA10   50
C        PURPOSE                                                       QA10   60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X  QA10   70
C                              FROM 0 TO INFINITY).                    QA10   80
C                                                                      QA10   90
C        USAGE                                                         QA10  100
C           CALL QA10 (FCT,Y)                                          QA10  110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT               QA10  120
C                                                                      QA10  130
C        DESCRIPTION OF PARAMETERS                                     QA10  140
C           FCT     - THE NAME OF AN EXTERNAL FUNCTION SUBPROGRAM USED. QA10 150
C           Y       - THE RESULTING INTEGRAL VALUE.                    QA10  160
C                                                                      QA10  170
C        REMARKS                                                       QA10  180
C           NONE                                                       QA10  190
C                                                                      QA10  200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 QA10  210
C           THE EXTERNAL FUNCTION SUBPROGRAM FCT(X) MUST BE FURNISHED  QA10  220
C           BY THE USER.                                               QA10  230
C                                                                      QA10  240
C        METHOD                                                        QA10  250
C           EVALUATION IS DONE BY MEANS OF 10-POINT GENERALIZED GAUSS- QA10  260
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY,     QA10  270
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 19.           QA10  280
C           FOR REFERENCE, SEE                                         QA10  290
C           CONCUS/CASSATT/JAEHNIG/MELBY, TABLES FOR THE EVALUATION OF QA10  300
C           INTEGRAL(X**BETA*EXP(-X)*F(X), SUMMED OVER X FROM 0 TO     QA10  310
C           INFINITY) BY GAUSS-LAGUERRE QUADRATURE, MTAC, VOL.17,      QA10  320
C           ISS.83 (1963), PP.245-256.                                 QA10  330
C                                                                      QA10  340
C     ...................................................................QA10  350
      SUBROUTINE QA10(FCT,Y)                                           QA10  360
C                                                                      QA10  370
C                                                                      QA10  380
      X=29.02495                                                       QA10  390
      Y=-.4458787E-12*FCT(X)                                           QA10  400
      X=21.19389                                                       QA10  410
      Y=Y+.8798682E-9*FCT(X)                                           QA10  420
      X=15.56116                                                       QA10  430
      Y=Y+.2172139E-6*FCT(X)                                           QA10  440
      X=11.20813                                                       QA10  450
      Y=Y+.1560511E-4*FCT(X)                                           QA10  460
      X=7.777439                                                       QA10  470
      Y=Y+.0004566773*FCT(X)                                           QA10  480
      X=5.084908                                                       QA10  490
      Y=Y+.006487547*FCT(X)                                            QA10  500
      X=3.022513                                                       QA10  510
      Y=Y+.04962104*FCT(X)                                             QA10  520
      X=1.522944                                                       QA10  530
      Y=Y+.2180344*FCT(X)                                              QA10  540
      X=.5438675                                                       QA10  550
      Y=Y+.5733510*FCT(X)                                              QA10  560
      X=.06019206                                                      QA10  570
      Y=Y+.9244873*FCT(X)                                              QA10  580
      RETURN                                                           QA10  590
      END                                                              QA10  600
                                                                       QA10  610
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C                                                                       DA12  10
C     ..................................................................DA12  20
C                                                                       DA12  30
C        SUBROUTINE DQA12                                               DA12  40
C                                                                       DA12  50
C        PURPOSE                                                        DA12  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   DA12  70
C                              FROM 0 TO INFINITY).                     DA12  80
C                                                                       DA12  90
C        USAGE                                                          DA12 100
C           CALL DQA12 (FCT,Y)                                          DA12 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DA12 120
C                                                                       DA12 130
C        DESCRIPTION OF PARAMETERS                                      DA12 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DA12 150
C                    SUBPROGRAM USED.                                   DA12 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DA12 170
C                                                                       DA12 180
C        REMARKS                                                        DA12 190
C           NONE                                                        DA12 200
C                                                                       DA12 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DA12 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DA12 230
C           MUST BE FURNISHED BY THE USER.                              DA12 240
C                                                                       DA12 250
C        METHOD                                                         DA12 260
C           EVALUATION IS DONE BY MEANS OF 12-POINT GENERALIZED GAUSS-  DA12 270
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY       DA12 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 23.            DA12 290
C           FOR REFERENCE, SEE                                          DA12 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DA12 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DA12 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DA12 330
C           TR00.1100 (MARCH 1964), PP.15-16.                           DA12 340
C                                                                       DA12 350
C     ..................................................................DA12 360
      SUBROUTINE DQA12(FCT,Y)                                           DA12 370
C                                                                       DA12 380
C                                                                       DA12 390
      DOUBLE PRECISION X,Y,FCT                                          DA12 400
C                                                                       DA12 410
      X=.3619136036061560202                                            DA12 420
      Y=.33287369929782177D-15*FCT(X)                                   DA12 430
      X=.2766110877984609002                                            DA12 440
      Y=Y+.13169240486156340D-11*FCT(X)                                 DA12 450
      X=.2139675593616109D2                                             DA12 460
      Y=Y+.60925085399751278D-9*FCT(X)                                  DA12 470
      X=.1643219508767531302                                            DA12 480
      Y=Y+.80379423498828590-7*FCT(X)                                   DA12 490
      X=.1239044796380947102                                            DA12 500
      Y=Y+.43164914098046673D-5*FCT(X)                                  DA12 510
      X=.9075434230961203D1                                             DA12 520
      Y=Y+.11377383272808760D-3*FCT(X)                                  DA12 530
      X=.6369975388030634901                                            DA12 540
      Y=Y+.16473849653768349D-2*FCT(X)                                  DA12 550
      X=.4198415644878413201                                            DA12 560
      Y=Y+.14096711620145342D-1*FCT(X)'                                 DA12 570
      X=.2509848097232128001                                            DA12 580
      Y=Y+.74890941006461490-1*FCT(X)                                   DA12 590
      X=.1269589940103961501                                            DA12 600
      Y=Y+.25547924356911832D0*FCT(X)                                   DA12 610
      X=.4545066815637802D0                                             DA12 620
      Y=Y+.57235907069288604D0*FCT(X)                                   DA12 630
      X=.5036188911729395ID-1                                           DA12 640
      Y=Y+.85386232773739850D0*FCT(X)                                   DA12 650
      RETURN                                                            DA12 660
      END                                                               DA12 670
                                                                        DA12 680
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C                                                                       DA16  10
C     ..................................................................DA16  20
C                                                                       DA16  30
C        SUBROUTINE DQA16                                               DA16  40
C                                                                       DA16  50
C        PURPOSE                                                        DA16  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   DA16  70
C                              FROM 0 TO INFINITY).                     DA16  80
C                                                                       DA16  90
C        USAGE                                                          DA16 100
C           CALL DQA16 (FCT,Y)                                          DA16 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DA16 120
C                                                                       DA16 130
C        DESCRIPTION OF PARAMETERS                                      DA16 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DA16 150
C                    SUBPROGRAM USED.                                   DA16 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DA16 170
C                                                                       DA16 180
C        REMARKS                                                        DA16 190
C           NONE                                                        DA16 200
C                                                                       DA16 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DA16 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DA16 230
C           MUST BE FURNISHED BY THE USER.                              DA16 240
C                                                                       DA16 250
C        METHOD                                                         DA16 260
C           EVALUATION IS DONE BY MEANS OF 16-POINT GENERALIZED GAUSS-  DA16 270
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY       DA16 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 31.            DA16 290
C           FOR REFERENCE, SEE                                          DA16 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DA16 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DA16 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DA16 330
C           TR00.1100 (MARCH 1964), PP.15-16.                           DA16 340
C                                                                       DA16 350
C     ..................................................................DA16 360
      SUBROUTINE DQA16(FCT,Y)                                           DA16 370
C                                                                       DA16 380
C                                                                       DA16 390
      DOUBLE PRECISION X,Y,FCT                                          DA16 400
C                                                                       DA16 410
      X=.5077722387753708002                                            DA16 420
      Y=.14621352854768325D-21*FCT(X)                                   DA16 430
      X=.4108166652549120202                                            DA16 440
      Y=Y+.18463473073036584D-17*FCT(X)                                 DA16 450
      X=.3378197048822616602                                            DA16 460
      Y=Y+.23946880341856973D-14*FCT(X)                                 DA16 470
      X=.2783143821132867602                                            DA16 480
      Y=Y+.84300204226528950-12*FCT(X)                                  DA16 490
      X=.2282130069352520802                                            DA16 500
      Y=Y+.11866582926793277D-9*FCT(X)                                  DA16 510
      X=.1853774317860669402                                            DA16 520
      Y=Y+.81976643295417930-8*FCT(X)                                   DA16 530
      X=.1485143134180125002                                            DA16 540
      Y=Y+.31483355850911881D-6*FCT(X)                                  DA16 550
      X=.1167703367397595702                                            DA16 560
      Y=Y+.73011702591247520-5*FCT(X)                                   DA16 570
      X=.8955001337723390001                                            DA16 580
      Y=Y+.10833168123639965D-3*FCT(X)                                  DA16 590
      X=.6642215179741444001                                            DA16 600
      Y=Y+.10725367310559441D-2*FCT(X)                                  DA16 610
      X=.4706726707667587201                                            DA16 620
      Y=Y+.73097806533088560-2*FCT(X)                                   DA16 630
      X=.3124601050702144301                                            DA16 640
      Y=Y+.35106857663146861D-1*FCT(X)                                  DA16 650
      X=.1877931507696074301                                            DA16 660
      Y=Y+.12091626191182523D0*FCT(X)                                   DA16 670
      X=.9535531553908655D0                                             DA16 680
      Y=Y+.30253946815328497D0*FCT(X)                                   DA16 690
      X=.3422001560109476800                                            DA16 700
      Y=Y+.55491628460505980D0*FCT(X)                                   DA16 710
      X=.3796291457531345501                                            DA16 720
      Y=Y+.75047670518560480*FCT(X)                                     DA16 730
      RETURN                                                            DA16 740
      END                                                               DA16 750
                                                                        DA16 760
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C                                                                       DA24  10
C     ..................................................................DA24  20
C                                                                       DA24  30
C        SUBROUTINE DQA24                                               DA24  40
C                                                                       DA24  50
C        PURPOSE                                                        DA24  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   DA24  70
C                              FROM 0 TO INFINITY).                     DA24  80
C                                                                       DA24  90
C        USAGE                                                          DA24 100
C           CALL DQA24 (FCT,Y)                                          DA24 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DA24 120
C                                                                       DA24 130
C        DESCRIPTION OF PARAMETERS                                      DA24 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DA24 150
C                    SUBPROGRAM USED.                                   DA24 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DA24 170
C                                                                       DA24 180
C        REMARKS                                                        DA24 190
C           NONE                                                        DA24 200
C                                                                       DA24 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DA24 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DA24 230
C           MUST BE FURNISHED BY THE USER.                              DA24 240
C                                                                       DA24 250
C        METHOD                                                         DA24 260
C           EVALUATION IS DONE BY MEANS OF 24-POINT GENERALIZED GAUSS-  DA24 270
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY       DA24 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 47.            DA24 290
C           FOR REFERENCE, SEE                                          DA24 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DA24 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DA24 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DA24 330
C           TR00.1100 (MARCH 1964), PP.15-16.                           DA24 340
C                                                                       DA24 350
C     ..................................................................DA24 360
C                                                                       DA24 370
      SUBROUTINE DQA24(FCT,Y)                                           DA24 380
C                                                                       DA24 390
C                                                                       DA24 400
      DOUBLE PRECISION X,Y,FCT                                          DA24 410
C                                                                       DA24 420
      X=.8055628081995041D2                                             DA24 430
      Y=.1587110292154799940-34*FCT(X)                                  DA24 440
      X=.6906860197530436902                                            DA24 450
      Y=Y+.1196922538662775 7D-29*FCT(X)                                DA24 460
      X=.6020666963057223D2                                             DA24 470
      Y=Y+.737007216030134 00-26*FCT(X)                                 DA24 480
      X=.5279543252728363002                                            DA24 490
      Y=Y+.1112915493780457 0D-22*FCT(X)                                DA24 500
      X=.4637697955754013302                                            DA24 510
      Y=Y+.6376774647010276 9D-20*FCT(X)                                DA24 520
      X=.4071159818554310702                                            DA24 530
      Y=Y+.1746031902373353D-17*FCT(X)                                  DA24 540
      X=.3565370351632821202                                            DA24 550
      Y=Y+.2630319245316817 0D-15*FCT(X)                                DA24 560
      X=.3110646470904656502                                            DA24 570
      Y=Y+.2395179730958358 7D-13*FCT(X)                                DA24 580
      X=.2700140605647235602                                            DA24 590
      Y=Y+.1409386516309178 8D-11*FCT(X)                                DA24 600
      X=.2328793282487991702                                            DA24 610
      Y=Y+.5630593075676376 2D-10*FCT(X)                                DA24 620
      X=.1992742587524624202                                            DA24 630
      Y=Y+.1586093499033076 5D-8*FCT(X)                                 DA24 640
      X=.1688967192852710802                                            DA24 650
      Y=Y+.3245028271791539 7D-7*FCT(X)                                 DA24 660
      X=.1415058618728575902                                            DA24 670
      Y=Y+.4937317987339501 00-6*FCT(X)                                 DA24 680
      X=.1169069592605607302                                            DA24 690
      Y=Y+.5694517383469696 20-5*FCT(X)                                 DA24 700
      X=.9494095330026488D1                                             DA24 710
      Y=Y+.5057198055496977 8D-4*FCT(X)                                 DA24 720
      X=.7547704680023454D1                                             DA24 730
      Y=Y+.3503008636023456 60-3*FCT(X)                                 DA24 740
      X=.5840733271323608001                                            DA24 750
      Y=Y+.1912784639638830 60-2*FCT(X)                                 DA24 760
      X=.4364280769353062D1                                             DA24 770
      Y=Y+.8306009823955105 0-2*FCT(X)                                  DA24 780
      X=.3111052455147713001                                            DA24 790
      Y=Y+.2888992314996219 9D-1*FCT(X)                                 DA24 800
      X=.2075112909852380601                                            DA24 810
      Y=Y+.8095935396920770 0-1*FCT(X)                                  DA24 820
      X=.1251740632627464D1                                             DA24 830
      Y=Y+.1836445941585703 6D0*FCT(X)                                  DA24 840
      X=.6372902787326687900                                            DA24 850
      Y=Y+.3384089438912822 1D0*FCT(X)                                  DA24 860
      X=.2291023164926243300                                            DA24 870
      Y=Y+.5079230853295182 0D0*FCT(X)                                  DA24 880
      X=.2543799658568935 90-1                                          DA24 890
      Y=Y+.6220020607559261 6D0*FCT(X)                                  DA24 900
      RETURN                                                            DA24 910
      END                                                               DA24 920
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C                                                                       DA32  10
C     ..................................................................DA32  20
C                                                                       DA32  30
C        SUBROUTINE DQA32                                               DA32  40
C                                                                       DA32  50
C        PURPOSE                                                        DA32  60
C           TO COMPUTE INTEGRAL(EXP(-X)*FCT(X)/SQRT(X), SUMMED OVER X   DA32  70
C                              FROM 0 TO INFINITY).                     DA32  80
C                                                                       DA32  90
C        USAGE                                                          DA32 100
C           CALL DQA32 (FCT,Y)                                          DA32 110
C           PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                DA32 120
C                                                                       DA32 130
C        DESCRIPTION OF PARAMETERS                                      DA32 140
C           FCT    - THE NAME OF AN EXTERNAL DOUBLE PRECISION FUNCTION  DA32 150
C                    SUBPROGRAM USED.                                   DA32 160
C           Y      - THE RESULTING DOUBLE PRECISION INTEGRAL VALUE.     DA32 170
C                                                                       DA32 180
C        REMARKS                                                        DA32 190
C           NONE                                                        DA32 200
C                                                                       DA32 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DA32 220
C           THE EXTERNAL DOUBLE PRECISION FUNCTION SUBPROGRAM FCT(X)    DA32 230
C           MUST BE FURNISHED BY THE USER.                              DA32 240
C                                                                       DA32 250
C        METHOD                                                         DA32 260
C           EVALUATION IS DONE BY MEANS OF 32-POINT GENERALIZED GAUSS-  DA32 270
C           LAGUERRE QUADRATURE FORMULA, WHICH INTEGRATES EXACTLY       DA32 280
C           WHENEVER FCT(X) IS A POLYNOMIAL UP TO DEGREE 63.            DA32 290
C           FOR REFERENCE, SEE                                          DA32 300
C           SHAO/CHEN/FRANK, TABLES OF ZEROS AND GAUSSIAN WEIGHTS OF    DA32 310
C           CERTAIN ASSOCIATED LAGUERRE POLYNOMIALS AND THE RELATED     DA32 320
C           GENERALIZED HERMITE POLYNOMIALS, IBM TECHNICAL REPORT       DA32 330
C           TR00.1100 (MARCH 1964), PP.15-16.                           DA32 340
C                                                                       DA32 350
C     ..................................................................DA32 360
C                                                                       DA32 370
      SUBROUTINE DQA32(FCT,Y)                                           DA32 380
C                                                                       DA32 390
C                                                                       DA32 400
      DOUBLE PRECISION X,Y,FCT                                          DA32 410
C                                                                       DA32 420
      X=.1107992689470757603                                            DA32 430
      Y=.1107141307171388 60-47*FCT(X)                                  DA32 440
      X=.9791671642606276D2                                             DA32 450
      Y=Y+.3359495980216318 4D-42*FCT(X)                                DA32 460
      X=.8785611994313352D2                                             DA32 470
      Y=Y+.6842276022511481 00-38*FCT(X)                                DA32 480
      X=.7933908652882320D2                                             DA32 490
      Y=Y+.3114791249259527 6D-34*FCT(X)                                DA32 500
      X=.7186849935955142 2D2                                           DA32 510
      Y=Y+.5099321798225998 5D-31*FCT(X)                                DA32 520
      X=.6518442637613578 2D2                                           DA32 530
      Y=Y+.3858207190929933 7D-28*FCT(X)                                DA32 540
      X=.5912902793439195 1D2                                           DA32 550
      Y=Y+.1572359557785182 1D-25*FCT(X)                                DA32 560
      X=.5359723182614851 2D2                                           DA32 570
      Y=Y+.3823413766601285 7D-23*FCT(X)                                DA32 580
      X=.4851458386741604 8D2                                           DA32 590
      Y=Y+.5965725568559702 3D-21*FCT(X)                                DA32 600
      X=.4382588636990390 2D2                                           DA32 610
      Y=Y+.6304509133007562 8D-19*FCT(X)                                DA32 620
      X=.3948879712336812 7D2                                           DA32 630
      Y=Y+.4703769421351638 2D-17*FCT(X)                                DA32 640
      X=.3546996139617328 3D2                                           DA32 650
      Y=Y+.2560186782644876 1D-15*FCT(X)                                DA32 660
      X=.3174254379061660 6D2                                           DA32 670
      Y=Y+.1043724745318169 5D-13*FCT(X)                                DA32 680
      X=.2828458319497053 1D2                                           DA32 690
      Y=Y+.3256681461419440 7D-12*FCT(X)                                DA32 700
      X=.2507785654419805 3D2                                           DA32 710
      Y=Y+.7918355533895448 0D-11*FCT(X)                                DA32 720
      X=.2210707038220600 7D2                                           DA32 730
      Y=Y+.1523043450029090 3D-9*FCT(X)                                 DA32 740
      X=.1935927108726871 4D2                                           DA32 750
      Y=Y+.2347233486430987 0D-8*FCT(X)                                 DA32 760
      X=.1698234053629536 4D2                                           DA32 770
      Y=Y+.2930250632952218 7D-7*FCT(X)                                 DA32 780
      X=.1448998669078027 4D2                                           DA32 790
      Y=Y+.2991065873454494 1D-6*FCT(X)                                 DA32 800
      X=.1235083821771477 0D2                                           DA32 810
      Y=Y+.2516680502062369 2D-5*FCT(X)                                 DA32 820
      X=.1039889190555626 2D2                                           DA32 830
      Y=Y+.1757699846170071 8D-4*FCT(X)                                 DA32 840
      X=.8628029857405929 0D1                                           DA32 850
      Y=Y+.1025185827157254 9D-3*FCT(X)                                 DA32 860
      X=.7032957798283893 6D1                                           DA32 870
      Y=Y+.5019673970261249 7D-3*FCT(X)                                 DA32 880
      X=.5609103457496151 3D1                                           DA32 890
      Y=Y+.2072658199C151 553D-2*FCT(X)                                 DA32 900
      X=.4352534529330141 0D1                                           DA32 910
      Y=Y+.7245173957068918D-2*FCT(X)                                   DA32 920
      X=.3259892256456941 9D1                                           DA32 930
      Y=Y+.2151208101975827 4D-1*FCT(X)                                 DA32 940
      X=.2328337668210397 0D1                                           DA32 950
      Y=Y+.5440625790737783 7D-1*FCT(X)                                 DA32 960
      X=.1555508231478938 0D1                                           DA32 970
      Y=Y+.1174799639281988 7D0*FCT(X)                                  DA32 980
      X=.9394832145007343 00                                            DA32 990
      Y=Y+.2169966986123736 8D0*FCT(X)                                  DA321000
      X=.4787564772774888 500                                           DA321010
      Y=Y+.3433716846998167 9D0*FCT(X)                                  DA321020
      X=.1722157241453955 8D0                                           DA321030
      Y=Y+.4659895721253560 9D0*FCT(X)                                  DA321040
      X=.1912751096844685 60-1                                          DA321050
      Y=Y+.5427548498826079 6D0*FCT(X)                                  DA321060
      RETURN                                                            DA321070
      END                                                               DA321080
```

Numerical Differentiation

Subroutines DGT3 and DDGT3

These subroutines compute a vector $Z=(z_1,\ldots,z_n)$ of derivative values, given vectors $X=(x_1,\ldots,x_n)$ of argument values and $Y=(y_1,\ldots y_n)$ of corresponding function values. Except at the endpoints x_1 and x_n, z_i is the derivative at x_i of the Lagrangian interpolation polynomial of degree 2 relevant to the three successive points (x_{i-1}, y_{i-1}), (x_i, y_i) and (x_{i+1}, y_{i+1}).

1. Mathematical background

For $i = 1,\ldots, n-2$ we must find a_i, b_i, and c_i such that

$$\bar{y}_i(x) = a_i x^2 + b_i x + c_i$$

passes through (x_i, y_i), (x_{i+1}, y_{i+1}), and (x_{i+2}, y_{i+2}).

The desired derivative values z_i are given by:

$$z_i = \begin{cases} y_1'(x_1) = 2a_1x_1 + b_1 & \text{if } i=1 \\ y_{i-1}'(x_i) = 2a_{i-1}x_i + b_{i-1} & \text{if } i=2,\ldots,n-1 \\ y_{n-2}'(x_n) = 2a_{n-2}x_n + b_{n-2} & \text{if } i=n \end{cases}$$

An easy computation yields:

$$z_i = \begin{cases} \dfrac{y_2-y_1}{x_2-x_1} + \dfrac{y_3-y_1}{x_3-x_1} - \dfrac{y_3-y_2}{x_3-x_2} & \text{if } i=1 \\ \dfrac{y_i-y_{i-1}}{x_i-x_{i-1}} + \dfrac{y_{i+1}-y_i}{x_{i+1}-x_i} - \dfrac{y_{i+1}-y_{i-1}}{x_{i+1}-x_{i-1}} & \text{if } i=2,\ldots,n-1 \\ \dfrac{y_n-y_{n-1}}{x_n-x_{n-1}} + \dfrac{y_n-y_{n-2}}{x_n-x_{n-2}} - \dfrac{y_{n-1}-y_{n-2}}{x_{n-1}-x_{n-2}} & \text{if } i=n \end{cases} \quad (1)$$

Assuming that the vectors X and Y represent a portion of a three-times differentiable function, z_i involves a truncation error T_i where:

$$T_i = \begin{cases} \frac{1}{6}(x_1-x_2)(x_1-x_3)y'''(\xi_1) & \text{if } i=1 \\ \frac{1}{6}(x_i-x_{i-1})(x_i-x_{i+1})y'''(\xi_i) & \text{if } i=2,\ldots,n-1 \\ \frac{1}{6}(x_n-x_{n-2})(x_n-x_{n-1})y'''(\xi_n) & \text{if } i=n \end{cases}$$

and ξ_i is in the closed interval determined by the three argument values used in computing z_i, $i = 1,\ldots,n$.

2. Programming considerations

The subroutines compute the z_i in serial order according to (1). If $n < 3$, there is no computation, and the error parameter is set to -1. If two of the three arguments x_{j-2}, x_{j-i}, x_j are identical, $j=3,\ldots,n$, the computation is prematurely terminated, and the error parameter IER is set to j. However, $z_1,\ldots,z_{j-1}$ are returned if $j > 3$. In this case z_{j-i} is computed treating x_{j-1} as the right-hand endpoint. If there is no error, IER is set to zero at the end of the computation. The output vector Z can have the same storage allocation as X or Y.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 64-68.

```
C                                                                       DGT3  10
C     ...................................................................DGT3  20
C                                                                       DGT3  30
C        SUBROUTINE DGT3                                                DGT3  40
C                                                                       DGT3  50
C        PURPOSE                                                        DGT3  60
C           TO COMPUTE A VECTOR OF DERIVATIVE VALUES GIVEN VECTORS OF   DGT3  70
C           ARGUMENT VALUES AND CORRESPONDING FUNCTION VALUES.          DGT3  80
C                                                                       DGT3  90
C        USAGE                                                          DGT3 100
C           CALL DGT3(X,Y,Z,NDIM,IER)                                   DGT3 110
C                                                                       DGT3 120
C        DESCRIPTION OF PARAMETERS                                      DGT3 130
C           X      -  GIVEN VECTOR OF ARGUMENT VALUES (DIMENSION NDIM)  DGT3 140
C           Y      -  GIVEN VECTOR OF FUNCTION VALUES CORRESPONDING TO X DGT3 150
C                     (DIMENSION NDIM)                                  DGT3 160
C           Z      -  RESULTING VECTOR OF DERIVATIVE VALUES (DIMENSION  DGT3 170
C                     NDIM)                                             DGT3 180
C           NDIM   -  DIMENSION OF VECTORS X,Y AND Z                    DGT3 190
C           IER    -  RESULTING ERROR PARAMETER                         DGT3 200
C                     IER  = -1  - NDIM IS LESS THAN 3                  DGT3 210
C                     IER  =  0  - NO ERROR                             DGT3 220
C                     IER POSITIVE  - X(IER) = X(IER-1) OR X(IER) =     DGT3 230
C                                     X(IER-2)                          DGT3 240
C                                                                       DGT3 250
C        REMARKS                                                        DGT3 260
C           (1)   IF IER = -1,2,3, THEN THERE IS NO COMPUTATION.        DGT3 270
C           (2)   IF IER = 4,...,N, THEN THE DERIVATIVE VALUES Z(1)     DGT3 280
C                 ,...., Z(IER-1) HAVE BEEN COMPUTED.                   DGT3 290
C           (3)   Z CAN HAVE THE SAME STORAGE ALLOCATION AS X OR Y.  IF DGT3 300
C                 X OR Y IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.  DGT3 310
C                                                                       DGT3 320
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DGT3 330
C           NONE                                                        DGT3 340
C                                                                       DGT3 350
C        METHOD                                                         DGT3 360
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), Z(I) IS THE       DGT3 370
C           DERIVATIVE AT X(I) OF THE LAGRANGIAN INTERPOLATION          DGT3 380
C           POLYNOMIAL OF DEGREE 2 RELEVANT TO THE 3 SUCCESSIVE POINTS  DGT3 390
C           (X(I+K),Y(I+K)) K = -1,0,1. (SEE HILDEBRAND, F.B.,          DGT3 400
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/ DGT3 410
C           TORONTO/LONDON, 1956, PP. 64-68.)                           DGT3 420
C                                                                       DGT3 430
C     ...................................................................DGT3 440
C                                                                       DGT3 450
      SUBROUTINE DGT3(X,Y,Z,NDIM,IER)                                   DGT3 460
C                                                                       DGT3 470
C     DIMENSION X(1),Y(1),Z(1)                                          DGT3 480
C                                                                       DGT3 490
C        TEST OF DIMENSION AND ERROR EXIT IN CASE NDIM IS LESS THAN 3   DGT3 500
      IER=-1                                                            DGT3 510
      IF(NDIM-3)8,1,1                                                   DGT3 520
C                                                                       DGT3 530
C        PREPARE DIFFERENTIATION LOOP                                   DGT3 540
    1 A=X(1)                                                            DGT3 550
      B=Y(1)                                                            DGT3 560
      I=2                                                               DGT3 570
      DY2=X(2)-A                                                        DGT3 580
      IF(DY2)2,9,2                                                      DGT3 590
    2 DY2=(Y(2)-B)/DY2                                                  DGT3 600
C                                                                       DGT3 610
C        START DIFFERENTIATION LOOP                                     DGT3 620
      DO 6 I=3,NDIM                                                     DGT3 630
      A=X(I)-A                                                          DGT3 640
      IF(A)3,9,3                                                        DGT3 650
    3 A=(Y(I)-B)/A                                                      DGT3 660
      B=X(I)-X(I-1)                                                     DGT3 670
      IF(B)4,9,4                                                        DGT3 680
    4 DY1=DY2                                                           DGT3 690
      DY2=(Y(I)-Y(I-1))/B                                               DGT3 700
      DY3=A                                                             DGT3 710
      A=X(I-1)                                                          DGT3 720
      B=Y(I-1)                                                          DGT3 730
      IF(I-3)5,5,6                                                      DGT3 740
    5 Z(1)=DY1+DY3-DY2                                                  DGT3 750
    6 Z(I-1)=DY1+DY2-DY3                                                DGT3 760
C        END DIFFERENTIATION LOOP                                       DGT3 770
C                                                                       DGT3 780
C        NORMAL EXIT                                                    DGT3 790
      IER=0                                                             DGT3 800
      I=NDIM                                                            DGT3 810
    7 Z(I)=DY2+DY3-DY1                                                  DGT3 820
    8 RETURN                                                            DGT3 830
C                                                                       DGT3 840
C        ERROR EXIT IN CASE OF IDENTICAL ARGUMENTS                      DGT3 850
    9 IER=I                                                             DGT3 860
      I=I-1                                                             DGT3 870
      IF(I-2)8,8,7                                                      DGT3 880
      END                                                               DGT3 890
                                                                        DGT3 900
```

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C                                                                       DDGT  10
C     ...................................................................DDGT  20
C                                                                       DDGT  30
C        SUBROUTINE DDGT3                                               DDGT  40
C                                                                       DDGT  50
C        PURPOSE                                                        DDGT  60
C           TO COMPUTE A VECTOR OF DERIVATIVE VALUES GIVEN VECTORS OF   DDGT  70
C           ARGUMENT VALUES AND CORRESPONDING FUNCTION VALUES.          DDGT  80
C                                                                       DDGT  90
C        USAGE                                                          DDGT 100
C           CALL DDGT3(X,Y,Z,NDIM,IER)                                  DDGT 110
C                                                                       DDGT 120
C        DESCRIPTION OF PARAMETERS                                      DDGT 130
C           X      -  GIVEN VECTOR OF DOUBLE PRECISION ARGUMENT VALUES  DDGT 140
C                     (DIMENSION NDIM)                                  DDGT 150
C           Y      -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES  DDGT 160
C                     CORRESPONDING TO X (DIMENSION NDIM)               DDGT 170
C           Z      -  RESULTING VECTOR OF DOUBLE PRECISION DERIVATIVE   DDGT 180
C                     VALUES (DIMENSION NDIM)                           DDGT 190
C           NDIM   -  DIMENSION OF VECTORS X,Y AND Z                    DDGT 200
C           IER    -  RESULTING ERROR PARAMETER                         DDGT 210
C                     IER  = -1  - NDIM IS LESS THAN 3                  DDGT 220
C                     IER  =  0  - NO ERROR                             DDGT 230
C                     IER POSITIVE  - X(IER) = X(IER-1) OR X(IER) =     DDGT 240
C                                     X(IER-2)                          DDGT 250
C                                                                       DDGT 260
C        REMARKS                                                        DDGT 270
C           (1)   IF IER = -1,2,3, THEN THERE IS NO COMPUTATION.        DDGT 280
C           (2)   IF IER =  4,...,N, THEN THE DERIVATIVE VALUES Z(1)    DDGT 290
C                 ,..., Z(IER-1) HAVE BEEN COMPUTED.                    DDGT 300
C           (3)   Z CAN HAVE THE SAME STORAGE ALLOCATION AS X OR Y.  IF DDGT 310
C                 X OR Y IS DISTINCT FROM Z, THEN IT IS NOT DESTROYED.  DDGT 320
C                                                                       DDGT 330
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DDGT 340
C           NONE                                                        DDGT 350
C                                                                       DDGT 360
C        METHOD                                                         DDGT 370
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), Z(I) IS THE       DDGT 380
C           DERIVATIVE AT X(I) OF THE LAGRANGIAN INTERPOLATION          DDGT 390
C           POLYNOMIAL OF DEGREE 2 RELEVANT TO THE 3 SUCCESSIVE POINTS  DDGT 400
C           (X(I+K),Y(I+K)) K = -1,0,1. (SEE HILDEBRAND, F.B.,          DDGT 410
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/ DDGT 420
C           TORONTO/LONDON, 1956, PP. 64-68.)                           DDGT 430
C                                                                       DDGT 440
C     ...................................................................DDGT 450
C                                                                       DDGT 460
      SUBROUTINE DDGT3(X,Y,Z,NDIM,IER)                                  DDGT 470
C                                                                       DDGT 480
C                                                                       DDGT 490
      DIMENSION X(1),Y(1),Z(1)                                          DDGT 500
      DOUBLE PRECISION X,Y,Z,DY1,DY2,DY3,A,B                            DDGT 510
C                                                                       DDGT 520
C        TEST OF DIMENSION AND ERROR EXIT IN CASE NDIM IS LESS THAN 3   DDGT 530
      IER=-1                                                            DDGT 540
      IF(NDIM-3)8,1,1                                                   DDGT 550
C                                                                       DDGT 560
C        PREPARE DIFFERENTIATION LOOP                                   DDGT 570
    1 A=X(1)                                                            DDGT 580
      B=Y(1)                                                            DDGT 590
      I=2                                                               DDGT 600
      DY2=X(2)-A                                                        DDGT 610
      IF(DY2)2,9,2                                                      DDGT 620
    2 DY2=(Y(2)-B)/DY2                                                  DDGT 630
C                                                                       DDGT 640
C        START DIFFERENTIATION LOOP                                     DDGT 650
      DO 6 I=3,NDIM                                                     DDGT 660
      A=X(I)-A                                                          DDGT 670
      IF(A)3,9,3                                                        DDGT 680
    3 A=(Y(I)-B)/A                                                      DDGT 690
      B=X(I)-X(I-1)                                                     DDGT 700
      IF(B)4,9,4                                                        DDGT 710
    4 DY1=DY2                                                           DDGT 720
      DY2=(Y(I)-Y(I-1))/B                                               DDGT 730
      DY3=A                                                             DDGT 740
      A=X(I-1)                                                          DDGT 750
      B=Y(I-1)                                                          DDGT 760
      IF(I-3)5,5,6                                                      DDGT 770
    5 Z(1)=DY1+DY3-DY2                                                  DDGT 780
    6 Z(I-1)=DY1+DY2-DY3                                                DDGT 790
C        END OF DIFFERENTIATION LOOP                                    DDGT 800
C                                                                       DDGT 810
C        NORMAL EXIT                                                    DDGT 820
      IER=0                                                             DDGT 830
      I=NDIM                                                            DDGT 840
    7 Z(I)=DY2+DY3-DY1                                                  DDGT 850
    8 RETURN                                                            DDGT 860
C                                                                       DDGT 870
C        ERROR EXIT IN CASE OF IDENTICAL ARGUMENTS                      DDGT 880
    9 IER=I                                                             DDGT 890
      I=I-1                                                             DDGT 900
      IF(I-2)8,8,7                                                      DDGT 910
      END                                                               DDGT 920
```

Subroutines DET3 and DDET3

These subroutines compute a vector $Z=(z_1,\ldots,z_n)$ of derivative values, given a vector $Y=(y_1,\ldots,y_n)$ of function values whose entries y_i correspond to n equidistantly spaced argument values x_i, with $x_i - x_{i-1} = h$ for $i=2,\ldots,n$. Except at the endpoints x_1 and x_n, z_i is the derivative at x_i of the Lagrangian interpolation polynomial of degree 2 relevant to the three successive points (x_{i-1}, y_{i-1}), (x_i, y_i), and (x_{i+1}, y_{i+1}).

1. Mathematical background

The procedure is that described for subroutines DGT3 and DDGT3, but here we have the additional relation $x_i - x_{i-1} = h$, a constant, for $i=2,\ldots,n$. This leads to the following expression for the z_i:

$$z_i = \begin{cases} \frac{1}{2h}(-y_3 + 4y_2 - 3y_1) & \text{if } i=1 \\ \frac{1}{2h}(y_{i+1} - y_{i-1}) & \text{if } i=2,\ldots,n-1 \\ \frac{1}{2h}(3y_n - 4y_{n-1} + y_{n-2}) & \text{if } i=n \end{cases} \qquad (1)$$

Assuming that the vector Y represents the function values of a portion of a three-times differentiable function, z_i involves a truncation error T_i where:

$$T_i = \begin{cases} \frac{h^2}{3} y'''(\xi_1),\ \xi_1 \in [x_1, x_3] & \text{if } i=1 \\ \frac{-h^2}{6} y'''(\xi_i),\ \xi_i \in [x_{i-1}, x_{i+1}] & \text{if } i=2,\ldots,n-1 \\ \frac{h^2}{3} y'''(\xi_n),\ \xi_n \in [x_{n-2}, x_n] & \text{if } i=n \end{cases}$$

In addition to these truncation errors, roundoff errors may be of considerable magnitude. Supposing that each of the ordinates y_i can be in error by $\pm\epsilon$, $\epsilon > 0$, the magnitude $|R_i|$ of the corresponding error R_i in the calculation of z_i can be as large as:

$$|R_i| = \begin{cases} \frac{4\epsilon}{|h|} & \text{if } i=1, n \\ \frac{\epsilon}{|h|} & \text{if } i=2,\ldots,n-1 \end{cases}$$

Since small truncation errors generally require small $|h|$, while small roundoff errors generally require large $|h|$, it is reasonable to choose h so that $|T_i| \approx |R_i|$.

If $M = \sup y'''(\xi)$, where $\xi \in [x_1, x_n]$, and if we regard only the inner points $x_2, \ldots, x_{n-1}$, we find that

$$h_{\text{optimum}} \approx \pm 1.8 \sqrt[3]{\epsilon/M},$$

and the magnitude $|E_i|$ of the total possible error E_i in z_i is given by:

$$|E_i| \approx \begin{cases} 3.3 \sqrt[3]{\epsilon^2 M} & \text{if } i = 1, n \\ 1.1 \sqrt[3]{\epsilon^2 M} & \text{if } i = 2, \ldots, n-1 \end{cases}$$

2. Programming considerations

The subroutines compute the z_i in serial order according to (1). If $n < 3$ or if $h = 0$, there is no computation, and the error parameter IER is set to -1 or 1 respectively. Otherwise IER is set to zero at the end of the computation. The output vector Z can have the same storage allocation as Y.

For reference see F. B. Hildebrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 82-84.

```
C                                                                       DET3  10
C     ...................................................................DET3  20
C                                                                       DET3  30
C        SUBROUTINE DET3                                                DET3  40
C                                                                       DET3  50
C        PURPOSE                                                        DET3  60
C           TO COMPUTE A VECTOR OF DERIVATIVE VALUES GIVEN A VECTOR OF  DET3  70
C           FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO EQUIDISTANTLY   DET3  80
C           SPACED ARGUMENT VALUES.                                     DET3  90
C                                                                       DET3 100
C        USAGE                                                          DET3 110
C           CALL DET3(H,Y,Z,NDIM,IER)                                   DET3 120
C                                                                       DET3 130
C        DESCRIPTION OF PARAMETERS                                      DET3 140
C           H      -  CONSTANT DIFFERENCE BETWEEN SUCCESSIVE ARGUMENT   DET3 150
C                     VALUES (H IS POSITIVE IF THE ARGUMENT VALUES      DET3 160
C                     INCREASE AND NEGATIVE OTHERWISE)                  DET3 170
C           Y      -  GIVEN VECTOR OF FUNCTION VALUES (DIMENSION NDIM)  DET3 180
C           Z      -  RESULTING VECTOR OF DERIVATIVE VALUES (DIMENSION  DET3 190
C                     NDIM)                                             DET3 200
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      DET3 210
C           IER    -  RESULTING ERROR PARAMETER                         DET3 220
C                     IER = -1  - NDIM IS LESS THAN 3                   DET3 230
C                     IER =  0  - NO ERROR                              DET3 240
C                     IER =  1  - H = 0                                 DET3 250
C                                                                       DET3 260
C        REMARKS                                                        DET3 270
C           (1)    IF IER = -1,1, THEN THERE IS NO COMPUTATION.         DET3 280
C           (2)    Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y. IF Y IS DET3 290
C                  DISTINCT FROM Z, THEN IT IS NOT DESTROYED.           DET3 300
C                                                                       DET3 310
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DET3 320
C           NONE                                                        DET3 330
C                                                                       DET3 340
C        METHOD                                                         DET3 350
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    DET3 360
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), Z(I) IS THE       DET3 370
C           DERIVATIVE AT X(I) OF THE LAGRANGIAN INTERPOLATION          DET3 380
C           POLYNOMIAL OF DEGREE 2 RELEVANT TO THE 3 SUCCESSIVE POINTS  DET3 390
C           (X(I+K),Y(I+K)) K = -1,0,1.  (SEE HILDEBRAND, F.B.,         DET3 400
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC-GRAW-HILL, NEW YORK/ DET3 410
C           TORONTO/LONDON, 1956, PP.82-84.)                            DET3 420
C                                                                       DET3 430
C     ...................................................................DET3 440
      SUBROUTINE DET3(H,Y,Z,NDIM,IER)                                   DET3 450
C                                                                       DET3 460
C                                                                       DET3 470
      DIMENSION Y(1),Z(1)                                               DET3 480
C                                                                       DET3 490
C        TEST OF DIMENSION                                              DET3 500
      IF(NDIM-3)4,1,1                                                   DET3 510
C                                                                       DET3 520
C        TEST OF STEPSIZE                                               DET3 530
    1 IF(H)2,5,2                                                        DET3 540
C                                                                       DET3 550
C        PREPARE DIFFERENTIATION LOOP                                   DET3 560
    2 HH=.5/H                                                           DET3 570
      YY=Y(NDIM-2)                                                      DET3 580
      B=Y(2)+Y(2)                                                       DET3 590
      B=HH*(B+B-Y(3)-Y(1)-Y(1)-Y(1))                                    DET3 600
C                                                                       DET3 610
C        START DIFFERENTIATION LOOP                                     DET3 620
      DO 3 I=3,NDIM                                                     DET3 630
      A=B                                                               DET3 640
      B=HH*(Y(I)-Y(I-2))                                                DET3 650
    3 Z(I-2)=A                                                          DET3 660
C        END OF DIFFERENTIATION LOOP                                    DET3 670
C                                                                       DET3 680
C        NORMAL EXIT                                                    DET3 690
C                                                                       DET3 700
      IER=0                                                             DET3 710
      A=Y(NDIM-1)+Y(NDIM-1)                                             DET3 720
      Z(NDIM)=HH*(Y(NDIM)+Y(NDIM)+Y(NDIM)-A-A+YY)                       DET3 730
      Z(NDIM-1)=B                                                       DET3 740
      RETURN                                                            DET3 750
C                                                                       DET3 760
C        ERROR EXIT IN CASE NDIM IS LESS THAN 3                         DET3 770
    4 IER=-1                                                            DET3 780
      RETURN                                                            DET3 790
C                                                                       DET3 800
C        ERROR EXIT IN CASE OF ZERO STEPSIZE                            DET3 810
    5 IER=1                                                             DET3 820
      RETURN                                                            DET3 830
      END                                                               DET3 840
```

```
C                                                                       DDT3  10
C     ...................................................................DDT3  20
C                                                                       DDT3  30
C        SUBROUTINE DDET3                                               DDT3  40
C                                                                       DDT3  50
C        PURPOSE                                                        DDT3  60
C           TO COMPUTE A VECTOR OF DERIVATIVE VALUES GIVEN A VECTOR OF  DDT3  70
C           FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO EQUIDISTANTLY   DDT3  80
C           SPACED ARGUMENT VALUES.                                     DDT3  90
C                                                                       DDT3 100
C        USAGE                                                          DDT3 110
C           CALL DDET3(H,Y,Z,NDIM,IER)                                  DDT3 120
C                                                                       DDT3 130
C        DESCRIPTION OF PARAMETERS                                      DDT3 140
C           H      -  DOUBLE PRECISION CONSTANT DIFFERENCE BETWEEN      DDT3 150
C                     SUCCESSIVE ARGUMENT VALUES (H IS POSITIVE IF THE  DDT3 160
C                     ARGUMENT VALUES INCREASE AND NEGATIVE OTHERWISE)  DDT3 170
C           Y      -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES  DDT3 180
C                     (DIMENSION NDIM)                                  DDT3 190
C           Z      -  RESULTING VECTOR OF DOUBLE PRECISION DERIVATIVE   DDT3 200
C                     VALUES (DIMENSION NDIM)                           DDT3 210
C           NDIM   -  DIMENSION OF VECTORS Y AND Z                      DDT3 220
C           IER    -  RESULTING ERROR PARAMETER                         DDT3 230
C                     IER = -1  - NDIM IS LESS THAN 3                   DDT3 240
C                     IER =  0  - NO ERROR                              DDT3 250
C                     IER =  1  - H = 0                                 DDT3 260
C                                                                       DDT3 270
C        REMARKS                                                        DDT3 280
C           (1)    IF IER = -1,1, THEN THERE IS NO COMPUTATION.         DDT3 290
C           (2)    Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y. IF Y IS DDT3 300
C                  DISTINCT FROM Z, THEN IT IS NOT DESTROYED.           DDT3 310
C                                                                       DDT3 320
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DDT3 330
C           NONE                                                        DDT3 340
C                                                                       DDT3 350
C        METHOD                                                         DDT3 360
C           IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN    DDT3 370
C           EXCEPT AT THE ENDPOINTS X(1) AND X(NDIM), Z(I) IS THE       DDT3 380
C           DERIVATIVE AT X(I) OF THE LAGRANGIAN INTERPOLATION          DDT3 390
C           POLYNOMIAL OF DEGREE 2 RELEVANT TO THE 3 SUCCESSIVE POINTS  DDT3 400
C           (X(I+K),Y(I+K)) K = -1,0,1.  (SEE HILDEBRAND, F.B.,         DDT3 410
C           INTRODUCTION TO NUMERICAL ANALYSIS, MC-GRAW-HILL, NEW YORK/ DDT3 420
C           TORONTO/LONDON, 1956, PP.82-84.)                            DDT3 430
C                                                                       DDT3 440
C     ...................................................................DDT3 450
C                                                                       DDT3 460
      SUBROUTINE DDET3(H,Y,Z,NDIM,IER)                                  DDT3 470
C                                                                       DDT3 480
C                                                                       DDT3 490
      DIMENSION Y(1),Z(1)                                               DDT3 500
      DOUBLE PRECISION H,Y,Z,HH,YY,A,B                                  DDT3 510
C                                                                       DDT3 520
C        TEST OF DIMENSION                                              DDT3 530
      IF(NDIM-3)4,1,1                                                   DDT3 540
C                                                                       DDT3 550
C        TEST OF STEPSIZE                                               DDT3 560
    1 IF(H)2,5,2                                                        DDT3 570
C                                                                       DDT3 580
C        PREPARE DIFFERENTIATION LOOP                                   DDT3 590
    2 HH=.500/H                                                         DDT3 600
      YY=Y(NDIM-2)                                                      DDT3 610
      B=Y(2)+Y(2)                                                       DDT3 620
      B=HH*(B+B-Y(3)-Y(1)-Y(1)-Y(1))                                    DDT3 630
C                                                                       DDT3 640
C        START DIFFERENTIATION LOOP                                     DDT3 650
      DO 3 I=3,NDIM                                                     DDT3 660
      A=B                                                               DDT3 670
      B=HH*(Y(I)-Y(I-2))                                                DDT3 680
    3 Z(I-2)=A                                                          DDT3 690
C        END OF DIFFERENTIATION LOOP                                    DDT3 700
C                                                                       DDT3 710
C        NORMAL EXIT                                                    DDT3 720
      IER=0                                                             DDT3 730
      A=Y(NDIM-1)+Y(NDIM-1)                                             DDT3 740
      Z(NDIM)=HH*(Y(NDIM)+Y(NDIM)+Y(NDIM)-A-A+YY)                       DDT3 750
      Z(NDIM-1)=B                                                       DDT3 760
      RETURN                                                            DDT3 770
C                                                                       DDT3 780
C        ERROR EXIT IN CASE NDIM IS LESS THAN 3                         DDT3 790
    4 IER=-1                                                            DDT3 800
      RETURN                                                            DDT3 810
C                                                                       DDT3 820
C        ERROR EXIT IN CASE OF ZERO STEPSIZE                            DDT3 830
    5 IER=1                                                             DDT3 840
      RETURN                                                            DDT3 850
      END                                                               DDT3 860
```

Subroutines DET5 and DDET5

These subroutines compute a vector $Z=(z_1,\ldots,z_n)$ of derivative values, given a vector $Y=(y_1,\ldots,y_n)$ of function values whose entries y_i correspond to n equidistantly spaced argument values x_i, with $x_i - x_{i-1} = h$ for $i=2,\ldots,n$. Except at the points x_1, x_2, x_{n-1}, and x_n, z_i is the derivative at x_i of the Lagrangian interpolation polynomial of degree 4 relevant to the five successive points (x_{i+k}, y_{i+k}), $k=-2,-1,\ldots,2$.

1. Mathematical background

For $i=1,\ldots,n-4$ we must find a_i, b_i, c_i, d_i, and e_i such that

$$\bar{y}_i(x) = a_i x^4 + b_i x^3 + c_i x^2 + d_i x + e_i$$

passes through (x_{i+k}, y_{i+k}) for $k=0,\ldots,4$.

The desired derivative values z_i are given by:

$$z_i = \begin{cases} \bar{y}_1'(x_i) = 4a_1x_i^3 + 3b_1x_i^2 + 2c_1x_i + d_1 & \text{if } i=1,2 \\ \bar{y}_{i-2}'(x_i) = 4a_{i-2}x_i^3 + 3b_{i-2}x_i^2 + 2c_{i-2}x_i + d_{i-2} & \text{if } i=3,\ldots,n-2 \\ \bar{y}_{n-4}'(x_i) = 4a_{n-4}x_i^3 + 3b_{n-4}x_i^2 + 2c_{n-4}x_i + d_{n-4} & \text{if } i=n-1,n \end{cases}$$

Using the fact that $x_i - x_{i-1} = h$, a constant, for $i=2,\ldots,n$, we get:

$$z_i = \begin{cases} \frac{1}{12h}(-25y_1 + 48y_2 - 36y_3 + 16y_4 - 3y_5) & \text{if } i=1 \\ \frac{1}{12h}(-3y_1 - 10y_2 + 18y_3 - 6y_4 + y_5) & \text{if } i=2 \\ \frac{1}{12h}(y_{i-2} - 8y_{i-1} + 8y_{i+1} - y_{i+2}) & \text{if } i=3,\ldots,n-2 \\ \frac{1}{12h}(-y_{n-4} + 6y_{n-3} - 18y_{n-2} + 10_{n-1} + 3y_n) & \text{if } i=n-1 \\ \frac{1}{12h}(3y_{n-4} - 16y_{n-3} + 36y_{n-2} - 48y_{n-1} + 25y_n) & \text{if } i=n \end{cases} \quad (1)$$

Assuming that the vector Y represents the function values of a portion of a five-times differentiable function, z_i involves a truncation error T_i where:

$$T_i = \begin{cases} \frac{h^4}{5}y^v(\xi_1), & \xi_1 \epsilon [x_1, x_5] & \text{if } i=1 \\ -\frac{h^4}{20}y^v(\xi_2), & \xi_2 \epsilon [x_1, x_5] & \text{if } i=2 \\ \frac{h^4}{30}y^v(\xi_i), & \xi_i \epsilon [x_{i-2}, x_{i+2}] & \text{if } i=3,\ldots,n-2 \\ -\frac{h^4}{20}y^v(\xi_{n-1}), & \xi_{n-i} \epsilon [x_{n-4}, x_n] & \text{if } i=n-1 \\ \frac{h^4}{5}y^v(\xi_n), & \xi_n \epsilon [x_{n-4}, x_n] & \text{if } i=n \end{cases}$$

In addition to the truncation errors, roundoff errors may be of considerable magnitude. Supposing that the ordinates y_i can be in error by $\pm\epsilon$, $\epsilon > 0$, the magnitude $|R_i|$ of the corresponding error R_i in the computation of z_i can be as large as:

$$|R_i| = \begin{cases} \frac{32\epsilon}{3|h|} & \text{if } i=1,n \\ \frac{19\epsilon}{6|h|} & \text{if } i=2,n-1 \\ \frac{3\epsilon}{2|h|} & \text{if } i=3,\ldots,n-2 \end{cases}$$

Since small truncation errors generally require small $|h|$, while small roundoff errors generally require large $|h|$, it is reasonable to choose h so that $|T_i| \approx |R_i|$.

If $M = \sup_{\xi \in [x_1, x_n]} y^{v}(\xi)$, and if we regard only the inner points $x_3, \ldots, x_{n-2}$, we find that

$$h_{optimum} \approx 2.1 \sqrt[5]{\epsilon/M}$$

and the magnitude $|E_i|$ of the total possible error E_i in z_i is given by:

$$|E_i| \approx \begin{cases} 9 \sqrt[5]{\epsilon^4 M} & \text{if } i=1, n \\ 2.5 \sqrt[5]{\epsilon^4 M} & \text{if } i=2, n-1 \\ 1.4 \sqrt[5]{\epsilon^4 M} & \text{if } i=3, \ldots, n-2 \end{cases}$$

2. Programming considerations

The subroutines compute the z_i in serial order according to (1). If $n < 5$ or if $h = 0$, there is no computation, and the error parameter IER is set to -1 or 1, respectively. Otherwise IER is set to zero at the end of the computation. The output vector Z may have the same storage allocation as Y.

For reference see F. B. Hilderbrand, Introduction to Numerical Analysis. McGraw-Hill, New York/Toronto/London, 1956, pp. 82-84.

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C                                                                       DET5  10
C  ...................................................................DET5  20
C                                                                       DET5  30
C     SUBROUTINE DET5                                                   DET5  40
C                                                                       DET5  50
C     PURPOSE                                                           DET5  60
C        TO COMPUTE A VECTOR OF DERIVATIVE VALUES GIVEN A VECTOR OF     DET5  70
C        FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO EQUIDISTANTLY      DET5  80
C        SPACED ARGUMENT VALUES.                                        DET5  90
C                                                                       DET5 100
C     USAGE                                                             DET5 110
C        CALL DET5(H,Y,Z,NDIM,IER)                                      DET5 120
C                                                                       DET5 130
C     DESCRIPTION OF PARAMETERS                                         DET5 140
C        H     -  CONSTANT DIFFERENCE BETWEEN SUCCESSIVE ARGUMENT       DET5 150
C                 VALUES (H IS POSITIVE IF THE ARGUMENT VALUES          DET5 160
C                 INCREASE AND NEGATIVE OTHERWISE)                      DET5 170
C        Y     -  GIVEN VECTOR OF FUNCTION VALUES (DIMENSION NDIM)      DET5 180
C        Z     -  RESULTING VECTOR OF DERIVATIVE VALUES (DIMENSION      DET5 190
C                 NDIM)                                                 DET5 200
C        NDIM  -  DIMENSION OF VECTORS Y AND Z                          DET5 210
C        IER   -  RESULTING ERROR PARAMETER                             DET5 220
C                 IER = -1  - NDIM IS LESS THAN 5                       DET5 230
C                 IER =  0  - NO ERROR                                  DET5 240
C                 IER =  1  - H = 0                                     DET5 250
C                                                                       DET5 260
C     REMARKS                                                           DET5 270
C        (1)   IF IER = -1,1, THERE IS NO COMPUTATION.                  DET5 280
C        (2)   Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y IS    DET5 290
C              DISTINCT FROM Z, THEN IT IS NOT DESTROYED.               DET5 300
C                                                                       DET5 310
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DET5 320
C        NONE                                                           DET5 330
C                                                                       DET5 340
C     METHOD                                                            DET5 350
C        IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN       DET5 360
C        EXCEPT AT THE POINTS X(1),X(2),X(NDIM-1) AND X(NDIM), Z(I)     DET5 370
C        IS THE DERIVATIVE AT X(I) OF THE LAGRANGIAN INTERPOLATION      DET5 380
C        POLYNOMIAL OF DEGREE 4 RELEVANT TO THE 5 SUCCESSIVE POINTS     DET5 390
C        (X(I+K),Y(I+K)) K = -2,-1,...,2.  (SEE HILDEBRAND, F.B.,       DET5 400
C        INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/    DET5 410
C        TORONTO/LONDON, 1956, PP. 82-84.)                              DET5 420
C                                                                       DET5 430
C  ...................................................................DET5 440
C                                                                       DET5 450
      SUBROUTINE DET5(H,Y,Z,NDIM,IER)                                   DET5 460
C                                                                       DET5 470
C                                                                       DET5 480
      DIMENSION Y(1),Z(1)                                               DET5 490
C                                                                       DET5 500
C     TEST OF DIMENSION                                                 DET5 510
      IF(NDIM-5)4,1,1                                                   DET5 520
C                                                                       DET5 530
C        TEST OF STEPSIZE                                               DET5 540
    1 IF(H)2,5,2                                                        DET5 550
C                                                                       DET5 560
C        PREPARE DIFFERENTIATION LOOP                                   DET5 570
    2 HH=.083333333/H                                                   DET5 580
      YY=Y(NDIM-4)                                                      DET5 590
      B=HH*(-25.*Y(1)+48.*Y(2)-36.*Y(3)+16.*Y(4)-3.*Y(5))               DET5 600
      C=HH*(-3.*Y(1)-10.*Y(2)+18.*Y(3)-6.*Y(4)+Y(5))                    DET5 610
C                                                                       DET5 620
C        START DIFFERENTIATION LOOP                                     DET5 630
      DO 3 I=5,NDIM                                                     DET5 640
      A=B                                                               DET5 650
      B=C                                                               DET5 660
      C=HH*(Y(I-4)-Y(I)+8.*(Y(I-1)-Y(I-3)))                             DET5 670
    3 Z(I-4)=A                                                          DET5 680
C        END OF DIFFERENTIATION LOOP                                    DET5 690
C                                                                       DET5 700
C        NORMAL EXIT                                                    DET5 710
      IER=0                                                             DET5 720
      A=HH*(-YY+6.*Y(NDIM-3)-18.*Y(NDIM-2)+10.*Y(NDIM-1)+3.*Y(NDIM))    DET5 730
     0Z(NDIM)=HH*(3.*YY-16.*Y(NDIM-3)+36.*Y(NDIM-2)-48.*Y(NDIM-1)       DET5 740
     1           +25.*Y(NDIM))                                          DET5 750
      Z(NDIM-1)=A                                                       DET5 760
      Z(NDIM-2)=C                                                       DET5 770
      Z(NDIM-3)=B                                                       DET5 780
      RETURN                                                            DET5 790
C                                                                       DET5 800
C        ERROR EXIT IN CASE NDIM IS LESS THAN 5                         DET5 810
    4 IER=-1                                                            DET5 820
      RETURN                                                            DET5 830
C                                                                       DET5 840
C        ERROR EXIT IN CASE OF ZERO STEPSIZE                            DET5 850
    5 IER=1                                                             DET5 860
      RETURN                                                            DET5 870
      END                                                               DET5 880
```

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C                                                                       DDT5  10
C  ...................................................................DDT5  20
C                                                                       DDT5  30
C     SUBROUTINE DDET5                                                  DDT5  40
C                                                                       DDT5  50
C     PURPOSE                                                           DDT5  60
C        TO COMPUTE A VECTOR OF DERIVATIVE VALUES GIVEN A VECTOR OF     DDT5  70
C        FUNCTION VALUES WHOSE ENTRIES CORRESPOND TO EQUIDISTANTLY      DDT5  80
C        SPACED ARGUMENT VALUES.                                        DDT5  90
C                                                                       DDT5 100
C     USAGE                                                             DDT5 110
C        CALL DDET5(H,Y,Z,NDIM,IER)                                     DDT5 120
C                                                                       DDT5 130
C     DESCRIPTION OF PARAMETERS                                         DDT5 140
C        H     -  DOUBLE PRECISION CONSTANT DIFFERENCE BETWEEN          DDT5 150
C                 SUCCESSIVE ARGUMENT VALUES (H IS POSITIVE IF THE      DDT5 160
C                 ARGUMENT VALUES INCREASE AND NEGATIVE OTHERWISE)      DDT5 170
C        Y     -  GIVEN VECTOR OF DOUBLE PRECISION FUNCTION VALUES      DDT5 180
C                 (DIMENSION NDIM)                                      DDT5 190
C        Z     -  RESULTING VECTOR OF DOUBLE PRECISION DERIVATIVE       DDT5 200
C                 VALUES (DIMENSION NDIM)                               DDT5 210
C        NDIM  -  DIMENSION OF VECTORS Y AND Z                          DDT5 220
C        IER   -  RESULTING ERROR PARAMETER                             DDT5 230
C                 IER = -1  - NDIM IS LESS THAN 5                       DDT5 240
C                 IER =  0  - NO ERROR                                  DDT5 250
C                 IER =  1  - H = 0                                     DDT5 260
C                                                                       DDT5 270
C     REMARKS                                                           DDT5 280
C        (1)   IF IER = -1,1, THEN THERE IS NO COMPUTATION.             DDT5 290
C        (2)   Z CAN HAVE THE SAME STORAGE ALLOCATION AS Y.  IF Y IS    DDT5 300
C              DISTINCT FROM Z, THEN IT IS NOT DESTROYED.               DDT5 310
C                                                                       DDT5 320
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DDT5 330
C        NONE                                                           DDT5 340
C                                                                       DDT5 350
C     METHOD                                                            DDT5 360
C        IF X IS THE (SUPPRESSED) VECTOR OF ARGUMENT VALUES, THEN       DDT5 370
C        EXCEPT AT THE POINTS X(1),X(2),X(NDIM-1) AND X(NDIM), Z(I)     DDT5 380
C        IS THE DERIVATIVE AT X(I) OF THE LAGRANGIAN INTERPOLATION      DDT5 390
C        POLYNOMIAL OF DEGREE 4 RELEVANT TO THE 5 SUCCESSIVE POINTS     DDT5 400
C        (X(I+K),Y(I+K)) K = -2,-1,...,2.  (SEE HILDEBRAND, F.B.,       DDT5 410
C        INTRODUCTION TO NUMERICAL ANALYSIS, MC GRAW-HILL, NEW YORK/    DDT5 420
C        TORONTO/LONDON, 1956, PP. 82-84.)                              DDT5 430
C                                                                       DDT5 440
C  ...................................................................DDT5 450
C                                                                       DDT5 460
      SUBROUTINE DDET5(H,Y,Z,NDIM,IER)                                  DDT5 470
C                                                                       DDT5 480
C                                                                       DDT5 490
      DIMENSION Y(1),Z(1)                                               DDT5 500
      DOUBLE PRECISION H,Y,Z,HH,YY,A,B,C                                DDT5 510
C                                                                       DDT5 520
C     TEST OF DIMENSION                                                 DDT5 530
      IF(NDIM-5)4,1,1                                                   DDT5 540
C                                                                       DDT5 550
C     TEST OF STEPSIZE                                                  DDT5 560
    1 IF(H)2,5,2                                                        DDT5 570
C                                                                       DDT5 580
C     PREPARE DIFFERENTIATION LOOP                                      DDT5 590
    2 HH=.0833333333333333333D0/H                                       DDT5 600
      YY=Y(NDIM-4)                                                      DDT5 610
      B=HH*(-25.D0*Y(1)+48.D0*Y(2)-36.D0*Y(3)+16.D0*Y(4)-3.D0*Y(5))     DDT5 620
      C=HH*(-3.D0*Y(1)-10.D0*Y(2)+18.D0*Y(3)-6.D0*Y(4)+Y(5))            DDT5 630
C                                                                       DDT5 640
C     START DIFFERENTIATION LOOP                                        DDT5 650
      DO 3 I=5,NDIM                                                     DDT5 660
      A=B                                                               DDT5 670
      B=C                                                               DDT5 680
      C=HH*(Y(I-4)-Y(I)+8.D0*(Y(I-1)-Y(I-3)))                           DDT5 690
    3 Z(I-4)=A                                                          DDT5 700
C        END OF DIFFERENTIATION LOOP                                    DDT5 710
C                                                                       DDT5 720
C     NORMAL EXIT                                                       DDT5 730
      IER=0                                                             DDT5 740
      0A=HH*(-YY+6.D0*Y(NDIM-3)-18.D0*Y(NDIM-2)+10.D0*Y(NDIM-1)         DDT5 750
     1      +3.D0*Y(NDIM))                                             DDT5 760
     0Z(NDIM)=HH*(3.D0*YY-16.D0*Y(NDIM-3)+36.D0*Y(NDIM-2)               DDT5 770
     1           -48.D0*Y(NDIM-1)+25.D0*Y(NDIM))                        DDT5 780
      Z(NDIM-1)=A                                                       DDT5 790
      Z(NDIM-2)=C                                                       DDT5 800
      Z(NDIM-3)=B                                                       DDT5 810
      RETURN                                                            DDT5 820
C                                                                       DDT5 830
C     ERROR EXIT IN CASE NDIM IS LESS THAN 5                            DDT5 840
    4 IER=-1                                                            DDT5 850
      RETURN                                                            DDT5 860
C                                                                       DDT5 870
C     ERROR EXIT IN CASE OF ZERO STEPSIZE                               DDT5 880
    5 IER=1                                                             DDT5 890
      RETURN                                                            DDT5 900
      END                                                               DDT5 910
```

Subroutines DCAR and DDCAR

Suppose that $y = y(t)$ is eleven-times differentiable in a neighborhood of radius $R > 0$ of the point x. These subroutines compute an approximation Z to $y'(x)$ by applying Richardson's and Romberg's extrapolation method to successively computed central divided differences, using function values in a closed interval of radius $|h|$ about the point x, $0 < |h| < R$.

1. Mathematical background

Suppose, first, that $y = y(t)$ is analytic at x; that is, y has a Taylor series expansion about the point x with radius of convergence $R > 0$. Let h be such that $0 < |h| < R$. For each positive integer n a step size h_1 with $0 < h_1 \leq |h|$ is computed as described below, and a sequence h_k of increments is generated, where

$$h_k = \frac{n-k+1}{n} h_1 \qquad \text{for } k=2,\ldots,n.$$

From the sequence $(x-h_k, x+h_k)$ of point pairs $(k=1,\ldots,n)$, the sequence of central divided differences

$$T_{0,k} = \frac{y(x+h_k) - y(x-h_k)}{2h_k} \qquad \text{for } k=1,\ldots,n \qquad (1)$$

is computed, which forms the first column of the triangular Romberg scheme. The central divided differences $T_{0,k}$ represent the slopes of the secants s_k in Figure 26.

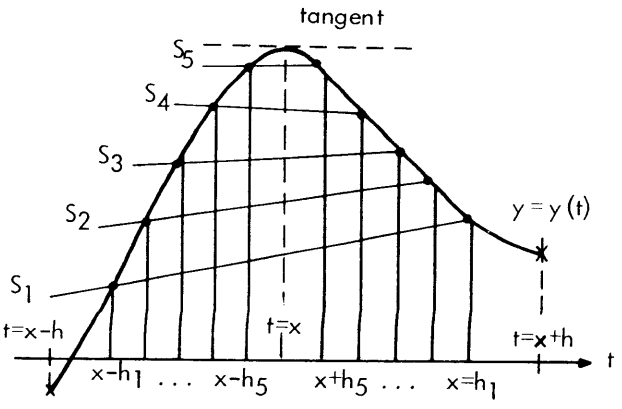

Figure 26. A sequence of secants for a given function $y = y(t)$ and a given argument $t = x$ for the case $n = 5$, $h > 0$

From the Taylor series expansions of $y(x+h_k)$ and $y(x-h_k)$ it follows that

$$T_{0,k} = y'(x) + \frac{h_k^2}{3!} y'''(x) + \frac{h_k^4}{5!} y^{v}(x) + \ldots \text{ for } k=1,\ldots,n$$

so that, as an approximation to $y'(x)$, $T_{0,k}$ involves a truncation error of order h_k^2.

Knowing the two divided differences $T_{0,k}$ and $T_{0,k+1}$, we are able to generate the extrapolated value

$$T_{1,k} = T_{0,k+1} + \frac{T_{0,k+1} - T_{0,k}}{a_{1,k} - 1}$$

where (2)

$$a_{1,k} = \left(1 + \frac{1}{n-k}\right)^2$$

$T_{1,k}$ is a better approximation to $y'(x)$ since

$$T_{1,k} = y'(x) - \frac{1}{5!} \frac{1}{a_{1,k}} h_k^4 y^{v}(x) - \frac{1}{7!} \frac{1}{a_{1,k}} \left(1 + \frac{1}{a_{1,k}}\right) h_k^6 y^{vii}(x) - \ldots,$$

which involves a truncation error of order h_k^4.

If we also know $T_{0,k+2}$, then we can generate $T_{1,k+1}$ using formula (2), and further, we can compute the extrapolated value

$$T_{2,k} = T_{1,k+1} + \frac{T_{1,k+1} - T_{1,k}}{a_{2,k} - 1}$$

where (3)

$$a_{2,k} = \left(1 + \frac{2}{n-(k+1)}\right)^2$$

which involves a truncation error of order h_k^6.

Generally, the order of the truncation error is increased by 2 with each new extrapolation step; in particular, $T_{i,j}$ will involve a truncation error of order

$$h_j^{2i+2}, \quad i = 0,\ldots,n-1, \quad j = 1,\ldots,n.$$

Figure 27 shows the arrangement of the T-values in the triangular Romberg scheme. The T-values are computed following the upward diagonals, using the general formula:

$$T_{m,k-m} = T_{m-1,k-m+1} + \frac{T_{m-1,k-m+1} - T_{m-1,k-m}}{\frac{m}{n-(k+1)}\left(2+\frac{m}{n-(k+1)}\right)}$$

for m = 1, . . . , k-1 for fixed k, k = 2, . . . , n (4)

Truncation error		$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$	$O(h_k^{10})$
Stepsize	m / k	0	1	2	3	4
h_1	1	$T_{0,1}$	$T_{1,1}$	$T_{2,1}$	$T_{3,1}$	$T_{4,1}$
$h_2=0.8h_1$	2	$T_{0,2}$	$T_{1,2}$	$T_{2,2}$	$T_{3,2}$	
$h_2=0.6h_1$	3	$T_{0,3}$	$T_{1,3}$	$T_{2,3}$		
$h_4=0.4h_1$	4	$T_{0,4}$	$T_{1,4}$			
$h_5=0.2h_1$	5	$T_{0,5}$				

Figure 27. The triangular Romberg scheme of T-values for the case n = 5

Numerical experience shows that the accuracy of the results depends heavily on roundoff errors in the central divided differences $T_{0,k}$. Therefore, the choice of the absolutely smallest step size, h_n, is based on the following considerations.
Let

$$v = \begin{cases} 1 & \text{in single-precision computation} \\ 3 & \text{in double-precision computation} \end{cases},$$

$$h_0 = \min\,(n \cdot 10^{-v}, |h|)$$

Set

$$Y = \tfrac{1}{2}(y(x+h_0) + y(x-h_0))$$

and

$$T = \tfrac{1}{2}(y(x+h_0) - y(x-h_0))/h_0$$

Y and T are approximations to y(x) and y'(x), respectively.

Assuming that the errors in the function values y(t) for $t \in [x-|h|, x+|h|]$ are bounded by

$$\epsilon = \begin{cases} Y \cdot 10^{-D} & \text{if } |Y| > 1 \\ 10^{-D} & \text{if } |Y| \le 1 \end{cases}$$

formula (1) shows that the roundoff error in the computation of $T_{0,n}$ is bounded by

$$R(T_{0,n}) = \frac{\epsilon}{h_n} = \begin{cases} \dfrac{Y \cdot 10^{-D}}{h_n} & \text{if } |Y| > 1 \\ \dfrac{10^{-D}}{h_n} & \text{if } |Y| \le 1 \end{cases}$$

where D is the number of significant digits in the floating-point representation of numbers. Suppose, also, that we are willing to tolerate a roundoff error

$$R'(T_{0,n}) = \begin{cases} T \cdot 10^{-D+v} & \text{if } |T| > 1 \\ 10^{-D+v} & \text{if } |T| \le 1 \end{cases}$$

Then we must have $R(T_{0,n}) \le R'(T_{0,n})$, which is satisfied when

$$h_n = \frac{\max(1, |Y|)}{\max(1, |T|)} \cdot 10^{-v} \qquad (5)$$

Finally we set

$$h_1 = \min(n \cdot h_n, |h|) \qquad (6)$$

guaranteeing that the evaluation of the function y = y(t) is restricted to the closed interval $[x-|h|, x+|h|]$.

2. Programming considerations

Numerical experience shows that, because of increasing roundoff errors, it is generally fruitless to perform more than five extrapolations. Thus, the subroutines use n = 5, and consequently it is only necessary that y = y(t) be eleven-times differentiable, rather than analytic. It is easy to see that in the case n = 5, y = y(t) must be evaluated at twelve points in the closed interval $[x-|h|, x+|h|]$.

The parameter lists of both subroutines contain the decision parameter IH. If the user wants the maximum step size to equal |h|, he must set IH = 0. In all other cases (IH ≠ 0) the procedure determines the maximum step size by itself, using formulas (5) and (6) with n = 5. Step size h_1 and all the other step sizes h_k (k = 2, . . . , 5) are successively stored in the single storage location HH.

As previously explained, the computation of the T-values is performed along the upward diagonals of the triangular Romberg scheme. Therefore, only a one-dimensional internal storage vector,

named AUX, with five storage locations is necessary. Figure 28 shows the storage administration and the sequence of computations (numbers in parentheses).

AUX(1)	$T_{0,5}^{(11)}$				
AUX(2)	$T_{0,4}^{(7)}$	$T_{1,4}^{(12)}$			
AUX(3)	$T_{0,3}^{(4)}$	$T_{1,3}^{(8)}$	$T_{2,3}^{(13)}$		
AUX(4)	$T_{0,2}^{(2)}$	$T_{1,2}^{(5)}$	$T_{2,2}^{(9)}$	$T_{3,2}^{(14)}$	
AUX(5)	$T_{0,1}^{(1)}$	$T_{1,1}^{(3)}$	$T_{2,1}^{(6)}$	$T_{3,1}^{(10)}$	$T_{4,1}^{(15)}$

Figure 28. Storage administration and order of computation

Each extrapolation loop, the computation of the elements on an upward diagonal, is terminated as soon as the absolute values of the differences between adjacent diagonal elements stop decreasing, showing the influence of roundoff errors. The computed T-value that differs least in absolute value from its immediately preceding diagonal neighbor is the desired value Z.

3. Accuracy of results

Tests of the single-precision (double-precision) subroutine on the functions $y(t) = t^2$, $1/t$, e^t, tan t, and sin t showed that the accuracy obtained using the step size determined by the subroutine was 3-4 (11-12) significant digits near poles, 5-6(13-14) decimal places near points with horizontal tangents, and 5-6(13-14) significant digits otherwise.

For reference see S. Fillipi and H. Engels, "Altes und Neues zur numerischen Differentiation," Elektronische Datenverarbeitung, iss. 2(1966) pp. 57-65.

```
C                                                                       DCAR  10
C     .................................................................DCAR  20
C                                                                       DCAR  30
C        SUBROUTINE DCAR                                                DCAR  40
C                                                                       DCAR  50
C     PURPOSE                                                           DCAR  60
C        TO COMPUTE, AT A GIVEN POINT X, AN APPROXIMATION Z TO THE      DCAR  70
C        DERIVATIVE OF AN ANALYTICALLY GIVEN FUNCTION FCT THAT IS 11-   DCAR  80
C        TIMES DIFFERENTIABLE IN A DOMAIN CONTAINING A CLOSED, 2-SIDED  DCAR  90
C        SYMMETRIC INTERVAL OF RADIUS ABSOLUTE H ABOUT X, USING FUNCTIONDCAR 100
C        VALUES ONLY ON THAT CLOSED INTERVAL.                           DCAR 110
C                                                                       DCAR 120
C     USAGE                                                             DCAR 130
C        CALL DCAR (X,H,IH,FCT,Z)                                       DCAR 140
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DCAR 150
C                                                                       DCAR 160
C     DESCRIPTION OF PARAMETERS                                         DCAR 170
C        X   - THE POINT AT WHICH THE DERIVATIVE IS TO BE COMPUTED      DCAR 180
C        H   - THE NUMBER WHOSE ABSOLUTE VALUE DEFINES THE CLOSED,      DCAR 190
C              SYMMETRIC 2-SIDED INTERVAL ABOUT X (SEE PURPOSE)         DCAR 200
C        IH  - INPUT PARAMETER (SEE REMARKS AND METHOD)                 DCAR 210
C              IH NON-ZERO - THE SUBROUTINE GENERATES THE INTERNAL      DCAR 220
C                            VALUE HH                                   DCAR 230
C              IH    =  0  - THE INTERNAL VALUE HH IS SET TO ABSOLUTE H DCAR 240
C        FCT - THE NAME OF THE EXTERNAL FUNCTION SUBPROGRAM THAT WILL   DCAR 250
C              GENERATE THE NECESSARY FUNCTION VALUES                   DCAR 260
C        Z   - RESULTING DERIVATIVE VALUE                               DCAR 270
C                                                                       DCAR 280
C     REMARKS                                                           DCAR 290
C        (1)  IF H = 0, THEN THERE IS NO COMPUTATION.                   DCAR 300
C        (2)  THE INTERNAL VALUE HH, WHICH IS DETERMINED ACCORDING TO   DCAR 310
C             IH, IS THE MAXIMUM STEP-SIZE USED IN THE COMPUTATION OF   DCAR 320
C             THE CENTRAL DIVIDED DIFFERENCES (SEE METHOD.)  IF IH IS   DCAR 330
C             NON-ZERO, THEN THE SUBROUTINE GENERATES HH ACCORDING TO   DCAR 340
C             CRITERIA THAT BALANCE ROUND-OFF AND TRUNCATION ERROR.  HH DCAR 350
C             IS ALWAYS LESS THAN OR EQUAL TO ABSOLUTE H IN ABSOLUTE    DCAR 360
C             VALUE, SO THAT ALL COMPUTATION OCCURS WITHIN A RADIUS     DCAR 370
C             ABSOLUTE H OF X.                                          DCAR 380
C                                                                       DCAR 390
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DCAR 400
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(I) MUST BE FURNISHED BY   DCAR 410
C        THE USER.                                                      DCAR 420
C                                                                       DCAR 430
C     METHOD                                                            DCAR 440
C        THE COMPUTATION OF Z IS BASED ON RICHARDSON'S AND ROMBERG'S    DCAR 450
C        EXTRAPOLATION METHOD AS APPLIED TO THE SEQUENCE OF CENTRAL     DCAR 460
C        DIVIDED DIFFERENCES ASSOCIATED WITH THE POINT PAIRS            DCAR 470
C        (X-(K*HH)/5,X+(K*HH)/5) K=1,...,5.  (SEE FILLIPI, S. AND       DCAR 480
C        ENGELS, H., ALTES UND NEUES ZUR NUMERISCHEN DIFFERENTIATION,   DCAR 490
C        ELECTRONISCHE DATENVERARBEITUNG, ISS. 2 (1966), PP. 57-65.)    DCAR 500
C                                                                       DCAR 510
C     .................................................................DCAR 520
C                                                                       DCAR 530
      SUBROUTINE DCAR(X,H,IH,FCT,Z)                                     DCAR 540
C                                                                       DCAR 550
C                                                                       DCAR 560
      DIMENSION AUX(5)                                                  DCAR 570
C                                                                       DCAR 580
C        NO ACTION IN CASE OF ZERO INTERVAL LENGTH                      DCAR 590
      IF(H)1,17,1                                                       DCAR 600
C                                                                       DCAR 610
C        GENERATE STEPSIZE HH FOR DIVIDED DIFFERENCES                   DCAR 620
    1 C=ABS(H)                                                          DCAR 630
      IF(IH)2,9,2                                                       DCAR 640
    2 HH=.5                                                             DCAR 650
      IF(C-HH)3,4,4                                                     DCAR 660
    3 HH=C                                                              DCAR 670
    4 A=FCT(X+HH)                                                       DCAR 680
      B=FCT(X-HH)                                                       DCAR 690
      Z=ABS((A-B)/(HH+HH))                                              DCAR 700
      A=.5*ABS(A+B)                                                     DCAR 710
      HH=.5                                                             DCAR 720
      IF(A-1.)6,6,5                                                     DCAR 730
    5 HH=HH*A                                                           DCAR 740
    6 IF(Z-1.)8,8,7                                                     DCAR 750
    7 HH=HH/Z                                                           DCAR 760
    8 IF(HH-C)10,10,9                                                   DCAR 770
    9 HH=C                                                              DCAR 780
C                                                                       DCAR 790
C        INITIALIZE DIFFERENTIATION LOOP                                DCAR 800
   10 Z=(FCT(X+HH)-FCT(X-HH))/(HH+HH)                                   DCAR 810
      J=5                                                               DCAR 820
      JJ=J-1                                                            DCAR 830
      AUX(J)=Z                                                          DCAR 840
      DH=HH/FLOAT(J)                                                    DCAR 850
      DZ=1.E75                                                          DCAR 860
C                                                                       DCAR 870
C        START DIFFERENTIATION LOOP                                     DCAR 880
   11 J=J-1                                                             DCAR 890
      C=J                                                               DCAR 900
      HH=C*DH                                                           DCAR 910
      AUX(J)=(FCT(X+HH)-FCT(X-HH))/(HH+HH)                              DCAR 920
C                                                                       DCAR 930
C        INITIALIZE EXTRAPOLATION LOOP                                  DCAR 940
      D2=1.E75                                                          DCAR 950
      B=0.                                                              DCAR 960
      A=1./C                                                            DCAR 970
C                                                                       DCAR 980
C        START EXTRAPOLATION LOOP                                       DCAR 990
      DO 12 I=J,JJ                                                      DCAR1000
      D1=D2                                                             DCAR1010
      B=B+A                                                             DCAR1020
      HH=(AUX(I)-AUX(I+1))/(B*(2.+B))                                   DCAR1030
      AUX(I+1)=AUX(I)+HH                                                DCAR1040
C                                                                       DCAR1050
C        TEST ON OSCILLATING INCREMENTS                                 DCAR1060
      D2=ABS(HH)                                                        DCAR1070
      IF(D2-D1)12,13,13                                                 DCAR1080
   12 CONTINUE                                                          DCAR1090
C        END OF EXTRAPOLATION LOOP                                      DCAR1100
C                                                                       DCAR1110
C        UPDATE RESULT VALUE Z                                          DCAR1120
      I=JJ+1                                                            DCAR1130
      GO TO 14                                                          DCAR1140
   13 D2=D1                                                             DCAR1150
      JJ=I                                                              DCAR1160
   14 IF(D2-DZ)15,16,16                                                 DCAR1170
   15 DZ=D2                                                             DCAR1180
      Z=AUX(I)                                                          DCAR1190
   16 IF(J-1)17,17,11                                                   DCAR1200
C        END OF DIFFERENTIATION LOOP                                    DCAR1210
C                                                                       DCAR1220
   17 RETURN                                                            DCAR1230
      END                                                               DCAR1240
```

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C                                                                       DDCA  10
C     ..................................................................DDCA  20
C                                                                       DDCA  30
C     SUBROUTINE DDCAR                                                  DDCA  40
C                                                                       DDCA  50
C     PURPOSE                                                           DDCA  60
C        TO COMPUTE, AT A GIVEN POINT X, AN APPROXIMATION Z TO THE      DDCA  70
C        DERIVATIVE OF AN ANALYTICALLY GIVEN FUNCTION FCT THAT IS 11-   DDCA  80
C        TIMES DIFFERENTIABLE IN A DOMAIN CONTAINING A CLOSED, 2-SIDED  DDCA  90
C        SYMMETRIC INTERVAL OF RADIUS ABSOLUTE H ABOUT X, USING FUNCTIONDDCA 100
C        VALUES ONLY ON THAT CLOSED INTERVAL.                           DDCA 110
C                                                                       DDCA 120
C     USAGE                                                             DDCA 130
C        CALL DDCAR(X,H,IH,FCT,Z)                                       DDCA 140
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DDCA 150
C                                                                       DDCA 160
C     DESCRIPTION OF PARAMETERS                                         DDCA 170
C        X   - THE POINT AT WHICH THE DERIVATIVE IS TO BE COMPUTED      DDCA 180
C              X IS IN DOUBLE PRECISION.                                DDCA 190
C        H   - THE NUMBER WHOSE ABSOLUTE VALUE DEFINES THE CLOSED,      DDCA 200
C              SYMMETRIC 2-SIDED INTERVAL ABOUT X (SEE PURPOSE)         DDCA 210
C              H IS IN SINGLE PRECISION                                 DDCA 220
C        IH  - INPUT PARAMETER (SEE REMARKS AND METHOD)                 DDCA 230
C              IH NON-ZERO - THE SUBROUTINE GENERATES THE INTERNAL      DDCA 240
C                            VALUE HH                                   DDCA 250
C              IH    =   0 - THE INTERNAL VALUE HH IS SET TO ABSOLUTE H DDCA 260
C        FCT - THE NAME OF THE EXTERNAL DOUBLE PRECISION FUNCTION       DDCA 270
C              SUPPROGRAM THAT WILL GENERATE THE NECESSARY FUNCTION     DDCA 280
C              VALUES.                                                  DDCA 290
C        Z   - RESULTING DERIVATIVE VALUE - DOUBLE PRECISION            DDCA 300
C                                                                       DDCA 310
C     REMARKS                                                           DDCA 320
C        (1)  IF H = 0, THEN THERE IS NO COMPUTATION.                   DDCA 330
C        (2)  THE INTERNAL VALUE HH, WHICH IS DETERMINED ACCORDING TO   DDCA 340
C             IH, IS THE MAXIMUM STEP-SIZE USED IN THE COMPUTATION OF   DDCA 350
C             THE CENTRAL DIVIDED DIFFERENCES (SEE METHOD.)  IF IH IS   DDCA 360
C             NON-ZERO, THEN THE SUBROUTINE GENERATES HH ACCORDING TO   DDCA 370
C             CRITERIA THAT BALANCE ROUND-OFF AND TRUNCATION ERROR.  HH DDCA 380
C             IS ALWAYS LESS THAN OR EQUAL TO ABSOLUTE H IN ABSOLUTE    DDCA 390
C             VALUE, SO THAT ALL COMPUTATION OCCURS WITHIN A RADIUS     DDCA 400
C             ABSOLUTE H OF X.                                          DDCA 410
C                                                                       DDCA 420
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DDCA 430
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(T) MUST BE FURNISHED BY   DDCA 440
C        THE USER. FCT(T) IS IN DOUBLE PRECISION                        DDCA 450
C                                                                       DDCA 460
C     METHOD                                                            DDCA 470
C        THE COMPUTATION OF Z IS BASED ON RICHARDSON'S AND ROMBERG'S    DDCA 480
C        EXTRAPOLATION METHOD AS APPLIED TO THE SEQUENCE OF CENTRAL     DDCA 490
C        DIVIDED DIFFERENCES ASSOCIATED WITH THE POINT PAIRS            DDCA 500
C        (X-(K+HH)/5,X+(K+HH)/5) K=1,...,5.  (SEE FILLIPI, S. AND      DDCA 510
C        ENGELS, H., ALTES UND NEUES ZUR NUMERISCHEN DIFFERENTIATION,   DDCA 520
C        ELECTRONISCHE DATENVERARBEITUNG, 1SS. 2 (1966), PP. 57-65.)    DDCA 530
C                                                                       DDCA 540
C     ..................................................................DDCA 550
C                                                                       DDCA 560
      SUBROUTINE DDCAR(X,H,IH,FCT,Z)                                    DDCA 570
C                                                                       DDCA 580
C                                                                       DDCA 590
      DIMENSION AUX(5)                                                  DDCA 600
      DOUBLE PRECISION X,FCT,Z,AUX,A,B,C,DH,HH                          DDCA 610
C                                                                       DDCA 620
C        NO ACTION IN CASE OF ZERO INTERVAL LENGTH                      DDCA 630
      IF(H)1,17,1                                                       DDCA 640
C                                                                       DDCA 650
C        GENERATE STEPSIZE HH FOR DIVIDED DIFFERENCES                   DDCA 660
    1 C=ABS(H)                                                          DDCA 670
      IF(IH)2,9,2                                                       DDCA 680
    2 HH=.5D-2                                                          DDCA 690
      IF(C-HH)3,4,4                                                     DDCA 700
    3 HH=C                                                              DDCA 710
    4 A=FCT(X+HH)                                                       DDCA 720
      B=FCT(X-HH)                                                       DDCA 730
      Z=DABS((A-B)/(HH+HH))                                             DDCA 740
      A=.5D0*DABS(A+B)                                                  DDCA 750
      HH=.5D-2                                                          DDCA 760
      IF(A-1.D0)6,6,5                                                   DDCA 770
    5 HH=HH*A                                                           DDCA 780
    6 IF(Z-1.D0)8,8,7                                                   DDCA 790
    7 HH=HH/Z                                                           DDCA 800
    8 IF(HH-C)10,10,9                                                   DDCA 810
    9 HH=C                                                              DDCA 820
C                                                                       DDCA 830
C        INITIALIZE DIFFERENTIATION LOOP                                DDCA 840
   10 Z=(FCT(X+HH)-FCT(X-HH))/(HH+HH)                                   DDCA 850
      J=5                                                               DDCA 860
      JJ=J-1                                                            DDCA 870
      AUX(J)=Z                                                          DDCA 880
      DH=HH/DFLOAT(J)                                                   DDCA 890
      DZ=1.E75                                                          DDCA 900
C                                                                       DDCA 910
C        START DIFFERENTIATION LOOP                                     DDCA 920
   11 J=J-1                                                             DDCA 930
      C=J                                                               DDCA 940
      HH=C*DH                                                           DDCA 950
      AUX(J)=(FCT(X+HH)-FCT(X-HH))/(HH+HH)                              DDCA 960
C                                                                       DDCA 970
C        INITIALIZE EXTRAPOLATION LOOP                                  DDCA 980
      D2=1.E75                                                          DDCA 990
      B=0.D0                                                            DDCA1000
      A=1.D0/C                                                          DDCA1010
C                                                                       DDCA1020
C        START EXTRAPOLATION LOOP                                       DDCA1030
      DO 12 I=J,JJ                                                      DDCA1040
      D1=D2                                                             DDCA1050
      B=B+A                                                             DDCA1060
      HH=(AUX(I)-AUX(I+1))/(B+(2.D0+B))                                 DDCA1070
      AUX(I+1)=AUX(I)+HH                                                DDCA1080
C                                                                       DDCA1090
C        TEST ON OSCILLATING INCREMENTS                                 DDCA1100
      D2=DABS(HH)                                                       DDCA1110
      IF(D2-D1)12,13,13                                                 DDCA1120
   12 CONTINUE                                                          DDCA1130
C        END OF EXTRAPOLATION LOOP                                      DDCA1140
C                                                                       DDCA1150
C        UPDATE RESULT VALUE Z                                          DDCA1160
      I=JJ+1                                                            DDCA1170
      GO TO 14                                                          DDCA1180
   13 D2=D1                                                             DDCA1190
      JJ=I                                                              DDCA1200
   14 IF(D2-DZ)15,16,16                                                 DDCA1210
   15 DZ=D2                                                             DDCA1220
      Z=AUX(I)                                                          DDCA1230
   16 IF(J-1)17,17,11                                                   DDCA1240
C        END OF DIFFERENTIATION LOOP                                    DDCA1250
C                                                                       DDCA1260
   17 RETURN                                                            DDCA1270
      END                                                               DDCA1280
```

Subroutines DBAR and DDBAR

Suppose that $y = y(t)$ is eleven-times differentiable in a neighborhood of radius $R > 0$ of the point x. These subroutines compute an approximation Z to $y'(x)$ by applying Richardson's and Romberg's extrapolation method to successively computed one-sided divided differences, using function values in a closed interval $[x, x+h]$, $0 < |h| < R$.

1. Mathematical background

Suppose, first, that $y = y(t)$ is analytic at x; that is, y has a Taylor series expansion about the point x with radius of convergence $R > 0$. Let h be such that $0 < |h| < R$. For each positive integer n, a step size h_1 with $0 < |h_1| \leq |h|$ is computed as described below, and a sequence h_k of increments is generated, where

$$h_k = \frac{n-k+1}{n} h_1$$

for $k = 2, \ldots, n$.

From the sequence $(x, x+h_k)$ of point pairs $(k = 1, \ldots, n)$, the sequence of one-sided divided differences

$$T_{0,k} = \frac{y(x+h_k) - y(x)}{h_k} \quad \text{for } k = 1, \ldots, n \qquad (1)$$

is computed, which forms the first column of the triangular Romberg scheme. These one-sided divided differences $T_{0,k}$ represent the slopes of the secants s_k in Figure 29, in the case $h > 0$.

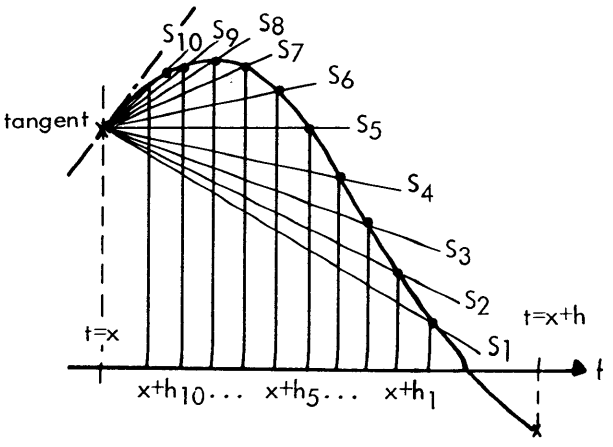

Figure 29. A sequence of secants for a given function $y = y(t)$ and a given argument $t = x$ for the case $n = 10$, $h > 0$

From the Taylor series expansion of $y(x+h_k)$ it follows that

$$T_{0,k} = y'(x) + \frac{h_k}{2!}y''(x) + \frac{h_k^2}{3!}y'''(x) + \ldots \text{ for } k = 1, \ldots, n$$

so that, as an approximation to $y'(x)$, $T_{0,k}$ involves a truncation error of order h_k. Knowing the two divided differences $T_{0,k}$ and $T_{0,k+1}$, we are able to generate the extrapolated value

$$T_{1,k} = T_{0,k+1} + \frac{T_{0,k+1} - T_{0,k}}{a_{1,k} - 1} \qquad (2)$$

where

$$a_{1,k} = \left(1 + \frac{1}{n-k}\right)$$

$T_{1,k}$ is a better approximation to $y'(x)$ since

$$T_{1,k} = y'(x) = \frac{1}{3!}\frac{1}{a_{i,k}-1}h_k^2 y'''(x)$$

$$- \frac{1}{4!}\frac{1}{a_{i,k}}\left(1 + \frac{1}{a_{i,k}}\right)h_k^3 y^{iv}(x)$$

..., which involves a truncation error of order h_k^2.

If we also know $T_{0,k+2}$, then we can generate $T_{1,k+1}$ using formula (2), and further, we can compute the extrapolated value

$$T_{2,k} = T_{1,k+1} + \frac{T_{1,k+1} - T_{1,k}}{a_{2,k} - 1}$$

where

$$a_{2,k} = \left(1 + \frac{2}{n-(k+1)}\right)$$

which involves a truncation error of order h_k^3.

Generally, the order of the truncation error is increased by 1 with each new extrapolation step; in particular, $T_{i,j}$ will involve a truncation error of order

$$h_j^{i+1},\ i = 0, \ldots, n-1,\ j = 1, \ldots, n.$$

Figure 30 shows the arrangement of the T-values in the triangular Romberg scheme. The T-values are computed following the upward diagonals, using the general formula

$$T_{m,k-m} = T_{m-1,k-m+1} + \frac{T_{m-1,k-m+1} - T_{m-1,k-m}}{\frac{m}{n-k+1}}$$

for $m = 1, \ldots, k-1$ for fixed k, $k = 2, \ldots, n$ (3)

Truncation error		$O(h_k)$	$O(h_k^2)$	$O(h_k^3)$	$O(h_k^4)$	$O(h_k^5)$	$O(h_k^6)$	$O(h_k^7)$	$O(h_k^8)$	$O(h_k^9)$	$O(h_k^{10})$
Stepsize	k \ m	0	1	2	3	4	5	6	7	8	9
h_1	1	$T_{0,1}$	$T_{1,1}$	$T_{2,1}$	$T_{3,1}$	$T_{4,1}$	$T_{5,1}$	$T_{6,1}$	$T_{7,1}$	$T_{8,1}$	$T_{9,1}$
$h_2=0.9h_1$	2	$T_{0,2}$	$T_{1,2}$	$T_{2,2}$	$T_{3,2}$	$T_{4,2}$	$T_{5,2}$	$T_{6,2}$	$T_{7,2}$	$T_{8,2}$	
$h_3=0.8h_1$	3	$T_{0,3}$	$T_{1,3}$	$T_{2,3}$	$T_{3,3}$	$T_{4,3}$	$T_{5,3}$	$T_{6,3}$	$T_{7,3}$		
$h_4=0.7h_1$	4	$T_{0,4}$	$T_{1,4}$	$T_{2,4}$	$T_{3,4}$	$T_{4,4}$	$T_{5,4}$	$T_{6,4}$			
$h_5=0.6h_1$	5	$T_{0,5}$	$T_{1,5}$	$T_{2,5}$	$T_{3,5}$	$T_{4,5}$	$T_{5,5}$				
$h_6=0.5h_1$	6	$T_{0,6}$	$T_{1,6}$	$T_{2,6}$	$T_{3,6}$	$T_{4,6}$					
$h_7=0.4h_1$	7	$T_{0,7}$	$T_{1,7}$	$T_{2,7}$	$T_{3,7}$						
$h_8=0.3h_1$	8	$T_{0,8}$	$T_{1,8}$	$T_{2,8}$							
$h_9=0.2h_1$	9	$T_{0,9}$	$T_{1,9}$								
$h_{10}=0.1h_1$	10	$T_{0,10}$									

Figure 30. The triangular Romberg scheme of T-values for the case n = 10

Numerical experience shows that the accuracy of the results depends heavily on roundoff errors in the one-sided divided differences $T_{0,k}$. Therefore, the choice of the absolutely smallest step size, h_n, is based on the following considerations.

Let

$$v = \begin{cases} 1 & \text{in single-precision computation} \\ 3 & \text{in double-precision computation} \end{cases}$$

Set

$$n_0 = \operatorname{sgn}(h) \cdot \min\left(\frac{n}{2} \cdot 10^{-v}, |h|\right)$$

$$T = (y(x+h_0) - y(x))/h_0.$$

T is an approximation to y'(x).

Assuming that the errors in the function values y(t) for $t \in [x, x+h]$ are bounded by

$$\epsilon = \begin{cases} |y(x)| \cdot 10^{-D} & \text{if } |y(x)| > 1 \\ 10^{-D} & \text{if } |y(x)| \le 1 \end{cases}$$

formula (1) shows that the roundoff error in the computation of $T_{0,n}$ is bounded by

$$R(T_{0,n}) = \frac{2\epsilon}{|h_n|} = \begin{cases} \dfrac{2\,|y(x)|\,10^{-D}}{|h_n|} & \text{if } |y(x)| > 1 \\ 2\dfrac{10^{-D}}{|h_n|} & \text{if } |y(x)| \le 1 \end{cases}$$

where D is the number of significant digits in the floating-point representation of numbers. Suppose, also, that we are willing to tolerate a roundoff error

$$R'(T_{0,n}) = \begin{cases} 2T \cdot 10^{-D+v} & \text{if } |T| > 1 \\ 2 \cdot 10^{-D+v} & \text{if } |T| \le 1 \end{cases}$$

Then we must have $R(T_{0,n}) \le R'(T_{0,n})$, which is satisfied when

$$h_n = \frac{\max(1, |y(x)|)}{\max(1, |T|)} \cdot 10^{-v} \qquad (4)$$

Finally, we set

$$h_1 = \operatorname{sgn}(h) \cdot \min(n \cdot |h_n|, |h|) \qquad (5)$$

guaranteeing that the evaluation of the function y = y(t) is restricted to the closed interval $[x, x+h]$.

2. Programming considerations

Numerical experience shows that, because of increasing roundoff errors, it is generally fruitless to perform more than ten extrapolations. Thus, the subroutines use n = 10, and consequently, it is only necessary that y = y(t) be eleven-times differentiable, rather than analytic. It is easy to see that in the case n = 10, y = y(t) must be evaluated at twelve points in the closed interval $[x, x+h]$.

The parameter lists of both subroutines contain the decision parameter IH. If the user wants the maximum step size to equal |h|, he must set IH = 0. In all other cases (IH ≠ 0) the procedure determines the maximum step size by itself, using formulas (4) and (5) with n = 10. Step size h_1 and all the other step sizes h_k (k = 2, . . . , 10) are successively stored in the single storage location HH.

As previously explained, the computation of the T-values is performed along the upward diagonals of the triangular Romberg scheme. Therefore, only a one-dimensional internal storage vector, named AUX, with ten storage locations is necessary. Figure 31 shows the storage administration and the sequence of computations (numbers in parentheses).

AUX(1)	$T_{0,10}^{(46)}$						
AUX(2)	$T_{0,9}^{(37)}$	$T_{1,9}^{(47)}$					
AUX(3)	$T_{0,8}^{(29)}$	$T_{1,8}^{(38)}$	$T_{2,8}^{(48)}$				
AUX(4)	$T_{0,7}^{(22)}$	$T_{1,7}^{(30)}$	$T_{2,7}^{(39)}$	...			
AUX(5)	$T_{0,6}^{(16)}$	$T_{1,6}^{(23)}$	$T_{2,6}^{(31)}$	...			
AUX(6)	$T_{0,5}^{(11)}$	$T_{1,5}^{(17)}$	$T_{2,5}^{(24)}$	...			
AUX(7)	$T_{0,4}^{(7)}$	$T_{1,4}^{(12)}$	$T_{2,4}^{(18)}$	...			
AUX(8)	$T_{0,3}^{(4)}$	$T_{1,3}^{(8)}$	$T_{2,3}^{(13)}$	...	$T_{7,3}^{(53)}$		
AUX(9)	$T_{0,2}^{(2)}$	$T_{1,2}^{(5)}$	$T_{2,2}^{(9)}$	...	$T_{7,2}^{(44)}$	$T_{8,2}^{(54)}$	
AUX(10)	$T_{0,1}^{(1)}$	$T_{1,1}^{(3)}$	$T_{2,1}^{(6)}$	...	$T_{7,1}^{(36)}$	$T_{8,1}^{(45)}$	$T_{9,1}^{(55)}$

Figure 31. Storage administration and sequence of calculations

Each extrapolation loop, the computation of the elements on an upward diagonal, is terminated as soon as the absolute values of the differences between adjacent diagonal elements stop decreasing, showing the influence of roundoff errors. The computed T-value that differs least in absolute value from its immediately preceding diagonal neighbor is the desired value Z.

3. Accuracy of results

Tests of the single-precision (double-precision) subroutine on the functions $y(t) = t^2$, 1/t, e^t, tan t, and sin t showed that the accuracy obtained using the step size determined by the subroutine was 2-4 (10-12) significant digits near poles, 4-6(13-14) decimal places near points with horizontal tangents, and 4-6(11-13) significant digits otherwise.

For reference see S. Fillipi and H. Engles, "Altes und Neues zur numerischen Differentiation," Elektronische Datenverarbeitung, iss. 2 (1966) pp. 57-65.

```
C                                                                       DBAR  10
C     ..................................................................DBAR  20
C                                                                       DBAR  30
C     SUBROUTINE DBAR                                                   DBAR  40
C                                                                       DBAR  50
C     PURPOSE                                                           DBAR  60
C        TO COMPUTE, AT A GIVEN POINT X, AN APPROXIMATION Z TO THE      DBAR  70
C        DERIVATIVE OF AN ANALYTICALLY GIVEN FUNCTION FCT THAT IS N1-   DBAR  80
C        TIMES DIFFERENTIABLE IN A DOMAIN CONTAINING A CLOSED INTERVAL -DBAR  90
C        THE SET OF T BETWEEN X AND X+H (H POSITIVE OR NEGATIVE) - USINGDBAR 100
C        FUNCTION VALUES ONLY ON THAT INTERVAL.                         DBAR 110
C                                                                       DBAR 120
C     USAGE                                                             DBAR 130
C        CALL DBAR(X,H,IH,FCT,Z)                                        DBAR 140
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DBAR 150
C                                                                       DBAR 160
C     DESCRIPTION OF PARAMETERS                                         DBAR 170
C        X   - THE POINT AT WHICH THE DERIVATIVE IS TO BE COMPUTED      DBAR 180
C        H   - THE NUMBER THAT DEFINES THE CLOSED INTERVAL WHOSE END-   DBAR 190
C              POINTS ARE X AND X+H (SEE PURPOSE)                       DBAR 200
C        IH  - INPUT PARAMETER (SEE REMARKS AND METHOD)                 DBAR 210
C              IH NON-ZERO - THE SUBROUTINE GENERATES THE INTERNAL      DBAR 220
C                            VALUE HH                                   DBAR 230
C              IH    =   0 - THE INTERNAL VALUE HH IS SET TO H          DBAR 240
C        FCT - THE NAME OF THE EXTERNAL FUNCTION SUBPROGRAM THAT WILL   DBAR 250
C              GENERATE THE NECESSARY FUNCTION VALUES                   DBAR 260
C        Z   - RESULTING DERIVATIVE VALUE                               DBAR 270
C                                                                       DBAR 280
C     REMARKS                                                           DBAR 290
C        (1)  IF H = 0, THEN THERE IS NO COMPUTATION.,                  DBAR 300
C        (2)  THE (MAGNITUDE OF THE) INTERNAL VALUE HH, WHICH IS DETER- DBAR 310
C             MINED ACCORDING TO IH, IS THE MAXIMUM STEP-SIZE USED IN   DBAR 320
C             THE COMPUTATION OF THE ONE-SIDED DIVIDED DIFFERENCES (SEE DBAR 330
C             METHOD.)  IF IH IS NON-ZERO, THEN THE SUBROUTINE GENERATESDBAR 340
C             HH ACCORDING TO CRITERIA THAT BALANCE ROUND-OFF AND TRUN- DBAR 350
C             CATION ERROR.  HH ALWAYS HAS THE SAME SIGN AS H AND IT IS DBAR 360
C             ALWAYS LESS THAN OR EQUAL TO THE MAGNITUDE OF H IN AB-    DBAR 370
C             SOLUTE VALUE, SO THAT ALL COMPUTATION OCCURS IN THE CLOSEDDBAR 380
C             INTERVAL DETERMINED BY H.                                 DBAR 390
C                                                                       DBAR 400
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DBAR 410
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(T) MUST BE FURNISHED BY   DBAR 420
C        THE USER.                                                      DBAR 430
C                                                                       DBAR 440
C     METHOD                                                            DBAR 450
C        THE COMPUTATION OF Z IS BASED ON RICHARDSON'S AND ROMBERG'S    DBAR 460
C        EXTRAPOLATION METHOD AS APPLIED TO THE SEQUENCE OF ONE-SIDED   DBAR 470
C        DIVIDED DIFFERENCES ASSOCIATED WITH THE POINT PAIRS            DBAR 480
C        (X,X+(K*HH)/10)K=1,...,10.  (SEE FILLIPI, S. AND ENGELS, H.,   DBAR 490
C        ALTES UND NEUES ZUR NUMERISCHEN DIFFERENTIATION, ELECTRONISCHE DBAR 500
C        DATENVERARBEITUNG, ISS. 2 (1966), PP. 57-65.)                  DBAR 510
C                                                                       DBAR 520
C     ..................................................................DBAR 530
C                                                                       DBAR 540
      SUBROUTINE DBAR(X,H,IH,FCT,Z)                                     DBAR 550
C                                                                       DBAR 560
C                                                                       DBAR 570
      DIMENSION AUX(10)                                                 DBAR 580
C                                                                       DBAR 590
C        NO ACTION IN CASE OF ZERO INTERVAL LENGTH                      DBAR 600
      IF(H)1,17,1                                                       DBAR 610
C                                                                       DBAR 620
C        GENERATE STEPSIZE HH FOR DIVIDED DIFFERENCES                   DBAR 630
    1 C=ABS(H)                                                          DBAR 640
      B=H                                                               DBAR 650
      D=X                                                               DBAR 660
      D=FCT(D)                                                          DBAR 670
      IF(IH)2,9,2                                                       DBAR 680
    2 HH=.5                                                             DBAR 690
      IF(C-HH)3,4,4                                                     DBAR 700
    3 HH=B                                                              DBAR 710
    4 HH=SIGN(HH,B)                                                     DBAR 720
      Z=ABS((FCT(X+HH)-D)/HH)                                           DBAR 730
      A=ABS(D)                                                          DBAR 740
      HH=1.                                                             DBAR 750
      IF(A-1.)6,6,5                                                     DBAR 760
    5 HH=HH*A                                                           DBAR 770
    6 IF(Z-1.)8,8,7                                                     DBAR 780
    7 HH=HH/Z                                                           DBAR 790
    8 IF(HH-C)10,10,9                                                   DBAR 800
    9 HH=B                                                              DBAR 810
   10 HH=SIGN(HH,B)                                                     DBAR 820
C                                                                       DBAR 830
C        INITIALIZE DIFFERENTIATION LOOP                                DBAR 840
      Z=(FCT(X+HH)-D)/HH                                                DBAR 850
      J=10                                                              DBAR 860
      JJ=J-1                                                            DBAR 870
      AUX(J)=Z                                                          DBAR 880
      DH=HH/FLOAT(J)                                                    DBAR 890
      DZ=1.E75                                                          DBAR 900
C                                                                       DBAR 910
C        START DIFFERENTIATION LOOP                                     DBAR 920
   11 J=J-1                                                             DBAR 930
      C=J                                                               DBAR 940
      HH=C*DH                                                           DBAR 950
      AUX(J)=(FCT(X+HH)-D)/HH                                           DBAR 960
C                                                                       DBAR 970
C        INITIALIZE EXTRAPOLATION LOOP                                  DBAR 980
      D2=1.E75                                                          DBAR 990
      B=0.                                                              DBAP1000
      A=1./C                                                            DBAR1010
C                                                                       DBAR1020
C        START EXTRAPOLATION LOOP                                       DBAR1030
      DO 12 I=J,JJ                                                      DBAP1040
      D1=D2                                                             DBAR1050
      B=B+A                                                             DBAR1060
      HH=(AUX(I)-AUX(I+1))/B                                            DBAR1070
      AUX(I+1)=AUX(I)+HH                                                DBAR1080
C                                                                       DBAR1090
C        TEST ON OSCILLATING INCREMENTS                                 DBAR1100
      D2=ABS(HH)                                                        DBAR1110
      IF(D2-D1)12,13,13                                                 DBAR1120
   12 CONTINUE                                                          DBAR1130
C        END OF EXTRAPOLATION LOOP                                      DBAR1140
C                                                                       DBAR1150
C        UPDATE RESULT VALUE Z                                          DBAR1160
      I=JJ+1                                                            DBAR1170
      GO TO 14                                                          DBAR1180
   13 D2=D1                                                             DBAR1190
      JJ=I                                                              DBAR1200
   14 IF(D2-DZ)15,16,16                                                 DBAR1210
   15 DZ=D2                                                             DBAR1220
      Z=AUX(I)                                                          DBAR1230
   16 IF(J-1)17,17,11                                                   DBAR1240
C        END OF DIFFERENTIATION LOOP                                    DBAR1250
C                                                                       DBAR1260
   17 RETURN                                                            DBAR1270
      END                                                               DBAR1280
```

```
C                                                                       DDBA  10
C     ..................................................................DDBA  20
C                                                                       DDBA  30
C     SUBROUTINE DDBAR                                                  DDBA  40
C                                                                       DDBA  50
C     PURPOSE                                                           DDBA  60
C        TO COMPUTE, AT A GIVEN POINT X, AN APPROXIMATION Z TO THE      DDBA  70
C        DERIVATIVE OF AN ANALYTICALLY GIVEN FUNCTION FCT THAT IS N1-   DDBA  80
C        TIMES DIFFERENTIABLE IN A DOMAIN CONTAINING A CLOSED INTERVAL -DDBA  90
C        THE SET OF T BETWEEN X AND X+H (H POSITIVE OR NEGATIVE) - USINGDDBA 100
C        FUNCTION VALUES ONLY ON THAT INTERVAL.                         DDBA 110
C                                                                       DDBA 120
C     USAGE                                                             DDBA 130
C        CALL DDBAR(X,H,IH,FCT,Z,)                                      DDBA 140
C        PARAMETER FCT REQUIRES AN EXTERNAL STATEMENT                   DDBA 150
C                                                                       DDBA 160
C     DESCRIPTION OF PARAMETERS                                         DDBA 170
C        X   - THE POINT AT WHICH THE DERIVATIVE IS TO BE COMPUTED      DDBA 180
C              X IS IN DOUBLE PRECISION                                 DDBA 190
C        H   - THE NUMBER THAT DEFINES THE CLOSED INTERVAL WHOSE END-   DDBA 200
C              POINTS ARE X AND X+H (SEE PURPOSE)                       DDBA 210
C              H IS IN SINGLE PRECISION                                 DDBA 220
C        IH  - INPUT PARAMETER (SEE REMARKS AND METHOD)                 DDBA 230
C              IH NON-ZERO - THE SUBROUTINE GENERATES THE INTERNAL      DDBA 240
C                            VALUE HH                                   DDBA 250
C              IH    =   0 - THE INTERNAL VALUE HH IS SET TO H          DDBA 260
C        FCT - THE NAME OF THE EXTERNAL DOUBLE PRECISION FUNCTION       DDBA 270
C              SUBPROGRAM THAT WILL GENERATE THE NECESSARY FUNCTION     DDBA 280
C              VALUES.                                                  DDBA 290
C        Z   - RESULTING DERIVATIVE VALUE - DOUBLE PRECISION            DDBA 300
C                                                                       DDBA 310
C     REMARKS                                                           DDBA 320
C        (1)  IF H = 0, THEN THERE IS NO COMPUTATION.                   DDBA 330
C        (2)  THE (MAGNITUDE OF THE) INTERNAL VALUE HH, WHICH IS DETER- DDBA 340
C             MINED ACCORDING TO IH, IS THE MAXIMUM STEP-SIZE USED IN   DDBA 350
C             THE COMPUTATION OF THE ONE-SIDED DIVIDED DIFFERENCES (SEE DDBA 360
C             METHOD.)  IF IH IS NON-ZERO, THEN THE SUBROUTINE GENERATESDDBA 370
C             HH ACCORDING TO CRITERIA THAT BALANCE ROUND-OFF AND TRUN- DDBA 380
C             CATION ERROR.  HH ALWAYS HAS THE SAME SIGN AS H AND IT IS DDBA 390
C             ALWAYS LESS THAN OR EQUAL TO THE MAGNITUDE OF H IN AB-    DDBA 400
C             SOLUTE VALUE, SO THAT ALL COMPUTATION OCCURS IN THE CLOSEDDDBA 410
C             INTERVAL DETERMINED BY H.                                 DDBA 420
C                                                                       DDBA 430
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     DDBA 440
C        THE EXTERNAL FUNCTION SUBPROGRAM FCT(T) MUST BE FURNISHED BY   DDBA 450
C        THE USER. FCT(T) IS IN DOUBLE PRECISION                        DDBA 460
C                                                                       DDBA 470
C     METHOD                                                            DDBA 480
C        THE COMPUTATION OF Z IS BASED ON RICHARDSON'S AND ROMBERG'S    DDBA 490
C        EXTRAPOLATION METHOD AS APPLIED TO THE SEQUENCE OF ONE-SIDED   DDBA 500
C        DIVIDED DIFFERENCES ASSOCIATED WITH THE POINT PAIRS            DDBA 510
C        (X,X+(K*HH)/10)K=1,...,10.  (SEE FILLIPI, S. AND ENGELS, H.,   DDBA 520
C        ALTES UND NEUES ZUR NUMERISCHEN DIFFERENTIATION, ELECTRONISCHE DDBA 530
C        DATENVERARBEITUNG, ISS. 2 (1966), PP. 57-65.)                  DDBA 540
C                                                                       DDBA 550
C     ..................................................................DDBA 560
C                                                                       DDBA 570
      SUBROUTINE DDBAR(X,H,IH,FCT,Z)                                    DDBA 580
C                                                                       DDBA 590
C                                                                       DDBA 600
      DIMENSION AUX(10)                                                 DDBA 610
      DOUBLE PRECISION X,FCT,Z,AUX,A,B,C,D,DH,HH                        DDBA 620
C                                                                       DDBA 630
C        NO ACTION IN CASE OF ZERO INTERVAL LENGTH                      DDBA 640
      IF(H)1,17,1                                                       DDBA 650
C                                                                       DDBA 660
C        GENERATE STEPSIZE HH FOR DIVIDED DIFFERENCES                   DDBA 670
    1 C=ABS(H)                                                          DDBA 680
      B=H                                                               DDBA 690
      D=X                                                               DDBA 700
      D=FCT(D)                                                          DDBA 710
      IF(IH)2,9,2                                                       DDBA 720
    2 HH=.5D-2                                                          DDBA 730
      IF(C-HH)3,4,4                                                     DDBA 740
    3 HH=B                                                              DDBA 750
    4 HH=DSIGN(HH,B)                                                    DDBA 760
      Z=DABS((FCT(X+HH)-D)/HH)                                          DDBA 770
      A=DABS(D)                                                         DDBA 780
      HH=1.D-2                                                          DDBA 790
      IF(A-1.D0)6,6,5                                                   DDBA 800
    5 HH=HH*A                                                           DDBA 810
    6 IF(Z-1.D0)8,8,7                                                   DDBA 820
    7 HH=HH/Z                                                           DDBA 830
    8 IF(HH-C)10,10,9                                                   DDBA 840
    9 HH=B                                                              DDBA 850
   10 HH=DSIGN(HH,B)                                                    DDBA 860
C                                                                       DDBA 870
C        INITIALIZE DIFFERENTIATION LOOP                                DDBA 880
      Z=(FCT(X+HH)-D)/HH                                                DDBA 890
      J=10                                                              DDBA 900
      JJ=J-1                                                            DDBA 910
      AUX(J)=Z                                                          DDBA 920
      DH=HH/DFLOAT(J)                                                   DDBA 930
      DZ=1.E75                                                          DDBA 940
C                                                                       DDBA 950
C        START DIFFERENTIATION LOOP                                     DDBA 960
   11 J=J-1                                                             DDBA 970
      C=J                                                               DDBA 980
      HH=C*DH                                                           DDBA 990
      AUX(J)=(FCT(X+HH)-D)/HH                                           DDBA1000
C                                                                       DDBA1010
C        INITIALIZE EXTRAPOLATION LOOP                                  DDBA1020
      D2=1.E75                                                          DDBA1030
      B=0.D0                                                            DDBA1040
      A=1.D0/C                                                          DDBA1050
C                                                                       DDBA1060
C        START EXTRAPOLATION LOOP                                       DDBA1070
      DO 12 I=J,JJ                                                      DDBA1080
      D1=D2                                                             DDBA1090
      B=B+A                                                             DDBA1100
      HH=(AUX(I)-AUX(I+1))/B                                            DDBA1110
      AUX(I+1)=AUX(I)+HH                                                DDBA1120
C                                                                       DDBA1130
C        TEST ON OSCILLATING INCREMENTS                                 DDBA1140
      D2=DABS(HH)                                                       DDBA1150
      IF(D2-D1)12,13,13                                                 DDBA1160
   12 CONTINUE                                                          DDBA1170
C        END OF EXTRAPOLATION LOOP                                      DDBA1180
C                                                                       DDBA1190
C        UPDATE RESULT VALUE Z                                          DDBA1200
      I=JJ+1                                                            DDBA1210
      GO TO 14                                                          DDBA1220
   13 D2=D1                                                             DDBA1230
      JJ=I                                                              DDBA1240
   14 IF(D2-DZ)15,16,16                                                 DDBA1250
   15 DZ=D2                                                             DDBA1260
      Z=AUX(I)                                                          DDBA1270
   16 IF(J-1)17,17,11                                                   DDBA1280
C        END OF DIFFERENTIATION LOOP                                    DDBA1290
C                                                                       DDBA1300
   17 RETURN                                                            DDBA1310
      END                                                               DDBA1320
```

Subroutine RK1

This subroutine integrates a given function using the Runge-Kutta technique and produces the final computed value of the integral.

The ordinary differential equation:

$$\frac{dy}{dx} = f(x,y) \tag{1}$$

with initial condition $y(x_0) = y_0$ is solved numerically using a fourth-order Runge-Kutta integration process. This is a single-step method in which the value of y at $x = x_n$ is used to compute $y_{n+1} = y(x_{n+1})$ and earlier values yn-1, yn-2, etc. are not used.

The relevant formulas are:

$$y_{n+1} = y_n + 1/6\,[k_0 + 2k_1 + 2k_2 + k_3] \tag{2}$$

where, for step size h:

$$\begin{cases} k_0 = h f(x_n, y_n) \\ k_1 = h f(x_n + h/2,\ y_n + k_0/2) \\ k_2 = h f(x_n + h/2,\ y_n + k_1/2) \\ k_3 = h f(x_n + h,\ y_n + k_2) \end{cases} \tag{3}$$

```
C                                                                       RK1   10
C     ..................................................................RK1   20
C                                                                       RK1   30
C        SUBROUTINE RK1                                                 RK1   40
C                                                                       RK1   50
C        PURPOSE                                                        RK1   60
C           INTEGRATES A FIRST ORDER DIFFERENTIAL EQUATION              RK1   70
C           DY/DX=FUN(X,Y) OF TO A SPECIFIED FINAL VALUE                RK1   80
C                                                                       RK1   90
C        USAGE                                                          RK1  100
C           CALL RK1(FUN,HI,XI,YI,XF,YF,ANSX,ANSY,IER)                  RK1  110
C                                                                       RK1  120
C        DESCRIPTION OF PARAMETERS                                      RK1  130
C           FUN -USER-SUPPLIED FUNCTION SUBPROGRAM WITH ARGUMENTS X,Y   RK1  140
C                WHICH GIVES DY/DX                                      RK1  150
C           HI  -THE STEP SIZE                                          RK1  160
C           XI  -INITIAL VALUE OF X                                     RK1  170
C           YI  -INITIAL VALUE OF Y WHERE YI=Y(XI)                      RK1  180
C           XF  -FINAL VALUE OF X                                       RK1  190
C           YF  -FINAL VALUE OF Y                                       RK1  200
C           ANSX-RESULTANT FINAL VALUE OF X                             RK1  210
C           ANSY-RESULTANT FINAL VALUE OF Y                             RK1  220
C                EITHER ANSX WILL EQUAL XF OR ANSY WILL EQUAL YF        RK1  230
C                DEPENDING ON WHICH IS REACHED FIRST                    RK1  240
C           IER -ERROR CODE                                             RK1  250
C                IER=0 NO ERROR                                         RK1  260
C                IER=1 STEP SIZE IS ZERO                                RK1  270
C                                                                       RK1  280
C                                                                       RK1  290
C        REMARKS                                                        RK1  300
C           IF XI IS GREATER THAN XF, ANSX=XI AND ANSY=YI               RK1  310
C           IF H IS ZERO, IER IS SET TO ONE, ANSX IS SET TO XI, AND     RK1  320
C           ANSY IS SET TO ZERO                                         RK1  330
C                                                                       RK1  340
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RK1  350
C           FUN IS A TWO ARGUMENT FUNCTION SUBPROGRAM FURNISHED BY THE  RK1  360
C           USER.  DY/DX=FUN (X,Y)                                      RK1  370
C           CALLING PROGRAM MUST HAVE FORTRAN EXTERNAL STATEMENT        RK1  380
C           CONTAINING NAMES OF FUNCTION SUBPROGRAMS LISTED IN CALL TO  RK1  390
C           RK1                                                         RK1  400
C                                                                       RK1  410
C        METHOD                                                         RK1  420
C           USES FOURTH ORDER RUNGE-KUTTA INTEGRATION PROCESS ON A      RK1  430
C           RECURSIVE BASIS AS SHOWN IN F.B. HILDEBRAND, 'INTRODUCTION  RK1  440
C           TO NUMERICAL ANALYSIS',MCGRAW-HILL,1956. PROCESS IS         RK1  450
C           TERMINATED AND FINAL VALUE ADJUSTED WHEN EITHER XF OR YF    RK1  460
C           IS REACHED.                                                 RK1  470
C     ..................................................................RK1  480
C                                                                       RK1  490
      SUBROUTINE RK1(FUN,HI,XI,YI,XF,YF,ANSX,ANSY,IER)                  RK1  500
C                                                                       RK1  510
C     ..................................................................RK1  520
C                                                                       RK1  530
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  RK1  540
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      RK1  550
C        STATEMENT WHICH FOLLOWS.                                       RK1  560
C                                                                       RK1  570
C     DOUBLE PRECISION HI,XI,YI,XF,YF,ANSX,ANSY,H,XN,YN,YNEW,XN1,YN1,   RK1  580
C    1                 XX,YY,XNEW,YNEW,H2,T1,T2,T3,T4,FUN             RK1  590
C                                                                       RK1  600
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    RK1  610
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      RK1  620
C        ROUTINE.                                                       RK1  630
C                                                                       RK1  640
C        USER FUNCTION SUBPROGRAM, FUN, MUST BE IN DOUBLE PRECISION.    RK1  650
C                                                                       RK1  660
C        ..............................................................RK1  670
C                                                                       RK1  680
C     IF XF IS LESS THAN OR EQUAL TO XI, RETURN XI,YI AS ANSWER         RK1  690
C                                                                       RK1  700
      IER=0                                                             RK1  705
      IF(XF-XI) 11,11,12                                                RK1  710
   11 ANSX=XI                                                           RK1  720
      ANSY=YI                                                           RK1  730
      RETURN                                                            RK1  740
C                                                                       RK1  750
C     TEST INTERVAL VALUE                                               RK1  760
C                                                                       RK1  770
   12 H=HI                                                              RK1  780
      IF(H) 13,14,20                                                    RK1  790
   13 IER=1                                                             RK1  800
      ANSX=XI                                                           RK1  810
      ANSY=0.0                                                          RK1  820
      RETURN                                                            RK1  830
   14 H=-H                                                              RK1  840
                                                                        RK1  850
C     SET XN=INITIAL X,YN=INITIAL Y                                     RK1  860
C                                                                       RK1  870
   20 XN=XI                                                             RK1  880
      YN=YI                                                             RK1  890
                                                                        RK1  900
C     INTEGRATE ONE TIME STEP                                           RK1  910
C                                                                       RK1  920
      HNEW=H                                                            RK1  930
      JUMP=1                                                            RK1  940
      GO TO 170                                                         RK1  950
   25 XN1=XX                                                            RK1  960
      YN1=YY                                                            RK1  970
                                                                        RK1  980
C     COMPARE XN1 (=X(N+1)) TO X FINAL AND BRANCH ACCORDINGLY           RK1  990
C                                                                       RK1 1000
      IF(XN1-XF)35C,3C,4C                                               RK1 1010
C                                                                       RK1 1020
C     XN1=XF, RETURN (XF,YN1) AS ANSWER                                 RK1 1030
C                                                                       RK1 1040
   3C ANSX=XF                                                           RK1 1050
      ANSY=YN1                                                          RK1 1060
      GO TO 16C                                                         RK1 1070
                                                                        RK1 1080
C     XN1 GREATER THAN XF, SET NEW STEP SIZE AND INTEGRATE ONE STEP     RK1 1090
C     RETURN RESULTS OF INTEGRATION AS ANSWER                           RK1 1100
C                                                                       RK1 1110
   4C HNEW=XF-XN                                                        RK1 1120
      JUMP=2                                                            RK1 1130
      GO TO 170                                                         RK1 1140
   45 ANSX=XX                                                           RK1 1150
      ANSY=YY                                                           RK1 1160
      GO TO 16C                                                         RK1 1170
                                                                        RK1 1180
C     XN1 LESS THAN X FINAL, CHECK IF (YN,YN1) SPAN Y FINAL             RK1 1190
C                                                                       RK1 1200
                                                                        RK1 1210
   5C IF((YN1-YF)*(YF-YN))6C,7C,11C                                     RK1 1220
                                                                        RK1 1230
C     YN1 AND YN DO NOT SPAN YF. SET (XN,YN) AS (XN1,YN1) AND REPEAT    RK1 1240
C                                                                       RK1 1250
   6C YN=YN1                                                            RK1 1260
      XN=XN1                                                            RK1 1270
      GO TO 17C                                                         RK1 1280
                                                                        RK1 1290
C     EITHER YN OR YN1 =YF. CHECK WHICH AND SET PROPER (X,Y) AS ANSWER  RK1 1300
C                                                                       RK1 1310
   7C IF(YN1-YF)8C,1CC,6C                                               RK1 1320
   8C ANSY=YN                                                           RK1 1330
      ANSX=XN                                                           RK1 1340
      GO TO 16C                                                         RK1 1350
  1CC ANSY=YN1                                                          RK1 1360
      ANSX=XN1                                                          RK1 1370
      GO TO 16C                                                         RK1 1380
                                                                        RK1 1390
C     YN AND YN1 SPAN YF. TRY TO FIND X VALUE ASSOCIATED WITH YF        RK1 1400
C                                                                       RK1 1410
  11C DO 14C I=1,1C                                                     RK1 1420
C                                                                       RK1 1430
C     INTERPOLATE TO FIND NEW TIME STEP AND INTEGRATE ONE STEP          RK1 1440
C     TRY TEN INTERPOLATIONS AT MOST                                    RK1 1450
C                                                                       RK1 1460
      HNEW=((YF-YN )/(YN1-YN))*(XN1-XN)                                 RK1 1470
      JUMP=3                                                            RK1 1480
      GO TO 17C                                                         RK1 1490
  115 XNEW=XX                                                           RK1 1500
      YNEW=YY                                                           RK1 1510
C                                                                       RK1 1520
C     COMPARE COMPUTED Y VALUE WITH YF AND BRANCH                       RK1 1530
C                                                                       RK1 1540
      IF(YNEW-YF)12C,15C,12C                                            RK1 1550
C                                                                       RK1 1560
C     ADVANCE, YF IS BETWEEN YNEW AND YN1                               RK1 1570
C                                                                       RK1 1580
  12C YN=YNEW                                                           RK1 1590
      XN=XNEW                                                           RK1 1600
      GO TO 14C                                                         RK1 1610
C                                                                       RK1 1620
C     ADVANCE, YF IS BETWEEN YN AND YNEW                                RK1 1630
C                                                                       RK1 1640
  13C YN1=YNEW                                                          RK1 1650
      XN1=XNEW                                                          RK1 1660
  14C CONTINUE                                                          RK1 1670
C                                                                       RK1 1680
C     RETURN (XNEW,YF) AS ANSWER                                        RK1 1690
C                                                                       RK1 1700
  15C ANSX=XNEW                                                         RK1 1710
      ANSY=YF                                                           RK1 1720
  16C RETURN                                                            RK1 1730
C                                                                       RK1 1740
  17C H2=HNEW/2.0                                                       RK1 1750
      T1=HNEW*FUN(XN,YN)                                                RK1 1760
      T2=HNEW*FUN(XN+H2,YN+T1/2.0)                                      RK1 1770
      T3=HNEW*FUN(XN+H2,YN+T2/2.0)                                      RK1 1780
      T4=HNEW*FUN(XN+HNEW,YN+T3)                                        RK1 1790
      YY=YN+(T1+2.0*T2+2.0*T3+T4)/6.0                                   RK1 1800
      XX=XN+HNEW                                                        RK1 1810
      GO TO (25,45,115), JUMP                                           RK1 1820
C                                                                       RK1 1830
      END                                                               RK1 1840
```

Subroutine RK2

This subroutine integrates a given function using the Runge-Kutta technique and produces tabulated values of the computed integral.

The ordinary differential equation:

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

with initial condition $y(x_0) = y_0$ is solved numerically using a fourth-order Runge-Kutta integration process. This is a single-step method in which the value of y at $x = x_n$ is used to compute $y_{n+1} = y(x_{n+1})$ and earlier values y_{n-1}, y_{n-2}, etc. are not used

The relevant formulas are:

$$y_{n+1} = y_n + 1/6\,[k_0 + 2k_1 + 2k_2 + k_3] \tag{2}$$

where, for step size h:

$$\begin{cases} k_0 = h f(x_n, y_n) \\ k_1 = h f(x_n + h/2,\ y_n + k_0/2) \\ k_2 = h f(x_n + h/2,\ y_n + k_1/2) \\ k_3 = h f(x_n + h,\ y_n + k_2) \end{cases} \tag{3}$$

```
C                                                                       RK2   10
C     ..................................................................RK2   20
C                                                                       RK2   30
C        SUBROUTINE RK2                                                 RK2   40
C                                                                       RK2   50
C        PURPOSE                                                        RK2   60
C           INTEGRATES A FIRST ORDER DIFFERENTIAL EQUATION              RK2   70
C           DY/DX=FUN(X,Y) AND PRODUCES A TABLE OF INTEGRATED VALUES    RK2   80
C                                                                       RK2   90
C        USAGE                                                          RK2  100
C           CALL RK2(FUN,H,XI,YI,K,N,VEC)                               RK2  110
C                                                                       RK2  120
C        DESCRIPTION OF PARAMETERS                                      RK2  130
C           FUN-USER-SUPPLIED FUNCTION SUBPROGRAM WITH ARGUMENTS X,Y    RK2  140
C               WHICH GIVES DY/DX                                       RK2  150
C           H  -STEP SIZE                                               RK2  160
C           XI -INITIAL VALUE OF X                                      RK2  170
C           YI -INITIAL VALUE OF Y WHERE YI=Y(XI)                       RK2  180
C           K  -THE INTERVAL AT WHICH COMPUTED VALUES ARE TO BE STORED  RK2  190
C           N  -THE NUMBER OF VALUES TO BE STORED                       RK2  200
C           VEC-THE RESULTANT VECTOR OF LENGTH N IN WHICH COMPUTED      RK2  210
C               VALUES OF Y ARE TO BE STORED                            RK2  220
C                                                                       RK2  230
C        REMARKS                                                        RK2  240
C           NONE                                                        RK2  250
C                                                                       RK2  260
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  RK2  270
C           FUN - USER-SUPPLIED FUNCTION SUBPROGRAM FOR DY/DX           RK2  280
C           CALLING PROGRAM MUST HAVE FORTRAN EXTERNAL STATEMENT        RK2  290
C           CONTAINING NAMES OF FUNCTION SUBPROGRAMS LISTED IN CALL TO  RK2  300
C           RK2                                                         RK2  310
C                                                                       RK2  320
C        METHOD                                                         RK2  330
C           FOURTH ORDER RUNGE-KUTTA INTEGRATION ON A RECURSIVE BASIS AS RK2  340
C           SHOWN IN F.B. HILDEBRAND, 'INTRODUCTION TO NUMERICAL        RK2  350
C           ANALYSIS', MCGRAW-HILL, NEW YORK, 1956                      RK2  360
C                                                                       RK2  370
C     ..................................................................RK2  380
      SUBROUTINE RK2(FUN,H,XI,YI,K,N,VEC)                               RK2  390
C                                                                       RK2  400
C     ..................................................................RK2  410
C                                                                       RK2  420
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  RK2  430
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      RK2  440
C        STATEMENT WHICH FOLLOWS.                                       RK2  450
C                                                                       RK2  460
C     DOUBLE PRECISION H,XI,YI,VEC,H2,Y,X,T1,T2,T3,T4,FUN               RK2  470
C                                                                       RK2  480
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    RK2  490
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      RK2  500
C        ROUTINE.                                                       RK2  510
C                                                                       RK2  520
C                                                                       RK2  530
C        USER FUNCTION SUBPROGRAM, FUN, MUST BE IN DOUBLE PRECISION.    RK2  540
C                                                                       RK2  550
C     ..................................................................RK2  560
C                                                                       RK2  570
      DIMENSION VEC(1)                                                  RK2  580
      H2=H/2.                                                           RK2  590
      Y=YI                                                              RK2  600
      X=XI                                                              RK2  610
      DO 2 I=1,N                                                        RK2  620
      DO 1 J=1,K                                                        RK2  630
      T1=H*FUN(X,Y)                                                     RK2  640
      T2=H*FUN(X+H2,Y+T1/2.)                                            RK2  650
      T3=H*FUN(X+H2,Y+T2/2.)                                            RK2  660
      T4=H*FUN(X+H,Y+T3)                                                RK2  670
      Y= Y+(T1+2.*T2+2.*T3+T4)/6.                                       RK2  680
    1 X=X+H                                                             RK2  690
    2 VEC(I)=Y                                                          RK2  700
      RETURN                                                            RK2  710
      END                                                               RK2  720
```

Subroutines RKGS and DRKGS

These subroutines use the Runge-Kutta method for the solution of initial-value problems.

The purpose of the Runge-Kutta method is to obtain an approximate solution of a system of first-order ordinary differential equations with given initial values. It is a fourth-order integration procedure which is stable and self-starting; that is, only the functional values at a single previous point are required to obtain the functional values ahead. For this reason it is easy to change the step size h at any step in the calculations. On the other hand, each Runge-Kutta step requires the evaluation of the right-hand side of the system four times, which is a great disadvantage compared with other methods of the same order of accuracy, especially predictor-corrector methods. Another disadvantage of the method is that neither the truncation errors nor estimates of them are obtained in the calculation procedure. Therefore, control of accuracy and adjustment of the step size h is done by comparison of the results due to double and single step size 2h and h.

Given the system of first-order ordinary differential equations:

$$y_1' = \frac{dy_1}{dx} = f_1(x, y_1, y_2, \ldots, y_n)$$

$$y_2' = \frac{dy_2}{dx} = f_2(x, y_1, y_2, \ldots, y_n)$$

$$\ldots\ldots\ldots\ldots$$

$$y_n' = \frac{dy_n}{dx} = f_n(x, y_1, y_2, \ldots, y_n)$$

and the initial values:

$$y_1(x_0) = y_{1,0},\ y_2(x_0) = y_{2,0},\ \ldots,\ y_n(x_0) = y_{n,0}$$

and using the following vector notations:

$$Y(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \cdot \\ \cdot \\ \cdot \\ y_n(x) \end{pmatrix},\quad F(x, Y) = \begin{pmatrix} f_1(x, Y) \\ f_2(x, Y) \\ \cdot \\ \cdot \\ \cdot \\ f_n(x, Y) \end{pmatrix},\quad Y_0 = \begin{pmatrix} y_{1,0} \\ y_{2,0} \\ \cdot \\ \cdot \\ \cdot \\ y_{n,0} \end{pmatrix}$$

where Y, F and Y_0 are column vectors, the given problem appears as follows:

$$Y' = \frac{dY}{dx} = F(x, Y) \text{ with } Y(x_0) = Y_0$$

With respect to storage requirements and compensation of accumulated roundoff errors, Gill's modification of the classical Runge-Kutta formulas is preferred. Thus, starting at x_0 with $Y(x_0) = Y_0$ and vector $Q_0 = 0$, the resulting vector $Y_4 = Y(x_0 + h)$ is computed by the following formulas:

$$K_1 = h \cdot F(x_0, Y_0) \quad ; \quad Y_1 = Y_0 + \frac{1}{2}(K_1 - 2Q_0) \quad ;$$

$$Q_1 = Q_0 + 3\left[\frac{1}{2}(K_1 - 2Q_0)\right] - \frac{1}{2}K_1$$

$$K_2 = h \cdot F\left(x_0 + \frac{h}{2}, Y_1\right) \quad ; \quad Y_2 = Y_1 + \left(1 - \sqrt{\frac{1}{2}}\right)(K_2 - Q_1) \quad ;$$

$$Q_2 = Q_1 + 3\left[\left(1 - \sqrt{\frac{1}{2}}\right)(K_2 - Q_1)\right] - \left(1 - \sqrt{\frac{1}{2}}\right)K_2 \qquad (1)$$

$$K_3 = h \cdot F\left(x_0 + \frac{h}{2}, Y_2\right) \quad ; \quad Y_3 = Y_2 + \left(1 + \sqrt{\frac{1}{2}}\right)(K_3 - Q_2) \quad ;$$

$$Q_3 = Q_2 + 3\left[\left(1 + \sqrt{\frac{1}{2}}\right)(K_3 - Q_2)\right] - \left(1 + \sqrt{\frac{1}{2}}\right)K_3$$

$$K_4 = h \cdot F(x_0 + h, Y_3) \quad ; \quad Y_4 = Y_3 + \frac{1}{6}(K_4 - 2Q_3) \quad ;$$

$$Q_4 = Q_3 + 3\left[\frac{1}{6}(K_4 - 2Q_3)\right] - \frac{1}{2}K_4$$

where K_1, K_2, K_3, K_4, Y_1, Y_2, Y_3, Y_4, Q_1, Q_2, Q_3, Q_4 are all column vectors with n components. If the procedure were carried out with infinite precision (that is, no rounding errors), vector Q_4 defined above would be zero. In practice this is not true, and Q_4 represents approximately three times the roundoff error in Y_4 accumulated during one step. To compensate for this accumulated roundoff, Q_4 is used as Q_0 for the next step. Also $(x_0 + h)$ and Y_4 serve as x_0 and Y_0 respectively at the next step.

For initial control of accuracy, an approximation for $Y(x_0 + 2h)$ called $Y^{(2)}(x_0 + 2h)$ is computed using the step size 2h, and then an approximation called $Y^{(1)}(x_0 + 2h)$, using two times the step size h. From these two approximations, a test value δ for accuracy is generated in the following way:

$$\delta = \frac{1}{15}\sum_{i=1}^{n} a_i \cdot \left| y_i^{(1)} - y_i^{(2)} \right| \qquad (2)$$

where the coefficients a_i are error-weights specified in the input of the procedure.

Test value δ is an approximate measure for the local truncation error at point x_0+2h. If δ is greater than a given tolerance ϵ_2, increment h is halved and the procedure starts again at the point x_0. If δ is less than ϵ_2, the results $Y^{(1)}(x_0+h)$ and $Y^{(1)}(x_0+2h)$

are assumed to be correct. They are then handed, together with $x_0 + h$ and $x_0 + 2h$ and the derivatives at these points -- that is, the values of $F[x_0 + h, Y^{(1)}(x_0+h)]$ and $F[x_0+2h, Y^{(1)}(x_0+2h)]$ respectively -- to a user-supplied output subroutine.

If δ is less than $\epsilon_1 = \epsilon_2/50$, the next step is carried out with the doubled increment. However, care is taken in the procedure that the increment never becomes greater than the increment h specified as an input parameter, and further that all points $x_0 + j \cdot h$ (where $j = 1, 2, \ldots$) which are situated between the lower and upper bound of the integration interval are included in the output. Finally, the increment of the last step of the procedure is chosen in such a way that the upper bound of the integration interval is reached exactly.

The entire input of the procedure is:

1. Lower and upper bound of the integration interval, initial increment of the independent variable, upper bound ϵ_2 of the local truncation error
2. Initial values of the dependent variables and weights for the local truncation errors in each component of the dependent variables
3. The number of differential equations in the system
4. As external subroutine subprograms, the computation of the right-hand side of the system of differential equations; for flexibility in output, an output subroutine
5. An auxiliary storage array named AUX with 8 rows and n columns

Output is done in the following way. If a set of approximations to the dependent variables Y(x) is found to be of sufficient accuracy, it is handed -- together with x, the derivative $F[x, Y(x)]$, the number of bisections of the initial increment, the number of differential equations, the lower and upper bound of the interval, the initial step size, error bound ϵ_2, and a parameter for terminating subroutine RKGS or DRKGS -- to the output subroutine. Because of this output subroutine, the user has the opportunity to choose his own output format, to handle the output values as he wants, to change the upper error bound, and to terminate subroutine RKGS or DRKGS at any output point. In particular, the user is able to drop the output of some intermediate points, printing only the result values at the special points $x_0 + n \cdot h$ ($n = 0, 1, 2, \ldots$). The user may also perform intermediate computation using the integration results before continuing the process.

For better understanding of the flowchart and of the FORTRAN program, Figure 32 shows the allocation of special intermediate result vectors within the storage array AUX.

For reference see A. Ralston/H. S. Wilf, Mathematical Methods for Digital Computers , Wiley, New York/London, 1960, pp. 110-120.

AUX

function vector Y(x)	1. row (AUX (1) in flowchart)
derivative vector F(x, Y(x))	2. row (AUX (2) in flowchart)
vector of accumulated roundoff at point x	3. row (AUX (3) in flowchart)
function vector Y(x+2h) for testing purposes	4. row (AUX (4) in flowchart)
function vector Y(x+h)	5. row (AUX (5) in flowchart)
vector of accumulated roundoff at point x+h	6. row (AUX (6) in flowchart)
derivative vector F(x+h, Y(x+h))	7. row (AUX (7) in flowchart)
vector of error weights multiplied by 1/15	8. row (AUX (8) in flowchart)

Figure 32. Storage allocation in auxiliary storage array AUX (RKGS-DRKGS)

```
C                                                                       RKGS  10
C     .....................................................................RKGS  20
C                                                                       RKGS  30
C        SUBROUTINE RKGS                                                RKGS  40
C                                                                       RKGS  50
C        PURPOSE                                                        RKGS  60
C           TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY DIFFERENTIAL      RKGS  70
C           EQUATIONS WITH GIVEN INITIAL VALUES.                        RKGS  80
C                                                                       RKGS  90
C        USAGE                                                          RKGS 100
C           CALL RKGS (PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)              RKGS 110
C           PARAMETERS FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT.      RKGS 120
C                                                                       RKGS 130
C        DESCRIPTION OF PARAMETERS                                      RKGS 140
C           PRMT   - AN INPUT AND OUTPUT VECTOR WITH DIMENSION GREATER  RKGS 150
C                    OR EQUAL TO 5, WHICH SPECIFIES THE PARAMETERS OF   RKGS 160
C                    THE INTERVAL AND OF ACCURACY AND WHICH SERVES FOR  RKGS 170
C                    COMMUNICATION BETWEEN OUTPUT SUBROUTINE (FURNISHED RKGS 180
C                    BY THE USER) AND SUBROUTINE RKGS. EXCEPT PRMT(5)   RKGS 190
C                    THE COMPONENTS ARE NOT DESTROYED BY SUBROUTINE     RKGS 200
C                    RKGS AND THEY ARE                                  RKGS 210
C           PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT).               RKGS 220
C           PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT).               RKGS 230
C           PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE      RKGS 240
C                    (INPUT).                                           RKGS 250
C           PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS    RKGS 260
C                    GREATER THAN PRMT(4), INCREMENT GETS HALVED.       RKGS 270
C                    IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE     RKGS 280
C                    ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.RKGS 290
C                    THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS        RKGS 300
C                    OUTPUT SUBROUTINE.                                 RKGS 310
C           PRMT(5)- NO INPUT PARAMETER. SUBROUTINE RKGS INITIALIZES    RKGS 320
C                    PRMT(5)=0. IF THE USER WANTS TO TERMINATE          RKGS 330
C                    SUBROUTINE RKGS AT ANY OUTPUT POINT, HE HAS TO     RKGS 340
C                    CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE  RKGS 350
C                    OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE        RKGS 360
C                    FEASIBLE IF ITS DIMENSION IS DEFINED GREATER       RKGS 370
C                    THAN 5. HOWEVER SUBROUTINE RKGS DOES NOT REQUIRE   RKGS 380
C                    AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL   RKGS 390
C                    FOR HANDING RESULT VALUES TO THE MAIN PROGRAM      RKGS 400
C                    (CALLING RKGS) WHICH ARE OBTAINED BY SPECIAL       RKGS 410
C                    MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP. RKGS 420
C           Y      - INPUT VECTOR OF INITIAL VALUES.  (DESTROYED)       RKGS 430
C                    LATERON Y IS THE RESULTING VECTOR OF DEPENDENT     RKGS 440
C                    VARIABLES COMPUTED AT INTERMEDIATE POINTS X.       RKGS 450
C           DERY   - INPUT VECTOR OF ERROR WEIGHTS.  (DESTROYED)        RKGS 460
C                    THE SUM OF ITS COMPONENTS MUST BE EQUAL TO 1.      RKGS 470
C                    LATERON DERY IS THE VECTOR OF DERIVATIVES, WHICH   RKGS 480
C                    BELONG TO FUNCTION VALUES Y AT A POINT X.          RKGS 490
C           NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF      RKGS 500
C                    EQUATIONS IN THE SYSTEM.                           RKGS 510
C           IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF     RKGS 520
C                    BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS   RKGS 530
C                    GREATER THAN 10, SUBROUTINE RKGS RETURNS WITH      RKGS 540
C                    ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM. ERROR     RKGS 550
C                    MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE         RKGS 560
C                    PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-RKGS 570
C                    PRMT(1)) RESPECTIVELY.                             RKGS 580
C           FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. THIS      RKGS 590
C                    SUBROUTINE COMPUTES THE RIGHT HAND SIDES DERY OF   RKGS 600
C                    THE SYSTEM TO GIVEN VALUES X AND Y. ITS PARAMETER  RKGS 610
C                    LIST MUST BE X,Y,DERY. SUBROUTINE FCT SHOULD       RKGS 620
C                    NOT DESTROY X AND Y.                               RKGS 630
C           OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.    RKGS 640
C                    ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.RKGS 650
C                    NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,    RKGS 660
C                    PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY          RKGS 670
C                    SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,RKGS 680
C                    SUBROUTINE RKGS IS TERMINATED.                     RKGS 690
C           AUX    - AN AUXILIARY STORAGE ARRAY WITH 8 ROWS AND NDIM    RKGS 700
C                    COLUMNS.                                           RKGS 710
C                                                                       RKGS 720
C        REMARKS                                                        RKGS 730
C           THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF RKGS 740
C           (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE    RKGS 750
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C              NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE      RKGS 760
C              IHLF=11),                                                  RKGS 770
C           (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN         RKGS 780
C              (ERROR MESSAGES IHLF=12 OR IHLF=13),                       RKGS 790
C           (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,         RKGS 800
C           (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.          RKGS 810
C                                                                         RKGS 820
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                    RKGS 830
C           THE EXTERNAL SUBROUTINES FCT(X,Y,DERY) AND                    RKGS 840
C           OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.  RKGS 850
C                                                                         RKGS 860
C        METHOD                                                           RKGS 870
C           EVALUATION IS DONE BY MEANS OF FOURTH ORDER RUNGE-KUTTA       RKGS 880
C           FORMULAE IN THE MODIFICATION DUE TO GILL. ACCURACY IS         RKGS 890
C           TESTED COMPARING THE RESULTS OF THE PROCEDURE WITH SINGLE     RKGS 900
C           AND DOUBLE INCREMENT.                                         RKGS 910
C           SUBROUTINE RKGS AUTOMATICALLY ADJUSTS THE INCREMENT DURING    RKGS 920
C           THE WHOLE COMPUTATION BY HALVING OR DOUBLING. IF MORE THAN    RKGS 930
C           10 BISECTIONS OF THE INCREMENT ARE NECESSARY TO GET           RKGS 940
C           SATISFACTORY ACCURACY, THE SUBROUTINE RETURNS WITH            RKGS 950
C           ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.                      RKGS 960
C           TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE       RKGS 970
C           MUST BE FURNISHED BY THE USER.                                RKGS 980
C           FOR REFERENCE, SEE                                            RKGS 990
C           RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL COMPUTERS,     RKGS1000
C           WILEY, NEW YORK/LONDON, 1960, PP.110-120.                     RKGS1010
C                                                                         RKGS1020
C     ..................................................................RKGS1030
C                                                                         RKGS1040
      SUBROUTINE RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)                 RKGS1050
C                                                                         RKGS1060
C                                                                         RKGS1070
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(1)              RKGS1080
      DO 1 I=1,NDIM                                                       RKGS1090
    1 AUX(8,I)=.06666667*DERY(I)                                          RKGS1100
      X=PRMT(1)                                                           RKGS1110
      XEND=PRMT(2)                                                        RKGS1120
      H=PRMT(3)                                                           RKGS1130
      PRMT(5)=0.                                                          RKGS1140
      CALL FCT(X,Y,DERY)                                                  RKGS1150
C                                                                         RKGS1160
C     ERROR TEST                                                          RKGS1170
      IF(H*(XEND-X))38,37,2                                               RKGS1180
C                                                                         RKGS1190
C     PREPARATIONS FOR RUNGE-KUTTA METHOD                                 RKGS1200
    2 A(1)=.5                                                             RKGS1210
      A(2)=.2928932                                                       RKGS1220
      A(3)=1.707107                                                       RKGS1230
      A(4)=.1666667                                                       RKGS1240
      B(1)=2.                                                             RKGS1250
      B(2)=1.                                                             RKGS1260
      B(3)=1.                                                             RKGS1270
      B(4)=2.                                                             RKGS1280
      C(1)=.5                                                             RKGS1290
      C(2)=.2928932                                                       RKGS1300
      C(3)=1.707107                                                       RKGS1310
      C(4)=.5                                                             RKGS1320
C                                                                         RKGS1330
C     PREPARATIONS OF FIRST RUNGE-KUTTA STEP                              RKGS1340
      DO 3 I=1,NDIM                                                       RKGS1350
      AUX(1,I)=Y(I)                                                       RKGS1360
      AUX(2,I)=DERY(I)                                                    RKGS1370
      AUX(3,I)=0.                                                         RKGS1380
    3 AUX(6,I)=0.                                                         RKGS1390
      IREC=0                                                              RKGS1400
      H=H+H                                                               RKGS1410
      IHLF=-1                                                             RKGS1420
      ISTEP=0                                                             RKGS1430
      IEND=0                                                              RKGS1440
C                                                                         RKGS1450
C                                                                         RKGS1460
C     START OF A RUNGE-KUTTA STEP                                         RKGS1470
    4 IF((X+H-XEND)*H)17,6,5                                              RKGS1480
    5 H=XEND-X                                                            RKGS1490
    6 IEND=1                                                              RKGS1500
C                                                                         RKGS1510
C     RECORDING OF INITIAL VALUES OF THIS STEP                            RKGS1520
    7 CALL OUTP(X,Y,DERY,IREC,NDIM,PRMT)                                  RKGS1530
      IF(PRMT(5))40,8,40                                                  RKGS1540
    8 ITEST=0                                                             RKGS1550
    9 ISTEP=ISTEP+1                                                       RKGS1560
C                                                                         RKGS1570
C                                                                         RKGS1580
C     START OF INNERMOST RUNGE-KUTTA LOOP                                 RKGS1590
      J=1                                                                 RKGS1600
   10 AJ=A(J)                                                             RKGS1610
      BJ=B(J)                                                             RKGS1620
      CJ=C(J)                                                             RKGS1630
      DO 11 I=1,NDIM                                                      RKGS1640
      R1=H*DERY(I)                                                        RKGS1650
      R2=AJ*(R1-BJ*AUX(6,I))                                              RKGS1660
      Y(I)=Y(I)+R2                                                        RKGS1670
      R2=R2+R2+R2                                                         RKGS1680
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1                                          RKGS1690
      IF(J-4)12,15,15                                                     RKGS1700
   12 J=J+1                                                               RKGS1710
      IF(J-3)13,14,13                                                     RKGS1720
   13 X=X+.5*H                                                            RKGS1730
   14 CALL FCT(X,Y,DERY)                                                  RKGS1740
      GOTO 10                                                             RKGS1750
C     END OF INNERMOST RUNGE-KUTTA LOOP                                   RKGS1760
C                                                                         RKGS1770
C                                                                         RKGS1780
C     TEST OF ACCURACY                                                    RKGS1790
   15 IF(ITEST)16,16,20                                                   RKGS1800
C                                                                         RKGS1810
C     IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING OF ACCURACY     RKGS1820
   16 DO 17 I=1,NDIM                                                      RKGS1830
   17 AUX(4,I)=Y(I)                                                       RKGS1840
      ITEST=1                                                             RKGS1850
      ISTEP=ISTEP+ISTEP-2                                                 RKGS1860
   18 IHLF=IHLF+1                                                         RKGS1870
      X=X-H                                                               RKGS1880
      H=.5*H                                                              RKGS1890
      DO 19 I=1,NDIM                                                      RKGS1900
      Y(I)=AUX(1,I)                                                       RKGS1910
      DERY(I)=AUX(2,I)                                                    RKGS1920
   19 AUX(6,I)=AUX(3,I)                                                   RKGS1930
      GOTO 9                                                              RKGS1940
C                                                                         RKGS1950
C     IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE                     RKGS1960
   20 IMOD=ISTEP/2                                                        RKGS1970
      IF(ISTEP-IMOD-IMOD)21,23,21                                         RKGS1980
   21 CALL FCT(X,Y,DERY)                                                  RKGS1990
      DO 22 I=1,NDIM                                                      RKGS2000
      AUX(5,I)=Y(I)                                                       RKGS2010
   22 AUX(7,I)=DERY(I)                                                    RKGS2020
      GOTO 9                                                              RKGS2030
C                                                                         RKGS2040
C     COMPUTATION OF TEST VALUE DELT                                      RKGS2050
   23 DELT=0.                                                             RKGS2060
      DO 24 I=1,NDIM                                                      RKGS2070
   24 DELT=DELT+AUX(8,I)*ABS(AUX(4,I)-Y(I))                               RKGS2080
      IF(DELT-PRMT(4))28,28,25                                            RKGS2090
C                                                                         RKGS2100
C     ERROR IS TOO GREAT                                                  RKGS2110
   25 IF(IHLF-10)26,36,36                                                 RKGS2120
   26 DO 27 I=1,NDIM                                                      RKGS2130
   27 AUX(4,I)=AUX(5,I)                                                   RKGS2140
      ISTEP=ISTEP+ISTEP-4                                                 RKGS2150
      X=X-H                                                               RKGS2160
      IEND=0                                                              RKGS2170
      GOTO 18                                                             RKGS2180
C                                                                         RKGS2190
C     RESULT VALUES ARE GOOD                                              RKGS2200
   28 CALL FCT(X,Y,DERY)                                                  RKGS2210
      DO 29 I=1,NDIM                                                      RKGS2220
      AUX(1,I)=Y(I)                                                       RKGS2230
      AUX(2,I)=DERY(I)                                                    RKGS2240
      AUX(3,I)=AUX(6,I)                                                   RKGS2250
      Y(I)=AUX(5,I)                                                       RKGS2260
   29 DERY(I)=AUX(7,I)                                                    RKGS2270
      CALL OUTP(X-H,Y,DERY,IHLF,NDIM,PRMT)                                RKGS2280
      IF(PRMT(5))40,30,40                                                 RKGS2290
   30 DO 31 I=1,NDIM                                                      RKGS2300
      Y(I)=AUX(1,I)                                                       RKGS2310
   31 DERY(I)=AUX(2,I)                                                    RKGS2320
      IREC=IHLF                                                           RKGS2330
      IF(IEND)32,32,39                                                    RKGS2340
C                                                                         RKGS2350
C     INCREMENT GETS DOUBLED                                              RKGS2360
   32 IHLF=IHLF-1                                                         RKGS2370
      ISTEP=ISTEP/2                                                       RKGS2380
      H=H+H                                                               RKGS2390
      IF(IHLF)4,33,33                                                     RKGS2400
   33 IMOD=ISTEP/2                                                        RKGS2410
      IF(ISTEP-IMOD-IMOD)4,34,4                                           RKGS2420
   34 IF(DELT-.02*PRMT(4))35,35,4                                         RKGS2430
   35 IHLF=IHLF-1                                                         RKGS2440
      ISTEP=ISTEP/2                                                       RKGS2450
      H=H+H                                                               RKGS2460
      GOTO 4                                                              RKGS2470
C                                                                         RKGS2480
C                                                                         RKGS2490
C     RETURNS TO CALLING PROGRAM                                          RKGS2500
   36 IHLF=11                                                             RKGS2510
      CALL FCT(X,Y,DERY)                                                  RKGS2520
      GOTO 39                                                             RKGS2530
   37 IHLF=12                                                             RKGS2540
      GOTO 39                                                             RKGS2550
   38 IHLF=13                                                             RKGS2560
   39 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                  RKGS2570
   40 RETURN                                                              RKGS2580
      END                                                                 RKGS2590
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C                                                                         DRKG  10
C     ..................................................................DRKG  20
C                                                                         DRKG  30
C        SUBROUTINE DRKGS                                                 DRKG  40
C                                                                         DRKG  50
C        PURPOSE                                                          DRKG  60
C           TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY DIFFERENTIAL        DRKG  70
C           EQUATIONS WITH GIVEN INITIAL VALUES.                          DRKG  80
C                                                                         DRKG  90
C        USAGE                                                            DRKG 100
C           CALL DRKGS (PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)               DRKG 110
C           PARAMETERS FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT.        DRKG 120
C                                                                         DRKG 130
C        DESCRIPTION OF PARAMETERS                                        DRKG 140
C           PRMT   - DOUBLE PRECISION INPUT AND OUTPUT VECTOR WITH        DRKG 150
C                    DIMENSION GREATER THAN OR EQUAL TO 5, WHICH          DRKG 160
C                    SPECIFIES THE PARAMETERS OF THE INTERVAL AND OF      DRKG 170
C                    ACCURACY AND WHICH SERVES FOR COMMUNICATION BETWEENDRKG 180
C                    OUTPUT SUBROUTINE (FURNISHED BY THE USER) AND        DRKG 190
C                    SUBROUTINE DRKGS. EXCEPT PRMT(5) THE COMPONENTS      DRKG 200
C                    ARE NOT DESTROYED BY SUBROUTINE DRKGS AND THEY ARE   DRKG 210
C           PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT),                 DRKG 220
C           PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT),                 DRKG 230
C           PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE        DRKG 240
C                    (INPUT),                                             DRKG 250
C           PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS      DRKG 260
C                    GREATER THAN PRMT(4), INCREMENT GETS HALVED.         DRKG 270
C                    IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE       DRKG 280
C                    ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.  DRKG 290
C                    THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS          DRKG 300
C                    OUTPUT SUBROUTINE.                                   DRKG 310
C           PRMT(5)- NO INPUT PARAMETER. SUBROUTINE DRKGS INITIALIZES     DRKG 320
C                    PRMT(5)=0. IF THE USER WANTS TO TERMINATE            DRKG 330
C                    SUBROUTINE DRKGS AT ANY OUTPUT POINT, HE HAS TO      DRKG 340
C                    CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE    DRKG 350
C                    OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE          DRKG 360
C                    FEASIBLE IF ITS DIMENSION IS DEFINED GREATER         DRKG 370
C                    THAN 5. HOWEVER SUBROUTINE DRKGS DOES NOT REQUIRE    DRKG 380
C                    AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL     DRKG 390
C                    FOR HANDING RESULT VALUES TO THE MAIN PROGRAM        DRKG 400
C                    (CALLING DRKGS) WHICH ARE OBTAINED BY SPECIAL        DRKG 410
C                    MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP.    DRKG 420
C           Y      - DOUBLE PRECISION INPUT VECTOR OF INITIAL VALUES      DRKG 430
C                    (DESTROYED). LATERON Y IS THE RESULTING VECTOR OF     DRKG 440
C                    DEPENDENT VARIABLES COMPUTED AT INTERMEDIATE         DRKG 450
C                    POINTS X.                                            DRKG 460
C           DERY   - DOUBLE PRECISION INPUT VECTOR OF ERROR WEIGHTS       DRKG 470
C                    (DESTROYED). THE SUM OF ITS COMPONENTS MUST BE       DRKG 480
C                    EQUAL TO 1. LATERON DERY IS THE VECTOR OF            DRKG 490
C                    DERIVATIVES, WHICH BELONG TO FUNCTION VALUES Y AT    DRKG 500
C                    INTERMEDIATE POINTS X.                               DRKG 510
C           NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF        DRKG 520
C                    EQUATIONS IN THE SYSTEM.                             DRKG 530
C           IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF       DRKG 540
C                    BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS     DRKG 550
C                    GREATER THAN 10, SUBROUTINE DRKGS RETURNS WITH       DRKG 560
C                    ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM. ERROR       DRKG 570
C                    MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE           DRKG 580
C                    PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-DRKG 590
C                    PRMT(1)) RESPECTIVELY.                               DRKG 600
C           FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. THIS       DRKG 610
C                    SUBROUTINE COMPUTES THE RIGHT HAND SIDES DERY OF     DRKG 620
C                    THE SYSTEM TO GIVEN VALUES X AND Y. ITS PARAMETER    DRKG 630
C                    LIST MUST BE X,Y,DERY. SUBROUTINE FCT SHOULD         DRKG 640
C                    NOT DESTROY X AND Y.                                 DRKG 650
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C           OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.      DRKG 660
C                    ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.DRKG 670
C                    NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,     DRKG 680
C                    PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY           DRKG 690
C                    SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,DRKG 700
C                    SUBROUTINE DRKGS IS TERMINATED.                     DRKG 710
C           AUX    - DOUBLE PRECISION AUXILIARY STORAGE ARRAY WITH 8     DRKG 720
C                    ROWS AND NDIM COLUMNS.                              DRKG 730
C                                                                        DRKG 740
C        REMARKS                                                         DRKG 750
C           THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF  DRKG 760
C           (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE     DRKG 770
C               NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE    DRKG 780
C               IHLF=11),                                                DRKG 790
C           (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN        DRKG 800
C               (ERROR MESSAGES IHLF=12 OR IHLF=13),                     DRKG 810
C           (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,        DRKG 820
C           (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.         DRKG 830
C                                                                        DRKG 840
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DRKG 850
C           THE EXTERNAL SUBROUTINES FCT(X,Y,DERY) AND                   DRKG 860
C           OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.DRKG 870
C                                                                        DRKG 880
C        METHOD                                                          DRKG 890
C           EVALUATION IS DONE BY MEANS OF FOURTH ORDER RUNGE-KUTTA      DRKG 900
C           FORMULAE IN THE MODIFICATION DUE TO GILL. ACCURACY IS        DRKG 910
C           TESTED COMPARING THE RESULTS OF THE PROCEDURE WITH SINGLE    DRKG 920
C           AND DOUBLE INCREMENT.                                        DRKG 930
C           SUBROUTINE DRKGS AUTOMATICALLY ADJUSTS THE INCREMENT DURING  DRKG 940
C           THE WHOLE COMPUTATION BY HALVING OR DOUBLING. IF MORE THAN   DRKG 950
C           10 BISECTIONS OF THE INCREMENT ARE NECESSARY TO GET          DRKG 960
C           SATISFACTORY ACCURACY, THE SUBROUTINE RETURNS WITH           DRKG 970
C           ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.                     DRKG 980
C           TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE      DRKG 990
C           MUST BE FURNISHED BY THE USER.                               DRKG1000
C           FOR REFERENCE, SEE                                           DRKG1010
C           RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL COMPUTERS,    DRKG1020
C           WILEY, NEW YORK/LONDON, 1960, PP.110-120.                    DRKG1030
C                                                                        DRKG1040
C     ..................................................................DRKG1050
C                                                                        DRKG1060
      SUBROUTINE DRKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)               DRKG1070
C                                                                        DRKG1080
C                                                                        DRKG1090
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(1)             DRKG1100
      DOUBLE PRECISION PRMT,Y,DERY,AUX,A,B,C,X,XEND,H,AJ,BJ,CJ,R1,R2,    DRKG1110
     1DELT                                                               DRKG1120
      DO 1 I=1,NDIM                                                      DRKG1130
    1 AUX(8,I)=.06666666666666667D0*DERY(I)                              DRKG1140
      X=PRMT(1)                                                          DRKG1150
      XEND=PRMT(2)                                                       DRKG1160
      H=PRMT(3)                                                          DRKG1170
      PRMT(5)=0.D0                                                       DRKG1180
      CALL FCT(X,Y,DERY)                                                 DRKG1190
C                                                                        DRKG1200
C     ERROR TEST                                                         DRKG1210
      IF(H*(XEND-X))38,37,2                                              DRKG1220
C                                                                        DRKG1230
C     PREPARATIONS FOR RUNGE-KUTTA METHOD                                DRKG1240
    2 A(1)=.5D0                                                          DRKG1250
      A(2)=.29289321881345248D0                                          DRKG1260
      A(3)=1.7071067811865475D0                                          DRKG1270
      A(4)=.16666666666666667D0                                          DRKG1280
      B(1)=2.D0                                                          DRKG1290
      B(2)=1.D0                                                          DRKG1300
      B(3)=1.D0                                                          DRKG1310
      B(4)=2.D0                                                          DRKG1320
      C(1)=.5D0                                                          DRKG1330
      C(2)=.29289321881345248D0                                          DRKG1340
      C(3)=1.7071067811865475D0                                          DRKG1350
      C(4)=.5D0                                                          DRKG1360
C                                                                        DRKG1370
C     PREPARATIONS OF FIRST RUNGE-KUTTA STEP                             DRKG1380
      DO 3 I=1,NDIM                                                      DRKG1390
      AUX(1,I)=Y(I)                                                      DRKG1400
      AUX(2,I)=DERY(I)                                                   DRKG1410
      AUX(3,I)=0.D0                                                      DRKG1420
    3 AUX(6,I)=0.D0                                                      DRKG1430
      IREC=0                                                             DRKG1440
      H=H+H                                                              DRKG1450
      IHLF=-1                                                            DRKG1460
      ISTEP=0                                                            DRKG1470
      IEND=0                                                             DRKG1480
C                                                                        DRKG1490
C                                                                        DRKG1500
C     START OF A RUNGE-KUTTA STEP                                        DRKG1510
    4 IF((X+H-XEND)*H)7,6,5                                              DRKG1520
    5 H=XEND-X                                                           DRKG1530
    6 IEND=1                                                             DRKG1540
C                                                                        DRKG1550
C     RECORDING OF INITIAL VALUES OF THIS STEP                           DRKG1560
    7 CALL OUTP(X,Y,DERY,IREC,NDIM,PRMT)                                 DRKG1570
      IF(PRMT(5))40,8,40                                                 DRKG1580
    8 ITEST=0                                                            DRKG1590
    9 ISTEP=ISTEP+1                                                      DRKG1600
C                                                                        DRKG1610
C                                                                        DRKG1620
C     START OF INNERMOST RUNGE-KUTTA LOOP                                DRKG1630
      J=1                                                                DRKG1640
   10 AJ=A(J)                                                            DRKG1650
      BJ=B(J)                                                            DRKG1660
      CJ=C(J)                                                            DRKG1670
      DO 11 I=1,NDIM                                                     DRKG1680
      R1=H*DERY(I)                                                       DRKG1690
      R2=AJ*(R1-BJ*AUX(6,I))                                             DRKG1700
      Y(I)=Y(I)+R2                                                       DRKG1710
      R2=R2+R2+R2                                                        DRKG1720
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1                                         DRKG1730
      IF(J-4)12,15,15                                                    DRKG1740
   12 J=J+1                                                              DRKG1750
      IF(J-3)13,14,13                                                    DRKG1760
   13 X=X+.5D0*H                                                         DRKG1770
   14 CALL FCT(X,Y,DERY)                                                 DRKG1780
      GOTO 10                                                            DRKG1790
C     END OF INNERMOST RUNGE-KUTTA LOOP                                  DRKG1800
C                                                                        DRKG1810
C                                                                        DRKG1820
C     TEST OF ACCURACY                                                   DRKG1830
   15 IF(ITEST)16,16,20                                                  DRKG1840
C                                                                        DRKG1850
C     IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING OF ACCURACY    DRKG1860
   16 DO 17 I=1,NDIM                                                     DRKG1870
   17 AUX(4,I)=Y(I)                                                      DRKG1880
      ITEST=1                                                            DRKG1890
      ISTEP=ISTEP+ISTEP-2                                                DRKG1900
   18 IHLF=IHLF+1                                                        DRKG1910
      X=X-H                                                              DRKG1920
      H=.5D0*H                                                           DRKG1930
      DO 19 I=1,NDIM                                                     DRKG1940
      Y(I)=AUX(1,I)                                                      DRKG1950
      DERY(I)=AUX(2,I)                                                   DRKG1960
   19 AUX(6,I)=AUX(3,I)                                                  DRKG1970
      GOTO 9                                                             DRKG1980
C                                                                        DRKG1990
C     IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE                    DRKG2000
   20 IMOD=ISTEP/2                                                       DRKG2010
      IF(ISTEP-IMOD-IMOD)21,23,21                                        DRKG2020
   21 CALL FCT(X,Y,DERY)                                                 DRKG2030
      DO 22 I=1,NDIM                                                     DRKG2040
      AUX(5,I)=Y(I)                                                      DRKG2050
   22 AUX(7,I)=DERY(I)                                                   DRKG2060
      GOTO 9                                                             DRKG2070
C                                                                        DRKG2080
C     COMPUTATION OF TEST VALUE DELT                                     DRKG2090
   23 DELT=0.D0                                                          DRKG2100
      DO 24 I=1,NDIM                                                     DRKG2110
   24 DELT=DELT+AUX(8,I)*DABS(AUX(4,I)-Y(I))                             DRKG2120
      IF(DELT-PRMT(4))28,28,25                                           DRKG2130
C                                                                        DRKG2140
C     ERROR IS TOO GREAT                                                 DRKG2150
   25 IF(IHLF-10)26,36,36                                                DRKG2160
   26 DO 27 I=1,NDIM                                                     DRKG2170
   27 AUX(4,I)=AUX(5,I)                                                  DRKG2180
      ISTEP=ISTEP+ISTEP-4                                                DRKG2190
      X=X-H                                                              DRKG2200
      IEND=0                                                             DRKG2210
      GOTO 18                                                            DRKG2220
C                                                                        DRKG2230
C     RESULT VALUES ARE GOOD                                             DRKG2240
   28 CALL FCT(X,Y,DERY)                                                 DRKG2250
      DO 29 I=1,NDIM                                                     DRKG2260
      AUX(1,I)=Y(I)                                                      DRKG2270
      AUX(2,I)=DERY(I)                                                   DRKG2280
      AUX(3,I)=AUX(6,I)                                                  DRKG2290
      Y(I)=AUX(5,I)                                                      DRKG2300
   29 DERY(I)=AUX(7,I)                                                   DRKG2310
      CALL OUTP(X-H,Y,DERY,IHLF,NDIM,PRMT)                               DRKG2320
      IF(PRMT(5))40,30,40                                                DRKG2330
   30 DO 31 I=1,NDIM                                                     DRKG2340
      Y(I)=AUX(1,I)                                                      DRKG2350
   31 DERY(I)=AUX(2,I)                                                   DRKG2360
      IREC=IHLF                                                          DRKG2370
      IF(IEND)32,32,39                                                   DRKG2380
C                                                                        DRKG2390
C     INCREMENT GETS DOUBLED                                             DRKG2400
   32 IHLF=IHLF-1                                                        DRKG2410
      ISTEP=ISTEP/2                                                      DRKG2420
      H=H+H                                                              DRKG2430
      IF(IHLF)4,33,33                                                    DRKG2440
   33 IMOD=ISTEP/2                                                       DRKG2450
      IF(ISTEP-IMOD-IMOD)4,34,4                                          DRKG2460
   34 IF(DELT-.02D0*PRMT(4))35,35,4                                      DRKG2470
   35 IHLF=IHLF-1                                                        DRKG2480
      ISTEP=ISTEP/2                                                      DRKG2490
      H=H+H                                                              DRKG2500
      GOTO 4                                                             DRKG2510
C                                                                        DRKG2520
C                                                                        DRKG2530
C     RETURNS TO CALLING PROGRAM                                         DRKG2540
   36 IHLF=11                                                            DRKG2550
      CALL FCT(X,Y,DERY)                                                 DRKG2560
      GOTO 39                                                            DRKG2570
   37 IHLF=12                                                            DRKG2580
      GOTO 39                                                            DRKG2590
   38 IHLF=13                                                            DRKG2600
   39 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                 DRKG2610
   40 RETURN                                                             DRKG2620
      END                                                                DRKG2630
```

Subroutines HPCG and DHPCG

These subroutines use Hamming's modified predictor-corrector method for the solution of general initial-value problems.

The purpose of Hamming's modified predictor-corrector method is to obtain an approximate solution of a general system of first-order ordinary differential equations with given initial values. It is a stable fourth-order integration procedure that requires the evaluation of the right-hand side of the system only two times per step. This is a great advantage compared with other methods of the same order of accuracy, especially the Runge-Kutta method, which requires the evaluation of the right-hand side four times per step. Another advantage is that at each step the calculation procedure gives an estimate for the local truncation error; thus the procedure is able, without a significant amount of calculation time, to choose and change the step size h. On the other hand, Hamming's predictor-corrector method itself is not self-starting; that is, the functional values at a single previous point are not enough to get the functional values ahead. Therefore, to obtain the starting values, a special Runge-Kutta procedure followed by one iteration step is added to the predictor-corrector method.

Given the general system of first-order ordinary differential equations:

$$y_1' = \frac{dy_1}{dx} = f_1(x, y_1, y_2, \ldots, y_n)$$

$$y_2' = \frac{dy_2}{dx} = f_2(x, y_1, y_2, \ldots, y_n)$$

$$\ldots\ldots\ldots\ldots$$

$$y_n' = \frac{dy_n}{dx} = f_n(x, y_1, y_2, \ldots, y_n)$$

and the initial values:

$$y_1(x_0) = y_{1,0},\ y_2(x_0) = y_{2,0},\ \ldots,\ y_n(x_0) = y_{n,0}$$

and using the following vector notations:

$$Y(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_n(x) \end{pmatrix},\quad F(x,Y) = \begin{pmatrix} f_1(x,Y) \\ f_2(x,Y) \\ \vdots \\ f_n(x,Y) \end{pmatrix},\quad Y_0 = \begin{pmatrix} y_{1,0} \\ y_{2,0} \\ \vdots \\ y_{n,0} \end{pmatrix}$$

where Y, F, and Y_0 are column vectors, the given problem appears as follows:

$$Y' = \frac{dY}{dx} = F(x,Y) \text{ with } Y(x_0) = Y_0$$

For stability purposes, the modification by Hamming of Milne's classical modified predictor-corrector method is preferred. Thus, knowing the results at the equidistant points x_{j-3}, x_{j-2}, x_{j-1} and x_j, the results at point $x_{j+1} = x_j + h$ are computed by the formulas below.

Predictor:
$$P_{j+1} = Y_{j-3} + \frac{4h}{3}(2Y'_j - Y'_{j-1} + 2Y'_{j-2}) \quad (1)$$

Modifier:
$$M_{j+1} = P_{j+1} - \frac{112}{121}(P_j - C_j)\ ;$$
$$M'_{j+1} = F(x_{j+1}, M_{j+1}) \quad (2), (3)$$

Corrector:
$$C_{j+1} = \frac{1}{8}\left[9Y_j - Y_{j-2} + 3h(M'_{j+1} + 2Y'_j - Y'_{j-1})\right] \quad (4)$$

Final value:
$$Y_{j+1} = C_{j+1} + \frac{9}{121}(P_{j+1} - C_{j+1}) \quad (5)$$

where Y, Y', P, M, M', F and C are column vectors with n components. Formulas (1) and (4) have local truncation errors:

$$T_1 = \frac{14}{45} h^5 Y^{(5)}(\xi_1) \text{ with } \xi_1 \in (x_{j-3}, x_{j+1})$$

and

$$T_2 = -\frac{1}{40} h^5 Y^{(5)}(\xi_2) \text{ with } \xi_2 \in (x_{j-2}, x_{j+1})$$

respectively, such that

$$C_{j+1} - P_{j+1} = \frac{121}{360} h^5 Y^{(5)}(\xi) \quad [\xi \in (x_{j-3}, x_{j+1})]$$

Assuming that $Y^{(5)}(x)$ does not vary to any great extent in the interval (x_{j-3}, x_{j+1}), it follows that:

$$T_2 \approx \frac{9}{121} (P_{j+1} - C_{j+1})$$

This formula shows that the components of column vector $P_{j+1} - C_{j+1}$ are measures for the local truncation errors in the components of column vector Y_{j+1}, and therefore control of accuracy and adjustment of step size h can be done by generating the following test value:

$$\delta = \sum_{i=1}^{n} a_i \cdot |p_{j+1,i} - c_{j+1,i}| \qquad (6)$$

where the coefficients a_i (i = 1, 2, ..., n) are error-weights specified in the input of the procedure.

If δ is greater than a given tolerance ϵ†, increment h is halved and the procedure computes $Y_{j+1/2}$ -- that is, $Y(x_j + \frac{h}{2})$ -- after having interpolated $Y_{j-1/2} = Y(x_j - \frac{h}{2})$ and $Y_{j-3/2} = Y(x_j - \frac{3}{2}h)$, with previous increment h, using the following sixth-order interpolation formulas):

$$Y_{j-1/2} = \frac{1}{256} (80Y_j + 135Y_{j-1} + 40Y_{j-2} + Y_{j-3}) + \frac{h}{2} \cdot \frac{15}{128} (-Y'_j + 6Y'_{j-1} + Y'_{j-2}) \qquad (7)$$

$$Y_{j-3/2} = \frac{1}{256} (12Y_j + 135Y_{j-1} + 108Y_{j-2} + Y_{j-3}) + \frac{h}{2} \cdot \frac{3}{128} (-Y'_j - 18Y'_{j-1} + 9Y'_{j-2}) \qquad (8)$$

If δ is less than ϵ, the result Y_{j+1} is assumed to be correct and is handed, together with x_{j+1} and the vector of derivatives $Y'_{j+1} = F(x_{j+1}, Y_{j+1})$, to a user-supplied output subroutine.

†Numerical experience seems to show that the procedure does not exceed a global relative error approximately equal to ϵ.

If δ is less than $\epsilon/50$, the next step is carried out with the doubled increment; however, care is taken in the procedure that the increment never gets greater than the increment h specified as an input parameter, and further, that among the output are all points $x_0 + j \cdot h$ (where j = 0, 1, 2, ..., and h is the input step size) which are situated between the lower and the upper bound of the integration interval.

Changing the step size by halving or doubling requires changing of $P_j - C_j$ or $P_{j+1} - C_{j+1}$, respectively. Using the following interpolation formula:

$$Y_j = Y_{j-3} + \frac{3}{8} h(Y'_{j-3} + 3Y'_{j-2} + 3Y'_{j-1} + Y'_j) - \frac{3}{80} h^5 Y^{(5)}(\xi_3) \quad [\xi_3 \in (x_{j-3}, x_j)]$$

and assuming that $Y^{(5)}(x)$ does not vary to any great extent in this interval, $P_j - C_j$ can be written as:

$$P_j - C_j \approx \frac{242}{27} (Y_j - Y_{j-3}) - \frac{121}{36} h(Y'_j + 3Y'_{j-1} + 3Y'_{j-2} + Y'_{j-3})$$

When halving increment h, this formula becomes:

$$P_j - C_j \approx \frac{242}{27} (Y_j - Y_{j-3/2}) - \frac{121}{36} \cdot \frac{h}{2} (Y'_j + 3Y'_{j-1/2} + 3Y'_{j-1} + Y'_{j-3/2}) \qquad (9)$$

and when doubling:

$$P_{j+1} - C_{j+1} \approx \frac{242}{27} (Y_{j+1} - Y_{j-5}) - \frac{121}{36} \cdot 2h(Y'_{j+1} + 3Y'_{j-1} + 3Y'_{j-3} + Y'_{j-5}) \qquad (10)$$

Starting Hamming's modified predictor-corrector method requires the functional and derivative values at four preceding equidistant points; that is, x_0, x_1, x_2 and x_3. The values Y_0 and $Y'_0 = F(x_0, Y_0)$ are specified by input. For computation of Y_1, Y'_1, Y_2, Y'_2, Y_3 and Y'_3 and for adjustment of the step size h to accuracy requirements, a special Runge-Kutta procedure suggested by Ralston is used. Starting at x_j, result values at point $x_{j+1} = x_j + h$ are computed using the following formulas:

$$K_1 = h \cdot Y'_j \tag{11}$$

$$k_2 = h \cdot F(x_j + 0.4h,\ Y_j + 0.4K_1) \tag{12}$$

$$K_3 = h \cdot F(x_j + 0.45573725421878943\,h,\ Y_j + 0.29697760924775360\ K_1 + 0.15875964497103583\ K_2) \tag{13}$$

$$K_4 = h \cdot F(x_j + h,\ Y_j + 0.21810038822592047\ K_1 - 3.0509651486929308\ K_2 + 3.8328647604670103\ K_3) \tag{14}$$

$$Y_{j+1} = Y_j + 0.17476028226269037\ K_1 - 0.55148066287873294\ K_2 + 1.2055355993965235\ K_3 + 0.17118478121951903\ K_4 \tag{15}$$

where Y_j, Y_{j+1}, K_1, K_2, K_3 and K_4 are all column vectors with n components.

These formulas are not very stable, but this does not matter because they are used only in three successive steps (j = 0, 1, 2). On the other hand, they have the smallest bound of truncation error of all fourth-order Runge-Kutta procedures. Therefore they are best suited to start other integration methods which are not self-starting.

For initial control of accuracy and adjustment of step size h, in starting the procedure an approximation for $Y_2 = Y(x_0 + h)$, named $Y_2^{(1)}$, is computed using the step size h, and then an approximation named $Y_2^{(2)}$, using the step size h/2 twice. From these two approximations a test value for accuracy is generated in the following way:

$$\delta = \frac{1}{15} \sum_{i=1}^{n} a_i \cdot \left| y_{2,i}^{(1)} - y_{2,i}^{(2)} \right| \tag{16}$$

If δ is greater than ϵ, increment h is halved, and the procedure starts again at point x_0.

If δ is less than ϵ, the results $Y_1^{(2)} = Y(x_0 + \frac{h}{2})$ and $Y_2^{(2)} = Y(x_0 + h)$ are assumed to be correct, and a third step follows, which computes the results at point $x_0 + \frac{3}{2}h$ -- that is, $Y_3 = Y(x_0 + \frac{3}{2}h)$. The step size h/2 of these three steps is handed as initial step size h to the predictor-corrector method.

It is very important that the starting values be as accurate as possible, because errors in these starting values may increase during the following predictor-corrector procedure. Therefore the starting values computed by the Runge-Kutta method are refined by one iteration step using the following fourth-order interpolation formulas:

$$Y_1 = Y_0 + \frac{h}{24}(9\ Y'_0 + 19\ Y'_1 - 5\ Y'_2 + Y'_3) \tag{17}$$

$$Y_2 = Y_0 + \frac{h}{3}(Y'_0 + 4\ Y'_1 + Y'_2) \tag{18}$$

$$Y_3 = Y_0 + \frac{3h}{8}(Y'_0 + 3\ Y'_1 + 3\ Y'_2 + Y'_3) \tag{19}$$

Use of these must be considered an iteration procedure; that is, first the result values of the Runge-Kutta method are used in the right-hand side of formula (17) to compute a refined Y_1. After computing the refined $Y'_1 = F(x_1, Y_1)$, the refined vector Y_2 is generated using formula (18). Finally, the refined $Y'_2 = F(x_2, Y_2)$ is used, together with the other values, in the right-hand side of formula (19) to compute the refined vector Y_3. During this iteration, the refined data sets x_j, Y_j, Y'_j are handed, together with the number of bisections of the initial step size (specified by input), to the output subroutine.

It can be shown that, using this iterative procedure, the initial column vector $P_3 - C_3$ used in formula (2) for j=3 is equal to zero.

The entire input of the procedure is:

1. Lower and upper bound of the integration interval, initial step size h of the independent variable, and upper bound ϵ of the local truncation error
2. Initial values Y_0 of the dependent variables and weights a_i (i = 1, 2, ..., n) for the local truncation errors in each component of the dependent variables
3. The number n of differential equations in the system
4. As external subroutine subprograms, the computation of the right-hand side of the system of differential equations; for flexibility in output, an output subroutine
5. An auxiliary storage array named AUX with 16 rows and n columns

Output is done in the following way. If a set of approximations to the dependent variables Y(x) is found to be of sufficient accuracy, it is handed -- together with x, the derivative Y' (x), the number of bisections of the initial increment, the number of differential equations, the lower and upper bound of the interval, the initial step size, error bound ε, and a parameter for terminating subroutine HPCG or DHPCG -- to the output subroutine. By means of this output subroutine, the user has the opportunity to choose his own output format, to handle the output values as he wants, to change the upper error bound, and to terminate subroutine HPCG or DHPCG at any output point. In particular, the user is able to drop the output of some intermediate points, printing only the result values at the special points $x_0 + j \cdot h$(where j = 0, 1, 2, ..., and h is the initial step size specified by input). The user may also perform intermediate computations using the integration results before continuing the process.

For better understanding of the flowchart and of the FORTRAN program, the allocation of special intermediate-result vectors within the storage array AUX is given in Figure 33.

function vector $Y_{j-6} = Y(x_{j-6})$	1. row (AUX (1) in flowchart)
function vector $Y_{j-5} = Y(x_{j-5})$	2. row (AUX (2) in flowchart)
function vector $Y_{j-4} = Y(x_{j-4})$	3. row (AUX (3) in flowchart)
function vector $Y_{j-3} = Y(x_{j-3})$	4. row (AUX (4) in flowchart)
function vector $Y_{j-2} = Y(x_{j-2})$	5. row (AUX (5) in flowchart)
function vector $Y_{j-1} = Y(x_{j-1})$	6. row (AUX (6) in flowchart)
function vector $Y_j = Y(x_j)$	7. row (AUX (7) in flowchart)
derivative vector $Y'_{j-6} = Y'(x_{j-6})$	8. row (AUX (8) in flowchart)
derivative vector $Y'_{j-5} = Y'(x_{j-5})$	9. row (AUX (9) in flowchart)
derivative vector $Y'_{j-4} = Y'(x_{j-4})$	10. row (AUX (10) in flowchart)
derivative vector $Y'_{j-3} = Y'(x_{j-3})$	11. row (AUX (11) in flowchart)
derivative vector $Y'_{j-2} = Y'(x_{j-2})$	12. row (AUX (12) in flowchart)
derivative vector $Y'_{j-1} = Y'(x_{j-1})$	13. row (AUX (13) in flowchart)
derivative vector $Y'_j = Y'(x_j)$	14. row (AUX (14) in flowchart)
vector of error weights	15. row (AUX (15) in flowchart)
vector $P_j - C_j$	16. row (AUX (16) in flowchart)

Figure 33. Allocation of special intermediate-result vectors within the special array AUX

For reference see:

(1) A. Ralston/ H.S. Wilf, Mathematical Methods for Digital Computers, Wiley, New York/London, 1960, pp. 95 - 109.

(2) A. Ralston, "Runge-Kutta Methods with Minimum Error Bounds", MTAC, vol. 16, no. 80 (1962), pp. 431 - 437.


```
C                                                                       HPCG  10
C                                                                       HPCG  20
C  ....................................................................HPCG  30
C                                                                       HPCG  40
C     SUBROUTINE HPCG                                                   HPCG  50
C                                                                       HPCG  60
C     PURPOSE                                                           HPCG  70
C        TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY GENERAL              HPCG  80
C        DIFFERENTIAL EQUATIONS WITH GIVEN INITIAL VALUES.              HPCG  90
C                                                                       HPCG 100
C     USAGE                                                             HPCG 110
C        CALL HPCG (PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)                 HPCG 120
C        PARAMETERS FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT.         HPCG 130
C                                                                       HPCG 140
C     DESCRIPTION OF PARAMETERS                                         HPCG 150
C        PRMT   - AN INPUT AND OUTPUT VECTOR WITH DIMENSION GREATER     HPCG 160
C                 OR EQUAL TO 5, WHICH SPECIFIES THE PARAMETERS OF      HPCG 170
C                 THE INTERVAL AND OF ACCURACY AND WHICH SERVES FOR     HPCG 180
C                 COMMUNICATION BETWEEN OUTPUT SUBROUTINE (FURNISHED    HPCG 190
C                 BY THE USER) AND SUBROUTINE HPCG. EXCEPT PRMT(5)      HPCG 200
C                 THE COMPONENTS ARE NOT DESTROYED BY SUBROUTINE        HPCG 210
C                 HPCG AND THEY ARE                                     HPCG 220
C           PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT),               HPCG 230
C           PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT),               HPCG 240
C           PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE      HPCG 250
C                    (INPUT),                                           HPCG 260
C           PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS    HPCG 270
C                    GREATER THAN PRMT(4), INCREMENT GETS HALVED.       HPCG 280
C                    IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE     HPCG 290
C                    ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.HPCG 300
C                    THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS        HPCG 310
C                    OUTPUT SUBROUTINE.                                 HPCG 320
C           PRMT(5)- NO INPUT PARAMETER. SUBROUTINE HPCG INITIALIZES    HPCG 330
C                    PRMT(5)=0. IF THE USER WANTS TO TERMINATE          HPCG 340
C                    SUBROUTINE HPCG AT ANY OUTPUT POINT, HE HAS TO     HPCG 350
C                    CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE  HPCG 360
C                    OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE        HPCG 370
C                    FEASIBLE IF ITS DIMENSION IS DEFINED GREATER       HPCG 380
C                    THAN 5. HOWEVER SUBROUTINE HPCG DOES NOT REQUIRE   HPCG 390
C                    AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL   HPCG 400
C                    FOR HANDING RESULT VALUES TO THE MAIN PROGRAM       HPCG 410
C                    (CALLING HPCG) WHICH ARE OBTAINED BY SPECIAL       HPCG 420
C                    MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP. HPCG 430
C        Y      - INPUT VECTOR OF INITIAL VALUES. (DESTROYED)          HPCG 440
C                 LATERON Y IS THE RESULTING VECTOR OF DEPENDENT       HPCG 450
C                 VARIABLES COMPUTED AT INTERMEDIATE POINTS X.         HPCG 460
C        DERY   - INPUT VECTOR OF ERROR WEIGHTS. (DESTROYED)           HPCG 470
C                 THE SUM OF ITS COMPONENTS MUST BE EQUAL TO 1.        HPCG 480
C                 LATERON DERY IS THE VECTOR OF DERIVATIVES, WHICH     HPCG 490
C                 BELONG TO FUNCTION VALUES Y AT A POINT X.            HPCG 500
C        NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF        HPCG 510
C                 EQUATIONS IN THE SYSTEM.                             HPCG 520
C        IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF       HPCG 530
C                 BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS     HPCG 540
C                 GREATER THAN 10, SUBROUTINE HPCG RETURNS WITH        HPCG 550
C                 ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.             HPCG 560
C                 ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE     HPCG 570
C                 PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-HPCG 580
C                 PRMT(1)) RESPECTIVELY.                               HPCG 590
C        FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT          HPCG 600
C                 COMPUTES THE RIGHT HAND SIDES DERY OF THE SYSTEM     HPCG 610
C                 TO GIVEN VALUES OF X AND Y. ITS PARAMETER LIST       HPCG 620
C                 MUST BE X,Y,DERY. THE SUBROUTINE SHOULD NOT          HPCG 630
C                 DESTROY X AND Y.                                     HPCG 640
C        OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.      HPCG 650
C                 ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.HPCG 660
C                 NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,      HPCG 670
C                 PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY            HPCG 680
C                 SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,HPCG 690
C                 SUBROUTINE HPCG IS TERMINATED.                       HPCG 700
C        AUX    - AN AUXILIARY STORAGE ARRAY WITH 16 ROWS AND NDIM     HPCG 710
C                 COLUMNS.                                             HPCG 720
C                                                                      HPCG 730
C     REMARKS                                                          HPCG 740
C        THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF   HPCG 750
C        (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE      HPCG 760
C            NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE     HPCG 770
C            IHLF=11),                                                 HPCG 780
C        (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN         HPCG 790
C            (ERROR MESSAGES IHLF=12 OR IHLF=13),                      HPCG 800
C        (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,         HPCG 810
C        (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.          HPCG 820
C                                                                      HPCG 830
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                    HPCG 840
C        THE EXTERNAL SUBROUTINES FCT(X,Y,DERY) AND                    HPCG 850
C        OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.HPCG 860
C                                                                      HPCG 870
C     METHOD                                                           HPCG 880
C        EVALUATION IS DONE BY MEANS OF HAMMINGS MODIFIED PREDICTOR-   HPCG 890
C        CORRECTOR METHOD. IT IS A FOURTH ORDER METHOD, USING 4        HPCG 900
C        PRECEEDING POINTS FOR COMPUTATION OF A NEW VECTOR Y OF THE    HPCG 910
C        DEPENDENT VARIABLES.                                          HPCG 920
C        FOURTH ORDER RUNGE-KUTTA METHOD SUGGESTED BY RALSTON IS       HPCG 930
C        USED FOR ADJUSTMENT OF THE INITIAL INCREMENT AND FOR          HPCG 940
C        COMPUTATION OF STARTING VALUES.                               HPCG 950
C        SUBROUTINE HPCG AUTOMATICALLY ADJUSTS THE INCREMENT DURING    HPCG 960
C        THE WHOLE COMPUTATION BY HALVING OR DOUBLING.                 HPCG 970
C        TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE       HPCG 980
C        MUST BE CODED BY THE USER.                                    HPCG 990
C        FOR REFERENCE, SEE                                            HPCG1000
C        (1) RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL            HPCG1010
C            COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.       HPCG1020
C        (2) RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS,   HPCG1030
C            MTAC, VOL.16, ISS.80 (1962), PP.431-437.                  HPCG1040
C                                                                      HPCG1050
C  ....................................................................HPCG1060
      SUBROUTINE HPCG(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)              HPCG1070
C                                                                      HPCG1080
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C                                                                       HPCG1090
C                                                                       HPCG1100
      DIMENSION PRMT(1),Y(1),DERY(1),AUX(16,1)                          HPCG1110
      N=1                                                               HPCG1120
      IHLF=0                                                            HPCG1130
      X=PRMT(1)                                                         HPCG1140
      H=PRMT(3)                                                         HPCG1150
      PRMT(5)=0.                                                        HPCG1160
      DO 1 I=1,NDIM                                                     HPCG1170
      AUX(16,I)=0.                                                      HPCG1180
      AUX(15,I)=DERY(I)                                                 HPCG1190
    1 AUX(1,I)=Y(I)                                                     HPCG1200
      IF(H*(PRMT(2)-X))3,2,4                                            HPCG1210
C                                                                       HPCG1220
C     ERROR RETURNS                                                     HPCG1230
    2 IHLF=12                                                           HPCG1240
      GOTO 4                                                            HPCG1250
    3 IHLF=13                                                           HPCG1260
C                                                                       HPCG1270
C     COMPUTATION OF DERY FOR STARTING VALUES                           HPCG1280
    4 CALL FCT(X,Y,DERY)                                                HPCG1290
C                                                                       HPCG1300
C     RECORDING OF STARTING VALUES                                      HPCG1310
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                HPCG1320
      IF(PRMT(5))6,5,6                                                  HPCG1330
    5 IF(IHLF)7,7,6                                                     HPCG1340
    6 RETURN                                                            HPCG1350
    7 DO 8 I=1,NDIM                                                     HPCG1360
    8 AUX(8,I)=DERY(I)                                                  HPCG1370
C                                                                       HPCG1380
C     COMPUTATION OF AUX(2,I)                                           HPCG1390
      ISW=1                                                             HPCG1400
      GOTO 100                                                          HPCG1410
C                                                                       HPCG1420
    9 X=X+H                                                             HPCG1430
      DO 10 I=1,NDIM                                                    HPCG1440
   10 AUX(2,I)=Y(I)                                                     HPCG1450
C                                                                       HPCG1460
C     INCREMENT H IS TESTED BY MEANS OF BISECTION                       HPCG1470
   11 IHLF=IHLF+1                                                       HPCG1480
      X=X-H                                                             HPCG1490
      DO 12 I=1,NDIM                                                    HPCG1500
   12 AUX(4,I)=AUX(2,I)                                                 HPCG1510
      H=.5*H                                                            HPCG1520
      N=1                                                               HPCG1530
      ISW=2                                                             HPCG1540
      GOTO 100                                                          HPCG1550
C                                                                       HPCG1560
   13 X=X+H                                                             HPCG1570
      CALL FCT(X,Y,DERY)                                                HPCG1580
      N=2                                                               HPCG1590
      DO 14 I=1,NDIM                                                    HPCG1600
      AUX(2,I)=Y(I)                                                     HPCG1610
   14 AUX(9,I)=DERY(I)                                                  HPCG1620
      ISW=3                                                             HPCG1630
      GOTO 100                                                          HPCG1640
C                                                                       HPCG1650
C     COMPUTATION OF TEST VALUE DELT                                    HPCG1660
   15 DELT=0.                                                           HPCG1670
      DO 16 I=1,NDIM                                                    HPCG1680
   16 DELT=DELT+AUX(15,I)*ABS(Y(I)-AUX(4,I))                            HPCG1690
      DELT=.06666667*DELT                                               HPCG1700
      IF(DELT-PRMT(4))19,19,17                                          HPCG1710
   17 IF(IHLF-10)11,18,18                                               HPCG1720
C                                                                       HPCG1730
C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.      HPCG1740
   18 IHLF=11                                                           HPCG1750
      X=X+H                                                             HPCG1760
      GOTO 4                                                            HPCG1770
C                                                                       HPCG1780
C     THERE IS SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS.      HPCG1790
   19 X=X+H                                                             HPCG1800
      CALL FCT(X,Y,DERY)                                                HPCG1810
      DO 20 I=1,NDIM                                                    HPCG1820
      AUX(3,I)=Y(I)                                                     HPCG1830
   20 AUX(10,I)=DERY(I)                                                 HPCG1840
      N=3                                                               HPCG1850
      ISW=4                                                             HPCG1860
      GOTO 100                                                          HPCG1870
C                                                                       HPCG1880
   21 N=1                                                               HPCG1890
      X=X+H                                                             HPCG1900
      CALL FCT(X,Y,DERY)                                                HPCG1910
      X=PRMT(1)                                                         HPCG1920
      DO 22 I=1,NDIM                                                    HPCG1930
      AUX(11,I)=DERY(I)                                                 HPCG1940
   22CY(I)=AUX(1,I)+H*(.375*AUX(8,I)+.7916667*AUX(9,I)                  HPCG1950
     1-.2083333*AUX(10,I)+.04166667*DERY(I))                            HPCG1960
   23 X=X+H                                                             HPCG1970
      N=N+1                                                             HPCG1980
      CALL FCT(X,Y,DERY)                                                HPCG1990
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                HPCG2000
      IF(PRMT(5))6,24,6                                                 HPCG2010
   24 IF(N-4)25,20C,200                                                 HPCG2020
   25 DO 26 I=1,NDIM                                                    HPCG2030
      AUX(N,I)=Y(I)                                                     HPCG2040
   26 AUX(N+7,I)=DERY(I)                                                HPCG2050
      IF(N-3)27,29,200                                                  HPCG2060
C                                                                       HPCG2070
   27 DO 28 I=1,NDIM                                                    HPCG2080
      DELT=AUX(9,I)+AUX(9,I)                                            HPCG2090
      DELT=DELT+DELT                                                    HPCG2100
   28 Y(I)=AUX(1,I)+.3333333*H*(AUX(8,I)+DELT+AUX(10,I))                HPCG2110
      GOTO 23                                                           HPCG2120
C                                                                       HPCG2130
   29 DO 30 I=1,NDIM                                                    HPCG2140
      DELT=AUX(9,I)+AUX(10,I)                                           HPCG2150
      DELT=DELT+DELT+DELT                                               HPCG2160
   30 Y(I)=AUX(1,I)+.375*H*(AUX(8,I)+DELT+AUX(11,I))                    HPCG2170
      GOTO 23                                                           HPCG2180
C                                                                       HPCG2190
C     THE FOLLOWING PART OF SUBROUTINE HPCG COMPUTES BY MEANS OF        HPCG2200
C     RUNGE-KUTTA METHOD STARTING VALUES FOR THE NOT SELF-STARTING      HPCG2210
C     PREDICTOR-CORRECTOR METHOD.                                       HPCG2220
  100 DO 101 I=1,NDIM                                                   HPCG2230
      Z=H*AUX(N+7,I)                                                    HPCG2240
      AUX(5,I)=Z                                                        HPCG2250
  101 Y(I)=AUX(N,I)+.4*Z                                                HPCG2260
C     Z IS AN AUXILIARY STORAGE LOCATION                                HPCG2270
C                                                                       HPCG2280
      Z=X+.4*H                                                          HPCG2290
      CALL FCT(Z,Y,DERY)                                                HPCG2300
      DO 102 I=1,NDIM                                                   HPCG2310
      Z=H*DERY(I)                                                       HPCG2320
      AUX(6,I)=Z                                                        HPCG2330
  102 Y(I)=AUX(N,I)+.2969776*AUX(5,I)+.1587596*Z                        HPCG2340
C                                                                       HPCG2350
      Z=X+.4557372*H                                                    HPCG2360
      CALL FCT(Z,Y,DERY)                                                HPCG2370
      DO 103 I=1,NDIM                                                   HPCG2380
      Z=H*DERY(I)                                                       HPCG2390
      AUX(7,I)=Z                                                        HPCG2400
  103 Y(I)=AUX(N,I)+.2181004*AUX(5,I)-3.050965*AUX(6,I)+3.832865*Z      HPCG2410
C                                                                       HPCG2420
      Z=X+H                                                             HPCG2430
      CALL FCT(Z,Y,DERY)                                                HPCG2440
      DO 104 I=1,NDIM                                                   HPCG2450
  1040Y(I)=AUX(N,I)+.1747603*AUX(5,I)-.5514807*AUX(6,I)                 HPCG2460
     1+1.205536*AUX(7,I)+.1711848*H*DERY(I)                             HPCG2470
      GOTO(9,13,15,21),ISW                                              HPCG2480
C                                                                       HPCG2490
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  HPCG2500
C                                                                       HPCG2510
C     STARTING VALUES ARE COMPUTED.                                     HPCG2520
C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.           HPCG2530
  200 ISTEP=3                                                           HPCG2540
  201 IF(N-8)204,202,204                                                HPCG2550
C                                                                       HPCG2560
C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS      HPCG2570
  202 DO 203 N=2,7                                                      HPCG2580
      DO 203 I=1,NDIM                                                   HPCG2590
      AUX(N-1,I)=AUX(N,I)                                               HPCG2600
  203 AUX(N+6,I)=AUX(N+7,I)                                             HPCG2610
      N=7                                                               HPCG2620
C                                                                       HPCG2630
C     N LESS THAN 8 CAUSES N+1 TO GET N                                 HPCG2640
  204 N=N+1                                                             HPCG2650
C                                                                       HPCG2660
C     COMPUTATION OF NEXT VECTOR Y                                      HPCG2670
      DO 205 I=1,NDIM                                                   HPCG2680
      AUX(N-1,I)=Y(I)                                                   HPCG2690
  205 AUX(N+6,I)=DERY(I)                                                HPCG2700
      X=X+H                                                             HPCG2710
  206 ISTEP=ISTEP+1                                                     HPCG2720
      DO 207 I=1,NDIM                                                   HPCG2730
     0DELT=AUX(N-4,I)+1.333333*H*(AUX(N+6,I)+AUX(N+6,I)-AUX(N+5,I)+     HPCG2740
     1AUX(N+4,I)+AUX(N+4,I))                                            HPCG2750
      Y(I)=DELT-.9256198*AUX(16,I)                                      HPCG2760
  207 AUX(16,I)=DELT                                                    HPCG2770
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR   HPCG2780
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.               HPCG2790
C                                                                       HPCG2800
      CALL FCT(X,Y,DERY)                                                HPCG2810
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY             HPCG2820
C                                                                       HPCG2830
      DO 208 I=1,NDIM                                                   HPCG2840
     0DELT=.125*(9.*AUX(N-1,I)-AUX(N-3,I)+3.*H*(DERY(I)+AUX(N+6,I)+     HPCG2850
     1AUX(N+6,I)-AUX(N+5,I)))                                           HPCG2860
      AUX(16,I)=AUX(16,I)-DELT                                          HPCG2870
  208 Y(I)=DELT+.07438017*AUX(16,I)                                     HPCG2880
C                                                                       HPCG2890
C     TEST WHETHER H MUST BE HALVED OR DOUBLED                          HPCG2900
      DELT=0.                                                           HPCG2910
      DO 209 I=1,NDIM                                                   HPCG2920
  209 DELT=DELT+AUX(15,I)*ABS(AUX(16,I))                                HPCG2930
      IF(DELT-PRMT(4))210,222,222                                       HPCG2940
C                                                                       HPCG2950
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                   HPCG2960
  210 CALL FCT(X,Y,DERY)                                                HPCG2970
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                HPCG2980
      IF(PRMT(5))212,211,212                                            HPCG2990
  211 IF(IHLF-11)213,212,212                                            HPCG3000
  212 RETURN                                                            HPCG3010
  213 IF(H*(X-PRMT(2)))214,212,212                                      HPCG3020
  214 IF(ABS(X-PRMT(2))-.1*ABS(H))212,215,215                           HPCG3030
  215 IF(DELT-.02*PRMT(4))216,216,201                                   HPCG3040
C                                                                       HPCG3050
C                                                                       HPCG3060
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE         HPCG3070
C     AVAILABLE                                                         HPCG3080
  216 IF(IHLF)201,201,217                                               HPCG3090
  217 IF(N-7)201,218,218                                                HPCG3100
  218 IF(ISTEP-4)201,219,219                                            HPCG3110
  219 IMOD=ISTEP/2                                                      HPCG3120
      IF(ISTEP-IMOD-IMOD)201,220,201                                    HPCG3130
  220 H=H+H                                                             HPCG3140
      IHLF=IHLF-1                                                       HPCG3150
      ISTEP=0                                                           HPCG3160
      DO 221 I=1,NDIM                                                   HPCG3170
      AUX(N-1,I)=AUX(N-2,I)                                             HPCG3180
      AUX(N-2,I)=AUX(N-4,I)                                             HPCG3190
      AUX(N-3,I)=AUX(N-6,I)                                             HPCG3200
      AUX(N+6,I)=AUX(N+5,I)                                             HPCG3210
      AUX(N+5,I)=AUX(N+3,I)                                             HPCG3220
      AUX(N+4,I)=AUX(N+1,I)                                             HPCG3230
      DELT=AUX(N+6,I)+AUX(N+5,I)                                        HPCG3240
      DELT=DELT+DELT+DELT                                               HPCG3250
  221OAUX(16,I)=8.962963*(Y(I)-AUX(N-3,I))-3.361111*H*(DERY(I)+DELT     HPCG3260
     1+AUX(N+4,I))                                                      HPCG3270
      GOTO 201                                                          HPCG3280
C                                                                       HPCG3290
C                                                                       HPCG3300
C     H MUST BE HALVED                                                  HPCG3310
  222 IHLF=IHLF+1                                                       HPCG3320
      IF(IHLF-10)223,223,210                                            HPCG3330
  223 H=.5*H                                                            HPCG3340
      ISTEP=0                                                           HPCG3350
      DO 224 I=1,NDIM                                                   HPCG3360
     0Y(I)=.00390625*(80.*AUX(N-1,I)+135.*AUX(N-2,I)+40.*AUX(N-3,I)+    HPCG3370
     1AUX(N-4,I))-.1171875*(AUX(N+6,I)-6.*AUX(N+5,I)-AUX(N+4,I))*H      HPCG3380
     0AUX(N-4,I)=.0039625*(12.*AUX(N-1,I)+135.*AUX(N-2,I)+              HPCG3390
     1128.*AUX(N-3,I)+AUX(N-4,I))-.0234375*(AUX(N+6,I)+18.*AUX(N+5,I)-  HPCG3400
     29.*AUX(N+4,I))*H                                                  HPCG3410
      AUX(N-3,I)=AUX(N-2,I)                                             HPCG3420
  224 AUX(N+4,I)=AUX(N+5,I)                                             HPCG3430
      X=X-H                                                             HPCG3440
      DELT=-(H+H)                                                       HPCG3450
      CALL FCT(DELT,Y,DERY)                                             HPCG3460
      DO 225 I=1,NDIM                                                   HPCG3470
      AUX(N-2,I)=Y(I)                                                   HPCG3480
      AUX(N+5,I)=DERY(I)                                                HPCG3490
  225 Y(I)=AUX(N-4,I)                                                   HPCG3500
      DELT=DELT-(H+H)                                                   HPCG3510
      CALL FCT(DELT,Y,DERY)                                             HPCG3520
      DO 226 I=1,NDIM                                                   HPCG3530
      DELT=AUX(N+5,I)+AUX(N+4,I)                                        HPCG3540
      DELT=DELT+DELT+DELT                                               HPCG3550
     0AUX(16,I)=8.962963*(AUX(N-1,I)-Y(I))-3.361111*H*(AUX(N+6,I)+DELT  HPCG3560
     1+DERY(I))                                                         HPCG3570
  226 AUX(N+3,I)=DERY(I)                                                HPCG3580
      GOTO 206                                                          HPCG3590
      END                                                               HPCG3600
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C                                                                       DHCG  10
C     ..................................................................DHCG  20
C                                                                       DHCG  30
C        SUBROUTINE DHPCG                                               DHCG  40
C                                                                       DHCG  50
C        PURPOSE                                                        DHCG  60
C           TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY GENERAL           DHCG  70
C           DIFFERENTIAL EQUATIONS WITH GIVEN INITIAL VALUES.           DHCG  80
C                                                                       DHCG  90
C        USAGE                                                          DHCG 100
C           CALL DHPCG (PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)             DHCG 110
C           PARAMETERS FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT.      DHCG 120
C                                                                       DHCG 130
C        DESCRIPTION OF PARAMETERS                                      DHCG 140
C           PRMT   - DOUBLE PRECISION INPUT AND OUTPUT VECTOR WITH      DHCG 150
C                    DIMENSION GREATER THAN OR EQUAL TO 5, WHICH        DHCG 160
C                    SPECIFIES THE PARAMETERS OF THE INTERVAL AND OF    DHCG 170
C                    ACCURACY AND WHICH SERVES FOR COMMUNICATION BETWEENDHCG 180
C                    OUTPUT SUBROUTINE (FURNISHED BY THE USER) AND      DHCG 190
C                    SUBROUTINE DHPCG. EXCEPT PRMT(5) THE COMPONENTS    DHCG 200
C                    ARE NOT DESTROYED BY SUBROUTINE DHPCG AND THEY ARE DHCG 210
C           PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT),               DHCG 220
C           PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT),               DHCG 230
C           PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE      DHCG 240
C                    (INPUT),                                           DHCG 250
C           PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS    DHCG 260
C                    GREATER THAN PRMT(4), INCREMENT GETS HALVED.       DHCG 270
C                    IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE     DHCG 280
C                    ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.DHCG 290
C                    THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS        DHCG 300
C                    OUTPUT SUBROUTINE.                                 DHCG 310
C           PRMT(5)- NO INPUT PARAMETER. SUBROUTINE DHPCG INITIALIZES   DHCG 320
C                    PRMT(5)=0. IF THE USER WANTS TO TERMINATE          DHCG 330
C                    SUBROUTINE DHPCG AT ANY OUTPUT POINT, HE HAS TO    DHCG 340
C                    CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE  DHCG 350
C                    OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE        DHCG 360
C                    FEASIBLE IF ITS DIMENSION IS DEFINED GREATER       DHCG 370
C                    THAN 5. HOWEVER SUBROUTINE DHPCG DOES NOT REQUIRE  DHCG 380
C                    AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL   DHCG 390
C                    FOR HANDING RESULT VALUES TO THE MAIN PROGRAM       DHCG 400
C                    (CALLING DHPCG) WHICH ARE OBTAINED BY SPECIAL       DHCG 410
C                    MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP.  DHCG 420
C           Y      - DOUBLE PRECISION INPUT VECTOR OF INITIAL VALUES     DHCG 430
C                    (DESTROYED). LATERON Y IS THE RESULTING VECTOR OF   DHCG 440
C                    DEPENDENT VARIABLES COMPUTED AT INTERMEDIATE        DHCG 450
C                    POINTS X.                                          DHCG 460
C           DERY   - DOUBLE PRECISION INPUT VECTOR OF ERROR WEIGHTS     DHCG 470
C                    (DESTROYED). THE SUM OF ITS COMPONENTS MUST BE     DHCG 480
C                    EQUAL TO 1. LATERON DERY IS THE VECTOR OF          DHCG 490
C                    DERIVATIVES, WHICH BELONG TO FUNCTION VALUES Y AT  DHCG 500
C                    INTERMEDIATE POINTS X.                             DHCG 510
C           NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF      DHCG 520
C                    EQUATIONS IN THE SYSTEM.                           DHCG 530
C           IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF     DHCG 540
C                    BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS   DHCG 550
C                    GREATER THAN 10, SUBROUTINE DHPCG RETURNS WITH     DHCG 560
C                    ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.           DHCG 570
C                    ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE   DHCG 580
C                    PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-DHCG 590
C                    PRMT(1)) RESPECTIVELY.                             DHCG 600
C           FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        DHCG 610
C                    COMPUTES THE RIGHT HAND SIDES DERY OF THE SYSTEM   DHCG 620
C                    TO GIVEN VALUES OF X AND Y. ITS PARAMETER LIST     DHCG 630
C                    MUST BE X,Y,DERY. THE SUBROUTINE SHOULD NOT        DHCG 640
C                    DESTROY X AND Y.                                   DHCG 650
C           OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.    DHCG 660
C                    ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.DHCG 670
C                    NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,    DHCG 680
C                    PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY          DHCG 690
C                    SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,DHCG 700
C                    SUBROUTINE DHPCG IS TERMINATED.                    DHCG 710
C           AUX    - DOUBLE PRECISION AUXILIARY STORAGE ARRAY WITH 16   DHCG 720
C                    ROWS AND NDIM COLUMNS.                             DHCG 730
C                                                                       DHCG 740
C        REMARKS                                                        DHCG 750
C           THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF DHCG 760
C           (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE    DHCG 770
C               NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE   DHCG 780
C               IHLF=11),                                               DHCG 790
C           (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN       DHCG 800
C               (ERROR MESSAGES IHLF=12 OR IHLF=13),                    DHCG 810
C           (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,       DHCG 820
C           (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.        DHCG 830
C                                                                       DHCG 840
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DHCG 850
C           THE EXTERNAL SUBROUTINES FCT(X,Y,DERY) AND                  DHCG 860
C           OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.DHCG 870
C                                                                       DHCG 880
C        METHOD                                                         DHCG 890
C           EVALUATION IS DONE BY MEANS OF HAMMINGS MODIFIED PREDICTOR- DHCG 900
C           CORRECTOR METHOD. IT IS A FOURTH ORDER METHOD, USING 4      DHCG 910
C           PRECEEDING POINTS FOR COMPUTATION OF A NEW VECTOR Y OF THE  DHCG 920
C           DEPENDENT VARIABLES.                                        DHCG 930
C           FOURTH ORDER RUNGE-KUTTA METHOD SUGGESTED BY RALSTON IS     DHCG 940
C           USED FOR ADJUSTMENT OF THE INITIAL INCREMENT AND FOR        DHCG 950
C           COMPUTATION OF STARTING VALUES.                             DHCG 960
C           SUBROUTINE DHPCG AUTOMATICALLY ADJUSTS THE INCREMENT DURING DHCG 970
C           THE WHOLE COMPUTATION BY HALVING OR DOUBLING.               DHCG 980
C           TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE     DHCG 990
C           MUST BE CODED BY THE USER.                                  DHCG1000
C           FOR REFERENCE, SEE                                          DHCG1010
C           (1) RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL          DHCG1020
C               COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.     DHCG1030
C           (2) RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS, DHCG1040
C               MTAC, VOL.16, ISS.80 (1962), PP.431-437.                DHCG1050
C                                                                       DHCG1060
C     ..................................................................DHCG1070
C                                                                       DHCG1080
      SUBROUTINE DHPCG(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)              DHCG1090
C                                                                       DHCG1100
C                                                                       DHCG1110
      DIMENSION PRMT(1),Y(1),DERY(1),AUX(16,1)                          DHCG1120
      DOUBLE PRECISION Y,DERY,AUX,PRMT,X,H,Z,DELT                       DHCG1130
      N=1                                                               DHCG1140
      IHLF=0                                                            DHCG1150
      X=PRMT(1)                                                         DHCG1160
      H=PRMT(3)                                                         DHCG1170
      PRMT(5)=0.D0                                                      DHCG1180
      DO 1 I=1,NDIM                                                     DHCG1190
      AUX(16,I)=0.D0                                                    DHCG1200
      AUX(15,I)=DERY(I)                                                 DHCG1210
    1 AUX(1,I)=Y(I)                                                     DHCG1220
      IF(H*(PRMT(2)-X))3,2,4                                            DHCG1230
C                                                                       DHCG1240
C     ERROR RETURNS                                                     DHCG1250
    2 IHLF=12                                                           DHCG1260
      GOTO 4                                                            DHCG1270
    3 IHLF=13                                                           DHCG1280
C                                                                       DHCG1290
C        COMPUTATION OF DERY FOR STARTING VALUES                        DHCG1300
      4 CALL FCT(X,Y,DERY)                                              DHCG1310
C                                                                       DHCG1320
C        RECORDING OF STARTING VALUES                                   DHCG1330
        CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                              DHCG1340
        IF(PRMT(5))6,5,6                                                DHCG1350
      5 IF(IHLF)7,7,6                                                   DHCG1360
      6 RETURN                                                          DHCG1370
      7 DO 8 I=1,NDIM                                                   DHCG1380
      8 AUX(8,I)=DERY(I)                                                DHCG1390
C                                                                       DHCG1400
C        COMPUTATION OF AUX(2,I)                                        DHCG1410
        ISW=1                                                           DHCG1420
        GOTO 100                                                        DHCG1430
C                                                                       DHCG1440
      9 X=X+H                                                           DHCG1450
        DO 10 I=1,NDIM                                                  DHCG1460
     10 AUX(2,I)=Y(I)                                                   DHCG1470
C                                                                       DHCG1480
C        INCREMENT H IS TESTED BY MEANS OF BISECTION                    DHCG1490
     11 IHLF=IHLF+1                                                     DHCG1500
        X=X-H                                                           DHCG1510
        DO 12 I=1,NDIM                                                  DHCG1520
     12 AUX(4,I)=AUX(2,I)                                               DHCG1530
        H=.5D0*H                                                        DHCG1540
        N=1                                                             DHCG1550
        ISW=2                                                           DHCG1560
        GOTO 100                                                        DHCG1570
C                                                                       DHCG1580
     13 X=X+H                                                           DHCG1590
        CALL FCT(X,Y,DERY)                                              DHCG1600
        N=2                                                             DHCG1610
        DO 14 I=1,NDIM                                                  DHCG1620
        AUX(2,I)=Y(I)                                                   DHCG1630
     14 AUX(9,I)=DERY(I)                                                DHCG1640
        ISW=3                                                           DHCG1650
        GOTO 100                                                        DHCG1660
C                                                                       DHCG1670
C        COMPUTATION OF TEST VALUE DELT                                 DHCG1680
     15 DELT=0.D0                                                       DHCG1690
        DO 16 I=1,NDIM                                                  DHCG1700
     16 DELT=DELT+AUX(15,I)*DABS(Y(I)-AUX(4,I))                         DHCG1710
        DELT=.06666666666666667D0*DELT                                  DHCG1720
        IF(DELT-PRMT(4))19,19,17                                        DHCG1730
     17 IF(IHLF-10)11,18,18                                             DHCG1740
C                                                                       DHCG1750
C        NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.   DHCG1760
     18 IHLF=11                                                         DHCG1770
        X=X+H                                                           DHCG1780
        GOTO 4                                                          DHCG1790
C                                                                       DHCG1800
C        THERE IS SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS.   DHCG1810
     19 X=X+H                                                           DHCG1820
        CALL FCT(X,Y,DERY)                                              DHCG1830
        DO 20 I=1,NDIM                                                  DHCG1840
        AUX(3,I)=Y(I)                                                   DHCG1850
     20 AUX(10,I)=DERY(I)                                               DHCG1860
        N=3                                                             DHCG1870
        ISW=4                                                           DHCG1880
        GOTO 100                                                        DHCG1890
C                                                                       DHCG1900
     21 N=1                                                             DHCG1910
        X=X+H                                                           DHCG1920
        CALL FCT(X,Y,DERY)                                              DHCG1930
        X=PRMT(1)                                                       DHCG1940
        DO 22 I=1,NDIM                                                  DHCG1950
        AUX(11,I)=DERY(I)                                               DHCG1960
     22Y(I)=AUX(1,I)+H*(.375D0*AUX(8,I)+.79166666666666670D0*AUX(9,I)   DHCG1970
       1-.20833333333333330D0*AUX(10,I)+.04166666666666667D0*DERY(I))   DHCG1980
     23 X=X+H                                                           DHCG1990
        N=N+1                                                           DHCG2000
        CALL FCT(X,Y,DERY)                                              DHCG2010
        CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                              DHCG2020
        IF(PRMT(5))6,24,6                                               DHCG2030
     24 IF(N-4)25,200,200                                               DHCG2040
     25 DO 26 I=1,NDIM                                                  DHCG2050
        AUX(N,I)=Y(I)                                                   DHCG2060
     26 AUX(N+7,I)=DERY(I)                                              DHCG2070
        IF(N-3)27,29,200                                                DHCG2080
C                                                                       DHCG2090
     27 DO 28 I=1,NDIM                                                  DHCG2100
        DELT=AUX(9,I)+AUX(9,I)                                          DHCG2110
        DELT=DELT+DELT                                                  DHCG2120
     28 Y(I)=AUX(1,I)+.33333333333333330D0*H*(AUX(8,I)+DELT+AUX(10,I))  DHCG2130
        GOTO 23                                                         DHCG2140
C                                                                       DHCG2150
     29 DO 30 I=1,NDIM                                                  DHCG2160
        DELT=AUX(9,I)+AUX(10,I)                                         DHCG2170
        DELT=DELT+DELT+DELT                                             DHCG2180
     30 Y(I)=AUX(1,I)+.375D0*H*(AUX(8,I)+DELT+AUX(11,I))                DHCG2190
        GOTO 23                                                         DHCG2200
C                                                                       DHCG2210
C        THE FOLLOWING PART OF SUBROUTINE DHPCG COMPUTES BY MEANS OF    DHCG2220
C        RUNGE-KUTTA METHOD STARTING VALUES FOR THE NOT SELF-STARTING   DHCG2230
C        PREDICTOR-CORRECTOR METHOD.                                    DHCG2240
  100 DO 101 I=1,NDIM                                                   DHCG2250
        Z=H*AUX(N+7,I)                                                  DHCG2260
        AUX(5,I)=Z                                                      DHCG2270
  101 Y(I)=AUX(N,I)+.4D0*Z                                              DHCG2280
C       Z IS AN AUXILIARY STORAGE LOCATION                              DHCG2290
C                                                                       DHCG2300
        Z=X+.4D0*H                                                      DHCG2310
        CALL FCT(Z,Y,DERY)                                              DHCG2320
        DO 102 I=1,NDIM                                                 DHCG2330
        Z=H*DERY(I)                                                     DHCG2340
        AUX(6,I)=Z                                                      DHCG2350
  102 Y(I)=AUX(N,I)+.29697760924775360D0*AUX(5,I)+.15875964497103583D0*ZDHCG2360
C                                                                       DHCG2370
        Z=X+.45573725421878943D0*H                                      DHCG2380
        CALL FCT(Z,Y,DERY)                                              DHCG2390
        DO 103 I=1,NDIM                                                 DHCG2400
        Z=H*DERY(I)                                                     DHCG2410
        AUX(7,I)=Z                                                      DHCG2420
  103 Y(I)=AUX(N,I)+.21810038822592047D0*AUX(5,I)-3.05096514869293080D0*DHCG2430
       1AUX(6,I)+3.83286476046701030D0*Z                                DHCG2440
C                                                                       DHCG2450
        Z=X+H                                                           DHCG2460
        CALL FCT(Z,Y,DERY)                                              DHCG2470
        DO 104 I=1,NDIM                                                 DHCG2480
 1040Y(I)=AUX(N,I)+.17476028226269037D0*AUX(5,I)-.55148066287873294D0*  DHCG2490
       1AUX(6,I)+1.20553559396523500*AUX(7,I)+.17118478121951903D0*     DHCG2500
       2H*DERY(I)                                                       DHCG2510
        GOTO(9,13,15,21),ISW                                            DHCG2520
C                                                                       DHCG2530
C        POSSIBLE BREAK-POINT FOR LINKAGE                               DHCG2540
C                                                                       DHCG2550
C        STARTING VALUES ARE COMPUTED.                                  DHCG2560
C        NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.        DHCG2570
  200 ISTEP=3                                                           DHCG2580
```

```
  201 IF(N-8)204,202,204                                                DHCG2590
C                                                                       DHCG2600
C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS      DHCG2610
  202 DO 203 N=2,7                                                      DHCG2620
      DO 203 I=1,NDIM                                                   DHCG2630
      AUX(N-1,I)=AUX(N,I)                                               DHCG2640
  203 AUX(N+6,I)=AUX(N+7,I)                                             DHCG2650
      N=7                                                               DHCG2660
C                                                                       DHCG2670
C     N LESS THAN 8 CAUSES N+1 TO GET N                                 DHCG2680
  204 N=N+1                                                             DHCG2690
C                                                                       DHCG2700
C     COMPUTATION OF NEXT VECTOR Y                                      DHCG2710
      DO 205 I=1,NDIM                                                   DHCG2720
      AUX(N-1,I)=Y(I)                                                   DHCG2730
  205 AUX(N+6,I)=DERY(I)                                                DHCG2740
      X=X+H                                                             DHCG2750
  206 ISTEP=ISTEP+1                                                     DHCG2760
      DO 207 I=1,NDIM                                                   DHCG2770
     CDELT=AUX(N-4,I)+1.3333333333333333D0*H*(AUX(N+6,I)+AUX(N+6,I)-    DHCG2780
     1AUX(N+5,I)+AUX(N+4,I)+AUX(N+4,I))                                 DHCG2790
      Y(I)=DELT-.92561983471074380D0*AUX(16,I)                          DHCG2800
  207 AUX(16,I)=DELT                                                    DHCG2810
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR   DHCG2820
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.               DHCG2830
C                                                                       DHCG2840
      CALL FCT(X,Y,DERY)                                                DHCG2850
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY             DHCG2860
C                                                                       DHCG2870
      DO 208 I=1,NDIM                                                   DHCG2880
     0DELT=.12500*(9.00*AUX(N-1,I)-AUX(N-3,I)+3.00*H*(DERY(I)+AUX(N+6,I)DHCG2890
     1+AUX(N+6,I)-AUX(N+5,I)))                                          DHCG2900
      AUX(16,I)=AUX(16,I)-DELT                                          DHCG2910
  208 Y(I)=DELT+.07438016528925620D0*AUX(16,I)                          DHCG2920
C                                                                       DHCG2930
C     TEST WHETHER H MUST BE HALVED OR DOUBLED                          DHCG2940
      DELT=0.D0                                                         DHCG2950
      DO 209 I=1,NDIM                                                   DHCG2960
  209 DELT=DELT+AUX(15,I)*DABS(AUX(16,I))                               DHCG2970
      IF(DELT-PRMT(4))210,222,222                                       DHCG2980
C                                                                       DHCG2990
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                   DHCG3000
  210 CALL FCT(X,Y,DERY)                                                DHCG3010
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                DHCG3020
      IF(PRMT(5))212,211,212                                            DHCG3030
  211 IF(IHLF-11)213,212,212                                            DHCG3040
  212 RETURN                                                            DHCG3050
  213 IF(H*(X-PRMT(2)))214,212,212                                      DHCG3060
  214 IF(DABS(X-PRMT(2))-.100*DABS(H))212,215,215                       DHCG3070
  215 IF(DELT-.0200*PRMT(4))216,216,201                                 DHCG3080
C                                                                       DHCG3090
C                                                                       DHCG3100
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE         DHCG3110
C     AVAILABLE                                                         DHCG3120
  216 IF(IHLF)201,201,217                                               DHCG3130
  217 IF(N-7)201,218,218                                                DHCG3140
  218 IF(ISTEP-4)201,219,219                                            DHCG3150
  219 IMOD=ISTEP/2                                                      DHCG3160
      IF(ISTEP-IMOD-IMOD)201,220,201                                    DHCG3170
  220 H=H+H                                                             DHCG3180
      IHLF=IHLF-1                                                       DHCG3190
      ISTEP=0                                                           DHCG3200
      DO 221 I=1,NDIM                                                   DHCG3210
      AUX(N-1,I)=AUX(N-2,I)                                             DHCG3220
      AUX(N-2,I)=AUX(N-4,I)                                             DHCG3230
      AUX(N-3,I)=AUX(N-6,I)                                             DHCG3240
      AUX(N+6,I)=AUX(N+5,I)                                             DHCG3250
      AUX(N+5,I)=AUX(N+3,I)                                             DHCG3260
      AUX(N+4,I)=AUX(N+1,I)                                             DHCG3270
      DELT=AUX(N+6,I)+AUX(N+5,I)                                        DHCG3280
      DELT=DELT+DELT+DELT                                               DHCG3290
 2210AUX(16,I)=8.9629629629629630D0*(Y(I)-AUX(N-3,I))                   DHCG3300
     1-3.3611111111111111D0*H*(DERY(I)+DELT+AUX(N+4,I))                 DHCG3310
      GOTO 201                                                          DHCG3320
C                                                                       DHCG3330
C                                                                       DHCG3340
C     H MUST BE HALVED                                                  DHCG3350
  222 IHLF=IHLF+1                                                       DHCG3360
      IF(IHLF-10)223,223,210                                            DHCG3370
  223 H=.500*H                                                          DHCG3380
      ISTEP=0                                                           DHCG3390
      DO 224 I=1,NDIM                                                   DHCG3400
     0Y(I)=.3906250-2*(8.01*AUX(N-1,I)+135.00*AUX(N-2,I)+4.01*AUX(N-3,I)DHCG3410
     1+AUX(N-4,I))-.11718750D0*(AUX(N+6,I)-6.00*AUX(N+5,I)-AUX(N+4,I))*H DHCG3420
     0AUX(N-4,I)=.3906250-2*(12.00*AUX(N-1,I)+135.00*AUX(N-2,I)+        DHCG3430
     1108.00*AUX(N-3,I)+AUX(N-4,I))-.02343750D0*(AUX(N+6,I)+            DHCG3440
     218.00*AUX(N+5,I)-9.00*AUX(N+4,I))*H                               DHCG3450
      AUX(N-3,I)=AUX(N-2,I)                                             DHCG3460
  224 AUX(N+4,I)=AUX(N+5,I)                                             DHCG3470
      X=X-H                                                             DHCG3480
      DELT=X-(H+H)                                                      DHCG3490
      CALL FCT(DELT,Y,DERY)                                             DHCG3500
      DO 225 I=1,NDIM                                                   DHCG3510
      AUX(N-2,I)=Y(I)                                                   DHCG3520
      AUX(N+5,I)=DERY(I)                                                DHCG3530
  225 Y(I)=AUX(N-4,I)                                                   DHCG3540
      DELT=DELT-(H+H)                                                   DHCG3550
      CALL FCT(DELT,Y,DERY)                                             DHCG3560
      DO 226 I=1,NDIM                                                   DHCG3570
      DELT=AUX(N+5,I)+AUX(N+4,I)                                        DHCG3580
      DELT=DELT+DELT+DELT                                               DHCG3590
     0AUX(16,I)=8.9629629629629630D0*(AUX(N-1,I)-Y(I))                  DHCG3600
     1-3.3611111111111111D0*H*(AUX(N+6,I)+DELT+DERY(I))                 DHCG3610
  226 AUX(N+3,I)=DERY(I)                                                DHCG3620
      GOTO 206                                                          DHCG3630
      END                                                               DHCG3640
```

Subroutines HPCL and DHPCL

These subroutines use Hamming's modified predictor-corrector method for the solution of linear initial - value problems. The purpose of this version of Hamming's modified predictor-corrector method is to obtain an approximate solution of a linear system of first-order ordinary differential equations with given initial values.† It is a stable fourth-order integration procedure, requiring the evaluation of the right-hand side of the system only two times per step. This is a great advantage compared with other methods of the same order of accuracy, especially the Runge-Kutta method, which requires the evaluation of the right-hand side four times per step. Another advantage is that at each step the calculation procedure gives an estimate for the local truncation error; thus the procedure is able -- without a significant amount of calculation time -- to choose and change the step size h. On the other hand, Hamming's predictor-corrector method is not self-starting; that is, the functional values at a single previous point are not enough to obtain the functional values ahead. Therefore, to get the starting values, a special Runge-Kutta procedure followed by one iteration step is added to the predictor-corrector method.

Given the linear system of first-order ordinary differential equations:

$$y'_1 = \frac{dy_1}{dx} = a_{11}(x)\,y_1 + a_{12}(x)\,y_2 + \ldots + a_{1n}(x)\,y_n + f_1(x)$$

$$y'_2 = \frac{dy_2}{dx} = a_{21}(x)\,y_1 + a_{22}(x)\,y_2 + \ldots + a_{2n}(x)\,y_n + f_2(x)$$

$$\ldots\ldots\ldots\ldots\ldots\ldots$$

$$y'_n = \frac{dy_n}{dx} = a_{n1}(x)\,y_1 + a_{n2}(x)\,y_2 + \ldots + a_{nn}(x)\,y_n + f_n(x)$$

---

† Solution can be done with subroutines HPCG and DHPCG too. The main reason for this special version, suitable to systems of linear differential equations, is that external subroutines furnished by the user for the solution of linear boundary-value problems can be used without changes by subroutine HPCL or DHPCL for the solution of corresponding linear initial-value problems.

and the initial values:

$$y_1(x_0) = y_{1,0},\ y_2(x_0) = y_{2,0},\ \ldots,\ y_n(x_0) = y_{n,0}$$

and using the following vector and matrix notations:

$$Y(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_n(x) \end{pmatrix}, \qquad f(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_n(x) \end{pmatrix},$$

$$A(x) = \begin{pmatrix} a_{11}(x)\ a_{12}(x) \ldots a_{1n}(x) \\ a_{21}(x)\ a_{22}(x) \ldots a_{2n}(x) \\ \cdots\cdots \\ a_{n1}(x)\ a_{n2}(x) \ldots a_{nn}(x) \end{pmatrix}$$

$$\text{and } Y_0 = \begin{pmatrix} y_{1,0} \\ y_{2,0} \\ \vdots \\ y_{n,0} \end{pmatrix}$$

where Y, F and Y_0 are column vectors and A is an n by n square matrix, the given problem appears as follows:

$$Y' = \frac{dY}{dx} = A(x) * Y + F(x) \text{ with } Y(x_0) = Y_0$$

For stability purposes, the modification by Hamming of Milne's classical modified predictor-corrector method is preferred. Thus, knowing the results at the equidistant points x_{j-3}, x_{j-2}, x_{j-1} and x_j, the results at point $x_{j+1} = x_j + h$ are computed by the formulas given below.

Predictor:
$$P_{j+1} = Y_{j-3} + \frac{4h}{3}(2Y'_j - Y'_{j-1} + 2Y'_{j-2}) \qquad (1)$$

Modifier:
$$M_{j+1} = P_{j+1} - \frac{112}{121}(P_j - C_j) \qquad (2)$$

$$M'_{j+1} = A(x_{j+1}) * M_{j+1} + F(x_{j+1}) \qquad (3)$$

Corrector:
$$C_{j+1} = \frac{1}{8}\left[9Y_j - Y_{j-2} + 3h(M'_{j+1} + 2Y'_j - Y'_{j-1})\right] \qquad (4)$$

Final Value:
$$Y_{j+1} = C_{j+1} + \frac{9}{121}(P_{j+1} - C_{j+1}) \qquad (5)$$

where Y, Y', P, M, M' and C are all column vectors with n components, and A is an n by n square matrix. Formulas (1) and (4) have local truncation errors:

$$T_1 = \frac{14}{45}h^5 Y^{(5)}(\xi_1) \text{ with } \xi_1 \in (x_{j-3}, x_{j+1})$$

and

$$T_2 = -\frac{1}{40}h^5 Y^{(5)}(\xi_2) \text{ with } \xi_2 \in (x_{j-2}, x_{j+1})$$

respectively such that

$$C_{j+1} - P_{j+1} = \frac{121}{360}h^5 Y^{(5)}(\xi) \text{ with } \xi \in (x_{j-3}, x_{j+1})$$

Assuming that $Y^{(5)}(x)$ does not vary to any great extent in the interval (x_{j-3}, x_{j+1}), it follows that:

$$T_2 \approx \frac{9}{121}(P_{j+1} - C_{j+1})$$

This formula shows that the components of column vector $P_{j+1} - C_{j+1}$ are measures for the local truncation errors in the components of column vector Y_{j+1}. Therefore, control of accuracy and adjustment of step size h can be done by generating the following test value:

$$\delta = \sum_{i=1}^{n} a_i \cdot \left| P_{j+1,i} - c_{j+1,i} \right| \qquad (6)$$

where the coefficients a_i $(i = 1, 2, \ldots, n)$ are error-weights specified in the input of the procedure.

If δ is greater than a given tolerance ε†, increment h is halved and the procedure computes $Y_{j-\frac{1}{2}}$ -- that is, $Y(x_j + \frac{h}{2})$ -- after having interpolated $Y_{j-\frac{1}{2}} = Y(x_j - \frac{h}{2})$ and $Y_{j-\frac{3}{2}} = Y(x_j - \frac{3h}{2})$, with previous increment h, using the following sixth-order interpolation formulas:

$$Y_{j-\frac{1}{2}} = \frac{1}{256}(80Y_j + 135Y_{j-1} + 40Y_{j-2} + Y_{j-3}) + \frac{h}{2} \cdot \frac{15}{128}(-Y'_j + 6Y'_{j-1} + Y'_{j-2}) \qquad (7)$$

† Numerical experience seems to show that the procedure does not exceed a global relative error approximately equal to ε.

$$Y_{j-\frac{3}{2}} = \frac{1}{256}(12\,Y_j + 135\,Y_{j-1} + 108\,Y_{j-2} + Y_{j-3}) + \frac{h}{2} \cdot \frac{3}{128}(-Y'_j - 18\,Y'_{j-1} + 9\,Y'_{j-2}) \quad (8)$$

If δ is less than ε, the result Y_{j+1} is assumed to be correct and is handed, together with x_{j+1} and the vector of derivatives Y'_{j+1}, to a user-supplied output subroutine.

If δ is less than $\varepsilon/50$, the next step is carried out with the doubled increment. However, care is taken in the procedure, so that the increment never becomes greater than the increment h specified as an input parameter, and further that among the output are all points $x_0 + j \cdot h$ (where $j = 0, 1, 2, \ldots$, and h is the input step size) which are situated between the lower and the upper bound of the integration interval.

Changing the step size by halving or doubling requires changing of $P_j - C_j$ or $P_{j+1} - C_{j+1}$ respectively. Using the following interpolation formula:

$$Y_j = Y_{j-3} + \frac{3}{8}h\,(Y'_{j-3} + 3Y'_{j-2} + 3Y'_{j-1} + Y_j) - \frac{3}{80}h^5\,Y^{(5)}(\xi_3)$$

with

$$\xi_3\ \varepsilon(x_{j-3},\ x_j)$$

and assuming that $Y^{(5)}(x)$ does not vary to any great extent in this interval, $P_j - C_j$ can be written in the following form:

$$P_j - C_j \approx \frac{242}{27}(Y_j - Y_{j-3}) - \frac{121}{36}h\,(Y'_j + 3Y'_{j-1} + 3Y'_{j-2} + Y'_{j-3})$$

When halving increment h, this formula becomes:

$$P_j - C_j \approx \frac{242}{27}(Y_j - Y_{j-\frac{3}{2}}) - \frac{121}{36} \cdot \frac{h}{2}(Y'_j + 3Y'_{j-\frac{3}{2}} + 3Y'_{j-1} + Y'_{j-\frac{3}{2}}) \quad (9)$$

and when doubling:

$$P_{j+1} - C_{j+1} \approx \frac{242}{27}(Y_{j+1} - Y_{j-5}) - \frac{121}{36} \cdot 2h\,(Y'_{j+1} + 3Y'_{j-1} + 3Y'_{j-3} + Y'_{j-5}) \quad (10)$$

Starting Hamming's modified predictor-corrector method requires the functional and derivative values at four preceding equidistant points: x_0, x_1, x_2 and x_3. The values Y_0 and $Y'_0 = A(x_0) * Y_0 + F(x_0)$ are specified by input. For computation of Y_1, Y'_1, Y_2, Y'_2, Y_3 and Y'_3 and for adjustment of step size h to accuracy requirements, a special Runge-Kutta procedure suggested by Ralston is used. Starting at x_j, result values at point $x_{j+1} = x_j + h$ are computed using the following formulas:

$$K_1 = h \cdot Y'_j \quad (11)$$

$$K_2 = h \cdot [A(x_j + 0.4\,h) * (Y_j + 0.4\,K_1) + F(x_j + 0.4\,h)] \quad (12)$$

$$K_3 = h \cdot [A(x_j + 0.45573725421878943\,h) * (Y_j + 0.29697760924775360\,K_1 + 0.15875964497103583\,K_2) + F(x_j + 0.45573725421878943\,h)] \quad (13)$$

$$K_4 = h \cdot [A(x_j + h) * (Y_j + 0.21810038822592047\,K_1 - 3.0509651486929308\,K_2 + 3.8328647604670103\,K_3) + F(x_j + h)] \quad (14)$$

$$Y_{j+1} = Y_j + 0.17476028226269037\,K_1 - 0.55148066287873294\,K_2 + 1.2055355993965235\,K_3 + 0.17118478121951903\,K_4 \quad (15)$$

where Y_j, Y_{j+1}, Y'_j, K_1, K_2, K_3 and K_4 are all column vectors with n components, and A is an n by n square matrix. These formulas are not very stable, but this does not matter because they are used only in three successive steps ($j = 0, 1, 2$). On the other hand, they have the smallest bound of truncation errors of all fourth-order Runge-Kutta procedures. Therefore they are best suited to start other integration methods which are not self-starting.

For initial control of accuracy and adjustment of step size h, in starting the procedure an approximation for $Y_2 = Y(x_0 + h)$ called $Y_2^{(1)}$ is computed using the step size h, and then an approximation called $Y_2^{(2)}$, using the step size h/2 twice. From these two approximations, a test value δ for accuracy is generated in the following way:

$$\delta = \frac{1}{15} \sum_{i=1}^{n} a_i \cdot \left| y_{2,i}^{(1)} - y_{2,i}^{(2)} \right| \qquad (16)$$

If δ is greater than ε, increment h is halved and the procedure starts anew at point x_0.

If δ is less than ε, the results $Y_1^{(2)} = Y(x_0 + \frac{h}{2})$ and $Y_2^{(2)} = Y(x_0 + h)$ are assumed to be correct and a third step follows which computes the results at point $x_0 + \frac{3h}{2}$ -- that is, $Y_3 = Y(x_0 + \frac{3}{2}h)$.

The step size h/2 of these three steps is used as initial step size h in the predictor-corrector method.

It is very important that the starting values be as accurate as possible, because errors in these starting values may increase during the following predictor-corrector procedure. Therefore the starting values computed by the Runge-Kutta method are refined by one iteration step using the following fourth-order interpolation formulas:

$$Y_1 = Y_0 + \frac{h}{24}(9\,Y'_0 + 19\,Y'_1 - 5\,Y'_2 + Y'_3) \qquad (17)$$

$$Y_2 = Y_0 + \frac{h}{3}(Y'_0 + 4\,Y'_1 + Y'_2) \qquad (18)$$

$$Y_3 = Y_0 + \frac{3h}{8}(Y'_0 + 3\,Y'_1 + 3\,Y'_2 + Y'_3) \qquad (19)$$

which must be considered as an iteration procedure. That is, first the result values of the Runge-Kutta method are handed to the right-hand side of formula (17) to compute a refined Y_1. After having computed the refined Y'_1, the refined vector Y_2 is generated using formula (18). Finally, refined Y'_2 is used, together with the other values, in the right-hand side of formula (19) to compute the refined vector Y_3. During this iteration, the refined data sets x_j, Y_j, Y'_j are handed, together with the number of bisections of the initial step size (specified by input), to the output subroutine.

It can be shown that, using this iterative procedure, the initial column vector $P_3 - C_3$ used in formula (2) for j = 3 is equal to zero.

The entire input of the procedure is:

1. Lower and upper bound of the integration interval, initial step size h of the independent variable, and upper bound ε of the local truncation error

2. Initial values Y_0 of the dependent variables and weights a_i (i = 1,2, ..., n) for the local truncation errors in each component of the dependent variables

3. The number n of differential equations in the system

4. As external subroutine subprograms, the computation of the right-hand side matrix A of the system of linear differential equations and of the inhomogeneous vector F; for flexibility in output, an output subroutine

5. An auxiliary storage array with 16 rows and n columns

6. An n by n matrix as auxiliary storage array

Output is done in the following way. If a set of approximations to the dependent variables Y (x) is found to be of sufficient accuracy, it is handed -- together with x, the derivative Y' (x), the number of bisections of the initial increment, the number of differential equations, the lower and upper bound of the interval, the initial step size, error bound ε, and a parameter for terminating subroutine HPCL or DHPCL -- to the output subroutine. By means of this output subroutine, the user has the opportunity to choose his own output format, to handle the output values as he wants, to change the upper error bound and to terminate subroutine HPCL or DHPCL at any output point. In particular, the user is able to drop the output of some intermediate points, printing only the result values at the special points $x_0 + j \cdot h$, where j = 0, 1, 2, ..., and he is the initial step size specified by input. The user may also perform intermediate computation using the integration results before continuing the process. For better understanding of the flowchart and of the FORTRAN program, see the allocation of special intermediate result vectors within the storage array AUX, shown previously in Figure 12.

For reference see:

(1) A. Ralston/ H.S. Wilf, Mathematical Methods for Digital Computers, Wiley, New York/London, 1960, pp. 95 - 109.

(2) A. Ralston, "Runge-Kutta Methods with Minimum Error Bounds", MTAC, vol. 16, no. 80 (1962), pp. 431 - 437.

```
C                                                                       HPCL  10
C     ...................................................................HPCL  20
C                                                                       HPCL  30
C        SUBROUTINE HPCL                                                HPCL  40
C                                                                       HPCL  50
C        PURPOSE                                                        HPCL  60
C           TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY LINEAR            HPCL  70
C           DIFFERENTIAL EQUATIONS WITH GIVEN INITIAL VALUES.           HPCL  80
C                                                                       HPCL  90
C        USAGE                                                          HPCL 100
C           CALL HPCL (PRMT,Y,DERY,NDIM,IHLF,AFCT,FCT,OUTP,AUX,A)       HPCL 110
C           PARAMETERS AFCT,FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT. HPCL 120
C                                                                       HPCL 130
C        DESCRIPTION OF PARAMETERS                                      HPCL 140
C           PRMT   - AN INPUT AND OUTPUT VECTOR WITH DIMENSION GREATER  HPCL 150
C                    OR EQUAL TO 5, WHICH SPECIFIES THE PARAMETERS OF   HPCL 160
C                    THE INTERVAL AND OF ACCURACY AND WHICH SERVES FOR  HPCL 170
C                    COMMUNICATION BETWEEN OUTPUT SUBROUTINE (FURNISHED HPCL 180
C                    BY THE USER) AND SUBROUTINE HPCL. EXCEPT PRMT(5)   HPCL 190
C                    THE COMPONENTS ARE NOT DESTROYED BY SUBROUTINE     HPCL 200
C                    HPCL AND THEY ARE                                  HPCL 210
C              PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT),            HPCL 220
C              PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT),            HPCL 230
C              PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE    HPCL 240
C                       (INPUT),                                        HPCL 250
C              PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS HPCL 260
C                       GREATER THAN PRMT(4), INCREMENT GETS HALVED.    HPCL 270
C                       IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE  HPCL 280
C                       ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.HPCL 290
C                       THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS     HPCL 300
C                       OUTPUT SUBROUTINE.                              HPCL 310
C              PRMT(5)- NO INPUT PARAMETER. SUBROUTINE HPCL INITIALIZES HPCL 320
C                       PRMT(5)=0. IF THE USER WANTS TO TERMINATE       HPCL 330
C                       SUBROUTINE HPCL AT ANY OUTPUT POINT, HE HAS TO  HPCL 340
C                       CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE HPCL 350
C                       OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE     HPCL 360
C                       FEASIBLE IF ITS DIMENSION IS DEFINED GREATER    HPCL 370
C                       THAN 5. HOWEVER SUBROUTINE HPCL DOES NOT REQUIRE HPCL 380
C                       AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL HPCL 390
C                       FOR HANDING RESULT VALUES TO THE MAIN PROGRAM   HPCL 400
C                       (CALLING HPCL) WHICH ARE OBTAINED BY SPECIAL    HPCL 410
C                       MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP. HPCL 420
C              Y      - INPUT VECTOR OF INITIAL VALUES. (DESTROYED)     HPCL 430
C                       LATERON Y IS THE RESULTING VECTOR OF DEPENDENT  HPCL 440
C                       VARIABLES COMPUTED AT INTERMEDIATE POINTS X.    HPCL 450
C              DERY   - INPUT VECTOR OF ERROR WEIGHTS.  (DESTROYED)     HPCL 460
C                       THE SUM OF ITS COMPONENTS MUST BE EQUAL TO 1.   HPCL 470
C                       LATERON DERY IS THE VECTOR OF DERIVATIVES, WHICH HPCL 480
C                       BELONG TO FUNCTION VALUES Y AT A POINT X.       HPCL 490
C              NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF   HPCL 500
C                       EQUATIONS IN THE SYSTEM.                        HPCL 510
C              IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF  HPCL 520
C                       BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS HPCL 530
C                       GREATER THAN 10, SUBROUTINE HPCL RETURNS WITH   HPCL 540
C                       ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.        HPCL 550
C                       ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE HPCL 560
C                       PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-HPCL 570
C                       PRMT(1)) RESPECTIVELY.                          HPCL 580
C              AFCT   - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT     HPCL 590
C                       COMPUTES MATRIX A (FACTOR OF VECTOR Y ON THE    HPCL 600
C                       RIGHT HAND SIDE OF THE SYSTEM) FOR A GIVEN X-VALUE.HPCL 610
C                       ITS PARAMETER LIST MUST BE X,A. THE SUBROUTINE  HPCL 620
C                       SHOULD NOT DESTROY X.                           HPCL 630
C              FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT     HPCL 640
C                       COMPUTES VECTOR F (INHOMOGENEOUS PART OF THE    HPCL 650
C                       RIGHT HAND SIDE OF THE SYSTEM) FOR A GIVEN X-VALUE.HPCL 660
C                       ITS PARAMETER LIST MUST BE X,F. THE SUBROUTINE  HPCL 670
C                       SHOULD NOT DESTROY X.                           HPCL 680
C              OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED. HPCL 690
C                       ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.HPCL 700
C                       NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY, HPCL 710
C                       PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY       HPCL 720
C                       SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,HPCL 730
C                       SUBROUTINE HPCL IS TERMINATED.                  HPCL 740
C              AUX    - AN AUXILIARY STORAGE ARRAY WITH 16 ROWS AND NDIM HPCL 750
C                       COLUMNS.                                        HPCL 760
C              A      - AN NDIM BY NDIM MATRIX, WHICH IS USED AS AUXILIARY HPCL 770
C                       STORAGE ARRAY.                                  HPCL 780
C                                                                       HPCL 790
C        REMARKS                                                        HPCL 800
C           THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF HPCL 810
C           (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE    HPCL 820
C               NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE   HPCL 830
C               IHLF=11),                                               HPCL 840
C           (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN       HPCL 850
C               (ERROR MESSAGES IHLF=12 OR IHLF=13),                    HPCL 860
C           (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,       HPCL 870
C           (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.        HPCL 880
C                                                                       HPCL 890
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  HPCL 900
C           THE EXTERNAL SUBROUTINES AFCT(X,A), FCT(X,F) AND            HPCL 910
C           OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.HPCL 920
C                                                                       HPCL 930
C        METHOD                                                         HPCL 940
C           EVALUATION IS DONE BY MEANS OF HAMMINGS MODIFIED PREDICTOR- HPCL 950
C           CORRECTOR METHOD. IT IS A FOURTH ORDER METHOD, USING 4      HPCL 960
C           PRECEEDING POINTS FOR COMPUTATION OF A NEW VECTOR Y OF THE  HPCL 970
C           DEPENDENT VARIABLES.                                        HPCL 980
C           FOURTH ORDER RUNGE-KUTTA METHOD SUGGESTED BY RALSTON IS     HPCL 990
C           USED FOR ADJUSTMENT OF THE INITIAL INCREMENT AND FOR        HPCL1000
C           COMPUTATION OF STARTING VALUES.                             HPCL1010
C           SUBROUTINE HPCL AUTOMATICALLY ADJUSTS THE INCREMENT DURING  HPCL1020
C           THE WHOLE COMPUTATION BY HALVING OR DOUBLING.               HPCL1030
C           TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE     HPCL1040
C           MUST BE CODED BY THE USER.                                  HPCL1050
C           FOR REFERENCE, SEE                                          HPCL1060
C           (1) RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL          HPCL1070
C               COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.     HPCL1080
C           (2) RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS, HPCL1090
C               MTAC, VOL.16, ISS.80 (1962), PP.431-437.                HPCL1100
C                                                                       HPCL1110
C     ...................................................................HPCL1120
C                                                                       HPCL1130
      SUBROUTINE HPCL(PRMT,Y,DERY,NDIM,IHLF,AFCT,FCT,OUTP,AUX,A)        HPCL1140
C                                                                       HPCL1150
C                                                                       HPCL1160
C     THE FOLLOWING FIRST PART OF SUBROUTINE HPCL (UNTIL FIRST BREAK-   HPCL1170
C     POINT FOR LINKAGE) HAS TO STAY IN CORE DURING THE WHOLE           HPCL1180
C     COMPUTATION                                                       HPCL1190
C                                                                       HPCL1200
      DIMENSION PRMT(1),Y(1),DERY(1),AUX(16,1),A(1)                     HPCL1210
      GOTO 100                                                          HPCL1220
C                                                                       HPCL1230
C     THIS PART OF SUBROUTINE HPCL COMPUTES THE RIGHT HAND SIDE DERY OF HPCL1240
C     THE GIVEN SYSTEM OF LINEAR DIFFERENTIAL EQUATIONS.                HPCL1250
C                                                                       HPCL1260
    1 CALL AFCT(X,A)                                                    HPCL1270
      CALL FCT(X,DERY)                                                  HPCL1280
      DO 3 M=1,NDIM                                                     HPCL1290
      LL=M-NDIM                                                         HPCL1300
      HS=0.                                                             HPCL1310
      DO 2 L=1,NDIM                                                     HPCL1320
      LL=LL+NDIM                                                        HPCL1330
    2 HS=HS+A(LL)*Y(L)                                                  HPCL1340
    3 DERY(M)=HS+DERY(M)                                                HPCL1350
      GOTO(105,202,204,206,115,122,125,308,312,327,329,128),ISW2        HPCL1360
C                                                                       HPCL1370
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  HPCL1380
C                                                                       HPCL1390
  100 N=1                                                               HPCL1400
      IHLF=0                                                            HPCL1410
      X=PRMT(1)                                                         HPCL1420
      H=PRMT(3)                                                         HPCL1430
      PRMT(5)=0.                                                        HPCL1440
      DO 101 I=1,NDIM                                                   HPCL1450
      AUX(16,I)=0.                                                      HPCL1460
      AUX(15,I)=DERY(I)                                                 HPCL1470
  101 AUX(1,I)=Y(I)                                                     HPCL1480
      IF(H*(PRMT(2)-X))103,102,104                                      HPCL1490
C                                                                       HPCL1500
C     ERROR RETURNS                                                     HPCL1510
  102 IHLF=12                                                           HPCL1520
      GOTO 104                                                          HPCL1530
  103 IHLF=13                                                           HPCL1540
C                                                                       HPCL1550
C     COMPUTATION OF DERY FOR STARTING VALUES                           HPCL1560
  104 ISW2=1                                                            HPCL1570
      GOTO 1                                                            HPCL1580
C                                                                       HPCL1590
C     RECORDING OF STARTING VALUES                                      HPCL1600
  105 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                HPCL1610
      IF(PRMT(5))107,106,107                                            HPCL1620
  106 IF(IHLF)108,108,107                                               HPCL1630
  107 RETURN                                                            HPCL1640
  108 DO 109 I=1,NDIM                                                   HPCL1650
  109 AUX(8,I)=DERY(I)                                                  HPCL1660
C                                                                       HPCL1670
C     COMPUTATION OF AUX(2,I)                                           HPCL1680
      ISW1=1                                                            HPCL1690
      GOTO 200                                                          HPCL1700
C                                                                       HPCL1710
  110 X=X+H                                                             HPCL1720
      DO 111 I=1,NDIM                                                   HPCL1730
  111 AUX(2,I)=Y(I)                                                     HPCL1740
C                                                                       HPCL1750
C     INCREMENT H IS TESTED BY MEANS OF BISECTION                       HPCL1760
  112 IHLF=IHLF+1                                                       HPCL1770
      X=X-H                                                             HPCL1780
      DO 113 I=1,NDIM                                                   HPCL1790
  113 AUX(4,I)=AUX(2,I)                                                 HPCL1800
      H=.5*H                                                            HPCL1810
      N=1                                                               HPCL1820
      ISW1=2                                                            HPCL1830
      GOTO 200                                                          HPCL1840
C                                                                       HPCL1850
  114 X=X+H                                                             HPCL1860
      ISW2=5                                                            HPCL1870
      GOTO 1                                                            HPCL1880
  115 N=2                                                               HPCL1890
      DO 116 I=1,NDIM                                                   HPCL1900
      AUX(2,I)=Y(I)                                                     HPCL1910
  116 AUX(9,I)=DERY(I)                                                  HPCL1920
      ISW1=3                                                            HPCL1930
      GOTO 200                                                          HPCL1940
C                                                                       HPCL1950
C     COMPUTATION OF TEST VALUE DELT                                    HPCL1960
  117 DELT=0.                                                           HPCL1970
      DO 118 I=1,NDIM                                                   HPCL1980
  118 DELT=DELT+AUX(15,I)*ABS(Y(I)-AUX(4,I))                            HPCL1990
      DELT=.06666667*DELT                                               HPCL2000
      IF(DELT-PRMT(4))121,121,119                                       HPCL2010
  119 IF(IHLF-10)112,120,120                                            HPCL2020
C                                                                       HPCL2030
C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.      HPCL2040
  120 IHLF=11                                                           HPCL2050
      X=X+H                                                             HPCL2060
      GOTO 104                                                          HPCL2070
C                                                                       HPCL2080
C     SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS               HPCL2090
  121 X=X+H                                                             HPCL2100
      ISW2=6                                                            HPCL2110
      GOTO 1                                                            HPCL2120
  122 DO 123 I=1,NDIM                                                   HPCL2130
      AUX(3,I)=Y(I)                                                     HPCL2140
  123 AUX(10,I)=DERY(I)                                                 HPCL2150
      N=3                                                               HPCL2160
      ISW1=4                                                            HPCL2170
      GOTO 200                                                          HPCL2180
C                                                                       HPCL2190
  124 N=1                                                               HPCL2200
      X=X+H                                                             HPCL2210
      ISW2=7                                                            HPCL2220
      GOTO 1                                                            HPCL2230
  125 X=PRMT(1)                                                         HPCL2240
      DO 126 I=1,NDIM                                                   HPCL2250
      AUX(11,I)=DERY(I)                                                 HPCL2260
1260Y(I,=AUX(1,I)+H*(.375*AUX(8,I)+.7916667*AUX(9,I)                    HPCL2270
     1-.2083333*AUX(10,I)+.04166667*DERY(I))                            HPCL2280
  127 X=X+H                                                             HPCL2290
      N=N+1                                                             HPCL2300
      ISW2=12                                                           HPCL2310
      GOTO 1                                                            HPCL2320
  128 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                HPCL2330
      IF(PRMT(5))107,129,107                                            HPCL2340
  129 IF(N-4)130,300,300                                                HPCL2350
  130 DO 131 I=1,NDIM                                                   HPCL2360
      AUX(N,I)=Y(I)                                                     HPCL2370
  131 AUX(N+7,I)=DERY(I)                                                HPCL2380
      IF(N-3)132,134,300                                                HPCL2390
C                                                                       HPCL2400
  132 DO 133 I=1,NDIM                                                   HPCL2410
      DELT=AUX(9,I)+AUX(9,I)                                            HPCL2420
      DELT=DELT+DELT                                                    HPCL2430
  133 Y(I)=AUX(1,I)+.3333333*H*(AUX(8,I)+DELT+AUX(10,I))                HPCL2440
      GOTO 127                                                          HPCL2660
C                                                                       HPCL2450
  134 DO 135 I=1,NDIM                                                   HPCL2460
      DELT=AUX(9,I)+AUX(10,I)                                           HPCL2470
      DELT=DELT+DELT+DELT                                               HPCL2480
  135 Y(I)=AUX(1,I)+.375*H*(AUX(8,I)+DELT+AUX(11,I))                    HPCL2490
      GOTO 127                                                          HPCL2500
C                                                                       HPCL2510
C     THE FOLLOWING PART OF SUBROUTINE HPCL COMPUTES BY MEANS OF        HPCL2520
C     RUNGE-KUTTA METHOD STARTING VALUES FOR THE NOT SELF-STARTING      HPCL2530
C     PREDICTOR-CORRECTOR METHOD.                                       HPCL2540
  200 Z=X                                                               HPCL2550
      DO 201 I=1,NDIM                                                   HPCL2560
      X=H*AUX(N+7,I)                                                    HPCL2570
      AUX(5,I)=X                                                        HPCL2580
```

```
  201 Y(I)=AUX(N,I)+.4*X                                                HPCL2590
C     X IS AN AUXILIARY STORAGE LOCATION                                HPCL2600
C                                                                       HPCL2610
      X=Z+.4*H                                                          HPCL2620
      ISW2=2                                                            HPCL2630
      GOTO 1                                                            HPCL2640
  202 DO 203 I=1,NDIM                                                   HPCL2650
      X=H*DERY(I)                                                       HPCL2660
      AUX(6,I)=X                                                        HPCL2670
  203 Y(I)=AUX(N,I)+.2969776*AUX(5,I)+.1587596*X                        HPCL2680
C                                                                       HPCL2690
      X=Z+.4557372*H                                                    HPCL2700
      ISW2=3                                                            HPCL2710
      GOTO 1                                                            HPCL2720
  204 DO 205 I=1,NDIM                                                   HPCL2730
      X=H*DERY(I)                                                       HPCL2740
      AUX(7,I)=X                                                        HPCL2750
  205 Y(I)=AUX(N,I)+.2181004*AUX(5,I)-3.050965*AUX(6,I)+3.832865*X      HPCL2760
C                                                                       HPCL2770
      X=Z+H                                                             HPCL2780
      ISW2=4                                                            HPCL2790
      GOTO 1                                                            HPCL2800
  206 DO 207 I=1,NDIM                                                   HPCL2810
  207DY(I)=AUX(N,I)+.1747603*AUX(5,I)-.5514807*AUX(6,I)                 HPCL2820
     1+1.205536*AUX(7,I)+.1711848*H*DERY(I)                             HPCL2830
      X=Z                                                               HPCL2840
      GOTO(110,114,117,124),ISW1                                        HPCL2850
C                                                                       HPCL2860
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  HPCL2870
C                                                                       HPCL2880
C     STARTING VALUES ARE COMPUTED.                                     HPCL2890
C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.           HPCL2900
  300 ISTEP=3                                                           HPCL2910
  301 IF(N-8)304,302,304                                                HPCL2920
C                                                                       HPCL2930
C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS      HPCL2940
  302 DO 303 N=2,7                                                      HPCL2950
      DO 303 I=1,NDIM                                                   HPCL2960
      AUX(N-1,I)=AUX(N,I)                                               HPCL2970
  303 AUX(N+6,I)=AUX(N+7,I)                                             HPCL2980
      N=7                                                               HPCL2990
C                                                                       HPCL3000
C     N LESS THAN 8 CAUSES N+1 TO GET N                                 HPCL3010
  304 N=N+1                                                             HPCL3020
C                                                                       HPCL3030
C     COMPUTATION OF NEXT VECTOR Y                                      HPCL3040
      DO 305 I=1,NDIM                                                   HPCL3050
      AUX(N-1,I)=Y(I)                                                   HPCL3060
  305 AUX(N+6,I)=DERY(I)                                                HPCL3070
      X=X+H                                                             HPCL3080
  306 ISTEP=ISTEP+1                                                     HPCL3090
      DO 307 I=1,NDIM                                                   HPCL3100
      ODELT=AUX(N-4,I)+1.333333*H*(AUX(N+6,I)+AUX(N+6,I)-AUX(N+5,I)+    HPCL3110
     1AUX(N+4,I)+AUX(N+4,I))                                            HPCL3120
      Y(I)=DELT-.9256198*AUX(16,I)                                      HPCL3130
  307 AUX(16,I)=DELT                                                    HPCL3140
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR   HPCL3150
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.               HPCL3160
      ISW2=8                                                            HPCL3170
      GOTO 1                                                            HPCL3180
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY             HPCL3190
C                                                                       HPCL3200
  308 DO 309 I=1,NDIM                                                   HPCL3210
      ODELT=.125*(9.*AUX(N-1,I)-AUX(N-3,I)+3.*H*(DERY(I)+AUX(N+6,I)+    HPCL3220
     1AUX(N+6,I)-AUX(N+5,I)))                                           HPCL3230
      AUX(16,I)=AUX(16,I)-DELT                                          HPCL3240
  309 Y(I)=DELT+.07438017*AUX(16,I)                                     HPCL3250
C                                                                       HPCL3260
C     TEST WHETHER H MUST BE HALVED OR DOUBLED                          HPCL3270
      DELT=0.                                                           HPCL3280
      DO 310 I=1,NDIM                                                   HPCL3290
  310 DELT=DELT+AUX(15,I)*ABS(AUX(16,I))                                HPCL3300
      IF(DELT-PRMT(4))311,324,324                                       HPCL3310
C                                                                       HPCL3320
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                   HPCL3330
  311 ISW2=9                                                            HPCL3340
      GOTO 1                                                            HPCL3350
  312 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                HPCL3360
      IF(PRMT(5))314,313,314                                            HPCL3370
  313 IF(IHLF-11)315,314,314                                            HPCL3380
  314 RETURN                                                            HPCL3390
  315 IF(H*(X-PRMT(2)))316,314,314                                      HPCL3400
  316 IF(ABS(X-PRMT(2))-.1*ABS(H))314,317,317                           HPCL3410
  317 IF(DELT-.02*PRMT(4))318,318,301                                   HPCL3420
C                                                                       HPCL3430
C                                                                       HPCL3440
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE         HPCL3450
C     AVAILABLE                                                         HPCL3460
  318 IF(IHLF)301,301,319                                               HPCL3470
  319 IF(N-7)301,320,320                                                HPCL3480
  320 IF(ISTEP-4)301,321,321                                            HPCL3490
  321 IMOD=ISTEP/2                                                      HPCL3500
      IF(ISTEP-IMOD-IMOD)301,322,301                                    HPCL3510
  322 H=H+H                                                             HPCL3520
      IHLF=IHLF-1                                                       HPCL3530
      ISTEP=0                                                           HPCL3540
      DO 323 I=1,NDIM                                                   HPCL3550
      AUX(N-1,I)=AUX(N-2,I)                                             HPCL3560
      AUX(N-2,I)=AUX(N-4,I)                                             HPCL3570
      AUX(N-3,I)=AUX(N-6,I)                                             HPCL3580
      AUX(N+6,I)=AUX(N+5,I)                                             HPCL3590
      AUX(N+5,I)=AUX(N+3,I)                                             HPCL3600
      AUX(N+4,I)=AUX(N+1,I)                                             HPCL3610
      DELT=AUX(N+6,I)+AUX(N+5,I)                                        HPCL3620
      DELT=DELT+DELT+DELT                                               HPCL3630
 3230AUX(16,I)=8.962963*(Y(I)-AUX(N-3,I))-3.361111*H*(DERY(I)+DELT      HPCL3640
     1+AUX(N+4,I))                                                      HPCL3650
      GOTO 301                                                          HPCL3660
C                                                                       HPCL3670
C                                                                       HPCL3680
C     H MUST BE HALVED                                                  HPCL3690
  324 IHLF=IHLF+1                                                       HPCL3700
      IF(IHLF-10)325,325,311                                            HPCL3710
  325 H=.5*H                                                            HPCL3720
      ISTEP=0                                                           HPCL3730
      DO 326 I=1,NDIM                                                   HPCL3740
      OY(I)=.00390625*(80.*AUX(N-1,I)+135.*AUX(N-2,I)+40.*AUX(N-3,I)+   HPCL3750
     1AUX(N-4,I))-.1171875*(AUX(N+6,I)-6.*AUX(N+5,I)-AUX(N+4,I))*H      HPCL3760
      OAUX(N-4,I)=.00390625*(12.*AUX(N-1,I)+135.*AUX(N-2,I)+            HPCL3770
     1108.*AUX(N-3,I)+AUX(N-4,I))-.0234375*(AUX(N+6,I)+18.*AUX(N+5,I)-  HPCL3780
     29.*AUX(N+4,I))*H                                                  HPCL3790
      AUX(N-3,I)=AUX(N-2,I)                                             HPCL3800
  326 AUX(N+4,I)=AUX(N+5,I)                                             HPCL3810
      DELT=X-H                                                          HPCL3820
      X=DELT-(H+H)                                                      HPCL3830
      ISW2=10                                                           HPCL3840
      GOTO 1                                                            HPCL3850
  327 DO 328 I=1,NDIM                                                   HPCL3860
      AUX(N-2,I)=Y(I)                                                   HPCL3870
      AUX(N+5,I)=DERY(I)                                                HPCL3880
  328 Y(I)=AUX(N-4,I)                                                   HPCL3890
      X=X-(H+H)                                                         HPCL3900
      ISW2=11                                                           HPCL3910
      GOTO 1                                                            HPCL3920
  329 X=DELT                                                            HPCL3930
      DO 330 I=1,NDIM                                                   HPCL3940
      DELT=AUX(N+5,I)+AUX(N+4,I)                                        HPCL3950
      DELT=DELT+DELT+DELT                                               HPCL3960
     OAUX(16,I)=8.962963*(AUX(N-1,I)-Y(I))-3.361111*H*(AUX(N+6,I)+DELT  HPCL3970
     1+DERY(I))                                                         HPCL3980
  330 AUX(N+3,I)=DERY(I)                                                HPCL3990
      GOTO 306                                                          HPCL4000
      END                                                               HPCL4010
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C                                                                       DHCL  10
C     ..................................................................DHCL  20
C                                                                       DHCL  30
C        SUBROUTINE DHPCL                                               DHCL  40
C                                                                       DHCL  50
C        PURPOSE                                                        DHCL  60
C           TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY LINEAR            DHCL  70
C           DIFFERENTIAL EQUATIONS WITH GIVEN INITIAL VALUES.           DHCL  80
C                                                                       DHCL  90
C        USAGE                                                          DHCL 100
C           CALL DHPCL (PRMT,Y,DERY,NDIM,IHLF,AFCT,FCT,OUTP,AUX,A)      DHCL 110
C           PARAMETERS AFCT,FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT. DHCL 120
C                                                                       DHCL 130
C        DESCRIPTION OF PARAMETERS                                      DHCL 140
C           PRMT   - DOUBLE PRECISION INPUT AND OUTPUT VECTOR WITH      DHCL 150
C                    DIMENSION GREATER THAN OR EQUAL TO 5, WHICH        DHCL 160
C                    SPECIFIES THE PARAMETERS OF THE INTERVAL AND OF    DHCL 170
C                    ACCURACY AND WHICH SERVES FOR COMMUNICATION BETWEENDHCL 180
C                    OUTPUT SUBROUTINE (FURNISHED BY THE USER) AND      DHCL 190
C                    SUBROUTINE DHPCL. EXCEPT PRMT(5) THE COMPONENTS    DHCL 200
C                    ARE NOT DESTROYED BY SUBROUTINE DHPCL AND THEY ARE DHCL 210
C           PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT),               DHCL 220
C           PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT),               DHCL 230
C           PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE      DHCL 240
C                    (INPUT),                                           DHCL 250
C           PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS    DHCL 260
C                    GREATER THAN PRMT(4), INCREMENT GETS HALVED.       DHCL 270
C                    IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE     DHCL 280
C                    ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.DHCL 290
C                    THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS        DHCL 300
C                    OUTPUT SUBROUTINE.                                 DHCL 310
C           PRMT(5)- NO INPUT PARAMETER. SUBROUTINE DHPCL INITIALIZES   DHCL 320
C                    PRMT(5)=0. IF THE USER WANTS TO TERMINATE          DHCL 330
C                    SUBROUTINE DHPCL AT ANY OUTPUT POINT, HE HAS TO    DHCL 340
C                    CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE  DHCL 350
C                    OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE        DHCL 360
C                    FEASIBLE IF ITS DIMENSION IS DEFINED GREATER       DHCL 370
C                    THAN 5. HOWEVER SUBROUTINE DHPCL DOES NOT REQUIRE  DHCL 380
C                    AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL   DHCL 390
C                    FOR HANDING RESULT VALUES TO THE MAIN PROGRAM      DHCL 400
C                    (CALLING DHPCL) WHICH ARE OBTAINED BY SPECIAL      DHCL 410
C                    MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP. DHCL 420
C           Y      - DOUBLE PRECISION INPUT VECTOR OF INITIAL VALUES    DHCL 430
C                    (DESTROYED). LATERON Y IS THE RESULTING VECTOR OF  DHCL 440
C                    DEPENDENT VARIABLES COMPUTED AT INTERMEDIATE       DHCL 450
C                    POINTS X.                                          DHCL 460
C           DERY   - DOUBLE PRECISION INPUT VECTOR OF ERROR WEIGHTS     DHCL 470
C                    (DESTROYED). THE SUM OF ITS COMPONENTS MUST BE     DHCL 480
C                    EQUAL TO 1. LATERON DERY IS THE VECTOR OF          DHCL 490
C                    DERIVATIVES, WHICH BELONG TO FUNCTION VALUES Y AT  DHCL 500
C                    INTERMEDIATE POINTS X.                             DHCL 510
C           NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF      DHCL 520
C                    EQUATIONS IN THE SYSTEM.                           DHCL 530
C           IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF     DHCL 540
C                    BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS   DHCL 550
C                    GREATER THAN 10, SUBROUTINE DHPCL RETURNS WITH     DHCL 560
C                    ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.           DHCL 570
C                    ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE   DHCL 580
C                    PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-DHCL 590
C                    PRMT(1)) RESPECTIVELY.                             DHCL 600
C           AFCT   - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        DHCL 610
C                    COMPUTES MATRIX A (FACTOR OF VECTOR Y ON THE       DHCL 620
C                    RIGHT HAND SIDE OF THE SYSTEM) FOR A GIVEN X-VALUE.DHCL 630
C                    ITS PARAMETER LIST MUST BE X,A. THE SUBROUTINE     DHCL 640
C                    SHOULD NOT DESTROY X.                              DHCL 650
C           FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        DHCL 660
C                    COMPUTES VECTOR F (INHOMOGENEOUS PART OF THE       DHCL 670
C                    RIGHT HAND SIDE OF THE SYSTEM) FOR A GIVEN X-VALUE.DHCL 680
C                    ITS PARAMETER LIST MUST BE X,F. THE SUBROUTINE     DHCL 690
C                    SHOULD NOT DESTROY X.                              DHCL 700
C           OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.    DHCL 710
C                    ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.DHCL 720
C                    NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,    DHCL 730
C                    PRMT(6),PRMT(5),...) SHOULD BE CHANGED BY          DHCL 740
C                    SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,DHCL 750
C                    SUBROUTINE DHPCL IS TERMINATED.                    DHCL 760
C           AUX    - DOUBLE PRECISION AUXILIARY STORAGE ARRAY WITH 16   DHCL 770
C                    ROWS AND NDIM COLUMNS.                             DHCL 780
C           A      - DOUBLE PRECISION NDIM BY NDIM MATRIX, WHICH IS USEDDHCL 790
C                    AS AUXILIARY STORAGE ARRAY.                        DHCL 800
C                                                                       DHCL 810
C        REMARKS                                                        DHCL 820
C           THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF DHCL 830
C           (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE    DHCL 840
C               NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE   DHCL 850
C               IHLF=11),                                               DHCL 860
C           (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN       DHCL 870
C               (ERROR MESSAGES IHLF=12 OR IHLF=13),                    DHCL 880
C           (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,       DHCL 890
C           (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.        DHCL 900
C                                                                       DHCL 910
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DHCL 920
C           THE EXTERNAL SUBROUTINES AFCT(X,A), FCT(X,F) AND            DHCL 930
C           OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.DHCL 940
C                                                                       DHCL 950
C        METHOD                                                         DHCL 960
C           EVALUATION IS DONE BY MEANS OF HAMMINGS MODIFIED PREDICTOR- DHCL 970
C           CORRECTOR METHOD. IT IS A FOURTH ORDER METHOD, USING 4      DHCL 980
C           PRECEEDING POINTS FOR COMPUTATION OF A NEW VECTOR Y OF THE  DHCL 990
C           DEPENDENT VARIABLES.                                        DHCL1000
C           FOURTH ORDER RUNGE-KUTTA METHOD SUGGESTED BY RALSTON IS     DHCL1010
C           USED FOR ADJUSTMENT OF THE INITIAL INCREMENT AND FOR        DHCL1020
C           COMPUTATION OF STARTING VALUES.                             DHCL1030
C           SUBROUTINE DHPCL AUTOMATICALLY ADJUSTS THE INCREMENT DURING DHCL1040
C           THE WHOLE COMPUTATION BY HALVING OR DOUBLING.               DHCL1050
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C           TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE     DHCL1060
C           MUST BE CODED BY THE USER.                                  DHCL1070
C           FOR REFERENCE, SEE                                          DHCL1080
C           (1)  RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL         DHCL1090
C                COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.    DHCL1100
C           (2)  RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS,DHCL1110
C                MTAC, VOL.16, ISS.80 (1962), PP.431-437.               DHCL1120
C                                                                       DHCL1130
C     ..................................................................DHCL1140
C                                                                       DHCL1150
      SUBROUTINE DHPCL(PRMT,Y,DERY,NDIM,IHLF,AFCT,FCT,OUTP,AUX,A)       DHCL1160
C                                                                       DHCL1170
C                                                                       DHCL1180
C     THE FOLLOWING FIRST PART OF SUBROUTINE DHPCL (UNTIL FIRST BREAK-  DHCL1190
C     POINT FOR LINKAGE) HAS TO STAY IN CORE DURING THE WHOLE           DHCL1200
C     COMPUTATION                                                       DHCL1210
C                                                                       DHCL1220
      DIMENSION PRMT(1),Y(1),DERY(1),AUX(16,1),A(1)                     DHCL1230
      DOUBLE PRECISION PRMT,Y,DERY,AUX,X,H,Z,DELT,A,HS                  DHCL1240
      GOTO 100                                                          DHCL1250
C                                                                       DHCL1260
C     THIS PART OF SUBROUTINE DHPCL COMPUTES THE RIGHT HAND SIDE DERY OFDHCL1270
C     THE GIVEN SYSTEM OF LINEAR DIFFERENTIAL EQUATIONS.                DHCL1280
    1 CALL AFCT(X,A)                                                    DHCL1290
      CALL FCT(X,DERY)                                                  DHCL1300
      DO 3 M=1,NDIM                                                     DHCL1310
      LL=M-NDIM                                                         DHCL1320
      HS=0.D0                                                           DHCL1330
      DO 2 L=1,NDIM                                                     DHCL1340
      LL=LL+NDIM                                                        DHCL1350
    2 HS=HS+A(LL)*Y(L)                                                  DHCL1360
    3 DERY(M)=HS+DERY(M)                                                DHCL1370
      GOTO(105,202,204,206,115,122,125,308,312,327,329,128),ISW2        DHCL1380
C                                                                       DHCL1390
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  DHCL1400
C                                                                       DHCL1410
  100 N=1                                                               DHCL1420
      IHLF=0                                                            DHCL1430
      X=PRMT(1)                                                         DHCL1440
      H=PRMT(3)                                                         DHCL1450
      PRMT(5)=0.D0                                                      DHCL1460
      DO 101 I=1,NDIM                                                   DHCL1470
      AUX(16,I)=0.D0                                                    DHCL1480
      AUX(15,I)=DERY(I)                                                 DHCL1490
  101 AUX(1,I)=Y(I)                                                     DHCL1500
      IF(H*(PRMT(2)-X))103,102,104                                      DHCL1510
C                                                                       DHCL1520
C     ERROR RETURNS                                                     DHCL1530
  102 IHLF=12                                                           DHCL1540
      GOTO 104                                                          DHCL1550
  103 IHLF=13                                                           DHCL1560
C                                                                       DHCL1570
C     COMPUTATION OF DERY FOR STARTING VALUES                           DHCL1580
  104 ISW2=1                                                            DHCL1590
      GOTO 1                                                            DHCL1600
C                                                                       DHCL1610
C     RECORDING OF STARTING VALUES                                      DHCL1620
  105 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                DHCL1630
      IF(PRMT(5))107,106,107                                            DHCL1640
  106 IF(IHLF)108,108,107                                               DHCL1650
  107 RETURN                                                            DHCL1660
  108 DO 109 I=1,NDIM                                                   DHCL1670
C                                                                       DHCL1680
  109 AUX(8,I)=DERY(I)                                                  DHCL1690
C     COMPUTATION OF AUX(2,I)                                           DHCL1700
      ISW1=1                                                            DHCL1710
      GOTO 200                                                          DHCL1720
  110 X=X+H                                                             DHCL1730
      DO 111 I=1,NDIM                                                   DHCL1740
  111 AUX(2,I)=Y(I)                                                     DHCL1750
C                                                                       DHCL1760
C     INCREMENT H IS TESTED BY MEANS OF BISECTION                       DHCL1770
  112 IHLF=IHLF+1                                                       DHCL1780
      X=X-H                                                             DHCL1790
      DO 113 I=1,NDIM                                                   DHCL1800
  113 AUX(4,I)=AUX(2,I)                                                 DHCL1810
      H=.5D0*H                                                          DHCL1820
      N=1                                                               DHCL1830
      ISW1=2                                                            DHCL1840
      GOTO 200                                                          DHCL1850
C                                                                       DHCL1860
  114 X=X+H                                                             DHCL1870
      ISW2=5                                                            DHCL1880
      GOTO 1                                                            DHCL1890
  115 N=2                                                               DHCL1900
      DO 116 I=1,NDIM                                                   DHCL1910
      AUX(2,I)=Y(I)                                                     DHCL1920
  116 AUX(9,I)=DERY(I)                                                  DHCL1930
      ISW1=3                                                            DHCL1940
      GOTO 200                                                          DHCL1950
C                                                                       DHCL1960
C     COMPUTATION OF TEST VALUE DELT                                    DHCL1970
  117 DELT=0.D0                                                         DHCL1980
      DO 118 I=1,NDIM                                                   DHCL1990
  118 DELT=DELT+AUX(15,I)*DABS(Y(I)-AUX(4,I))                           DHCL2000
      DELT=.06666666666666667D0*DELT                                    DHCL2010
      IF(DELT-PRMT(4))121,121,119                                       DHCL2020
  119 IF(IHLF-10)112,120,120                                            DHCL2030
C                                                                       DHCL2040
C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.      DHCL2050
  120 IHLF=11                                                           DHCL2060
      X=X+H                                                             DHCL2070
      GOTO 104                                                          DHCL2080
C                                                                       DHCL2090
C     SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS               DHCL2100
  121 X=X+H                                                             DHCL2110
      ISW2=6                                                            DHCL2120
      GOTO 1                                                            DHCL2130
  122 DO 123 I=1,NDIM                                                   DHCL2140
      AUX(3,I)=Y(I)                                                     DHCL2150
  123 AUX(10,I)=DERY(I)                                                 DHCL2160
      N=3                                                               DHCL2170
      ISW1=4                                                            DHCL2180
      GOTO 200                                                          DHCL2190
C                                                                       DHCL2200
  124 N=1                                                               DHCL2210
      X=X+H                                                             DHCL2220
      ISW2=7                                                            DHCL2230
      GOTO 1                                                            DHCL2240
  125 X=PRMT(1)                                                         DHCL2250
      DO 126 I=1,NDIM                                                   DHCL2260
      AUX(11,I)=DERY(I)                                                 DHCL2270
1260Y(I)=AUX(1,I)+H*(.375D0*AUX(8,I)+.7916666666666667D0*AUX(9,I)     DHCL2280
     1-.2083333333333333D0*AUX(10,I)+.04166666666666667D0*DERY(I))      DHCL2290
  127 X=X+H                                                             DHCL2300
      N=N+1                                                             DHCL2310
      ISW2=12                                                           DHCL2320
      GOTO 1                                                            DHCL2330
  128 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                DHCL2340
      IF(PRMT(5))107,129,107                                            DHCL2350
  129 IF(N-4)130,300,300                                                DHCL2360
  130 DO 131 I=1,NDIM                                                   DHCL2370
      AUX(N,I)=Y(I)                                                     DHCL2380
  131 AUX(N+7,I)=DERY(I)                                                DHCL2390
      IF(N-3)132,134,300                                                DHCL2400
C                                                                       DHCL2410
  132 DO 133 I=1,NDIM                                                   DHCL2420
      DELT=AUX(9,I)+AUX(9,I)                                            DHCL2430
      DELT=DELT+DELT                                                    DHCL2440
  133 Y(I)=AUX(1,I)+.3333333333333333D0*H*(AUX(8,I)+DELT+AUX(10,I))     DHCL2450
      GOTO 127                                                          DHCL2460
C                                                                       DHCL2470
  134 DO 135 I=1,NDIM                                                   DHCL2480
      DELT=AUX(9,I)+AUX(10,I)                                           DHCL2490
      DELT=DELT+DELT+DELT                                               DHCL2500
  135 Y(I)=AUX(1,I)+.375D0*H*(AUX(8,I)+DELT+AUX(11,I))                  DHCL2510
      GOTO 127                                                          DHCL2520
C                                                                       DHCL2530
C     THE FOLLOWING PART OF SUBROUTINE DHPCL COMPUTES BY MEANS OF       DHCL2540
C     RUNGE-KUTTA METHOD STARTING VALUES FOR THE NOT SELF-STARTING      DHCL2550
C     PREDICTOR-CORRECTOR METHOD.                                       DHCL2560
  200 Z=X                                                               DHCL2570
      DO 201 I=1,NDIM                                                   DHCL2580
      X=H*AUX(N+7,I)                                                    DHCL2590
      AUX(5,I)=X                                                        DHCL2600
  201 Y(I)=AUX(N,I)+.4D0*X                                              DHCL2610
C     X IS AN AUXILIARY STORAGE LOCATION                                DHCL2620
C                                                                       DHCL2630
      X=Z+.4D0*H                                                        DHCL2640
      ISW2=2                                                            DHCL2650
      GOTO 1                                                            DHCL2660
  202 DO 203 I=1,NDIM                                                   DHCL2670
      X=H*DERY(I)                                                       DHCL2680
      AUX(6,I)=X                                                        DHCL2690
  203 Y(I)=AUX(N,I)+.2969776092477536OD0*AUX(5,I)+.1587596449710358300D0*XDHCL2700
C                                                                       DHCL2710
      X=Z+.45573725421878943OD0*H                                       DHCL2720
      ISW2=3                                                            DHCL2730
      GOTO 1                                                            DHCL2740
  204 DO 205 I=1,NDIM                                                   DHCL2750
      X=H*DERY(I)                                                       DHCL2760
      AUX(7,I)=X                                                        DHCL2770
  205 Y(I)=AUX(N,I)+.2181003882259204700D0*AUX(5,I)-3.050965148692930800D0* DHCL2780
     1AUX(6,I)+3.832864760467010300D0*X                                 DHCL2790
C                                                                       DHCL2800
      X=Z+H                                                             DHCL2810
      ISW2=4                                                            DHCL2820
      GOTO 1                                                            DHCL2830
  206 DO 207 I=1,NDIM                                                   DHCL2840
  207Y(I)=AUX(N,I)+.1747602822626903700*AUX(5,I)-.5514806628787329400* DHCL2850
     1AUX(6,I)+1.205535599396523500*AUX(7,I)+.1711847812195190300*      DHCL2860
     2H*DERY(I)                                                         DHCL2870
      X=Z                                                               DHCL2880
      GOTO(110,114,117,124),ISW1                                        DHCL2890
C                                                                       DHCL2900
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  DHCL2910
C                                                                       DHCL2920
C     STARTING VALUES ARE COMPUTED.                                     DHCL2930
C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.           DHCL2940
  300 ISTEP=3                                                           DHCL2950
  301 IF(N-8)304,302,304                                                DHCL2960
C                                                                       DHCL2970
C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS      DHCL2980
  302 DO 303 N=2,7                                                      DHCL2990
      DO 303 I=1,NDIM                                                   DHCL3000
      AUX(N-1,I)=AUX(N,I)                                               DHCL3010
  303 AUX(N+6,I)=AUX(N+7,I)                                             DHCL3020
      N=7                                                               DHCL3030
C                                                                       DHCL3040
C     N LESS THAN 8 CAUSES N+1 TO GET N                                 DHCL3050
  304 N=N+1                                                             DHCL3060
C                                                                       DHCL3070
C     COMPUTATION OF NEXT VECTOR Y                                      DHCL3080
      DO 305 I=1,NDIM                                                   DHCL3090
      AUX(N-1,I)=Y(I)                                                   DHCL3100
  305 AUX(N+6,I)=DERY(I)                                                DHCL3110
      X=X+H                                                             DHCL3120
  306 ISTEP=ISTEP+1                                                     DHCL3130
      DO 307 I=1,NDIM                                                   DHCL3140
      ODELT=AUX(N-4,I)+1.333333333333333D0*H*(AUX(N+6,I)+AUX(N+6,I)-    DHCL3150
     1AUX(N+5,I)+AUX(N+4,I)+AUX(N+4,I))                                 DHCL3160
      Y(I)=DELT-.9256198347107438D0*AUX(16,I)                           DHCL3170
  307 AUX(16,I)=DELT                                                    DHCL3180
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR   DHCL3190
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.               DHCL3200
      ISW2=8                                                            DHCL3210
      GOTO 1                                                            DHCL3220
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY             DHCL3230
C                                                                       DHCL3240
  308 DO 309 I=1,NDIM                                                   DHCL3250
     0DELT=.125D0*(9.D0*AUX(N-1,I)-AUX(N-3,I)+3.D0*H*(DERY(I)+AUX(N+6,I))DHCL3260
     1+AUX(N+6,I)-AUX(N+5,I)))                                          DHCL3270
      AUX(16,I)=AUX(16,I)-DELT                                          DHCL3280
  309 Y(I)=DELT+.9743801652892562D0*AUX(16,I)                           DHCL3290
C                                                                       DHCL3300
C     TEST WHETHER H MUST BE HALVED OR DOUBLED                          DHCL3310
      DELT=0.D0                                                         DHCL3320
      DO 310 I=1,NDIM                                                   DHCL3330
  310 DELT=DELT+AUX(15,I)*DABS(AUX(16,I))                               DHCL3340
      IF(DELT-PRMT(4))311,324,324                                       DHCL3350
C                                                                       DHCL3360
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                   DHCL3370
  311 ISW2=9                                                            DHCL3380
      GOTO 1                                                            DHCL3390
  312 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                DHCL3400
      IF(PRMT(5))314,313,314                                            DHCL3410
  313 IF(IHLF-11)315,314,314                                            DHCL3420
  314 RETURN                                                            DHCL3430
  315 IF(H*(X-PRMT(2)))316,314,314                                      DHCL3440
  316 IF(DABS(X-PRMT(2))-.1D0*DABS(H))314,317,317                       DHCL3450
  317 IF(DELT-.02D0*PRMT(4))318,318,301                                 DHCL3460
C                                                                       DHCL3470
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE         DHCL3480
C     AVAILABLE                                                         DHCL3490
  318 IF(IHLF)301,301,319                                               DHCL3500
  319 IF(N-7)301,320,320                                                DHCL3510
  320 IF(ISTEP-4)301,321,321                                            DHCL3520
  321 IMOD=ISTEP/2                                                      DHCL3530
      IF(ISTEP-IMOD-IMOD)301,322,301                                    DHCL3540
  322 H=H+H                                                             DHCL3550
      IHLF=IHLF-1                                                       DHCL3560
      ISTEP=0                                                           DHCL3570
      DO 323 I=1,NDIM                                                   DHCL3580
      AUX(N-1,I)=AUX(N-2,I)                                             DHCL3590
      AUX(N-2,I)=AUX(N-4,I)                                             DHCL3600
      AUX(N-3,I)=AUX(N-6,I)                                             DHCL3610
      AUX(N+6,I)=AUX(N+5,I)                                             DHCL3620
      AUX(N+5,I)=AUX(N+3,I)                                             DHCL3630
```

```
      AUX(N+4,I)=AUX(N+1,I)                                          DHCL3640
      DELT=AUX(N+6,I)+AUX(N+5,I)                                     DHCL3650
      DELT=DELT+DELT+DELT                                            DHCL3660
 3230AUX(16,I)=8.9629629629629630D0*(Y(I)-AUX(N-3,I))                DHCL3670
     1-3.3611111111111111100*H*(DERY(I)+DELT+AUX(N+4,I))             DHCL3680
      GOTO 301                                                       DHCL3690
C     .                                                             DHCL3700
C     H MUST BE HALVED                                              DHCL3710
  324 IHLF=IHLF+1                                                    DHCL3720
      IF(IHLF-10)325,325,311                                         DHCL3730
  325 H=.500*H                                                       DHCL3740
      ISTEP=0                                                        DHCL3750
      DO 326 I=1,NDIM                                                DHCL3760
     0Y(I)=-.3906250-2*(8.01*AUX(N-1,I)+135.00*AUX(N-2,I)+4.01*AUX(N-3,I) DHCL3770
     1+AUX(N-4,I))-.1171875D0*(AUX(N+6,I)-6.00*AUX(N+5,I)-AUX(N+4,I))*H DHCL3780
     0AUX(N-4,I)=.3906250-2*(12.00*AUX(N-1,I)+135.00*AUX(N-2,I)+      DHCL3790
     1108.00*AUX(N-3,I)+AUX(N-4,I))-.0234375D0*(AUX(N+6,I)+           DHCL3800
     218.00*AUX(N+5,I)-9.00*AUX(N+4,I))*H                            DHCL3810
      AUX(N-3,I)=AUX(N-2,I)                                          DHCL3820
  326 AUX(N+4,I)=AUX(N+5,I)                                          DHCL3830
      DELT=X-H                                                       DHCL3840
      X=DELT-(H+H)                                                   DHCL3850
      ISW2=10                                                        DHCL3860
      GOTO 1                                                         DHCL3870
  327 DO 328 I=1,NDIM                                                DHCL3880
      AUX(N-2,I)=Y(I)                                                DHCL3890
      AUX(N+5,I)=DERY(I)                                             DHCL3900
  328 Y(I)=AUX(N-4,I)                                                DHCL3910
      X=X-(H+H)                                                      DHCL3920
      ISW2=11                                                        DHCL3930
      GOTO 1                                                         DHCL3940
  329 X=DELT                                                         DHCL3950
      DO 330 I=1,NDIM                                                DHCL3960
      DELT=AUX(N+5,I)+AUX(N+4,I)                                     DHCL3970
      DELT=DELT+DELT+DELT                                            DHCL3980
     0AUX(16,I)=8.9629629629629630D0*(AUX(N-1,I)-Y(I))               DHCL3990
     1-3.3611111111111111100*H*(AUX(N+6,I)+DELT+DERY(I))             DHCL4000
  330 AUX(N+3,I)=DERY(I)                                             DHCL4010
      GOTO 306                                                       DHCL4020
      END                                                            DHCL4030
```

Subroutines LBVP and DLBVP

These subroutines generate an approximate solution of a given linear boundary-value problem consisting of a system of linear first-order ordinary differential equations with linear boundary conditions. Solution is done by the method of adjoint equations, which generates successively adjoint initial-value problems. By means of the solutions of these adjoint initial-value problems (done by Hamming's modified predictor-corrector method) it is possible to generate missing boundary conditions, which are necessary to compute initial values suitable to the given boundary-value problem (done by subroutine GELG or DGELG: solution of simultaneous linear equations by means of Gauss elimination). Thus the boundary-value problem is reduced to a linear initial-value problem, which is finally solved by Hamming's modified predictor-corrector method also.

Given the system of n linear first-order ordinary differential equations:

$$\left.\begin{aligned}
y'_1 \equiv \frac{dy_1}{dx} &= a_{11}(x)y_1 + a_{12}(x)y_2 + \cdots \\
&\quad + a_{1n}(x)y_n + f_1(x) \\
y'_2 \equiv \frac{dy_2}{dx} &= a_{21}(x)y_1 + a_{22}(x)y_2 + \cdots \\
&\quad + a_{2n}(x)y_n + f_2(x) \\
&\cdots\cdots \\
y'_n \equiv \frac{dy_n}{dx} &= a_{n1}(x)y_1 + a_{n2}(x)y_2 + \cdots \\
&\quad + a_{nn}(x)y_n + f_n(x)
\end{aligned}\right\}$$

together with n boundary conditions:

$$\left.\begin{aligned}
&b_{11}y_1(x_l)+b_{12}y_2(x_l)+\cdots+b_{1n}y_n(x_l)+c_{11}y_1(x_u) \\
&+c_{12}y_2(x_u)+\cdots+c_{1n}y_n(x_u) = r_1 \\
&b_{21}y_1(x_l)+b_{22}y_2(x_l)+\cdots+b_{2n}y_n(x_l)+c_{21}y_1(x_u) \\
&\quad +c_{22}y_2(x_u)+\cdots+c_{2n}y_n(x_u) = r_2 \\
&\cdots\cdots \\
&b_{n1}y_1(x_l)+b_{n2}y_2(x_l)+\cdots+b_{nn}y_n(x_l)+c_{n1}y_1(x_u) \\
&\quad +c_{n2}y_2(x_u)+\cdots+c_{nn}y_n(x_u) = r_n
\end{aligned}\right\}$$

where x_l and x_u are the lower and upper bound respectively of the integration interval, and using the following vector and matrix notations:

$$Y(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_n(x) \end{pmatrix}, \quad F(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_n(x) \end{pmatrix},$$

$$Y_l = \begin{pmatrix} y_1(x_l) \\ y_2(x_l) \\ \vdots \\ y_n(x_l) \end{pmatrix}, \quad Y_u = \begin{pmatrix} y_1(x_u) \\ y_2(x_u) \\ \vdots \\ y_n(x_u) \end{pmatrix},$$

$$R = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix},$$

$$A(x) = \begin{pmatrix} a_{11}(x)a_{12}(x)\ldots a_{1n}(x) \\ a_{21}(x)a_{22}(x)\ldots a_{2n}(x) \\ \ldots \\ a_{n1}(x)a_{n2}(x)\ldots a_{nn}(x) \end{pmatrix}$$

$$B = \begin{pmatrix} b_{11}b_{12}\ldots b_{1n} \\ b_{21}b_{22}\ldots b_{2n} \\ \ldots \\ b_{n1}b_{n2}\ldots b_{nn} \end{pmatrix} \quad \text{and}$$

$$C = \begin{pmatrix} c_{11}c_{12}\ldots c_{1n} \\ c_{21}c_{22}\ldots c_{2n} \\ \ldots \\ c_{n1}c_{n2}\ldots c_{nn} \end{pmatrix}$$

where Y(x), F(x), Y_l, Y_u and R are column vectors with n components, and A(x), and B and C are n by n square matrices, the given problem appears as follows:

$$Y' \equiv \frac{dY}{dx} = A(x) * Y + F(x) \tag{1}$$

with

$$B * Y_l + C * Y_u = R \tag{2}$$

The first problem is to generate new boundary conditions. Assuming that B has fewer zero-columns than C†, the procedure eliminates Y_u from the boundary conditions and generates a system of simultaneous linear equations for the unknown initial values $y_1(x_l)$, $y_2(x_l)$, ..., $y_n(x_l)$. This is done in the following way.

Assuming that the k^{th} column of matrix C (k = 1, 2, ..., n) contains at least one nonzero element (that is, $y_k(x_u)$ appears in the boundary conditions), the following adjoint linear initial-value problem is generated and solved by Hamming's modified predictor-corrector method:

$$\left.\begin{aligned} z'_1(x) &\equiv \frac{dz_1}{dx} = -a_{11}(x)z_1 - a_{21}(x)z_2 - \ldots \\ &\quad - a_{n1}(x)z_n \\ z'_2(x) &\equiv \frac{dz_2}{dx} = -a_{12}(x)z_1 - a_{22}(x)z_2 - \ldots \\ &\quad - a_{n2}(x)z_n \\ &\ldots \\ z'_n(x) &\equiv \frac{dz_n}{dx} = -a_{1n}(x)z_1 - a_{2n}(x)z_2 - \ldots \\ &\quad - a_{nn}(x)z_n \end{aligned}\right\}$$

with initial values:

$$z_1(x_u) = 0, \; z_2(x_u) = 0, \ldots, z_{k-1}(x_u) = 0, \; z_k(x_u) = 1, \; z_{k+1}(x_u) = 0, \ldots, z_n(x_u)$$

or in vector and matrix notations††:

$$Z' \equiv \frac{dZ}{dx} = -A^T(x) * Z \tag{3}$$

with initial values $Z(x_u) = E_k$ (4)

† If this is not the case, the procedure interchanges x_l with x_u and B with C, in order to get a minimum number of adjoint initial-value problems.

†† As vectors Z and Z' are actually stored in the same storage arrays as Y and Y', in the flowchart and the FORTRAN program they are also named Y and DERY.

where $A^T(x)$ is the transpose of $A(x)$, and E_k is the column vector with only one nonzero element; that is, 1 as k^{th} element.

Assuming that $Z_k(x)$ is the solution of this k^{th} adjoint initial-value problem, and using equations (1) and (3), then:

$$\frac{d}{dx}\left[\sum_{i=1}^{n} z_i^{(k)}(x) \cdot y_i(x)\right] = \frac{d}{dx}\left[Z_k^T(x) * Y(x)\right]$$

$$= Z_k^T(x) * Y'(x) + Z'^T(x) * Y(x)$$

$$= Z_k^T * (A * Y + F) + (-A^T * Z_k)^T * Y$$

$$= Z_k^T * A * Y + Z_k^T * F - Z_k^T * A * Y$$

$$= Z_k^T * F$$

from which it follows that:

$$\frac{d}{dx}\left[\sum_{i=1}^{n} z_i^{(k)}(x) \cdot y_i(x)\right] = \left[\sum_{i=1}^{n} z_i^{(k)}(x) \cdot f_i(x)\right]$$

Integrating this equation from x_l up to x_u the result is:

$$\sum_{i=1}^{n} z_i^{(k)}(x_u) \cdot y_i(x_u) - \sum_{i=1}^{n} z_i^{(k)}(x_l)\, y_i(x_l)$$

$$= \int_{x_l}^{x_u} \left[\sum_{i=1}^{n} z_i^{(k)}(x) \cdot f_i(x)\right] dx$$

or:

$$y_k(x_u) = \sum_{i=1}^{n} z_i^{(k)}(x_l) \cdot y_i(x_l) - sum_k(x_l) \qquad (5)$$

with:

$$sum_k(x_l) = \int_{x_u}^{x_l} \left[\sum_{i=1}^{n} z_i^{(k)}(x) \cdot f_i(x)\right] dx \qquad (6)$$

Elimination of $y_k(x_u)$ in the boundary conditions can be done by the following transformation formulas, which transform matrix B_{k-1} and column vector R_{k-1} into matrix B_k and column vector R_k (with $B_0 = B$ and $R_0 = R$) on the storage locations of B and R:

$$\left.\begin{aligned} b_{ij}^{(k)} &= b_{ij}^{(k-1)} + c_{ik} \cdot z_j^{(k)}(x_l) \quad (j = 1, 2, \ldots, n) \qquad (7) \\ r_i^{(k)} &= r_i^{(k-1)} + c_{ik} \cdot sum_k(x_l) \qquad (8) \end{aligned}\right\} (i = 1, 2, \ldots, n)$$

If the k^{th} column of matrix C contains only zero-elements (that is, $y_k(x_u)$ does not appear in the boundary conditions), elimination of $y_k(x_u)$ is not necessary, and k can at once be increased by one.

If at least all $y_k(x_u)$ ($k = 1, 2, \ldots, n$) in the boundary conditions are eliminated, the remaining system of simultaneous linear equations

$$B_n * Y_l = R_n \qquad (9)$$

is solved by Gauss elimination (subroutine GELG or DGELG). However, this is only possible if matrix B_n is not singular. In case of a singular matrix B_n (that is, the pivot element at any elimination step is exactly equal to zero), the procedure is bypassed, giving an error message which shows that the given boundary-value problem has no or more than one solution, or that the method of adjoint equations was not able to find a solution because one or more of the generated new boundary conditions were linear combinations of the given boundary conditions.

There is another critical case in the solution of equation (9), indicated by a warning given by subroutine GELG or DGELG which means possible loss of significance in the Gauss elimination of at least as many significant digits as specified by the upper bound ε of the local truncation error in the integration procedures. If this warning appears, it is highly probable that matrix B_n is singular too. But as this may not necessarily be the case, the procedure goes on after having given a warning to the user's output subroutine in the form of a negative number of bisections of the initial step size together with the resulting initial values of the finally generated initial-value problem (first set of output values). The absolute value of this "warning parameter" indicates the step of the Gauss algorithm immediately preceding the detection of the loss of significance.

After the vector of initial values Y_l is computed (that is after the boundary-value problem is reduced to an initial-value problem), the final step to solve the generated initial-value problem is done by

Hamming's modified predictor-corrector method, incorporated in subroutines LBVP and DLBVP.

Both the solution of adjoint linear initial-value problems described above and the solution of the finally generated linear initial-value problem equivalent to the given boundary-value problem are done by means of Hamming's modified predictor-corrector method for systems of linear differential equations. An extensive description of this method can be found in the mathematical description of subroutines HPCL and DHPCL (except that control of accuracy and adjustment of step size is done differently). Therefore it will be sufficient to give a short description of this method in the form of a notation of the formulas used.

1. Problem to be solved --
System of linear differential equations $Y' = L(x, Y)$ with initial values $Y(x_0) = Y_0$, $Y'(x_0) = L(x_0, Y_0) = Y'_0$
For adjoint initial-value problems, this is:

$$Y' \equiv L(x, Y) = -A^T(x) * Y$$

$$x_0 = x_u,\ Y(x_0) = E_k,\ Y'(x_0) = -A^T(x_0) * E_k,\ h = \frac{1}{16}(x_1 - x_u)$$

and for the finally generated initial-value problem:

$$Y' = L(x, Y) = A(x) * Y + F(x)$$

$$x_0 = x_1,\ Y_0 = Y_1,\ Y'_0 = A(x_1) * Y_1 + F(x_1)$$

2. Hamming's modified predictor-corrector formulas -- (h represents the step size adjusted to accuracy requirements) for j = 3, 4, 5, ... (that means at points $x_j = x_3, x_4, x_5, \ldots$)

Predictor:
$$P_{j+1} = Y_{j-3} + \frac{4}{3}h\,(2\,Y'_j - Y'_{j-1} + 2\,Y'_{j-2}) \quad (10)$$

Modifier:
$$M_{j+1} = P_{j+1} - \frac{112}{121}(P_j - C_j) \quad (11)$$

$$M'_{j+1} = L(x_{j+1}, M_{j+1}) \quad (12)$$

Corrector:
$$C_{j+1} = \frac{1}{8}\left[9\,Y_j - Y_{j-2} + 3\,h \cdot (M'_{j+1} + 2Y'_j - Y'_{j-1})\right] \quad (13)$$

Final value:
$$Y_{j+1} = C_{j+1} + \frac{9}{121}(P_{j+1} - C_{j+1}) \quad (14)$$

3. Test value for control of accuracy and adjustment of step size h in predictor-corrector part ("local truncation error")†:

$$\delta = \max_i \frac{a_i \cdot |p_{j+1,\,i} - c_{j+1,\,i}|}{\max(1, |y_{j+1,\,i}|)} \quad (15)$$

with error weights $a_i = 1$ $(i=1,2,\ldots,n)$ for the adjoint initial-value problems, and given by input for the finally generated initial-value problem.
Adjustment of step size h: halving, if $\delta > \varepsilon$
doubling, if $\delta \leqq \varepsilon/50$
with the upper bound ε for the local truncation error given by input.

4. Formulas for interpolating intermediate points in case of halving the step size h:

$$Y_{j-1/2} \equiv Y(x_j - \frac{h}{2}) = \frac{1}{256}(80Y_j + 135Y_{j-1} + 40Y_{j-2} + Y_{j-3}) - \frac{h}{2} \cdot \frac{15}{128} \cdot (Y'_j - 6Y'_{j-1} - Y'_{j-2}) \quad (16)$$

$$Y_{j-3/2} \equiv Y(x_j - \frac{3h}{2}) = \frac{1}{256}(12Y_j + 135Y_{j-1} + 108Y_{j-2} + Y_{j-3}) - \frac{h}{2} \cdot \frac{3}{128} \cdot (Y'_j + 18Y'_{j-1} - 9Y'_{j-2}) \quad (17)$$

5. Changing vectors $P_j - C_j$ in case of halving, or $P_{j+1} - C_{j+1}$ in case of doubling the step size h:

$$P_j - C_j = \frac{242}{27}(Y_j - Y_{j-3/2}) - \frac{121}{36} \cdot \frac{h}{2}(Y'_j + 3Y'_{j-1/2} + 3Y'_{j-1} + Y'_{j-3/2}) \quad (18)$$

$$P_{j+1} - C_{j+1} = \frac{242}{27}(Y_{j+1} - Y_{j-5}) - \frac{121}{36} \cdot 2h\,(Y'_{j+1} + 3Y'_{j-1} + 3Y'_{j-3} + Y'_{j-5}) \quad (19)$$

† The terms from which δ is generated by searching for the maximum are weighted relative errors if the absolute values of $y_{j+1,i}(x)$ are greater than 1, and weighted absolute errors if the absolute values are not greater than 1.

6. Starting Hamming's modified predictor-corrector method by means of three Runge-Kutta steps:

For $j = 0, 1, 2$

$$K_1 = h \cdot Y'_j \tag{20}$$

$$K_2 = h \cdot L(x_j + 0.4h,\ Y_j + 0.4K_1) \tag{21}$$

$$K_3 = h \cdot L(x_j + 0.4557372542187894\,3\ h,\ Y_j + 0.29697760924775360\ K_1 + 0.15875964497103583\ K_2) \tag{22}$$

$$K_4 = h \cdot L(x_j + h,\ Y_j + 0.21810038822592047\ K_1 - 3.0509651486929308\ K_2 + 3.8328647604670103\ K_3) \tag{23}$$

$$Y_{j+1} = Y_j + 0.17476028226269037\ K_1 - 0.55148066287873294\ K_2 + 1.2055355993965235\ K_3 + 0.17118478121951903\ K_4 \tag{24}$$

7. Test value for control of accuracy and adjustment of step size h in the Runge-Kutta part ("local truncation error")†:

$$\delta = \frac{1}{15} \cdot \max_i \frac{a_i \left| y^{(1)}_{2,i} - y^{(2)}_{2,i} \right|}{\max\left(1, \left| y^{(2)}_{2,i} \right|\right)} \tag{25}$$

with error weights $a_i = 1$ ($i = 1, 2, \ldots, n$) for adjoint initial-value problems and given by input for the finally generated initial-value problem. Step size h is adjusted by halving if $\delta > \varepsilon$, with the upper bound ε of the local truncation error given by input.

† The terms from which δ is generated by searching for the maximum are weighted relative errors if the absolute values of $y^{(2)}_{2,i}$ are greater than 1, and weighted absolute errors if the absolute values are not greater than 1.

8. Iteration formulas for refinement of Runge-Kutta results:

$$Y_1 = Y_0 + \frac{h}{24}(9\,Y'_0 + 19\,Y'_1 - 5\,Y'_2 + Y'_3) \tag{26}$$

$$Y_2 = Y_0 + \frac{h}{3}(Y'_0 + 4\,Y'_1 + Y'_2) \tag{27}$$

$$Y_3 = Y_0 + \frac{3h}{8}(Y'_0 + 3Y'_1 + 3Y'_2 + Y'_3) \tag{28}$$

As transformation formulas (7) and (8) show, the output of Hamming's modified predictor-corrector method for the solution of any adjoint initial-value problem must contain only the vector $Z_k(x_1)$ of function values at the lower bound x_1 (actually stored in vector Y) and the integral value $sum_k(x_1)$. With respect to the predictor-corrector method, which is a fourth-order integration procedure generating function vectors $Z_k(x)$ (in storage array Y) and derivative vectors $Z'_k(x)$ (in storage array DERY) at intermediate (not necessarily equidistant) points x, the following fourth-order Hermitian integration formula -- using the function and the first derivative values of the function to be integrated -- is suitable to accumulate integral values $sum_k(x)$ and finally $sum_k(x_1)$:

$$sum_k(x+h) = sum_k(x) + \frac{h}{2}\left\{ g_k(x) + g_k(x+h) + \frac{h}{6}\left[g'_k(x) - g'_k(x+h) \right] \right\} \tag{29}$$

using the instantaneous step size h of the predictor-corrector method, and with:

$$g_k(x) = \sum_{i=1}^{n} z_i^{(k)}(x)\, f_i(x) = Z_k^T(x) + F(x) \tag{30}$$

and:

$$g'_k(x) = \sum_{i=1}^{n} \left[\frac{dz_i^{(k)}}{dx} \cdot f_i(x) + z_i^{(k)}(x) \cdot \frac{df_i}{dx} \right] = \frac{dZ_k^T}{dx} * F(x) + Z_k^T(x) * \frac{dF}{dx} \tag{31}$$

Therefore, generation of sum_k (x+h) is done by means of the following formulas:

$$g_u^{(k)} = g_k(x+h) = \sum_{i=1}^{n} z_i^{(k)}(x+h)\, f_i(x+h)$$

$$= Z_k^T(x+h) * F(x+h) \tag{32}$$

$$dg_u^{(k)} = g'_k(x+h) = \sum_{i=1}^{n} \left[z'^{(k)}_i(x+h)\, f_i(x+h) + z_i^{(k)}(x+h)\, f'_i(x+h) \right] = Z'^T_k(x+h) * F(x+h)$$

$$+ Z_k^T(x+h) * F'(x+h) \tag{33}$$

$$sum_k(x+h) = sum_k(x) + \frac{h}{2}\left[g_1^{(k)} + g_u^{(k)} + \frac{h}{6}(dg_1^{(k)} - dg_u^{(k)}) \right] \tag{34}$$

After these three formulas have been evaluated, $g_u^{(k)}$ becomes $g_1^{(k)}$, and $dg_u^{(k)}$ becomes $dg_1^{(k)}$. Initial values of $g_1^{(k)}$ and $dg_1^{(k)}$ are generated, using formulas (30) and (31) at point $x = x_u$, leading to:

$$g_1^{(k)} = g_k(x_u) = f_k(x_u) \tag{35}$$

and:

$$dg_1^{(k)} = g'_k(x_u) = f'_k(x_u) - \sum_{i=1}^{n} a_{ki}(x_u) \cdot f_i(x_u) \tag{36}$$

The entire input of subroutines LBVP and DLBVP is:

1. Lower and upper bound x_l and x_u of the integration interval, initial step size h of the independent variable and upper bound ε (≤ 1) of the local "relative" truncation error in integration procedures

2. Coefficient matrices B and C of vectors Y_l and Y_u in boundary conditions and right-hand side vector R

3. Vector of error weights a_i (i = 1, 2, ..., n) for the local "relative" truncation error in each component of the dependent variables ($a_i \leq 1$ for all i)

4. The number n of differential equations and boundary conditions

5. As external subroutine subprograms, the computation of the right-hand side matrix A(x) of the system of linear differential equations, and the computation of the inhomogeneous vector F(x) and of its derivative F'(x); for flexibility in output, an output subroutine

6. A one-dimensional auxiliary storage array with n storage locations, an n by n auxiliary storage array, and a two-dimensional auxiliary storage array (named AUX in flowchart, FORTRAN subroutine, and mathematical description) with 20 rows and n columns

Output is done in the following way. If a set of approximations to the dependent variables Y(x) is found to be of sufficient accuracy (that is $\delta \leq \varepsilon$), it is handed -- together with x, the vector of derivatives Y' (x), the number of bisections of the initial increment, the number of differential equations, the lower and upper bound of the integration interval, the initial step size, error bound ε, and a parameter for terminating subroutine LBVP or DLBVP -- to the output subroutine. By means of this output subroutine, the user has the opportunity to choose his own output format, to handle the output values as he wants, to change the upper error bound and to terminate subroutine LBVP or DLBVP at any output point (for example, in case of possible loss of accuracy in Gauss elimination). In particular, the user is able to drop the output of some intermediate points, printing only the result values at the special points $x_0 + j \cdot h$, where j = 0, 1, 2, ..., and h is the initial step size specified by input. The user may also perform intermediate computations using the integration results before continuing the process.

For better understanding of the flowchart and of the FORTRAN program, Figure 34 shows the allocation of special intermediate result vectors within the storage array AUX.

For reference see:

(1) G.N. Lance, Numerical Methods for High Speed Computers, Iliffe, London, 1960, pp. 64 - 67.

(2) A. Ralston/H.S. Wilf, Mathematical Methods for Digital Computers, Wiley, New York/London, 1960, pp. 95 - 109.

(3) A. Ralston, "Runge-Kutta Methods with Minimum Error Bounds", MTAC, vol. 16, no. 80 (1962), pp. 431 - 437.

(4) R. Zurmühl, Praktische Mathematik für Ingenieure und Physiker, Springer, Berlin/Göttingen/Heidelberg, 1963, pp. 227 - 232.

function vector $Y_{j-6} = Y(x_{j-6})$	1. row (AUX (1) in flowchart)
function vector $Y_{j-5} = Y(x_{j-5})$	2. row (AUX (2) in flowchart)
function vector $Y_{j-4} = Y(x_{j-4})$	3. row (AUX (3) in flowchart)
function vector $Y_{j-3} = Y(x_{j-3})$	4. row (AUX (4) in flowchart)
function vector $Y_{j-2} = Y(x_{j-2})$	5. row (AUX (5) in flowchart)
function vector $Y_{j-1} = Y(x_{j-1})$	6. row (AUX (6) in flowchart)
function vector $Y_{j} = Y(x_{j})$	7. row (AUX (7) in flowchart)
derivative vector $Y'_{j-6} = Y'(x_{j-6})$	8. row (AUX (8) in flowchart)
derivative vector $Y'_{j-5} = Y'(x_{j-5})$	9. row (AUX (9) in flowchart)
derivative vector $Y'_{j-4} = Y'(x_{j-4})$	10. row (AUX (10) in flowchart)
derivative vector $Y'_{j-3} = Y'(x_{j-3})$	11. row (AUX (11) in flowchart)
derivative vector $Y'_{j-2} = Y'(x_{j-2})$	12. row (AUX (12) in flowchart)
derivative vector $Y'_{j-1} = Y'(x_{j-1})$	13. row (AUX (13) in flowchart)
derivative vector $Y'_{j} = Y'(x_{j})$	14. row (AUX (14) in flowchart)
vector of error weights	15. row (AUX (15) in flowchart)
vector $P_j - C_j$	16. row (AUX (16) in flowchart)
decision vector for zero-columns in Matrix C	17. row (AUX (17) in flowchart)
vector $F(x_u)$	18. row (AUX (18) in flowchart)
vector $F'(x_u)$	19. row (AUX (19) in flowchart)
right-hand side vector R	20. row (AUX (20) in flowchart)

Figure 34. Storage allocation in auxiliary storage array AUX (LBVP-DLBVP)

```
C                                                                       LBVP  10
C     ...................................................................LBVP  20
C                                                                       LBVP  30
C        SUBROUTINE LBVP                                                LBVP  40
C                                                                       LBVP  50
C        PURPOSE                                                        LBVP  60
C           TO SOLVE A LINEAR BOUNDARY VALUE PROBLEM, WHICH CONSISTS OF LBVP  70
C           A SYSTEM OF NDIM LINEAR FIRST ORDER DIFFERENTIAL EQUATIONS  LBVP  80
C                 DY/DX=A(X)*Y(X)+F(X)                                  LBVP  90
C           AND NDIM LINEAR BOUNDARY CONDITIONS                         LBVP 100
C                 B*Y(XL)+C*Y(XU)=R.                                    LBVP 110
C                                                                       LBVP 120
C        USAGE                                                          LBVP 130
C           CALL LBVP (PRMT,B,C,R,Y,DERY,NDIM,IHLF,AFCT,FCT,DFCT,OUTP,  LBVP 140
C                AUX,A)                                                 LBVP 150
C           PARAMETERS AFCT,FCT,DFCT,OUTP REQUIRE AN EXTERNAL STATEMENT.LBVP 160
C                                                                       LBVP 170
C        DESCRIPTION OF PARAMETERS                                      LBVP 180
C           PRMT   - AN INPUT AND OUTPUT VECTOR WITH DIMENSION GREATER  LBVP 190
C                    OR EQUAL TO 5, WHICH SPECIFIES THE PARAMETERS OF   LBVP 200
C                    THE INTERVAL AND OF ACCURACY AND WHICH SERVES FOR  LBVP 210
C                    COMMUNICATION BETWEEN OUTPUT SUBROUTINE (FURNISHED LBVP 220
C                    BY THE USER) AND SUBROUTINE LBVP.                  LBVP 230
C                    THE COMPONENTS ARE                                 LBVP 240
C              PRMT(1)- LOWER BOUND XL OF THE INTERVAL (INPUT),         LBVP 250
C              PRMT(2)- UPPER BOUND XU OF THE INTERVAL (INPUT),         LBVP 260
C              PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE   LBVP 270
C                       (INPUT),                                        LBVP 280
C              PRMT(4)- UPPER ERROR BOUND (INPUT). IF RELATIVE ERROR IS LBVP 290
C                       GREATER THAN PRMT(4), INCREMENT GETS HALVED.    LBVP 300
C                       IF INCREMENT IS LESS THAN PRMT(3) AND RELATIVE  LBVP 310
C                       ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.LBVP 320
C                       THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS     LBVP 330
C                       OUTPUT SUBROUTINE.                              LBVP 340
C              PRMT(5)- NO INPUT PARAMETER. SUBROUTINE LBVP INITIALIZES LBVP 350
C                       PRMT(5)=0. IF THE USER WANTS TO TERMINATE       LBVP 360
C                       SUBROUTINE LBVP AT ANY OUTPUT POINT, HE HAS TO  LBVP 370
C                       CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE LBVP 380
C                       OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE     LBVP 390
C                       FEASIBLE IF ITS DIMENSION IS DEFINED GREATER    LBVP 400
C                       THAN 5. HOWEVER SUBROUTINE LBVP DOES NOT REQUIRE LBVP 410
C                       AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL LBVP 420
C                       FOR HANDING RESULT VALUES TO THE MAIN PROGRAM   LBVP 430
C                       (CALLING LBVP) WHICH ARE OBTAINED BY SPECIAL    LBVP 440
C                       MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP. LBVP 450
C           B      - AN NDIM BY NDIM INPUT MATRIX.  (DESTROYED)         LBVP 460
C                    IT IS THE COEFFICIENT MATRIX OF Y(XL) IN           LBVP 470
C                    THE BOUNDARY CONDITIONS.                           LBVP 480
C           C      - AN NDIM BY NDIM INPUT MATRIX (POSSIBLY DESTROYED). LBVP 490
C                    IT IS THE COEFFICIENT MATRIX OF Y(XU) IN           LBVP 500
C                    THE BOUNDARY CONDITIONS.                           LBVP 510
C           R      - AN INPUT VECTOR WITH DIMENSION NDIM.  (DESTROYED)  LBVP 520
C                    IT SPECIFIES THE RIGHT HAND SIDE OF THE            LBVP 530
C                    BOUNDARY CONDITIONS.                               LBVP 540
C           Y      - AN AUXILIARY VECTOR WITH DIMENSION NDIM.           LBVP 550
C                    IT IS USED AS STORAGE LOCATION FOR THE RESULTING   LBVP 560
C                    VALUES OF DEPENDENT VARIABLES COMPUTED AT          LBVP 570
C                    INTERMEDIATE POINTS.                               LBVP 580
C           DERY   - INPUT VECTOR OF ERROR WEIGHTS.  (DESTROYED)        LBVP 590
C                    ITS MAXIMAL COMPONENT SHOULD BE EQUAL TO 1.        LBVP 600
C                    LATERON DERY IS THE VECTOR OF DERIVATIVES, WHICH   LBVP 610
C                    BELONG TO FUNCTION VALUES Y AT INTERMEDIATE POINTS.LBVP 620
C           NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF      LBVP 630
C                    DIFFERENTIAL EQUATIONS IN THE SYSTEM.              LBVP 640
C           IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF     LBVP 650
C                    BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS   LBVP 660
C                    GREATER THAN 10, SUBROUTINE LBVP RETURNS WITH      LBVP 670
C                    ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.           LBVP 680
C                    ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE   LBVP 690
C                    PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-LBVP 700
C                    PRMT(1)) RESPECTIVELY. FINALLY ERROR MESSAGE       LBVP 710
C                    IHLF=14 INDICATES, THAT THERE IS NO SOLUTION OR    LBVP 720
C                    THAT THERE ARE MORE THAN ONE SOLUTION OF THE       LBVP 730
C                    PROBLEM.                                           LBVP 740
C                    A NEGATIVE VALUE OF IHLF HANDED TO SUBROUTINE OUTP LBVP 750
C                    TOGETHER WITH INITIAL VALUES OF FINALLY GENERATED  LBVP 760
C                    INITIAL VALUE PROBLEM INDICATES, THAT THERE WAS    LBVP 770
C                    POSSIBLE LOSS OF SIGNIFICANCE IN THE SOLUTION OF   LBVP 780
C                    THE SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS FOR    LBVP 790
C                    THESE INITIAL VALUES. THE ABSOLUTE VALUE OF IHLF   LBVP 800
C                    SHOWS, AFTER WHICH ELIMINATION STEP OF GAUSS       LBVP 810
C                    ALGORITHM POSSIBLE LOSS OF SIGNIFICANCE WAS        LBVP 820
C                    DETECTED.                                          LBVP 830
C           AFCT   - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        LBVP 840
C                    COMPUTES THE COEFFICIENT MATRIX A OF VECTOR Y ON    LBVP 850
C                    THE RIGHT HAND SIDE OF THE SYSTEM OF DIFFERENTIAL  LBVP 860
C                    EQUATIONS FOR A GIVEN X-VALUE. ITS PARAMETER LIST  LBVP 870
C                    MUST BE X,A. SUBROUTINE AFCT SHOULD NOT DESTROY X. LBVP 880
C           FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        LBVP 890
C                    COMPUTES VECTOR F (INHOMOGENEOUS PART OF THE       LBVP 900
C                    RIGHT HAND SIDE OF THE SYSTEM OF DIFFERENTIAL      LBVP 910
C                    EQUATIONS) FOR A GIVEN X-VALUE. ITS PARAMETER LIST LBVP 920
C                    MUST BE X,F. SUBROUTINE FCT SHOULD NOT DESTROY X.  LBVP 930
C           DFCT   - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        LBVP 940
C                    COMPUTES VECTOR DF (DERIVATIVE OF THE INHOMOGENEOUSLBVP 950
C                    PART ON THE RIGHT HAND SIDE OF THE SYSTEM OF       LBVP 960
C                    DIFFERENTIAL EQUATIONS) FOR A GIVEN X-VALUE. ITS   LBVP 970
C                    PARAMETER LIST MUST BE X,DF. SUBROUTINE DFCT       LBVP 980
C                    SHOULD NOT DESTROY X.                              LBVP 990
C           OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.    LBVP1000
C                    ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.LBVP1010
C                    NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,    LBVP1020
C                    PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY          LBVP1030
C                    SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,LBVP1040
C                    SUBROUTINE LBVP IS TERMINATED.                     LBVP1050
C           AUX    - AN AUXILIARY STORAGE ARRAY WITH 20 ROWS AND        LBVP1060
C                    NDIM COLUMNS.                                      LBVP1070
C           A      - AN NDIM BY NDIM MATRIX, WHICH IS USED AS AUXILIARY LBVP1080
C                    STORAGE ARRAY.                                     LBVP1090
C                                                                       LBVP1100
C        REMARKS                                                        LBVP1110
C           THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF LBVP1120
C           (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE    LBVP1130
C               NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE   LBVP1140
C               IHLF=11),                                               LBVP1150
C           (2) INITIAL INCREMENT IS EQUAL TO 0 OR IF IT HAS WRONG SIGN LBVP1160
C               (ERROR MESSAGES IHLF=12 OR IHLF=13),                    LBVP1170
C           (3) THERE IS NO OR MORE THAN ONE SOLUTION OF THE PROBLEM    LBVP1180
C               (ERROR MESSAGE IHLF=14),                                LBVP1190
C           (4) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,       LBVP1200
C           (5) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.        LBVP1210
C                                                                       LBVP1220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  LBVP1230
C           SUBROUTINE GELG      SYSTEM OF LINEAR EQUATIONS.            LBVP1240
C           THE EXTERNAL SUBROUTINES AFCT(X,A), FCT(X,F), DFCT(X,DF),   LBVP1250
C           AND OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED         LBVP1260
C           BY THE USER.                                                LBVP1270
C                                                                       LBVP1280
C        METHOD                                                         LBVP1290
C           EVALUATION IS DONE USING THE METHOD OF ADJOINT EQUATIONS.   LBVP1300
C           HAMMINGS FOURTH ORDER MODIFIED PREDICTOR-CORRECTOR METHOD   LBVP1310
C           IS USED TO SOLVE THE ADJOINT INITIAL VALUE PROBLEMS AND FI- LBVP1320
C           NALLY TO SOLVE THE GENERATED INITIAL VALUE PROBLEM FOR Y(X).LBVP1330
C           THE INITIAL INCREMENT PRMT(3) IS AUTOMATICALLY ADJUSTED.    LBVP1340
C           FOR COMPUTATION OF INTEGRAL SUM, A FOURTH ORDER HERMITEAN   LBVP1350
C           INTEGRATION FORMULA IS USED.                                LBVP1360
C           FOR REFERENCE, SEE                                          LBVP1370
C           (1) LANCE, NUMERICAL METHODS FOR HIGH SPEED COMPUTERS,      LBVP1380
C               ILIFFE, LONDON, 1960, PP.64-67.                         LBVP1390
C           (2) RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL          LBVP1400
C               COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.     LBVP1410
C           (3) RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS, LBVP1420
C               MTAC, VOL.16, 1SS.80 (1962), PP.431-437.                LBVP1430
C           (4) ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND     LBVP1440
C               PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963, LBVP1450
C               PP.227-232.                                             LBVP1460
C                                                                       LBVP1470
C     ...................................................................LBVP1480
C                                                                       LBVP1490
      SUBROUTINE LBVP(PRMT,B,C,R,Y,DERY,NDIM,IHLF,AFCT,FCT,DFCT,OUTP,   LBVP1500
     1AUX,A)                                                            LBVP1510
C                                                                       LBVP1520
      DIMENSION PRMT(1),B(1),C(1),R(1),Y(1),DERY(1),AUX(20,1),A(1)      LBVP1530
C                                                                       LBVP1540
C     ERROR TEST                                                        LBVP1550
      IF(PRMT(3)*(PRMT(2)-PRMT(1)))2,1,3                                LBVP1560
    1 IHLF=12                                                           LBVP1570
      RETURN                                                            LBVP1580
    2 IHLF=13                                                           LBVP1590
      RETURN                                                            LBVP1600
C                                                                       LBVP1610
C     SEARCH FOR ZERO-COLUMNS IN MATRICES B AND C                       LBVP1620
    3 KK=-NDIM                                                          LBVP1630
      IB=0                                                              LBVP1640
      IC=0                                                              LBVP1650
      DO 7 K=1,NDIM                                                     LBVP1660
      AUX(15,K)=DERY(K)                                                 LBVP1670
      AUX(1,K)=1.                                                       LBVP1680
      AUX(17,K)=1.                                                      LBVP1690
      KK=KK+NDIM                                                        LBVP1700
      DO 4 I=1,NDIM                                                     LBVP1710
      II=KK+I                                                           LBVP1720
      IF(B(II))5,4,5                                                    LBVP1730
    4 CONTINUE                                                          LBVP1740
      IB=IB+1                                                           LBVP1750
      AUX(1,K)=0.                                                       LBVP1760
    5 DO 6 I=1,NDIM                                                     LBVP1770
      II=KK+I                                                           LBVP1780
      IF(C(II))7,6,7                                                    LBVP1790
    6 CONTINUE                                                          LBVP1800
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      IC=IC+1                                                           L8VP1810
      AUX(17,K)=0.                                                      L8VP1820
    7 CONTINUE                                                          L8VP1830
C                                                                       L8VP1840
C     DETERMINATION OF LOWER AND UPPER BOUND                            L8VP1850
      IF(IC-18)8,11,11                                                  L8VP1860
    8 H=PRMT(2)                                                         L8VP1870
      PRMT(2)=PRMT(1)                                                   L8VP1880
      PRMT(1)=H                                                         L8VP1890
      PRMT(3)=-PRMT(3)                                                  L8VP1900
      DO 9 I=1,NDIM                                                     L8VP1910
    9 AUX(17,I)=AUX(1,I)                                                L8VP1920
      II=NDIM*NDIM                                                      L8VP1930
      DO 10 I=1,II                                                      L8VP1940
      H=B(I)                                                            L8VP1950
      B(I)=C(I)                                                         L8VP1960
   10 C(I)=H                                                            L8VP1970
C                                                                       L8VP1980
C     PREPARATIONS FOR CONSTRUCTION OF ADJOINT INITIAL VALUE PROBLEMS   L8VP1990
   11 X=PRMT(2)                                                         L8VP2000
      CALL FCT(X,Y)                                                     L8VP2010
      CALL DFCT(X,DERY)                                                 L8VP2020
      DO 12 I=1,NDIM                                                    L8VP2030
      AUX(18,I)=Y(I)                                                    L8VP2040
   12 AUX(19,I)=DERY(I)                                                 L8VP2050
C                                                                       L8VP2060
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  L8VP2070
C                                                                       L8VP2080
C     THE FOLLOWING PART OF SUBROUTINE L8VP UNTIL NEXT BREAK-POINT FOR  L8VP2090
C     LINKAGE HAS TO REMAIN IN CORE DURING THE WHOLE REST OF THE        L8VP2100
C     COMPUTATIONS                                                      L8VP2110
C                                                                       L8VP2120
C     START LOOP FOR GENERATING ADJOINT INITIAL VALUE PROBLEMS          L8VP2130
      K=0                                                               L8VP2140
      KK=0                                                              L8VP2150
  100 K=K+1                                                             L8VP2160
      IF(AUX(17,K))108,108,101                                          L8VP2170
C                                                                       L8VP2180
C     INITIALIZATION OF ADJOINT INITIAL VALUE PROBLEM                   L8VP2190
  101 X=PRMT(2)                                                         L8VP2200
      CALL AFCT(X,A)                                                    L8VP2210
      SUM=0.                                                            L8VP2220
      GL=AUX(18,K)                                                      L8VP2230
      DGL=AUX(19,K)                                                     L8VP2240
      II=K                                                              L8VP2250
      DO 104 I=1,NDIM                                                   L8VP2260
      H=-A(II)                                                          L8VP2270
      DERY(I)=H                                                         L8VP2280
      AUX(20,I)=R(I)                                                    L8VP2290
      Y(I)=0.                                                           L8VP2300
      IF(I-K)103,102,103                                                L8VP2310
  102 Y(I)=1.                                                           L8VP2320
  103 DGL=DGL+H*AUX(18,I)                                               L8VP2330
  104 II=II+NDIM                                                        L8VP2340
      XEND=PRMT(1)                                                      L8VP2350
      H=.0625*(XEND-X)                                                  L8VP2360
      ISW=0                                                             L8VP2370
      GOTO 400                                                          L8VP2380
C     THIS IS BRANCH TO ADJOINT LINEAR INITIAL VALUE PROBLEM            L8VP2390
C                                                                       L8VP2400
C     THIS IS RETURN FROM ADJOINT LINEAR INITIAL VALUE PROBLEM          L8VP2410
  105 IF(IHLF-10)106,106,117                                            L8VP2420
C                                                                       L8VP2430
C     UPDATING OF COEFFICIENT MATRIX B AND VECTOR R                     L8VP2440
  106 DO 107 I=1,NDIM                                                   L8VP2450
      KK=KK+1                                                           L8VP2460
      H=C(KK)                                                           L8VP2470
      R(I)=AUX(20,I)+H*SUM                                              L8VP2480
      II=I                                                              L8VP2490
      DO 107 J=1,NDIM                                                   L8VP2500
      B(II)=B(II)+H*Y(J)                                                L8VP2510
  107 II=II+NDIM                                                        L8VP2520
      GOTO 109                                                          L8VP2530
  108 KK=KK+NDIM                                                        L8VP2540
  109 IF(K-NDIM)100,110,110                                             L8VP2550
C                                                                       L8VP2560
C     GENERATION OF LAST INITIAL VALUE PROBLEM                          L8VP2570
  110 X=PRMT(4)                                                         L8VP2580
      CALL GELG(R,B,NDIM,1,X,I)                                         L8VP2590
      IF(I)111,112,112                                                  L8VP2600
  111 IHLF=14                                                           L8VP2610
      RETURN                                                            L8VP2620
C                                                                       L8VP2630
  112 PRMT(5)=0.                                                        L8VP2640
      IHLF=-1                                                           L8VP2650
      X=PRMT(1)                                                         L8VP2660
      XEND=PRMT(2)                                                      L8VP2670
      H=PRMT(3)                                                         L8VP2680
      DO 113 I=1,NDIM                                                   L8VP2690
  113 Y(I)=R(I)                                                         L8VP2700
      ISW=1                                                             L8VP2710
  114 ISW2=12                                                           L8VP2720
      GOTO 200                                                          L8VP2730
  115 ISW3=-1                                                           L8VP2740
      GOTO 300                                                          L8VP2750
  116 IF(IHLF)400,400,117                                               L8VP2760
C     THIS WAS BRANCH INTO INITIAL VALUE PROBLEM                        L8VP2770
C                                                                       L8VP2780
C     THIS IS RETURN FROM INITIAL VALUE PROBLEM                         L8VP2790
  117 RETURN                                                            L8VP2800
C                                                                       L8VP2810
C     THIS PART OF LINEAR BOUNDARY VALUE PROBLEM COMPUTES THE RIGHT     L8VP2820
C     HAND SIDE DERY OF THE SYSTEM OF ADJOINT LINEAR DIFFERENTIAL       L8VP2830
C     EQUATIONS (IN CASE ISW=0) OR OF THE GIVEN SYSTEM (IN CASE ISW=1). L8VP2840
  200 CALL AFCT(X,A)                                                    L8VP2850
      IF(ISW)201,201,205                                                L8VP2860
C                                                                       L8VP2870
C     ADJOINT SYSTEM                                                    L8VP2880
  201 LL=0                                                              L8VP2890
      DO 203 M=1,NDIM                                                   L8VP2900
      HS=0.                                                             L8VP2910
      DO 202 L=1,NDIM                                                   L8VP2920
      LL=LL+1                                                           L8VP2930
  202 HS=HS-A(LL)*Y(L)                                                  L8VP2940
  203 DERY(M)=HS                                                        L8VP2950
  204 GOTO(502,504,506,407,415,418,608,617,632,634,421,115),ISW2        L8VP2960
C                                                                       L8VP2970
C     GIVEN SYSTEM                                                      L8VP2980
  205 CALL FCT(X,DERY)                                                  L8VP2990
      DO 207 M=1,NDIM                                                   L8VP3000
      LL=M-NDIM                                                         L8VP3010
      HS=0.                                                             L8VP3020
      DO 206 L=1,NDIM                                                   L8VP3030
      LL=LL+NDIM                                                        L8VP3040
  206 HS=HS+A(LL)*Y(L)                                                  L8VP3050
  207 DERY(M)=HS+DERY(M)                                                L8VP3060
      GOTO 204                                                          L8VP3070
C                                                                       L8VP3080
C     THIS PART OF LINEAR BOUNDARY VALUE PROBLEM COMPUTES THE VALUE OF  L8VP3090
C     INTEGRAL SUM, WHICH IS A PART OF THE OUTPUT OF ADJOINT INITIAL    L8VP3100
C     VALUE PROBLEM (IN CASE ISW=0) OR RECORDS RESULT VALUES OF THE     L8VP3110
C     FINAL INITIAL VALUE PROBLEM (IN CASE ISW=1).                      L8VP3120
  300 IF(ISW)301,301,305                                                L8VP3130
C                                                                       L8VP3140
C     ADJOINT PROBLEM                                                   L8VP3150
  301 CALL FCT(X,R)                                                     L8VP3160
      GU=0.                                                             L8VP3170
      DGU=0.                                                            L8VP3180
      DO 302 L=1,NDIM                                                   L8VP3190
      GU=GU+Y(L)*R(L)                                                   L8VP3200
  302 DGU=DGU+DERY(L)*R(L)                                              L8VP3210
      CALL DFCT(X,R)                                                    L8VP3220
      DO 303 L=1,NDIM                                                   L8VP3230
  303 DGU=DGU+Y(L)*R(L)                                                 L8VP3240
      SUM=SUM+.5*H*((GL+GU)+.1666667*H*(DGL-DGU))                       L8VP3250
      GL=GU                                                             L8VP3260
      DGL=DGU                                                           L8VP3270
  304 IF(ISW3)116,422,618                                               L8VP3280
C                                                                       L8VP3290
C     GIVEN PROBLEM                                                     L8VP3300
  305 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                L8VP3310
      IF(PRMT(5)+1.)117,304,117                                         L8VP3320
C                                                                       L8VP3330
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  L8VP3340
C                                                                       L8VP3350
C     THE FOLLOWING PART OF SUBROUTINE L8VP SOLVES IN CASE ISW=0 THE    L8VP3360
C     ADJOINT INITIAL VALUE PROBLEM. IT COMPUTES INTEGRAL SUM AND       L8VP3370
C     THE VECTOR Y OF DEPENDENT VARIABLES AT THE LOWER BOUND PRMT(1).   L8VP3380
C     IN CASE ISW=1 IT SOLVES FINALLY GENERATED INITIAL VALUE PROBLEM.   L8VP3390
  400 N=1                                                               L8VP3400
      XST=X                                                             L8VP3410
      IHLF=0                                                            L8VP3420
      DO 401 I=1,NDIM                                                   L8VP3430
      AUX(16,I)=0.                                                      L8VP3440
      AUX(1,I)=Y(I)                                                     L8VP3450
  401 AUX(8,I)=DERY(I)                                                  L8VP3460
      ISW1=1                                                            L8VP3470
      GOTO 500                                                          L8VP3480
C                                                                       L8VP3490
  402 X=X+H                                                             L8VP3500
      DO 403 I=1,NDIM                                                   L8VP3510
  403 AUX(2,I)=Y(I)                                                     L8VP3520
C                                                                       L8VP3530
C     INCREMENT H IS TESTED BY MEANS OF BISECTION                       L8VP3540
  404 IHLF=IHLF+1                                                       L8VP3550
      X=X-H                                                             L8VP3560
      DO 405 I=1,NDIM                                                   L8VP3570
  405 AUX(4,I)=AUX(2,I)                                                 L8VP3580
      H=.5*H                                                            L8VP3590
      N=1                                                               L8VP3600
      ISW1=2                                                            L8VP3610
      GOTO 500                                                          L8VP3620
C                                                                       L8VP3630
  406 X=X+H                                                             L8VP3640
      ISW2=4                                                            L8VP3650
      GOTO 200                                                          L8VP3660
  407 N=2                                                               L8VP3670
      DO 408 I=1,NDIM                                                   L8VP3680
      AUX(2,I)=Y(I)                                                     L8VP3690
  408 AUX(9,I)=DERY(I)                                                  L8VP3700
      ISW1=3                                                            L8VP3710
      GOTO 500                                                          L8VP3720
C                                                                       L8VP3730
C     TEST ON SATISFACTORY ACCURACY                                     L8VP3740
  409 DO 414 I=1,NDIM                                                   L8VP3750
      Z=ABS(Y(I))                                                       L8VP3760
      IF(Z-1.)410,411,411                                               L8VP3770
  410 Z=1.                                                              L8VP3780
  411 DELT=.06666667*ABS(Y(I)-AUX(4,I))                                 L8VP3790
      IF(ISW)413,413,412                                                L8VP3800
  412 DELT=AUX(15,I)+DELT                                               L8VP3810
  413 IF(DELT-Z*PRMT(4))414,414,429                                     L8VP3820
  414 CONTINUE                                                          L8VP3830
C                                                                       L8VP3840
C     SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS               L8VP3850
      X=X+H                                                             L8VP3860
      ISW2=5                                                            L8VP3870
      GOTO 200                                                          L8VP3880
  415 DO 416 I=1,NDIM                                                   L8VP3890
      AUX(3,I)=Y(I)                                                     L8VP3900
  416 AUX(10,I)=DERY(I)                                                 L8VP3910
      N=3                                                               L8VP3920
      ISW1=4                                                            L8VP3930
      GOTO 500                                                          L8VP3940
C                                                                       L8VP3950
  417 N=1                                                               L8VP3960
      X=X+H                                                             L8VP3970
      ISW2=6                                                            L8VP3980
      GOTO 200                                                          L8VP3990
  418 X=XST                                                             L8VP4000
      DO 419 I=1,NDIM                                                   L8VP4010
      AUX(11,I)=DERY(I)                                                 L8VP4020
  419 Y(I)=AUX(1,I)+H*(.375*AUX(8,I)+.7916667*AUX(9,I)                  L8VP4030
     1-.2083333*AUX(10,I)+.04166667*DERY(I))                            L8VP4040
  420 X=X+H                                                             L8VP4050
      N=N+1                                                             L8VP4060
      ISW2=11                                                           L8VP4070
      GOTO 200                                                          L8VP4080
  421 ISW3=0                                                            L8VP4090
      GOTO 300                                                          L8VP4100
  422 IF(N-4)423,600,600                                                L8VP4110
  423 DO 424 I=1,NDIM                                                   L8VP4120
      AUX(N,I)=Y(I)                                                     L8VP4130
  424 AUX(N+7,I)=DERY(I)                                                L8VP4140
      IF(N-3)425,427,600                                                L8VP4150
C                                                                       L8VP4160
  425 DO 426 I=1,NDIM                                                   L8VP4170
      DELT=AUX(9,I)+AUX(9,I)                                            L8VP4180
      DELT=DELT+DELT                                                    L8VP4190
  426 Y(I)=AUX(1,I)+.3333333*H*(AUX(8,I)+DELT+AUX(10,I))                L8VP4200
      GOTO 420                                                          L8VP4210
C                                                                       L8VP4220
  427 DO 428 I=1,NDIM                                                   L8VP4230
      DELT=AUX(9,I)+AUX(10,I)                                           L8VP4240
      DELT=DELT+DELT+DELT                                               L8VP4250
  428 Y(I)=AUX(1,I)+.375*H*(AUX(8,I)+DELT+AUX(11,I))                    L8VP4260
      GOTO 420                                                          L8VP4270
C                                                                       L8VP4280
C     NO SATISFACTORY ACCURACY. H MUST BE HALVED.                       L8VP4290
  429 IF(IHLF-10)404,430,430                                            L8VP4300
C                                                                       L8VP4310
C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.      L8VP4320
  430 IHLF=11                                                           L8VP4330
      X=X+H                                                             L8VP4340
      IF(ISW)105,105,114                                                L8VP4350
C                                                                       L8VP4360
C     THIS PART OF LINEAR INITIAL VALUE PROBLEM COMPUTES                L8VP4370
C     STARTING VALUES BY MEANS OF RUNGE-KUTTA METHOD.                   L8VP4380
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      500 Z=X                                                           LBVP4390
          DO 501 I=1,NDIM                                               LBVP4400
          X=H*AUX(N+7,I)                                                LBVP4410
          AUX(5,I)=X                                                    LBVP4420
      501 Y(I)=AUX(N,I)+.4*X                                            LBVP4430
C                                                                       LBVP4440
          X=Z+.4*H                                                      LBVP4450
          ISW2=1                                                        LBVP4460
          GOTO 200                                                      LBVP4470
      502 DO 503 I=1,NDIM                                               LBVP4480
          X=H*DERY(I)                                                   LBVP4490
          AUX(6,I)=X                                                    LBVP4500
      503 Y(I)=AUX(N,I)+.2969776*AUX(5,I)+.1587596*X                    LBVP4510
C                                                                       LBVP4520
          X=Z+.45573725*H                                               LBVP4530
          ISW2=2                                                        LBVP4540
          GOTO 200                                                      LBVP4550
      504 DO 505 I=1,NDIM                                               LBVP4560
          X=H*DERY(I)                                                   LBVP4570
          AUX(7,I)=X                                                    LBVP4580
      505 Y(I)=AUX(N,I)+.2181004*AUX(5,I)-3.050965*AUX(6,I)+3.832865*X  LBVP4590
C                                                                       LBVP4600
          X=Z+H                                                         LBVP4610
          ISW2=3                                                        LBVP4620
          GOTO 200                                                      LBVP4630
      506 DO 507 I=1,NDIM                                               LBVP4640
      5070Y(I)=AUX(N,I)+.1747603*AUX(5,I)-.5514807*AUX(6,I)             LBVP4650
         1+1.205536*AUX(7,I)+.1711848*H*DERY(I)                         LBVP4660
          X=Z                                                           LBVP4670
          GOTO(402,406,409,417),ISW1                                    LBVP4680
C                                                                       LBVP4690
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  LBVP4700
C                                                                       LBVP4710
C     STARTING VALUES ARE COMPUTED.                                     LBVP4720
C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.           LBVP4730
      600 ISTEP=3                                                       LBVP4740
      601 IF(N-8)604,602,604                                            LBVP4750
C                                                                       LBVP4760
C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS      LBVP4770
      602 DO 603 N=2,7                                                  LBVP4780
          DO 603 I=1,NDIM                                               LBVP4790
          AUX(N-1,I)=AUX(N,I)                                           LBVP4800
      603 AUX(N+6,I)=AUX(N+7,I)                                         LBVP4810
          N=7                                                           LBVP4820
C                                                                       LBVP4830
C     N LESS THAN 8 CAUSES N+1 TO GET N                                 LBVP4840
      604 N=N+1                                                         LBVP4850
C                                                                       LBVP4860
C     COMPUTATION OF NEXT VECTOR Y                                      LBVP4870
          DO 605 I=1,NDIM                                               LBVP4880
          AUX(N-1,I)=Y(I)                                               LBVP4890
      605 AUX(N+6,I)=DERY(I)                                            LBVP4900
          X=X+H                                                         LBVP4910
      606 ISTEP=ISTEP+1                                                 LBVP4920
          DO 607 I=1,NDIM                                               LBVP4930
          ODELT=AUX(N-4,I)+1.333333*H*(AUX(N+6,I)+AUX(N+6,I)-AUX(N+5,I)+LBVP4940
         1AUX(N+4,I)+AUX(N+4,I))                                        LBVP4950
          Y(I)=DELT-.9256198*AUX(16,I)                                  LBVP4960
      607 AUX(16,I)=DELT                                                LBVP4970
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR   LBVP4980
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.               LBVP4990
C                                                                       LBVP5000
          ISW2=7                                                        LBVP5010
          GOTO 200                                                      LBVP5020
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY.            LBVP5030
C                                                                       LBVP5040
      608 DO 609 I=1,NDIM                                               LBVP5050
          ODELT=.125*(9.*AUX(N-1,I)-AUX(N-3,I)+3.*H*(DERY(I)+AUX(N+6,I)+LBVP5060
         1AUX(N+6,I)-AUX(N+5,I)))                                       LBVP5070
          AUX(16,I)=AUX(16,I)-DELT                                      LBVP5080
      609 Y(I)=DELT+.07438017*AUX(16,I)                                 LBVP5090
C                                                                       LBVP5100
C     TEST WHETHER H MUST BE HALVED OR DOUBLED                          LBVP5110
          DELT=0.                                                       LBVP5120
          DO 616 I=1,NDIM                                               LBVP5130
          Z=ABS(Y(I))                                                   LBVP5140
          IF(Z-1.)610,611,611                                           LBVP5150
      610 Z=1.                                                          LBVP5160
      611 Z=ABS(AUX(16,I))/Z                                            LBVP5170
          IF(ISW)613,613,612                                            LBVP5180
      612 Z=AUX(15,I)*Z                                                 LBVP5190
      613 IF(Z-PRMT(4))614,614,628                                      LBVP5200
      614 IF(DELT-Z)615,616,616                                         LBVP5210
      615 DELT=Z                                                        LBVP5220
      616 CONTINUE                                                      LBVP5230
C                                                                       LBVP5240
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                   LBVP5250
          ISW2=8                                                        LBVP5260
          GOTO 200                                                      LBVP5270
      617 ISW3=1                                                        LBVP5280
          GOTO 300                                                      LBVP5290
      618 IF(H*(X-XEND))619,621,621                                     LBVP5300
      619 IF(ABS(X-XEND)-.1*ABS(H))621,620,620                          LBVP5310
      620 IF(DELT-.02*PRMT(4))622,622,601                               LBVP5320
      621 IF(ISW)105,105,117                                            LBVP5330
C                                                                       LBVP5340
C                                                                       LBVP5350
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE         LBVP5360
C     AVAILABLE.                                                        LBVP5370
      622 IF(IHLF)601,601,623                                           LBVP5380
      623 IF(N-7)601,624,624                                            LBVP5390
      624 IF(ISTEP-4)601,625,625                                        LBVP5400
      625 IMOD=ISTEP/2                                                  LBVP5410
          IF(ISTEP-IMOD-IMOD)601,626,601                                LBVP5420
      626 H=H+H                                                         LBVP5430
          IHLF=IHLF-1                                                   LBVP5440
          ISTEP=0                                                       LBVP5450
          DO 627 I=1,NDIM                                               LBVP5460
          AUX(N-1,I)=AUX(N-2,I)                                         LBVP5470
          AUX(N-2,I)=AUX(N-4,I)                                         LBVP5480
          AUX(N-3,I)=AUX(N-6,I)                                         LBVP5490
          AUX(N+6,I)=AUX(N+5,I)                                         LBVP5500
          AUX(N+5,I)=AUX(N+3,I)                                         LBVP5510
          AUX(N+4,I)=AUX(N+1,I)                                         LBVP5520
          DELT=AUX(N+6,I)+AUX(N+5,I)                                    LBVP5530
          DELT=DELT+DELT+DELT                                           LBVP5540
  6270AUX(16,I)=8.962963*(Y(I)-AUX(N-3,I))-3.361111*H*(DERY(I)+DELT     LBVP5550
         1+AUX(N+4,I))                                                  LBVP5560
          GOTO 601                                                      LBVP5570
C                                                                       LBVP5580
C                                                                       LBVP5590
C     H MUST BE HALVED                                                  LBVP5600
      628 IHLF=IHLF+1                                                   LBVP5610
          IF(IHLF-10)630,630,629                                        LBVP5620
      629 IF(ISW)105,105,114                                            LBVP5630
      630 H=.5*H                                                        LBVP5640
          ISTEP=0                                                       LBVP5650
          DO 631 I=1,NDIM                                               LBVP5660
          OY(I)=.00390625*(80.*AUX(N-1,I)+135.*AUX(N-2,I)+40.*AUX(N-3,I)+LBVP5670
         1AUX(N-4,I))-.1171875*(AUX(N+6,I)-6.*AUX(N+5,I)-AUX(N+4,I))*H  LBVP5680
          OAUX(N-4,I)=.00390625*(12.*AUX(N-1,I)+135.*AUX(N-2,I)+        LBVP5690
         1108.*AUX(N-3,I)+AUX(N-4,I))-.0234375*(AUX(N+6,I)+18.*AUX(N+5,I)-LBVP5700
         29.*AUX(N+4,I))*H                                              LBVP5710
          AUX(N-3,I)=AUX(N-2,I)                                         LBVP5720
      631 AUX(N+4,I)=AUX(N+5,I)                                         LBVP5730
          DELT=X-H                                                      LBVP5740
          X=DELT-(H+H)                                                  LBVP5750
          ISW2=9                                                        LBVP5760
          GOTO 200                                                      LBVP5770
      632 DO 633 I=1,NDIM                                               LBVP5780
          AUX(N-2,I)=Y(I)                                               LBVP5790
          AUX(N+5,I)=DERY(I)                                            LBVP5800
      633 Y(I)=AUX(N-4,I)                                               LBVP5810
          X=X-(H+H)                                                     LBVP5820
          ISW2=10                                                       LBVP5830
          GOTO 200                                                      LBVP5840
      634 X=DELT                                                        LBVP5850
          DO 635 I=1,NDIM                                               LBVP5860
          DELT=AUX(N+5,I)+AUX(N+4,I)                                    LBVP5870
          DELT=DELT+DELT+DELT                                           LBVP5880
          OAUX(16,I)=8.962963*(AUX(N-1,I)-Y(I))-3.361111*H*(AUX(N+6,I)+DELT LBVP5890
         1+DERY(I))                                                     LBVP5900
      635 AUX(N+3,I)=DERY(I)                                            LBVP5910
          GOTO 606                                                      LBVP5920
C                                                                       LBVP5930
C     END OF INITIAL VALUE PROBLEM                                      LBVP5940
          END                                                           LBVP5950
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C                                                                       DLBV  10
C  ***********************************************************************DLBV  20
C                                                                       DLBV  30
C     SUBROUTINE DLBVP                                                  DLBV  40
C                                                                       DLBV  50
C     PURPOSE                                                           DLBV  60
C        TO SOLVE A LINEAR BOUNDARY VALUE PROBLEM, WHICH CONSISTS OF    DLBV  70
C        A SYSTEM OF NDIM LINEAR FIRST ORDER DIFFERENTIAL EQUATIONS     DLBV  80
C              DY/DX=A(X)*Y(X)+F(X)                                     DLBV  90
C        AND NDIM LINEAR BOUNDARY CONDITIONS                            DLBV 100
C              B*Y(XL)+C*Y(XU)=R.                                       DLBV 110
C                                                                       DLBV 120
C     USAGE                                                             DLBV 130
C        CALL DLBVP (PRMT,B,C,R,Y,DERY,NDIM,IHLF,AFCT,FCT,DFCT,OUTP,    DLBV 140
C                    AUX,A)                                             DLBV 150
C        PARAMETERS AFCT,FCT,DFCT,OUTP REQUIRE AN EXTERNAL STATEMENT.   DLBV 160
C                                                                       DLBV 170
C     DESCRIPTION OF PARAMETERS                                         DLBV 180
C        PRMT   - DOUBLE PRECISION INPUT AND OUTPUT VECTOR WITH         DLBV 190
C                 DIMENSION GREATER THAN OR EQUAL TO 5, WHICH           DLBV 200
C                 SPECIFIES THE PARAMETERS OF THE INTERVAL AND OF       DLBV 210
C                 ACCURACY AND WHICH SERVES FOR COMMUNICATION BETWEEN   DLBV 220
C                 OUTPUT SUBROUTINE (FURNISHED BY THE USER) AND         DLBV 230
C                 SUBROUTINE DLBVP. EXCEPT PRMT(5) THE COMPONENTS       DLBV 240
C                 ARE NOT DESTROYED BY SUBROUTINE DLBVP AND THEY ARE    DLBV 250
C        PRMT(1)- LOWER BOUND XL OF THE INTERVAL (INPUT),               DLBV 260
C        PRMT(1)- UPPER BOUND XU OF THE INTERVAL (INPUT),               DLBV 270
C        PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE         DLBV 280
C                 (INPUT),                                              DLBV 290
C        PRMT(4)- UPPER ERROR BOUND (INPUT). IF RELATIVE ERROR IS       DLBV 300
C                 GREATER THAN PRMT(4), INCREMENT GETS HALVED.          DLBV 310
C                 IF INCREMENT IS LESS THAN PRMT(3) AND RELATIVE        DLBV 320
C                 ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.   DLBV 330
C                 THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS           DLBV 340
C                 OUTPUT SUBROUTINE.                                    DLBV 350
C        PRMT(5)- NO INPUT PARAMETER. SUBROUTINE DLBVP INITIALIZES      DLBV 360
C                 PRMT(5)=0. IF THE USER WANTS TO TERMINATE             DLBV 370
C                 SUBROUTINE DLBVP AT ANY OUTPUT POINT, HE HAS TO       DLBV 380
C                 CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE     DLBV 390
C                 OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE           DLBV 400
C                 FEASIBLE IF ITS DIMENSION IS DEFINED GREATER          DLBV 410
C                 THAN 5. HOWEVER SUBROUTINE DLBVP DOES NOT REQUIRE     DLBV 420
C                 AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL      DLBV 430
C                 FOR HANDING RESULT VALUES TO THE MAIN PROGRAM         DLBV 440
C                 (CALLING DLBVP) WHICH ARE OBTAINED BY SPECIAL         DLBV 450
C                 MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP.    DLBV 460
C        B      - DOUBLE PRECISION NDIM BY NDIM INPUT MATRIX           DLBV 470
C                 (DESTROYED). IT IS THE COEFFICIENT MATRIX OF Y(XL)    DLBV 480
C                 IN THE BOUNDARY CONDITIONS.                           DLBV 490
C        C      - DOUBLE PRECISION NDIM BY NDIM INPUT MATRIX           DLBV 500
C                 (POSSIBLY DESTROYED). IT IS THE COEFFICIENT MATRIX    DLBV 510
C                 OF Y(XU) IN THE BOUNDARY CONDITIONS.                  DLBV 520
C        R      - DOUBLE PRECISION INPUT VECTOR WITH DIMENSION NDIM     DLBV 530
C                 (DESTROYED). IT SPECIFIES THE RIGHT HAND SIDE OF      DLBV 540
C                 THE BOUNDARY CONDITIONS.                              DLBV 550
C        Y      - DOUBLE PRECISION AUXILIARY VECTOR WITH               DLBV 560
C                 DIMENSION NDIM. IT IS USED AS STORAGE LOCATION        DLBV 570
C                 FOR THE RESULTING VALUES OF DEPENDENT VARIABLES       DLBV 580
C                 COMPUTED AT INTERMEDIATE POINTS X.                    DLBV 590
C        DERY   - DOUBLE PRECISION INPUT VECTOR OF ERROR WEIGHTS       DLBV 600
C                 (DESTROYED). ITS MAXIMAL COMPONENT SHOULD BE          DLBV 610
C                 EQUAL TO 1. LATERON DERY IS THE VECTOR OF             DLBV 620
C                 DERIVATIVES, WHICH BELONG TO FUNCTION VALUES Y AT     DLBV 630
C                 INTERMEDIATE POINTS X.                                DLBV 640
C        NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF         DLBV 650
C                 DIFFERENTIAL EQUATIONS IN THE SYSTEM.                 DLBV 660
C        IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF        DLBV 670
C                 BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS      DLBV 680
C                 GREATER THAN 10, SUBROUTINE DLBVP RETURNS WITH        DLBV 690
C                 ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.              DLBV 700
C                 ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE      DLBV 710
C                 PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-   DLBV 720
C                 PRMT(1)) RESPECTIVELY. FINALLY ERROR MESSAGE          DLBV 730
C                 IHLF=14 INDICATES, THAT THERE IS NO SOLUTION OR       DLBV 740
C                 THAT THERE ARE MORE THAN ONE SOLUTION OF THE          DLBV 750
C                 PROBLEM.                                              DLBV 760
C                 A NEGATIVE VALUE OF IHLF HANDED TO SUBROUTINE OUTP    DLBV 770
C                 TOGETHER WITH INITIAL VALUES OF FINALLY GENERATED     DLBV 780
C                 INITIAL VALUE PROBLEM INDICATES, THAT THERE WAS       DLBV 790
C                 POSSIBLE LOSS OF SIGNIFICANCE IN THE SOLUTION OF      DLBV 800
C                 THE SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS FOR       DLBV 810
C                 THESE INITIAL VALUES. THE ABSOLUTE VALUE OF IHLF      DLBV 820
C                 SHOWS, AFTER WHICH ELIMINATION STEP OF GAUSS          DLBV 830
C                 ALGORITHM POSSIBLE LOSS OF SIGNIFICANCE WAS           DLBV 840
C                 DETECTED.                                             DLBV 850
C        AFCT   - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT           DLBV 860
C                 COMPUTES THE COEFFICIENT MATRIX A OF VECTOR Y ON      DLBV 870
C                 THE RIGHT HAND SIDE OF THE SYSTEM OF DIFFERENTIAL     DLBV 880
C                 EQUATIONS FOR A GIVEN X-VALUE. ITS PARAMETER LIST     DLBV 890
C                 MUST BE X,A. SUBROUTINE AFCT SHOULD NOT DESTROY X.    DLBV 900
C        FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT          DLBV 910
C                 COMPUTES VECTOR F (INHOMOGENEOUS PART OF THE          DLBV 920
C                 RIGHT HAND SIDE OF THE SYSTEM OF DIFFERENTIAL         DLBV 930
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C                EQUATIONS) FOR A GIVEN X-VALUE. ITS PARAMETER LIST      DLBV 940
C                MUST BE X,F. SUBROUTINE FCT SHOULD NOT DESTROY X.       DLBV 950
C          DFCT  - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT           DLBV 960
C                COMPUTES VECTOR OF (DERIVATIVE OF THE INHOMOGENEOUS     DLBV 970
C                PART ON THE RIGHT HAND SIDE OF THE SYSTEM OF            DLBV 980
C                DIFFERENTIAL EQUATIONS) FOR A GIVEN X-VALUE. ITS        DLBV 990
C                PARAMETER LIST MUST BE X,DF. SUBROUTINE DFCT            DLBV1000
C                SHOULD NOT DESTROY X.                                   DLBV1010
C          OUTP  - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.       DLBV1020
C                ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.     DLBV1030
C                NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,         DLBV1040
C                PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY               DLBV1050
C                SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,     DLBV1060
C                SUBROUTINE DLBVP IS TERMINATED.                         DLBV1070
C          AUX   - DOUBLE PRECISION AUXILIARY STORAGE ARRAY WITH 20      DLBV1080
C                ROWS AND NDIM COLUMNS.                                  DLBV1090
C          A     - DOUBLE PRECISION NDIM BY NDIM MATRIX, WHICH IS USED   DLBV1100
C                AS AUXILIARY STORAGE ARRAY.                             DLBV1110
C                                                                        DLBV1120
C       REMARKS                                                          DLBV1130
C          THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF   DLBV1140
C          (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE      DLBV1150
C              NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE     DLBV1160
C              IHLF=11),                                                 DLBV1170
C          (2) INITIAL INCREMENT IS EQUAL TO 0 OR IF IT HAS WRONG SIGN   DLBV1180
C              (ERROR MESSAGES IHLF=12 OR IHLF=13),                      DLBV1190
C          (3) THERE IS NO OR MORE THAN ONE SOLUTION OF THE PROBLEM      DLBV1200
C              (ERROR MESSAGE IHLF=14),                                  DLBV1210
C          (4) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,         DLBV1220
C          (5) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.          DLBV1230
C                                                                        DLBV1240
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                    DLBV1250
C          SUBROUTINE DGELG      SYSTEM OF LINEAR EQUATIONS.             DLBV1260
C          THE EXTERNAL SUBROUTINES AFCT(X,A), FCT(X,F), DFCT(X,DF),     DLBV1270
C          AND OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED           DLBV1280
C          BY THE USER.                                                  DLBV1290
C                                                                        DLBV1300
C       METHOD                                                           DLBV1310
C          EVALUATION IS DONE USING THE METHOD OF ADJOINT EQUATIONS.     DLBV1320
C          HAMMINGS FOURTH ORDER MODIFIED PREDICTOR-CORRECTOR METHOD     DLBV1330
C          IS USED TO SOLVE THE ADJOINT INITIAL VALUE PROBLEMS AND FI-   DLBV1340
C          NALLY TO SOLVE THE GENERATED INITIAL VALUE PROBLEM FOR Y(X).  DLBV1350
C          THE INITIAL INCREMENT PRMT(3) IS AUTOMATICALLY ADJUSTED.      DLBV1360
C          FOR COMPUTATION OF INTEGRAL SUM, A FOURTH ORDER HERMITEAN     DLBV1370
C          INTEGRATION FORMULA IS USED.                                  DLBV1380
C          FOR REFERENCE, SEE                                            DLBV1390
C          (1) LANCE, NUMERICAL METHODS FOR HIGH SPEED COMPUTERS,        DLBV1400
C              ILIFFE, LONDON, 1960, PP.64-67.                           DLBV1410
C          (2) RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL            DLBV1420
C              COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.       DLBV1430
C          (3) RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS,   DLBV1440
C              MTAC, VOL.16, 1SS.80 (1962), PP.431-437.                  DLBV1450
C          (4) ZURMUEHL, PRAKTISCHE MATHEMATIK FUER INGENIEURE UND       DLBV1460
C              PHYSIKER, SPRINGER, BERLIN/GOETTINGEN/HEIDELBERG, 1963,   DLBV1470
C              PP.227-232.                                               DLBV1480
C                                                                        DLBV1490
C  ..................................................................... DLBV1500
C                                                                        DLBV1510
      SUBROUTINE DLBVP(PRMT,B,C,R,Y,DERY,NDIM,IHLF,AFCT,FCT,DFCT,OUTP,   DLBV1520
     1AUX,A)                                                             DLBV1530
C                                                                        DLBV1540
C                                                                        DLBV1550
      DIMENSION PRMT(1),B(1),C(1),R(1),Y(1),DERY(1),AUX(20,1),A(1)       DLBV1560
      DOUBLE PRECISION PRMT,B,C,R,Y,DERY,AUX,A,H,X,Z,GL,HS,GU,SUM,       DLBV1570
     1DGL,DGU,XST,XEND,DELT                                              DLBV1580
C                                                                        DLBV1590
C     ERROR TEST                                                         DLBV1600
      IF(PRMT(3)*(PRMT(2)-PRMT(1)))2,1,3                                 DLBV1610
    1 IHLF=12                                                            DLBV1620
      RETURN                                                             DLBV1630
    2 IHLF=13                                                            DLBV1640
      RETURN                                                             DLBV1650
C                                                                        DLBV1660
C     SEARCH FOR ZERO-COLUMNS IN MATRICES B AND C                        DLBV1670
    3 KK=-NDIM                                                           DLBV1680
      IB=0                                                               DLBV1690
      IC=0                                                               DLBV1700
      DO 7 K=1,NDIM                                                      DLBV1710
      AUX(15,K)=DERY(K)                                                  DLBV1720
      AUX(1,K)=1.D0                                                      DLBV1730
      AUX(17,K)=1.D0                                                     DLBV1740
      KK=KK+NDIM                                                         DLBV1750
      DO 4 I=1,NDIM                                                      DLBV1760
      II=KK+I                                                            DLBV1770
      IF(B(II))5,4,5                                                     DLBV1780
    4 CONTINUE                                                           DLBV1790
      IB=IB+1                                                            DLBV1800
      AUX(1,K)=0.D0                                                      DLBV1810
    5 DO 6 I=1,NDIM                                                      DLBV1820
      II=KK+I                                                            DLBV1830
      IF(C(II))7,6,7                                                     DLBV1840
    6 CONTINUE                                                           DLBV1850
      IC=IC+1                                                            DLBV1860
      AUX(17,K)=0.D0                                                     DLBV1870
    7 CONTINUE                                                           DLBV1880
C                                                                        DLBV1890
C     DETERMINATION OF LOWER AND UPPER BOUND                             DLBV1900
      IF(IC-IB)8,11,11                                                   DLBV1910
    8 H=PRMT(2)                                                          DLBV1920
      PRMT(2)=PRMT(1)                                                    DLBV1930
      PRMT(1)=H                                                          DLBV1940
      PRMT(3)=-PRMT(3)                                                   DLBV1950
      DO 9 I=1,NDIM                                                      DLBV1960
    9 AUX(17,I)=AUX(1,I)                                                 DLBV1970
      II=NDIM*NDIM                                                       DLBV1980
      DO 10 I=1,II                                                       DLBV1990
      H=B(I)                                                             DLBV2000
      B(I)=C(I)                                                          DLBV2010
   10 C(I)=H                                                             DLBV2020
C                                                                        DLBV2030
C     PREPARATIONS FOR CONSTRUCTION OF ADJOINT INITIAL VALUE PROBLEMS    DLBV2040
   11 X=PRMT(2)                                                          DLBV2050
      CALL FCT(X,Y)                                                      DLBV2060
      CALL DFCT(X,DERY)                                                  DLBV2070
      DO 12 I=1,NDIM                                                     DLBV2080
      AUX(18,I)=Y(I)                                                     DLBV2090
   12 AUX(19,I)=DERY(I)                                                  DLBV2100
C                                                                        DLBV2110
C     POSSIBLE BREAK-POINT FOR LINKAGE                                   DLBV2120
C                                                                        DLBV2130
C     THE FOLLOWING PART OF SUBROUTINE DLBVP UNTIL NEXT BREAK-POINT FOR  DLBV2140
C     LINKAGE HAS TO REMAIN IN CORE DURING THE WHOLE REST OF THE         DLBV2150
C     COMPUTATIONS                                                       DLBV2160
C                                                                        DLBV2170
C     START LOOP FOR GENERATING ADJOINT INITIAL VALUE PROBLEMS           DLBV2180
      K=0                                                                DLBV2190
      KK=0                                                               DLBV2200
  100 K=K+1                                                              DLBV2210
      IF(AUX(17,K))108,108,101                                           DLBV2220
C                                                                        DLBV2230
C     INITIALIZATION OF ADJOINT INITIAL VALUE PROBLEM                    DLBV2240
  101 X=PRMT(2)                                                          DLBV2250
      CALL AFCT(X,A)                                                     DLBV2260
      SUM=0.D0                                                           DLBV2270
      GL=AUX(18,K)                                                       DLBV2280
      DGL=AUX(19,K)                                                      DLBV2290
      II=K                                                               DLBV2300
      DO 104 I=1,NDIM                                                    DLBV2310
      H=-A(II)                                                           DLBV2320
      DERY(I)=H                                                          DLBV2330
      AUX(20,I)=R(I)                                                     DLBV2340
      Y(I)=0.D0                                                          DLBV2350
      IF(I-K)103,102,103                                                 DLBV2360
  102 Y(I)=1.D0                                                          DLBV2370
  103 DGL=DGL+H*AUX(18,I)                                                DLBV2380
  104 II=II+NDIM                                                         DLBV2390
      XEND=PRMT(1)                                                       DLBV2400
      H=.0625D0*(XEND-X)                                                 DLBV2410
      ISW=0                                                              DLBV2420
      GOTO 400                                                           DLBV2430
C     THIS IS BRANCH TO ADJOINT LINEAR INITIAL VALUE PROBLEM             DLBV2440
C                                                                        DLBV2450
C     THIS IS RETURN FROM ADJOINT LINEAR INITIAL VALUE PROBLEM           DLBV2460
  105 IF(IHLF-10)106,106,117                                             DLBV2470
C                                                                        DLBV2480
C     UPDATING OF COEFFICIENT MATRIX B AND VECTOR R                      DLBV2490
  106 DO 107 I=1,NDIM                                                    DLBV2500
      KK=KK+1                                                            DLBV2510
      H=C(KK)                                                            DLBV2520
      R(I)=AUX(20,I)+H*SUM                                               DLBV2530
      II=I                                                               DLBV2540
      DO 107 J=1,NDIM                                                    DLBV2550
      B(II)=B(II)+H*Y(J)                                                 DLBV2560
  107 II=II+NDIM                                                         DLBV2570
      GOTO 109                                                           DLBV2580
  108 KK=KK+NDIM                                                         DLBV2590
  109 IF(K-NDIM)100,110,110                                              DLBV2600
C                                                                        DLBV2610
C                                                                        DLBV2620
C     GENERATION OF LAST INITIAL VALUE PROBLEM                           DLBV2630
  110 EPS=PRMT(4)                                                        DLBV2640
      CALL DGELG(R,B,NDIM,1,EPS,I)                                       DLBV2650
      IF(I)111,112,112                                                   DLBV2660
  111 IHLF=14                                                            DLBV2670
      RETURN                                                             DLBV2680
C                                                                        DLBV2690
  112 PRMT(5)=0.D0                                                       DLBV2700
      IHLF=-I                                                            DLBV2710
      X=PRMT(1)                                                          DLBV2720
      XEND=PRMT(2)                                                       DLBV2730
      H=PRMT(3)                                                          DLBV2740
      DO 113 I=1,NDIM                                                    DLBV2750
  113 Y(I)=R(I)                                                          DLBV2760
      ISW=1                                                              DLBV2770
  114 ISW2=12                                                            DLBV2780
      GOTO 200                                                           DLBV2790
  115 ISW3=-1                                                            DLBV2800
      GOTO 300                                                           DLBV2810
  116 IF(IHLF)400,400,117                                                DLBV2820
C     THIS WAS BRANCH INTO INITIAL VALUE PROBLEM                         DLBV2830
C                                                                        DLBV2840
C     THIS IS RETURN FROM INITIAL VALUE PROBLEM                          DLBV2850
  117 RETURN                                                             DLBV2860
C                                                                        DLBV2870
C     THIS PART OF LINEAR BOUNDARY VALUE PROBLEM COMPUTES THE RIGHT      DLBV2880
C     HAND SIDE DERY OF THE SYSTEM OF ADJOINT LINEAR DIFFERENTIAL        DLBV2890
C     EQUATIONS (IN CASE ISW=0) OR OF THE GIVEN SYSTEM (IN CASE ISW=1).  DLBV2900
  200 CALL AFCT(X,A)                                                     DLBV2910
      IF(ISW)201,201,205                                                 DLBV2920
C                                                                        DLBV2930
C     ADJOINT SYSTEM                                                     DLBV2940
  201 LL=0                                                               DLBV2950
      DO 203 M=1,NDIM                                                    DLBV2960
      HS=0.D0                                                            DLBV2970
      DO 202 L=1,NDIM                                                    DLBV2980
      LL=LL+1                                                            DLBV2990
  202 HS=HS-A(LL)*Y(L)                                                   DLBV3000
  203 DERY(M)=HS                                                         DLBV3010
  204 GOTO(502,504,506,407,415,418,608,617,632,634,421,115),ISW2         DLBV3020
C                                                                        DLBV3030
C     GIVEN SYSTEM                                                       DLBV3040
  205 CALL FCT(X,DERY)                                                   DLBV3050
      DO 207 M=1,NDIM                                                    DLBV3060
      LL=M-NDIM                                                          DLBV3070
      HS=0.D0                                                            DLBV3080
      DO 206 L=1,NDIM                                                    DLBV3090
      LL=LL+NDIM                                                         DLBV3100
  206 HS=HS+A(LL)*Y(L)                                                   DLBV3110
  207 DERY(M)=HS+DERY(M)                                                 DLBV3120
      GOTO 204                                                           DLBV3130
C                                                                        DLBV3140
C     THIS PART OF LINEAR BOUNDARY VALUE PROBLEM COMPUTES THE VALUE OF   DLBV3150
C     INTEGRAL SUM, WHICH IS A PART OF THE OUTPUT OF ADJOINT INITIAL     DLBV3160
C     VALUE PROBLEM (IN CASE ISW=0) OR RECORDS RESULT VALUES OF THE      DLBV3170
C     FINAL INITIAL VALUE PROBLEM (IN CASE ISW=1).                       DLBV3180
  300 IF(ISW)301,301,305                                                 DLBV3190
C                                                                        DLBV3200
C     ADJOINT PROBLEM                                                    DLBV3210
  301 CALL FCT(X,R)                                                      DLBV3220
      GU=0.D0                                                            DLBV3230
      DGU=0.D0                                                           DLBV3240
      DO 302 L=1,NDIM                                                    DLBV3250
      GU=GU+Y(L)*R(L)                                                    DLBV3260
  302 DGU=DGU+DERY(L)*R(L)                                               DLBV3270
      CALL DFCT(X,R)                                                     DLBV3280
      DO 303 L=1,NDIM                                                    DLBV3290
  303 DGU=DGU+Y(L)*R(L)                                                  DLBV3300
      SUM=SUM+.5D0*H*((GL+GU)+.16666666666666667D0*H*(DGL-DGU))          DLBV3310
      GL=GU                                                              DLBV3320
      DGL=DGU                                                            DLBV3330
  304 IF(ISW3)116,422,618                                                DLBV3340
C                                                                        DLBV3350
C     GIVEN PROBLEM                                                      DLBV3360
  305 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                 DLBV3370
      IF(PRMT(5))117,304,117                                             DLBV3380
C                                                                        DLBV3390
C     POSSIBLE BREAK-POINT FOR LINKAGE                                   DLBV3400
C                                                                        DLBV3410
C     THE FOLLOWING PART OF SUBROUTINE DLBVP SOLVES IN CASE ISW=0 THE    DLBV3420
C     ADJOINT INITIAL VALUE PROBLEM. IT COMPUTES INTEGRAL SUM AND        DLBV3430
C     THE VECTOR Y OF DEPENDENT VARIABLES AT THE LOWER BOUND PRMT(1).    DLBV3440
C     IN CASE ISW=1 IT SOLVES FINALLY GENERATED INITIAL VALUE PROBLEM.   DLBV3450
  400 N=1                                                                DLBV3460
      XST=X                                                              DLBV3470
      IHLF=0                                                             DLBV3480
      DO 401 I=1,NDIM                                                    DLBV3490
      AUX(16,I)=0.D0                                                     DLBV3500
      AUX(1,I)=Y(I)                                                      DLBV3510
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  401 AUX(8,I)=DERY(I)                                                  DLBV3520
      ISW1=1                                                            DLBV3530
      GOTO 500                                                          DLBV3540
C                                                                       DLBV3550
  402 X=X+H                                                             DLBV3560
      DO 403 I=1,NDIM                                                   DLBV3570
  403 AUX(2,I)=Y(I)                                                     DLBV3580
C                                                                       DLBV3590
C     INCREMENT H IS TESTED BY MEANS OF BISECTION                       DLBV3600
  404 IHLF=IHLF+1                                                       DLBV3610
      X=X-H                                                             DLBV3620
      DO 405 I=1,NDIM                                                   DLBV3630
  405 AUX(4,I)=AUX(2,I)                                                 DLBV3640
      H=.500*H                                                          DLBV3650
      N=1                                                               DLBV3660
      ISW1=2                                                            DLBV3670
      GOTO 500                                                          DLBV3680
C                                                                       DLBV3690
  406 X=X+H                                                             DLBV3700
      ISW2=4                                                            DLBV3710
      GOTO 200                                                          DLBV3720
  407 N=2                                                               DLBV3730
      DO 408 I=1,NDIM                                                   DLBV3740
      AUX(2,I)=Y(I)                                                     DLBV3750
  408 AUX(9,I)=DERY(I)                                                  DLBV3760
      ISW1=3                                                            DLBV3770
      GOTO 500                                                          DLBV3780
C                                                                       DLBV3790
C     TEST ON SATISFACTORY ACCURACY                                     DLBV3800
  409 DO 414 I=1,NDIM                                                   DLBV3810
      Z=DABS(Y(I))                                                      DLBV3820
      IF(Z-1.D0)410,411,411                                             DLBV3830
  410 Z=1.D0                                                            DLBV3840
  411 DELT=.0666666666666666670D0*DABS(Y(I)-AUX(4,I))                   DLBV3850
      IF(ISW)413,413,412                                                DLBV3860
  412 DELT=AUX(15,I)*DELT                                               DLBV3870
  413 IF(DELT-Z*PRMT(4))414,414,429                                     DLBV3880
  414 CONTINUE                                                          DLBV3890
C                                                                       DLBV3900
C     SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS               DLBV3910
      X=X+H                                                             DLBV3920
      ISW2=5                                                            DLBV3930
      GOTO 200                                                          DLBV3940
  415 DO 416 I=1,NDIM                                                   DLBV3950
      AUX(3,I)=Y(I)                                                     DLBV3960
  416 AUX(10,I)=DERY(I)                                                 DLBV3970
      N=3                                                               DLBV3980
      ISW1=4                                                            DLBV3990
      GOTO 500                                                          DLBV4000
C                                                                       DLBV4010
  417 N=1                                                               DLBV4020
      X=X+H                                                             DLBV4030
      ISW2=6                                                            DLBV4040
      GOTO 200                                                          DLBV4050
  418 X=XST                                                             DLBV4060
      DO 419 I=1,NDIM                                                   DLBV4070
      AUX(11,I)=DERY(I)                                                 DLBV4080
4190Y(I)=AUX(1,I)+H*(.375D0*AUX(8,I)+.79166666666666670D0*AUX(9,I)      DLBV4090
     1-.208333333333333330D0*AUX(10,I)+.041666666666666670D0*DERY(I))   DLBV4100
  420 X=X+H                                                             DLBV4110
      N=N+1                                                             DLBV4120
      ISW2=11                                                           DLBV4130
      GOTO 200                                                          DLBV4140
  421 ISW3=0                                                            DLBV4150
      GOTO 300                                                          DLBV4160
  422 IF(N-4)423,600,600                                                DLBV4170
  423 DO 424 I=1,NDIM                                                   DLBV4180
      AUX(N,I)=Y(I)                                                     DLBV4190
  424 AUX(N+7,I)=DERY(I)                                                DLBV4200
      IF(N-3)425,427,600                                                DLBV4210
C                                                                       DLBV4220
  425 DO 426 I=1,NDIM                                                   DLBV4230
      DELT=AUX(9,I)+AUX(9,I)                                            DLBV4240
      DELT=DELT+DELT                                                    DLBV4250
  426 Y(I)=AUX(1,I)+.33333333333333330D0*H*(AUX(8,I)+DELT+AUX(10,I))    DLBV4260
      GOTO 420                                                          DLBV4270
C                                                                       DLBV4280
  427 DO 428 I=1,NDIM                                                   DLBV4290
      DELT=AUX(9,I)+AUX(10,I)                                           DLBV4300
      DELT=DELT+DELT+DELT                                               DLBV4310
  428 Y(I)=AUX(1,I)+.375D0*H*(AUX(8,I)+DELT+AUX(11,I))                  DLBV4320
      GOTO 420                                                          DLBV4330
C                                                                       DLBV4340
C     NO SATISFACTORY ACCURACY. H MUST BE HALVED.                       DLBV4350
  429 IF(IHLF-10)404,430,430                                            DLBV4360
C                                                                       DLBV4370
C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.      DLBV4380
  430 IHLF=11                                                           DLBV4390
      X=X+H                                                             DLBV4400
      IF(ISW)105,105,114                                                DLBV4410
C                                                                       DLBV4420
C     THIS PART OF LINEAR INITIAL VALUE PROBLEM COMPUTES                DLBV4430
C     STARTING VALUES BY MEANS OF RUNGE-KUTTA METHOD.                   DLBV4440
  500 Z=X                                                               DLBV4450
      DO 501 I=1,NDIM                                                   DLBV4460
      X=H*AUX(N+7,I)                                                    DLBV4470
      AUX(5,I)=X                                                        DLBV4480
  501 Y(I)=AUX(N,I)+.400*X                                              DLBV4490
C                                                                       DLBV4500
      X=Z+.400*H                                                        DLBV4510
      ISW2=1                                                            DLBV4520
      GOTO 200                                                          DLBV4530
  502 DO 503 I=1,NDIM                                                   DLBV4540
      X=H*DERY(I)                                                       DLBV4550
      AUX(6,I)=X                                                        DLBV4560
  503 Y(I)=AUX(N,I)+.29697760924775360D0*AUX(5,I)+.15875964497103583D0*XDLBV4570
C                                                                       DLBV4580
      X=Z+.45573725421878943D0*H                                        DLBV4590
      ISW2=2                                                            DLBV4600
      GOTO 200                                                          DLBV4610
  504 DO 505 I=1,NDIM                                                   DLBV4620
      X=H*DERY(I)                                                       DLBV4630
      AUX(7,I)=X                                                        DLBV4640
  505 Y(I)=AUX(N,I)+.21810038822592047D0*AUX(5,I)-3.05096514869293080D0* DLBV4650
     1AUX(6,I)+3.83286476046701030D0*X                                  DLBV4660
C                                                                       DLBV4670
      X=Z+H                                                             DLBV4680
      ISW2=3                                                            DLBV4690
      GOTO 200                                                          DLBV4700
  506 DO 507 I=1,NDIM                                                   DLBV4710
  5070Y(I)=AUX(N,I)+.17476028226269037D0*AUX(5,I)-.55148066287873294D0* DLBV4720
     1AUX(6,I)+1.2055355993965235D0*AUX(7,I)+.17118478121951903D0*      DLBV4730
     2H*DERY(I)                                                         DLBV4740
      X=Z                                                               DLBV4750
      GOTO(402,406,409,417),ISW1                                        DLBV4760
C                                                                       DLBV4770
C     POSSIBLE BREAK-POINT FOR LINKAGE                                  DLBV4780
C                                                                       DLBV4790
C     STARTING VALUES ARE COMPUTED.                                     DLBV4800
C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.           DLBV4810
  600 ISTEP=3                                                           DLBV4820
  601 IF(N-8)604,602,604                                                DLBV4830
C                                                                       DLBV4840
C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS      DLBV4850
  602 DO 603 N=2,7                                                      DLBV4860
      DO 603 I=1,NDIM                                                   DLBV4870
      AUX(N-1,I)=AUX(N,I)                                               DLBV4880
  603 AUX(N+6,I)=AUX(N+7,I)                                             DLBV4890
      N=7                                                               DLBV4900
C                                                                       DLBV4910
C     N LESS THAN 8 CAUSES N+1 TO GET N                                 DLBV4920
  604 N=N+1                                                             DLBV4930
C                                                                       DLBV4940
C     COMPUTATION OF NEXT VECTOR Y                                      DLBV4950
      DO 605 I=1,NDIM                                                   DLBV4960
      AUX(N-1,I)=Y(I)                                                   DLBV4970
  605 AUX(N+6,I)=DERY(I)                                                DLBV4980
      X=X+H                                                             DLBV4990
  606 ISTEP=ISTEP+1                                                     DLBV5000
      DO 607 I=1,NDIM                                                   DLBV5010
      ODELT=AUX(N-4,I)+1.3333333333333333D0*H*(AUX(N+6,I)+AUX(N+6,I)-   DLBV5020
     1AUX(N+5,I)+AUX(N+4,I)+AUX(N+4,I))                                 DLBV5030
      Y(I)=DELT-.92561983471074380D0*AUX(16,I)                          DLBV5040
  607 AUX(16,I)=DELT                                                    DLBV5050
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR   DLBV5060
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.               DLBV5070
C                                                                       DLBV5080
      ISW2=7                                                            DLBV5090
      GOTO 200                                                          DLBV5100
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY.            DLBV5110
C                                                                       DLBV5120
  608 DO 609 I=1,NDIM                                                   DLBV5130
      ODELT=.125D0*(9.D0*AUX(N-1,I)-AUX(N-3,I)+3.D0*H*(DERY(I)+AUX(N+6,I)DLBV5140
     1+AUX(N+6,I)-AUX(N+5,I)))                                          DLBV5150
      AUX(16,I)=AUX(16,I)-DELT                                          DLBV5160
  609 Y(I)=DELT+.074380165289256200D0*AUX(16,I)                         DLBV5170
C                                                                       DLBV5180
C     TEST WHETHER H MUST BE HALVED OR DOUBLED                          DLBV5190
      DELT=0.D0                                                         DLBV5200
      DO 616 I=1,NDIM                                                   DLBV5210
      Z=DABS(Y(I))                                                      DLBV5220
      IF(Z-1.D0)610,611,611                                             DLBV5230
  610 Z=1.D0                                                            DLBV5240
  611 Z=DABS(AUX(16,I))/Z                                               DLBV5250
      IF(ISW)613,613,612                                                DLBV5260
  612 Z=AUX(15,I)*Z                                                     DLBV5270
  613 IF(Z-PRMT(4))614,614,628                                          DLBV5280
  614 IF(DELT-Z)615,616,616                                             DLBV5290
  615 DELT=Z                                                            DLBV5300
  616 CONTINUE                                                          DLBV5310
C                                                                       DLBV5320
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                   DLBV5330
      ISW2=8                                                            DLBV5340
      GOTO 200                                                          DLBV5350
  617 ISW3=1                                                            DLBV5360
      GOTO 300                                                          DLBV5370
  618 IF(H*(X-XEND))619,621,621                                         DLBV5380
  619 IF(DABS(X-XEND)-.100*DABS(H))621,620,620                          DLBV5390
  620 IF(DELT-.02D0*PRMT(4))622,622,601                                 DLBV5400
  621 IF(ISW)105,105,117                                                DLBV5410
C                                                                       DLBV5420
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE         DLBV5430
C     AVAILABLE.                                                        DLBV5440
  622 IF(IHLF)601,601,623                                               DLBV5450
  623 IF(N-7)601,624,624                                                DLBV5460
  624 IF(ISTEP-4)601,625,625                                            DLBV5470
  625 IMOD=ISTEP/2                                                      DLBV5480
      IF(ISTEP-IMOD-IMOD)601,626,601                                    DLBV5490
  626 H=H+H                                                             DLBV5500
      IHLF=IHLF-1                                                       DLBV5510
      ISTEP=0                                                           DLBV5520
      DO 627 I=1,NDIM                                                   DLBV5530
      AUX(N-1,I)=AUX(N-2,I)                                             DLBV5540
      AUX(N-2,I)=AUX(N-4,I)                                             DLBV5550
      AUX(N-3,I)=AUX(N-6,I)                                             DLBV5560
      AUX(N+6,I)=AUX(N+5,I)                                             DLBV5570
      AUX(N+5,I)=AUX(N+3,I)                                             DLBV5580
      AUX(N+4,I)=AUX(N+1,I)                                             DLBV5590
      DELT=AUX(N+6,I)+AUX(N+5,I)                                        DLBV5600
      DELT=DELT+DELT+DELT                                               DLBV5610
  627OAUX(16,I)=8.9629629629629630D0*(Y(I)-AUX(N-3,I))                  DLBV5620
     1-3.3611111111111111D0*H*(DERY(I)+DELT+AUX(N+4,I))                 DLBV5630
      GOTO 601                                                          DLBV5640
C                                                                       DLBV5650
C     H MUST BE HALVED                                                  DLBV5660
  628 IHLF=IHLF+1                                                       DLBV5670
      IF(IHLF-10)630,630,629                                            DLBV5680
  629 IF(ISW)105,105,114                                                DLBV5690
  630 H=.500*H                                                          DLBV5700
      ISTEP=0                                                           DLBV5710
      DO 631 I=1,NDIM                                                   DLBV5720
      OY(I)=.3906250-2*(8.D1*AUX(N-1,I)+135.D0*AUX(N-2,I)+4.D1*AUX(N-3,I)DLBV5730
     1+AUX(N-4,I))-.1171875D0*(AUX(N+6,I)-6.D0*AUX(N+5,I)-AUX(N+4,I))*H DLBV5740
     OAUX(N-4,I)=.3906250-2*(12.D0*AUX(N-1,I)+135.D0*AUX(N-2,I)+        DLBV5750
     1108.D0*AUX(N-3,I)+AUX(N-4,I))-.0234375D0*(AUX(N+6,I)+             DLBV5760
     218.D0*AUX(N+5,I)-9.D0*AUX(N+4,I))*H                               DLBV5770
      AUX(N-3,I)=AUX(N-2,I)                                             DLBV5780
  631 AUX(N+4,I)=AUX(N+5,I)                                             DLBV5790
      DELT=X-H                                                          DLBV5800
      X=DELT-(H+H)                                                      DLBV5810
      ISW2=9                                                            DLBV5820
      GOTO 200                                                          DLBV5830
  632 DO 633 I=1,NDIM                                                   DLBV5840
      AUX(N-2,I)=Y(I)                                                   DLBV5850
      AUX(N+5,I)=DERY(I)                                                DLBV5860
  633 Y(I)=AUX(N-4,I)                                                   DLBV5870
      X=X-(H+H)                                                         DLBV5880
      ISW2=10                                                           DLBV5890
      GOTO 200                                                          DLBV5900
  634 X=DELT                                                            DLBV5910
      DO 635 I=1,NDIM                                                   DLBV5920
      DELT=AUX(N+5,I)+AUX(N+4,I)                                        DLBV5930
      DELT=DELT+DELT+DELT                                               DLBV5940
     OAUX(16,I)=8.9629629629629630D0*(AUX(N-1,I)-Y(I))                  DLBV5950
     1-3.3611111111111111D0*H*(AUX(N+6,I)+DELT+DERY(I))                 DLBV5960
  635 AUX(N+3,I)=DERY(I)                                                DLBV5970
      GOTO 606                                                          DLBV5980
C     END OF INITIAL VALUE PROBLEM                                      DLBV5990
      END                                                               DLBV6000
```

Subroutine GMMMA

This subroutine computes the value of the gamma function for a given argument x.
The calculation of the gamma function, $\Gamma(x)$ is defined for $x > 0$ by:

$$\Gamma(x) = \int_0^{\infty} t^{x-1} \cdot e^{-t}\, dt \qquad (1)$$

This function satisfies the recurrence relation:

$$\Gamma(x) = (x-1) \cdot \Gamma(x-1) \qquad (2)$$

which defines $\Gamma(x)$ for any x not a negative integer.

Note that when x is a positive integer, $\Gamma(x) = (x-1)!$

To compute $\Gamma(x)$ for $x > 1$, apply the recurrence (2), r times until $1 < x - r = y \leq 2$. Thus, for $x > 1$:

$$\Gamma(x) = (x-1)\ (x-2)\ \ldots\ (x-r)\ \ \Gamma(y) \qquad (3)$$

$\Gamma(y)$ is computed from the following formula:

$$\begin{aligned}\Gamma(y) \approx 1 &- 0.57710166(y-1) + 0.98585399(y-1)^2 \\ &- 0.87642182(y-1)^3 + 0.83282120(y-1)^4 \\ &- 0.56847290(y-1)^5 + 0.25482049(y-1)^6 \\ &- 0.05149930(y-1)^7\end{aligned} \qquad (4)$$

For $x < 1$, the recurrence (2) is taken in the direction of decreasing n, giving:

$$\Gamma(x) = \frac{\Gamma(y)}{x(x+1)\ (x+2)\ \ldots\ (x+r-1)} \qquad (5)$$

where $1 < x + r = y \leq 2$.

As before, $\Gamma(y)$ is computed using equation (4).

```
C                                                                       GMMM  10
C     .................................................................GMMM  20
C                                                                       GMMM  30
C        SUBROUTINE GMMMA                                               GMMM  40
C                                                                       GMMM  50
C        PURPOSE                                                        GMMM  60
C           COMPUTES THE GAMMA FUNCTION FOR A GIVEN ARGUMENT            GMMM  70
C                                                                       GMMM  80
C        USAGE                                                          GMMM  90
C           CALL GMMMA(XX,GX,IER)                                       GMMM 100
C                                                                       GMMM 110
C        DESCRIPTION OF PARAMETERS                                      GMMM 120
C           XX -THE ARGUMENT FOR THE GAMMA FUNCTION                     GMMM 130
C           GX -THE RESULTANT GAMMA FUNCTION VALUE                      GMMM 140
C           IER-RESULTANT ERROR CODE WHERE                              GMMM 150
C               IER=0  NO ERROR                                         GMMM 160
C               IER=1  XX IS WITHIN .000001 OF BEING A NEGATIVE INTEGER GMMM 170
C               IER=2  XX GT 57, OVERFLOW, GX SET TO 1.0E75             GMMM 180
C                                                                       GMMM 190
C        REMARKS                                                        GMMM 200
C           NONE                                                        GMMM 210
C                                                                       GMMM 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  GMMM 230
C           NONE                                                        GMMM 240
C                                                                       GMMM 250
C        METHOD                                                         GMMM 260
C           THE RECURSION RELATION AND POLYNOMIAL APPROXIMATION         GMMM 270
C           BY C.HASTINGS,JR., 'APPROXIMATIONS FOR DIGITAL COMPUTERS',  GMMM 280
C           PRINCETON UNIVERSITY PRESS, 1955                            GMMM 290
C                                                                       GMMM 300
C     .................................................................GMMM 310
C                                                                       GMMM 320
      SUBROUTINE GMMMA(XX,GX,IER)                                       GMMM 330
      IF(XX-57.16,6,4                                                   GMMM 340
    4 IER=2                                                             GMMM 350
      GX=1.E75                                                          GMMM 360
      RETURN                                                            GMMM 370
    6 X=XX                                                              GMMM 380
      ERR=1.0E-6                                                        GMMM 390
      IER=0                                                             GMMM 400
      GX=1.0                                                            GMMM 410
      IF(X-2.0)50,50,15                                                 GMMM 420
   10 IF(X-2.0)110,110,15                                               GMMM 430
   15 X=X-1.0                                                           GMMM 440
      GX=GX*X                                                           GMMM 450
      GO TO 10                                                          GMMM 460
   50 IF(X-1.0)60,120,110                                               GMMM 470
C                                                                       GMMM 480
C        SEE IF X IS NEAR NEGATIVE INTEGER OR ZERO                      GMMM 490
C                                                                       GMMM 500
   60 IF(X-ERR)62,62,80                                                 GMMM 510
   62 Y=FLOAT(INT(X))-X                                                 GMMM 520
      IF(ABS(Y)-ERR)130,130,64                                          GMMM 530
   64 IF(1.0-Y-ERR)130,130,70                                           GMMM 540
C                                                                       GMMM 550
C        X NOT NEAR A NEGATIVE INTEGER OR ZERO                          GMMM 560
C                                                                       GMMM 570
   70 IF(X-1.0)80,80,110                                                GMMM 580
   80 GX=GX/X                                                           GMMM 590
      X=X+1.0                                                           GMMM 600
      GO TO 70                                                          GMMM 610
  110 Y=X-1.0                                                           GMMM 620
      GY=1.0+Y*(-0.5771017+Y*(+0.9858540+Y*(-0.8764218+Y*(+0.8328212+   GMMM 630
     1Y*(-0.5684729+Y*(+0.2548205+Y*(-0.0514993))))))                   GMMM 640
      GX=GX*GY                                                          GMMM 650
  120 RETURN                                                            GMMM 660
  130 IER=1                                                             GMMM 670
      RETURN                                                            GMMM 680
      END                                                               GMMM 690
```

Subroutine DLGAM

This subroutine computes the double-precision natural logarithm of the gamma function of a given double-precision argument, x, where $10^{-9} < x < 10^{70}$. The Euler-McLaurin expansion, to the seventh derivative term, is used. For $x > 0$:

$$\log \Gamma(x) \simeq (x - 1/2) \log x + 1/2 \log 2\pi - x + 1/12\, x - 1/360\, x^3 + 1/1260\, x^5 - 1/1680\, x^7 \qquad (1)$$

This expression is very accurate for $x > 18$. If $x \leq 18$, x is replaced by $z = k + x$, where k is an integer such that $z > 18$. Log $\Gamma(z)$ is then evaluated by (1), and $\log x + \log (x + 1) + \ldots + \log (x + k - 1)$ is subtracted to obtain the desired result.

If x is between 10^{10} and 10^{70}, terms of lowest order in (1) are neglected, and $\log \Gamma(x)$ is computed as:

$$\log \Gamma(x) = x (\log (x) - 1) \qquad (2)$$

Subroutine DLGAM is available in a double-precision format only. If the single-precision value of the log gamma function of a given single-precision argument is desired, subroutine GMMMA should be used along with the FORTRAN-supplied natural logarithm function.

For reference see M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions. U.S. Department of Commerce, National Bureau of Standards Applied Mathematics Series, 1966, equation 6.1.41.

```
C                                                                       DLGA  10
C     ..................................................................DLGA  20
C                                                                       DLGA  30
C        SUBROUTINE DLGAM                                               DLGA  40
C                                                                       DLGA  50
C        PURPOSE                                                        DLGA  60
C           COMPUTES THE DOUBLE PRECISION NATURAL LOGARITHM OF THE      DLGA  70
C           GAMMA FUNCTION OF A GIVEN DOUBLE PRECISION ARGUMENT.        DLGA  80
C                                                                       DLGA  90
C        USAGE                                                          DLGA 100
C           CALL DLGAM(XX,DLNG,IER)                                     DLGA 110
C                                                                       DLGA 120
C        DESCRIPTION OF PARAMETERS                                      DLGA 130
C           XX   - THE DOUBLE PRECISION ARGUMENT FOR THE LOG GAMMA      DLGA 140
C                  FUNCTION.                                            DLGA 150
C           DLNG - THE RESULTANT DOUBLE PRECISION LOG GAMMA FUNCTION    DLGA 160
C                  VALUE.                                               DLGA 170
C           IER  - RESULTANT ERROR CODE WHERE                           DLGA 180
C                  IER= 0----NO ERROR.                                  DLGA 190
C                  IER=-1----XX IS WITHIN 10**(-9) OF BEING ZERO OR XX  DLGA 200
C                            IS NEGATIVE.  DLNG IS SET TO -1.0D75.      DLGA 210
C                  IER=+1----XX IS GREATER THAN 10**70. DLNG IS SET TO  DLGA 220
C                            +1.0D75.                                   DLGA 230
C                                                                       DLGA 240
C        REMARKS                                                        DLGA 250
C           NONE                                                        DLGA 260
C                                                                       DLGA 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DLGA 280
C           NONE                                                        DLGA 290
C                                                                       DLGA 300
C        METHOD                                                         DLGA 310
C           THE EULER-MCLAURIN EXPANSION TO THE SEVENTH DERIVATIVE TERM DLGA 320
C           IS USED, AS GIVEN BY M. ABRAMOWITZ AND I.A. STEGUN,         DLGA 330
C           'HANDBOOK OF MATHEMATICAL FUNCTIONS', U. S. DEPARTMENT OF   DLGA 340
C           COMMERCE, NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS  DLGA 350
C           SERIES. 1966, EQUATION 6.1.41.                              DLGA 360
C                                                                       DLGA 370
C     ..................................................................DLGA 380
C                                                                       DLGA 390
      SUBROUTINE DLGAM(XX,DLNG,IER)                                     DLGA 400
      DOUBLE PRECISION XX,ZZ,TERM,RZZ,DLNG                              DLGA 410
      IER=0                                                             DLGA 420
      ZZ=XX                                                             DLGA 430
      IF(XX-1.D10) 2,2,1                                                DLGA 440
    1 IF(XX-1.D70) 8,9,9                                                DLGA 450
C                                                                       DLGA 460
C        SEE IF XX IS NEAR ZERO OR NEGATIVE                             DLGA 470
C                                                                       DLGA 480
    2 IF(XX-1.D-9) 3,3,4                                                DLGA 490
    3 IER=-1                                                            DLGA 500
      DLNG=-1.D75                                                       DLGA 510
      GO TO 10                                                          DLGA 520
C                                                                       DLGA 530
C        XX GREATER THAN ZERO AND LESS THAN OR EQUAL TO 1.D+10          DLGA 540
C                                                                       DLGA 550
    4 TERM=1.D0                                                         DLGA 560
    5 IF(ZZ-18.D0) 6,6,7                                                DLGA 570
    6 TERM=TERM*ZZ                                                      DLGA 580
      ZZ=ZZ+1.D0                                                        DLGA 590
      GO TO 5                                                           DLGA 600
    7 RZZ=1.D0/ZZ**2                                                    DLGA 610
      DLNG =(ZZ-.5D0)*DLOG(ZZ)-ZZ +0.9189385332046727 -DLOG(TERM)+      DLGA 620
     1(1.D0/ZZ)*(.8333333333333333D-1 -(RZZ*(.2777777777777777D-2 +(RZZ*DLGA 630
     2(.7936507936507936D-3 -(RZZ*(.5952380952380952D-3))))))))         DLGA 640
      GO TO 10                                                          DLGA 650
C                                                                       DLGA 660
C        XX GREATER THAN 1.D+10 AND LESS THAN 1.D+70                    DLGA 670
C                                                                       DLGA 680
    8 DLNG=ZZ*(DLOG(ZZ)-1.D0)                                           DLGA 690
      GO TO 10                                                          DLGA 700
C                                                                       DLGA 710
C        XX GREATER THAN OR EQUAL TO 1.D+70                             DLGA 720
C                                                                       DLGA 730
    9 IER=+1                                                            DLGA 740
      DLNG=1.D75                                                        DLGA 750
   10 RETURN                                                            DLGA 760
      END                                                               DLGA 770
```

Subroutine BESJ

This subroutine computes the J Bessel function for a given argument and integer order by using the recurrence relationship:

$$F_{n+1}(x) + F_{n-1}(x) = \left(\frac{2n}{x}\right) F_n(x) \qquad (1)$$

The desired Bessel function is:

$$J_n(x) = \frac{F_n(x)}{\alpha} \qquad (2)$$

where:

$$\alpha = F_0(x) + 2 \sum_{m=1}^{M-2} F_{2m}(x) \qquad (3)$$

M is initialized at M_0.

M_0 is the greater of M_A and M_B where;

$$M_A = \begin{cases} [x+6] & \text{if } x < 5 \\ [1.4x+60/x] & \text{if } x \geq 5 \end{cases}$$

$$M_B = [n+x/4+2]$$

F_{M-2}, F_{M-3}, ..., F_2, F_1, F_0 is evaluated using equation (1) with $F_M = 0$ and $F_{M-1} = 10^{-30}$. Values of α and $J_n(x)$ are then computed using equations (3) and (2) respectively.

The computation is repeated for M+3.

The values of $J_n(x)$ for M and M+3 are compared:

$$\text{If } \left| J_n(x)_M - J_n(x)_{M+3} \right| \leq \delta \left| J_n(x)_{M+3} \right|$$

this value is accepted as $J_n(x)$; if not, the computation is repeated by adding 3 to M and using this as a new value for M. If M reaches M_{MAX} before the desired accuracy is obtained, execution is terminated. M_{MAX} is defined as:

$$M_{MAX} = \begin{cases} \left[20 + 10x - \frac{x^2}{3}\right] & \text{for } x \leq 15 \\ [90 + x/2] & \text{for } x > 15 \end{cases} \qquad (4)$$

```
C                                                                       BESJ  10
C     ..................................................................BESJ  20
C                                                                       BESJ  30
C        SUBROUTINE BESJ                                                BESJ  40
C                                                                       BESJ  50
C        PURPOSE                                                        BESJ  60
C           COMPUTE THE J BESSEL FUNCTION FOR A GIVEN ARGUMENT AND ORDERBESJ  70
C                                                                       BESJ  80
C        USAGE                                                          BESJ  90
C           CALL BESJ(X,N,BJ,D,IER)                                     BESJ 100
C                                                                       BESJ 110
C        DESCRIPTION OF PARAMETERS                                      BESJ 120
C           X  -THE ARGUMENT OF THE J BESSEL FUNCTION DESIRED           BESJ 130
C           N  -THE ORDER OF THE J BESSEL FUNCTION DESIRED              BESJ 140
C           BJ -THE RESULTANT J BESSEL FUNCTION                         BESJ 150
C           D  -REQUIRED ACCURACY                                       BESJ 160
C           IER-RESULTANT ERROR CODE WHERE                              BESJ 170
C              IER=0  NO ERROR                                          BESJ 180
C              IER=1  N IS NEGATIVE                                     BESJ 190
C              IER=2  X IS NEGATIVE OR ZERO                             BESJ 200
C              IER=3  REQUIRED ACCURACY NOT OBTAINED                    BESJ 210
C              IER=4  RANGE OF N COMPARED TO X NOT CORRECT (SEE REMARKS)BESJ 220
C                                                                       BESJ 230
C        REMARKS                                                        BESJ 240
C           N MUST BE GREATER THAN OR EQUAL TO ZERO, BUT IT MUST BE     BESJ 250
C           LESS THAN                                                   BESJ 260
C              20+10*X-X** 2/3   FOR X LESS THAN OR EQUAL TO 15         BESJ 270
C              90+X/2            FOR X GREATER THAN 15                  BESJ 280
C                                                                       BESJ 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  BESJ 300
C           NONE                                                        BESJ 310
C                                                                       BESJ 320
C        METHOD                                                         BESJ 330
C           RECURRENCE RELATION TECHNIQUE DESCRIBED BY H. GOLDSTEIN AND BESJ 340
C           R.M. THALER,'RECURRENCE TECHNIQUES FOR THE CALCULATION OF   BESJ 350
C           BESSEL FUNCTIONS',M.T.A.C.,V.13,PP.102-108 AND I.A. STEGUN  BESJ 360
C           AND M. ABRAMOWITZ,'GENERATION OF BESSEL FUNCTIONS ON HIGH   BESJ 370
C           SPEED COMPUTERS',M.T.A.C.,V.11,1957,PP.255-257              BESJ 380
C                                                                       BESJ 390
C     ..................................................................BESJ 400
C                                                                       BESJ 410
      SUBROUTINE BESJ(X,N,BJ,D,IER)                                     BESJ 420
C                                                                       BESJ 430
      BJ=.0                                                             BESJ 440
      IF(N)10,20,20                                                     BESJ 450
   10 IER=1                                                             BESJ 460
      RETURN                                                            BESJ 470
   20 IF(X)30,30,31                                                     BESJ 480
   30 IER=2                                                             BESJ 490
      RETURN                                                            BESJ 500
   31 IF(X-15.)32,32,34                                                 BESJ 510
   32 NTEST=20.+10.*X-X** 2/3                                           BESJ 520
      GO TO 36                                                          BESJ 530
   34 NTEST=90.+X/2.                                                    BESJ 540
   36 IF(N-NTEST)40,38,38                                               BESJ 550
   38 IER=4                                                             BESJ 560
      RETURN                                                            BESJ 570
   40 IER=0                                                             BESJ 580
      N1=N+1                                                            BESJ 590
      BPREV=.0                                                          BESJ 600
C                                                                       BESJ 610
C     COMPUTE STARTING VALUE OF M                                       BESJ 620
C                                                                       BESJ 630
      IF(X-5.)50,60,60                                                  BESJ 640
   50 MA=X+6.                                                           BESJ 650
      GO TO 70                                                          BESJ 660
   60 MA=1.4*X+60./X                                                    BESJ 670
   70 MB=N+IFIX(X)/4+2                                                  BESJ 680
      MZERO=MAX0(MA,MB)                                                 BESJ 690
C                                                                       BESJ 700
C     SET UPPER LIMIT OF M                                              BESJ 710
C                                                                       BESJ 720
      MMAX=NTEST                                                        BESJ 730
  100 DO 190 M=MZERO,MMAX,3                                             BESJ 740
C                                                                       BESJ 750
C     SET F(M),F(M-1)                                                   BESJ 760
C                                                                       BESJ 770
      FM1=1.0E-28                                                       BESJ 780
      FM=.0                                                             BESJ 790
      ALPHA=.0                                                          BESJ 800
      IF(M-(M/2)*2)120,110,120                                          BESJ 810
  110 JT=-1                                                             BESJ 820
      GO TO 130                                                         BESJ 830
  120 JT=1                                                              BESJ 840
  130 M2=M-2                                                            BESJ 850
      DO 160 K=1,M2                                                     BESJ 860
      MK=M-K                                                            BESJ 870
      BMK=2.*FLOAT(MK)*FM1/X-FM                                         BESJ 880
      FM=FM1                                                            BESJ 890
      FM1=BMK                                                           BESJ 900
      IF(MK-N-1)150,140,150                                             BESJ 910
  140 BJ=BMK                                                            BESJ 920
  150 JT=-JT                                                            BESJ 930
      S=1+JT                                                            BESJ 940
  160 ALPHA=ALPHA+BMK*S                                                 BESJ 950
      BMK=2.*FM1/X-FM                                                   BESJ 960
      IF(N)180,170,180                                                  BESJ 970
  170 BJ=BMK                                                            BESJ 980
  180 ALPHA=ALPHA+BMK                                                   BESJ 990
      BJ=BJ/ALPHA                                                       BESJ1000
      IF(ABS(BJ-BPREV)-ABS(D*BJ))200,200,190                            BESJ1010
  190 BPREV=BJ                                                          BESJ1020
      IER=3                                                             BESJ1030
  200 RETURN                                                            BESJ1040
      END                                                               BESJ1050
```

Subroutine BESY

This subroutine computes the Y Bessel function for a given argument x and order n. The recurrence relation:

$$Y_{n+1}(x) = \left(\frac{2n}{x}\right) \cdot Y_n(x) - Y_{n-1}(x) \qquad (1)$$

is used for this evaluation.

For $x > 4$

$$Y_0(x) = \sqrt{\frac{2}{\pi x}} \left(P_0(x) \sin\left(x - \frac{\pi}{4}\right) + Q_0(x) \cos\left(x - \frac{\pi}{4}\right) \right) \qquad (2)$$

$$Y_1(x) = \sqrt{\frac{2}{\pi x}} \left(-P_1(x) \cos\left(x - \frac{\pi}{4}\right) + Q_1(x) \sin\left(x - \frac{\pi}{4}\right) \right) \qquad (3)$$

$P_0(x)$, $Q_0(x)$, $P_1(x)$, and $Q_1(x)$ are:

$$\frac{1}{\sqrt{2\pi}} P_0\left(\frac{4}{t}\right) = 0.3989422793 - 0.0017530620t^2 + 0.0001734300t^4 - 0.0000487613t^6 + 0.0000173565t^8 - 0.0000037043t^{10} \qquad (4)$$

$$t\frac{1}{\sqrt{2\pi}} Q_0\left(\frac{4}{t}\right) = -0.0124669441 + 0.0004564324t^2 - 0.0000869791t^4 + 0.0000342468t^6 - 0.0000142078t^8 + 0.0000032312t^{10} \qquad (5)$$

$$\frac{1}{\sqrt{2\pi}} P_1\left(\frac{4}{t}\right) = 0.3989422819 + 0.0029218256t^2 - 0.0002232030t^4 + 0.0000580759t^6 - 0.0000200920t^8 + 0.0000042414t^{10} \qquad (6)$$

$$t\frac{1}{\sqrt{2\pi}} Q_1\left(\frac{4}{t}\right) = 0.0374008364 - 0.0006390400t^2 - 0.0001064741t^4 - 0.0000398708t^6 - 0.0000162200t^8 - 0.0000042414t^{10} \qquad (7)$$

where $t = \frac{4}{x}$

For $x \leq 4$

$$Y_0(x) = \frac{2}{\pi} \sum_{m=0}^{15} (-1)^m \left(\frac{x}{2}\right)^{2m} \frac{1}{(m!)^2} \left[\log\frac{x}{2} + \gamma - H_m \right] \qquad (8)$$

where:

$$H_m = \begin{cases} \sum_{r=1}^{m} \frac{1}{r} & \text{if } m \geq 1 \\ 0 & \text{if } m = 0 \end{cases} \qquad (9)$$

and γ = Euler's constant = 0.5772156649

$$Y_1(x) = -\frac{2}{\pi x} + \frac{2}{\pi} \sum_{m=1}^{16} (-1)^{m+1} \left(\frac{x}{2}\right)^{2m-1} \frac{1}{m!\,(m-1)!} \cdot \left[\log\frac{x}{2} + \gamma - H_m + \frac{1}{2m} \right] \qquad (10)$$

```
C                                                                       BESY  10
C     .................................................................BESY  20
C                                                                       BESY  30
C        SUBROUTINE BESY                                                BESY  40
C                                                                       BESY  50
C        PURPOSE                                                        BESY  60
C           COMPUTE THE Y BESSEL FUNCTION FOR A GIVEN ARGUMENT AND ORDERBESY  70
C                                                                       BESY  80
C        USAGE                                                          BESY  90
C           CALL BESY(X,N,BY,IER)                                       BESY 100
C                                                                       BESY 110
C        DESCRIPTION OF PARAMETERS                                      BESY 120
C           X  -THE ARGUMENT OF THE Y BESSEL FUNCTION DESIRED           BESY 130
C           N  -THE ORDER OF THE Y BESSEL FUNCTION DESIRED              BESY 140
C           BY -THE RESULTANT Y BESSEL FUNCTION                         BESY 150
C           IER-RESULTANT ERROR CODE WHERE                              BESY 160
C              IER=0  NO ERROR                                          BESY 170
C              IER=1  N IS NEGATIVE                                     BESY 180
C              IER=2  X IS NEGATIVE OR ZERO                             BESY 190
C              IER=3  BY HAS EXCEEDED MAGNITUDE OF 10**70               BESY 200
C                                                                       BESY 210
C        REMARKS                                                        BESY 220
C           VERY SMALL VALUES OF X MAY CAUSE THE RANGE OF THE LIBRARY   BESY 230
C           FUNCTION ALOG TO BE EXCEEDED                                BESY 240
C           X MUST BE GREATER THAN ZERO                                 BESY 250
C           N MUST BE GREATER THAN OR EQUAL TO ZERO                     BESY 260
C                                                                       BESY 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  BESY 280
C           NONE                                                        BESY 290
C                                                                       BESY 300
C        METHOD                                                         BESY 310
C           RECURRENCE RELATION AND POLYNOMIAL APPROXIMATION TECHNIQUE  BESY 320
C           AS DESCRIBED BY A.J.M.HITCHCOCK,*POLYNOMIAL APPROXIMATIONS  BESY 330
C           TO BESSEL FUNCTIONS OF ORDER ZERO AND ONE AND TO RELATED    BESY 340
C           FUNCTIONS*, M.T.A.C., V.11,1957,PP.86-88, AND G.N. WATSON,  BESY 350
C           *A TREATISE ON THE THEORY OF BESSEL FUNCTIONS*, CAMBRIDGE    BESY 360
C           UNIVERSITY PRESS, 1958, P. 62                               BESY 370
C                                                                       BESY 380
C     .................................................................BESY 390
```

```
C
      SUBROUTINE BESY(X,N,BY,IER)
C
C     CHECK FOR ERRORS IN N AND X
C
      IF(N)180,10,10
   10 IER=0
      IF(X)190,190,20
C
C     BRANCH IF X LESS THAN OR EQUAL 4
C
   20 IF(X-4.0)40,40,30
C
C       COMPUTE Y0 AND Y1 FOR X GREATER THAN 4
C
   30 T1=4.0/X
      T2=T1*T1
      P0=((((-.000003704 3*T2+.0000173565)*T2-.0000487613)*T2
     1  +.00017343)*T2-.0017530621)*T2+.3989423
      Q0=((((.0000032312*T2-.0000142078)*T2+.0000342468)*T2
     1  -.0000869791)*T2+.0004564324)*T2-.01246694
      P1=((((.0000042414*T2-.0000200920)*T2+.0000580759)*T2
     1  -.0002232031)*T2+.0029218261)*T2+.3989423
      Q1=((((-.0000036594*T2+.0000162213)*T2-.0000398708)*T2
     1  +.0001064741)*T2-.0006390400)*T2+.03740084
      A=2.0/SQRT(X)
      B=A*T1
      C=X-.7853982
      Y0=A*P0*SIN(C)+B*Q0*COS(C)
      Y1=-A*P1*COS(C)+B*Q1*SIN(C)
      GO TO 90
C
C       COMPUTE Y0 AND Y1 FOR X LESS THAN OR EQUAL TO 4
C
   40 XX=X/2.
      X2=XX*XX
      T=ALOG(XX)+.5772157
      SUM=0.
      TERM=T
      Y0=T
      DO 70 L=1,15
      IF(L-1)50,60,50
   50 SUM=SUM+1./FLOAT(L-1)
   60 FL=L
      TS=T-SUM
      TERM=(TERM*(-X2)/FL**2)*(1.-1./(FL*TS))
   70 Y0=Y0+TERM
      TERM = XX*(T-.5)
      SUM=0.
      Y1=TERM
      DO 80 L=2,16
      SUM=SUM+1./FLOAT(L-1)
      FL=L
      FL1=FL-1.
      TS=T-SUM
      TERM=(TERM*(-X2)/(FL1*FL))*((TS-.5/FL)/(TS+.5/FL1))
   80 Y1=Y1+TERM
      PI2=.6366198
      Y0=PI2*Y0
      Y1=-PI2/X+PI2*Y1
C
C     CHECK IF ONLY Y0 OR Y1 IS DESIRED
C
   90 IF(N-1)100,100,130
C
C     RETURN EITHER Y0 OR Y1 AS REQUIRED
C
  100 IF(N)110,120,110
  110 BY=Y1
      GO TO 170
  120 BY=Y0
      GO TO 170
C
C    PERFORM RECURRENCE OPERATIONS TO FIND YN(X)
C
  130 YA=Y0
      YB=Y1
      K=1
  140 T=FLOAT(2*K)/X
      YC=T*YB-YA
      IF(ABS(YC)-1.0E70)145,145,141
  141 IER=3
      RETURN
  145 K=K+1
      IF(K-N)150,160,150
  150 YA=YB
      YB=YC
      GO TO 140
  160 BY=YC
  170 RETURN
  180 IER=1
      RETURN
  190 IER=2
      RETURN
      END
```

Subroutine I0

This subroutine computes the modified Bessel function $I_0(x)$ for a given argument (x).

For $-3.75 \leq x \leq 3.75$; $t = x/3.75$

$$I_0(x) = 1 + 3.515623t^2 + 3.089942t^4 + 1.206749t^6 + 0.2659732t^8 + 0.0360768t^{10} + 0.0045813t^{12} + \epsilon$$

with $|\epsilon| < 1.6 \cdot 10^{-7}$

For $3.75 \leq |x| < \infty$; $t = 3.75/|x|$

$$\sqrt{|x|}\, e^{-|x|} I_0(x) = 0.3989423 + 0.01328592t + 0.00225319t^2 - 0.00157565t^3 + 0.00916281t^4 - 0.02057706t^5 + 0.02635537t^6 - 0.01647633t^7 + 0.00392377t^8 + \epsilon$$

with $|\epsilon| < 1.9 \cdot 10^{-7}$

```
C                                                                       I0   10
C     ..................................................................I0   20
C                                                                       I0   30
C        SUBROUTINE IC                                                  I0   40
C                                                                       I0   50
C        PURPOSE                                                        I0   60
C           COMPUTE THE MODIFIED BESSEL FUNCTION I OF ORDER ZERO        I0   70
C                                                                       I0   80
C        USAGE                                                          I0   90
C           CALL IC(X,RIC)                                              I0  100
C                                                                       I0  110
C        DESCRIPTION OF PARAMETERS                                      I0  120
C           X    -GIVEN ARGUMENT OF THE BESSEL FUNCTION I OF ORDER 0    I0  130
C           RIC  -RESULTANT VALUE OF THE BESSEL FUNCTION I OF ORDER 0   I0  140
C                                                                       I0  150
C        REMARKS                                                        I0  160
C           LARGE VALUES OF THE ARGUMENT MAY CAUSE OVERFLOW IN THE      I0  170
C           BUILTIN EXP-FUNCTION                                        I0  180
C                                                                       I0  190
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  I0  200
C           NONE                                                        I0  210
C                                                                       I0  220
C        METHOD                                                         I0  230
C           POLYNOMIAL APPROXIMATIONS GIVEN BY E.E. ALLEN ARE USED FOR  I0  240
C           CALCULATION.                                                I0  250
C           FOR REFERENCE SEE                                           I0  260
C           M. ABRAMOWITZ AND I.A. STEGUN,'HANDBOOK OF MATHEMATICAL     I0  270
C           FUNCTIONS', U.S. DEPARTMENT OF COMMERCE, NATIONAL BUREAU OF I0  280
C           STANDARDS APPLIED MATHEMATICS SERIES, 1966, P.378.          I0  290
C                                                                       I0  300
C     ..................................................................I0  310
C                                                                       I0  320
      SUBROUTINE IC(X,RIC)                                              I0  330
      RIC=ABS(X)                                                        I0  340
      IF(RIC-3.75)1,1,2                                                 I0  350
    1 Z=X**2*7.111111E-2                                                I0  360
      RIC=(((((( 4.5813E-3*Z+3.60768E-2)*Z+2.659732E-1)*Z+1.206749E0)*Z I0  370
     1+3.0899422E0)*Z+3.515623E0)*Z+1.                                  I0  380
      RETURN                                                            I0  390
    2 Z=3.75/RIC                                                        I0  400
      RIC= EXP(RIC)/SQRT(RIC)*(((((((( 3.92377E-3*Z-1.647633E-2)*Z      I0  410
     1+2.62553E-2)*Z-2.0577C6E-2)*Z+5.16281E-3)*Z-1.57565E-3)*Z         I0  420
     2+2.25315E-3)*Z+1.328592E-2)*Z+3.989423E-1)                        I0  430
      RETURN                                                            I0  440
      END                                                               I0  450
```

Subroutine INUE

This subroutine computes the modified Bessel functions $I_1(x)$, $I_2(x)$, ..., $I_n(x)$ for a given argument x, where n is the given maximum order.

The recurrence relation

$$I_{k+1}(x) + \frac{2k}{x} I_k(x) - I_{k-1}(x) = 0 \qquad (1)$$

is used for this evaluation.

From (1) the values

$$G_k = I_k / I_{k-1} \qquad (2)$$

satisfy

$$G_k = \frac{1}{\frac{2k}{x} + G_{k+1}} \qquad (3)$$

Therefore, G_{n+1} may be calculated from the continued fraction

$$G_{n+1} = \frac{1}{\frac{2(n+1)}{x} + \frac{1}{\frac{2(n+2)}{x} + \frac{1}{\frac{2(n+3)}{x} + \cdots}}} \qquad (4)$$

This continued fraction is evaluated using the following forward A-B process:

Let $A_{-1} = 1$, $A_0 = 0$, $A_k = \frac{2(n+k)}{x} A_{k-1} + A_{k-2}$ (5)

$B_{-1} = 0$, $B_0 = 1$, $B_k = \frac{2(n+k)}{x} B_{k-1} + B_{k-2}$

for $k = 1, 2 \ldots$.

Then $G_{n+1} = \lim_{k \to \infty} \frac{A_k}{B_k}$ (6)

From G_{n+1} the values G_n, G_{n-1}, ..., G_1 are obtained

applying (3) successively, with $k = n, n-1, \ldots, 1$.

Finally the values I_1, I_2, ... I_n are computed using $I_k = G_k \cdot I_{k-1}$, where I_0 is the value of (7)
Bessel function I of order zero, for example, as obtained using subroutine I0.

```
C                                                                       INUE  10
C     ..................................................................INUE  20
C                                                                       INUE  30
C        SUBROUTINE INUE                                                INUE  40
C                                                                       INUE  50
C        PURPOSE                                                        INUE  60
C           COMPUTE THE MODIFIED BESSEL FUNCTIONS I FOR ORDERS 1 TO N   INUE  70
C                                                                       INUE  80
C        USAGE                                                          INUE  90
C           CALL INUE(X,N,ZI,RI)                                        INUE 100
C                                                                       INUE 110
C        DESCRIPTION OF PARAMETERS                                      INUE 120
C           X      -GIVEN ARGUMENT OF THE BESSEL FUNCTIONS I            INUE 130
C           N      -GIVEN MAXIMUM ORDER OF BESSEL FUNCTIONS I           INUE 140
C           ZI     -GIVEN VALUE OF BESSEL FUNCTION I OF ORDER ZERO      INUE 150
C                   FOR ARGUMENT X                                      INUE 160
C           RI     -RESULTANT VECTOR OF DIMENSION N, CONTAINING THE     INUE 170
C                   VALUES OF THE FUNCTIONS I FOR ORDERS 1 TO N         INUE 180
C                                                                       INUE 190
C        REMARKS                                                        INUE 200
C           THE VALUE OF ZI MAY BE CALCULATED USING SUBROUTINE I0.      INUE 210
C           USING A DIFFERENT VALUE HAS THE EFFECT THAT ALL VALUES OF   INUE 220
C           BESSEL FUNCTIONS I ARE MULTIPLIED BY THE  FACTOR ZI/I(0,X)  INUE 230
C           WHERE I(0,X) IS THE VALUE OF I FOR ORDER 0 AND ARGUMENT X.  INUE 240
C           THIS MAY BE USED DISADVANTAGEOUSLY IF ONLY THE RATIOS OF I  INUE 250
C           FOR DIFFERENT ORDERS ARE REQUIRED.                          INUE 260
C                                                                       INUE 270
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  INUE 280
C           NONE                                                        INUE 290
C                                                                       INUE 300
C        METHOD                                                         INUE 310
C           THE VALUES ARE OBTAINED USING BACKWARD RECURRENCE RELATION  INUE 320
C           TECHNIQUE. THE RATIO I(N+1,X)/I(N,X) IS OBTAINED FROM A     INUE 330
C           CONTINUED FRACTION.                                         INUE 340
C           FOR REFERENCE SEE                                           INUE 350
C           G. BLANCH,'NUMERICAL EVALUATION OF CONTINUED FRACTIONS',    INUE 360
C           SIAM REVIEW, VOL.6,NO.4,1964,PP.383-421.                    INUE 370
C                                                                       INUE 380
C     ..................................................................INUE 390
C                                                                       INUE 400
      SUBROUTINE INUE(X,N,ZI,RI)                                        INUE 410
      DIMENSION RI(1)                                                   INUE 420
      IF(N)10,10,1                                                      INUE 430
    1 FN=N+N                                                            INUE 440
      Q1=X/FN                                                           INUE 450
      IF(ABS(X)-5.E-4)6,6,2                                             INUE 460
    2 A0=1.                                                             INUE 470
      A1=0.                                                             INUE 480
      B0=0.                                                             INUE 490
      B1=1.                                                             INUE 500
      FI=FN                                                             INUE 510
    3 FI=FI+2.                                                          INUE 520
      AN=FI/ABS(X)                                                      INUE 530
      A=AN*A1+A0                                                        INUE 540
      B=AN*B1+B0                                                        INUE 550
      A0=A1                                                             INUE 560
      B0=B1                                                             INUE 570
      A1=A                                                              INUE 580
      B1=B                                                              INUE 590
      Q0=Q1                                                             INUE 600
      Q1=A/B                                                            INUE 610
      IF(ABS((Q1-Q0)/Q1)-1.E-6)4,4,3                                    INUE 620
    4 IF(X)5,6,6                                                        INUE 630
    5 C1=-Q1                                                            INUE 640
    6 K=N                                                               INUE 650
    7 Q1=X/(FN+X*Q1)                                                    INUE 660
      RI(K)=Q1                                                          INUE 670
      FN=FN-2.                                                          INUE 680
      K=K-1                                                             INUE 690
      IF(K)8,8,7                                                        INUE 700
    8 FI=ZI                                                             INUE 710
      DO 9 I=1,N                                                        INUE 720
      FI=FI*RI(I)                                                       INUE 730
    9 RI(I)=FI                                                          INUE 740
   10 RETURN                                                            INUE 750
      END                                                               INUE 760
```

Subroutine BESK

This subroutine computes the K Bessel function for a given argument x and order n. The recurrence relation:

$$K_{n+1}(x) = \frac{2n}{x} K_n(x) + K_{n-1}(x) \tag{1}$$

is used for this evaluation.

The initial values K_0 and K_1 are found as follows:

For x > 1:

$$K_0(x) = e^{-x}\sqrt{\frac{\pi}{2x}}\, G_0(x) \tag{2}$$

$$K_1(x) = e^{-x}\sqrt{\frac{\pi}{2x}}\, G_1(x) \tag{3}$$

where x = 1/t for t < 1:

$$G_0\left(\frac{1}{t}\right)\cdot\sqrt{\frac{\pi}{2}} = 1.2533141 - 0.1566642t + 0.08811128t^2 - 0.09139095t^3 + 0.1344596t^4 - 0.2299850t^5 + 0.3792410t^6 - 0.5247277t^7 + 0.5575368t^8 - 0.4262633t^9 + 0.2184518t^{10} - 0.06680977t^{11} + 0.009189383t^{12} \tag{4}$$

$$G_1\left(\frac{1}{t}\right)\cdot\sqrt{\frac{\pi}{2}} = 1.2533141 + 0.4699927t - 0.1468583t^2 + 0.1280427t^3 - 0.1736432t^4 + 0.2847618t^5 - 0.4594342t^6 + 0.6283381t^7 - 0.6632295t^8 + 0.5050239t^9 - 0.2581304t^{10} + 0.07880001t^{11} - 0.0108242t^{12} \tag{5}$$

For x ≤ 1:

γ = Euler's constant = 0.5772156649 (6)

$$K_0(x) = -\left(\gamma + \log\frac{x}{2}\right) + \sum_{s=1}^{6}\left(\frac{x}{2}\right)^{2s}\frac{1}{(s!)^2}\left[H_s - \left(\gamma + \log\frac{x}{2}\right)\right] \tag{7}$$

where:

$$H_s = \sum_{r=1}^{s}\frac{1}{r} \tag{8}$$

$$K_1(x) = \frac{1}{x} + \sum_{s=1}^{8}\left(\frac{x}{2}\right)^{2s-1}\frac{1}{(s!)^2}\left[\frac{1}{2} + s\cdot\left(\gamma + \log\frac{x}{2} - H_s\right)\right] \tag{9}$$

```
C                                                                       BESK  10
C     .................................................................BESK  20
C                                                                       BESK  30
C        SUBROUTINE BESK                                                BESK  40
C                                                                       BESK  50
C           COMPUTE THE K BESSEL FUNCTION FOR A GIVEN ARGUMENT AND ORDERBESK  60
C                                                                       BESK  70
C        USAGE                                                          BESK  80
C           CALL BESK(X,N,BK,IER)                                       BESK  90
C                                                                       BESK 100
C        DESCRIPTION OF PARAMETERS                                      BESK 110
C           X  -THE ARGUMENT OF THE K BESSEL FUNCTION DESIRED           BESK 120
C           N  -THE ORDER OF THE K BESSEL FUNCTION DESIRED              BESK 130
C           BK -THE RESULTANT K BESSEL FUNCTION                         BESK 140
C           IER-RESULTANT ERROR CODE WHERE                              BESK 150
C              IER=0  NO ERROR                                          BESK 160
C              IER=1  X IS NEGATIVE                                     BESK 170
C              IER=2  X IS ZERO OR NEGATIVE                             BESK 180
C              IER=3  X .GT. 170, MACHINE RANGE EXCEEDED                BESK 190
C              IER=4  BK .GT. 10**70                                    BESK 200
C                                                                       BESK 210
C        REMARKS                                                        BESK 220
C           N MUST BE GREATER THAN OR EQUAL TO ZERO                     BESK 230
C                                                                       BESK 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  BESK 250
C           NONE                                                        BESK 260
C                                                                       BESK 270
C        METHOD                                                         BESK 280
C           COMPUTES ZERO ORDER AND FIRST ORDER BESSEL FUNCTIONS USING  BESK 290
C           SERIES APPROXIMATIONS AND THEN COMPUTES N TH ORDER FUNCTION BESK 300
C           USING RECURRENCE RELATION.                                  BESK 310
C           RECURRENCE RELATION AND POLYNOMIAL APPROXIMATION TECHNIQUE  BESK 320
C           AS DESCRIBED BY A.J.M.HITCHCOCK,'POLYNOMIAL APPROXIMATIONS  BESK 330
C           TO BESSEL FUNCTIONS OF ORDER ZERO AND ONE AND TO RELATED    BESK 340
C           FUNCTIONS', M.T.A.C., V.11,1957,PP.86-88, AND C.A. WATSON,  BESK 350
C           'A TREATISE ON THE THEORY OF BESSEL FUNCTIONS', CAMBRIDGE   BESK 360
C           UNIVERSITY PRESS, 1958, P. 62                               BESK 370
C                                                                       BESK 380
C     .................................................................BESK 390
      SUBROUTINE BESK(X,N,BK,IER)                                       BESK 400
      DIMENSION T(12)                                                   BESK 410
      BK=0.0                                                            BESK 420
      IF(N)10,11,11                                                     BESK 430
   10 IER=1                                                             BESK 440
      RETURN                                                            BESK 450
   11 IF(X)12,12,20                                                     BESK 460
   12 IER=2                                                             BESK 470
      RETURN                                                            BESK 480
   20 IF(X-170.0)22,22,21                                               BESK 490
   21 IER=3                                                             BESK 500
      RETURN                                                            BESK 510
   22 IER=0                                                             BESK 520
      IF(X-1.0)24,36,25                                                 BESK 530
   25 A=EXP(-X)                                                         BESK 540
      B=1./X                                                            BESK 550
      C=SQRT(B)                                                         BESK 560
      T(1)=B                                                            BESK 570
      DO 26 L=2,12                                                      BESK 580
   26 T(L)=T(L-1)*B                                                     BESK 590
      IF(N-1)27,29,27                                                   BESK 600
C                                                                       BESK 610
C     COMPUTE KO USING POLYNOMIAL APPROXIMATION                         BESK 620
C                                                                       BESK 630
   27 CC=A*(1.2533141-.1566642*T(1)+.0881128*T(2)-.0913595*T(3)         BESK 640
     2+.1344596*T(4)-.2299850*T(5)+.3792410*T(6)-.5247277*T(7)          BESK 650
     3+.5575368*T(8)-.4262633*T(9)+.2184518*T(10)-.0668097*T(11)        BESK 660
     4+.0091893*T(12))*C                                                BESK 670
      IF(N)32,28,29                                                     BESK 680
   28 BK=CC                                                             BESK 690
      RETURN                                                            BESK 700
C                                                                       BESK 710
C     COMPUTE K1 USING POLYNOMIAL APPROXIMATION                         BESK 720
                                                                        BESK 730
```

```
C
   25 G1=A*(1.25331414+.46559278*T(1)-.11468563*T(2)+.12804278*T(3)
     2-.17326432*T(4)+.28478218*T(5)-.45594342*T(6)+.62833681*T(7)
     3-.66326256*T(8)+.50582364*T(9)-.25813648*T(10)+.07880001*T(11)
     4-.01062418*T(12))*C
      IF(N-1)2C,3C,31
   2C BK=G1
      RETURN
C
C     FROM KC,K1 COMPUTE KN USING RECURRENCE RELATION
C
   31 DO 35 J=2,N
      GJ=2.*(FLOAT(J)-1.)*G1/X+GC
      IF(GJ-1.0E70)33,33,32
   32 IER=4
      GO TO 34
   33 GC=G1
   35 G1=GJ
   34 BK=GJ
      RETURN
   36 B=X/2.
      A=.5772157+ALOG(B)
      C=B*B
      IF(N-1)37,43,37
C
C     COMPUTE KC USING SERIES EXPANSION
C
   37 GC=-A
      X2J=1.
      FACT=1.
      FJ=.0
      DO 4C J=1,6
      RJ=1./FLOAT(J)
      X2J=X2J*C
      FACT=FACT*RJ*RJ
      FJ=FJ+FJ
   4C GC=GC+X2J*FACT*(FJ-A)
      IF(N)43,42,43
   42 BK=GC
      RETURN
C
C     COMPUTE K1 USING SERIES EXPANSION
C
   43 X2J=B
      FACT=1.
      FJ=1.
      G1=1./X+X2J*(.5+A-FJ)
      DO 5C J=2,8
      X2J=X2J*C
      RJ=1./FLOAT(J)
      FACT=FACT*RJ*RJ
      FJ=FJ+RJ
   5C G1=G1+X2J*FACT*(.5+(A-FJ)*FLOAT(J))
      IF(N-1)51,52,51
   52 BK=G1
      RETURN
      END
```

BESK 740
BESK 750
BESK 760
BESK 770
BESK 780
BESK 790
BESK 800
BESK 810
BESK 820
BESK 830
BESK 840
BESK 850
BESK 860
BESK 870
BESK 880
BESK 890
BESK 900
BESK 910
BESK 920
BESK 930
BESK 940
BESK 950
BESK 960
BESK 970
BESK 980
BESK 990
BESK1000
BESK1010
BESK1020
BESK1030
BESK1040
BESK1050
BESK1060
BESK1070
BESK1080
BESK1090
BESK1100
BESK1110
BESK1120
BESK1130
BESK1140
BESK1150
BESK1160
BESK1170
BESK1180
BESK1190
BESK1200
BESK1210
BESK1220
BESK1230
BESK1240
BESK1250
BESK1260
BESK1270
BESK1280
BESK1290
BESK1300

Subroutine EXPI

This subroutine computes the exponential integral for a given value of the argument x.

The exponential integral is defined as:

$$E_1(x) = -Ei(-x) = \int_x^\infty \frac{e^{-t}}{t}\,dt = \int_0^x \frac{1-e^{-t}}{t}\,dt - C - \ln(x)$$

where C = 0.57 ... is Euler's constant.

The integral

$\int_x^\infty \frac{e^{-t}}{t}\,dt$ has a logarithmic singularity at x = 0.

Therefore, it must be evaluated in the Cauchy Principal Value sense for negative values of x.

For x = 0 the routine returns -1.E75 as value of $E_1(x)$.

For $x \geq 1$:

$$AUX = xe^x E_1(x)$$

$$= (x^4 + 8.5733287401x^3 + 18.0590169730x^2 + 8.6347608925x + 0.2677737343)/(x^4 + 9.5733223454x^3 + 25.6329561486x^2 + 21.0996530827x + 3.9584969228) + \epsilon$$

with $|\epsilon| < 2.E-8.$

For $-3 \leq x \leq 1$:

$$AUX = (E_1(x) + \ln|x| + C)/x$$

$$= 9.999999E-1 - 2.500001E-1 \cdot x + 5.555682E-2 \cdot x^2 - 1.041576E-2 \cdot x^3 + 1.664156E-3 \cdot x^4 - 2.335379E-4 \cdot x^5 + 2.928433E-5 \cdot x^6 - 1.766345E-6 \cdot x^7 + 7.122452E-7 \cdot x^7 + \epsilon$$

with $|\epsilon| < 7.3E-8.$

For $-9 \leq x \leq -3$:

$$AUX = xe^{x}E_1(x)$$

$$= 1-(248.6697 + 224.4234x + 32.43665x^2 + 3.061037x^3 + 0.05176245x^4)/(180.7837 + 22.63818x + 38.93944x^2 + 3.995161x^3 + x^4) + \epsilon$$

with $|\epsilon| < 1.3E-7$.

For $-174 \leq x \leq -9$:

$$AUX = xe^{x}E_1(x)$$

$$= 1-(674.567029 + 57.4118330x - 6.05529232x^2 - x^3)/(1699.06552 + 841.654932x + 49.3133893x^2 - 8.01957683x^3 - 0.999792040x^4) + \epsilon$$

with $|\epsilon| < 3.8E-7$.

```
C                                                                       EXPI  10
C  .....................................................................EXPI  20
C                                                                       EXPI  30
C     SUBROUTINE EXPI                                                   EXPI  40
C                                                                       EXPI  50
C     PURPOSE                                                           EXPI  60
C        COMPUTES THE EXPONENTIAL INTEGRAL -EI(-X)                      EXPI  70
C                                                                       EXPI  80
C     USAGE                                                             EXPI  90
C        CALL EXPI(X,RES)                                               EXPI 100
C                                                                       EXPI 110
C     DESCRIPTION OF PARAMETERS                                         EXPI 120
C        X    - ARGUMENT OF EXPONENTIAL INTEGRAL                        EXPI 130
C        RES  - RESULT VALUE                                            EXPI 140
C        ALX  - RESULTANT AUXILIARY VALUE                               EXPI 150
C                                                                       EXPI 160
C     REMARKS                                                           EXPI 170
C        X GT 170 (X LT -174) MAY CAUSE UNDERFLOW (OVERFLOW)            EXPI 180
C        WITH THE EXPONENTIAL FUNCTION                                  EXPI 190
C        FOR X = 0 THE RESULT VALUE IS SET TO -1.E75                    EXPI 200
C                                                                       EXPI 210
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     EXPI 220
C        NONE                                                           EXPI 230
C                                                                       EXPI 240
C     METHOD                                                            EXPI 250
C        DEFINITION                                                     EXPI 260
C        RES=INTEGRAL(EXP(-T)/T, SWPED OVER T FROM X TO INFINITY).      EXPI 270
C        EVALUATION                                                     EXPI 280
C        THREE DIFFERENT RATIONAL APPROXIMATIONS ARE USED IN THE        EXPI 290
C        RANGES 1 LE X, X LE -9 AND -9 LT X LE -3 RESPECTIVELY.         EXPI 300
C        A POLYNOMIAL APPROXIMATION IS USED IN -3 LT X LT 1.            EXPI 310
C                                                                       EXPI 320
C  .....................................................................EXPI 330
C                                                                       EXPI 340
      SUBROUTINE EXPI(X,RES,ALX)                                        EXPI 350
      IF(X-1.)2,1,1                                                     EXPI 360
    1 Y=1./X                                                            EXPI 370
      ALX=1.-Y*(((Y+3.37735EEC)*Y+2.C5215EEC)*Y+2.709479E-1)/((((Y+     EXPI 380
     11.C72553EC+5.716543EC)*Y+6.945235EC)*Y+2.593888EC)*Y+2.709456E-1) EXPI 390
      RES=ALX*Y*EXP(-X)                                                 EXPI 400
      RETURN                                                            EXPI 410
      IF(X+2.)6,6,3                                                     EXPI 420
    3 ALX=(((((((7.122452E-7*X-1.7EE345E-6)*X+2.926433E-5)*X-2.335379E-4EXPI 430
     1)*X+1.EE4156E-3)*X-1.041576E-2)*X+5.555682E-2)*X-2.5000C1E-1)*X   EXPI 440
     2+5.5555556E-1                                                     EXPI 450
      RES=-1.E75                                                        EXPI 460
      IF(X)4,5,4                                                        EXPI 470
    4 RES=X*ALX-ALOG(ABS(X))-5.772157E-1                                EXPI 480
    5 RETURN                                                            EXPI 490
    6 IF(X+5.)8,6,7                                                     EXPI 500
    7 ALX=1.-(((((5.176245E-2*X+3.CE1C37EC)*X+3.243665E1)*X+2.244234E2)*XEXPI 510
     1+2.466657E2)/((((X+3.595161EC)*X+2.893544E1)*X+2.263818E1)*X      EXPI 520
     2+1.EC7E37E2)                                                      EXPI 530
      GOTO 5                                                            EXPI 540
    8 Y=5./X                                                            EXPI 550
      ALX=1.-Y*(((Y+7.659824E-1)*Y-1.271015E-1)*Y-1.08C653EC)/((((Y     EXPI 560
     1+2.518755EC+1.122927E1)*Y+5.9214C5EC)*Y-8.66E702EC)*Y-9.724216EC) EXPI 570
    9 RES=ALX*EXP(-X)/X                                                 EXPI 580
      RETURN                                                            EXPI 590
      END                                                               EXPI 600
```

Subroutine SICI

This subroutine computes the sine and cosine integrals for a given value of the argument x.

These integrals are defined as:

$$si(x) = S_i(x) - \pi/2 = \int_0^x \frac{\sin(t)}{t}\,dt - \pi/2$$

$$ci(x) = C + \ln(x) + \int_0^x \frac{\cos(t)-1}{t}\,dt$$

where C is Euler's constant 0.57 ... .

The integral $\int \frac{\cos(t)}{t}\,dt$ has a logarithmic singularity at x = 0. Therefore, it must be evaluated in the Cauchy Principal Value sense for negative values of x.

For x = 0 the routine returns -1.E75 as value of ci(x).

For $x \leq 4$ and $t = 16-x^2$:

$$(si(x) + \pi/2)/x = 4.395509E\text{-}1 + 1.964882E\text{-}2\cdot t + 6.939889E\text{-}4\cdot t^2 + 1.374168E\text{-}5\cdot t^3 + 1.568988E\text{-}7\cdot t^4 + 1.753141E\text{-}9\cdot t^5 + \epsilon$$

with $|\epsilon| < 8.2E\text{-}8$

$$-(ci(x) - C - \ln|x|)/x^2 = 1.315308E\text{-}1 + 4.990920E\text{-}3\cdot t + 1.185999E\text{-}4\cdot t^2 + 1.725752E\text{-}6\cdot t^3 + 1.584996E\text{-}8\cdot t^4 + 1.386985E\text{-}10\cdot t^5 + \epsilon$$

with $|\epsilon| < 5.6E\text{-}9$.

For x > 4 and t = 4/x:

$$si(x) = -\left(\frac{4}{x}\right)(\cos(x)\cdot P(x) + \sin(x)\cdot Q(x)) + \epsilon$$

$$ci(x) = \left(\frac{4}{x}\right)(\sin(x)\cdot P(x) - \cos(x)\cdot Q(x)) + \epsilon$$

where:

$$|\epsilon| < \frac{1}{x} \cdot 2.3E\text{-}8 \text{ and}$$

$$P(x) = 2.500000E\text{-}1 - 6.646441E\text{-}7\cdot t - 3.122418E\text{-}2\cdot t^2 - 3.764000E\text{-}4\cdot t^3 + 2.601293E\text{-}2\cdot t^4 - 7.945556E\text{-}3\cdot t^5 - 4.400416E\text{-}2\cdot t^6 + 7.902034E\text{-}2\cdot t^7 - 6.537283E\text{-}2\cdot t^8 + 2.819179E\text{-}2\cdot t^9 - 5.108699E\text{-}3\cdot t^{10}$$

$$Q(x) = 2.583989E\text{-}10 + 6.250011E\text{-}2\cdot t - 1.134958E\text{-}5\cdot t^2 - 2.314617E\text{-}2\cdot t^3 - 3.332519E\text{-}3\cdot t^4 + 4.987716E\text{-}2\cdot t^5 - 7.261642E\text{-}2\cdot t^6 + 5.515070E\text{-}2\cdot t^7 - 2.279143E\text{-}2\cdot t^8 + 4.048069E\text{-}3\cdot t^9$$

```
C                                                                       SICI  10
C     .................................................................SICI  20
C                                                                       SICI  30
C        SUBROUTINE SICI                                                SICI  40
C                                                                       SICI  50
C        PURPOSE                                                        SICI  60
C           COMPUTES THE SINE AND COSINE INTEGRAL                       SICI  70
C                                                                       SICI  80
C        USAGE                                                          SICI  90
C           CALL SICI(SI,CI,X)                                          SICI 100
C                                                                       SICI 110
C        DESCRIPTION OF PARAMETERS                                      SICI 120
C           SI    - THE RESULTANT VALUE SI(X)                           SICI 130
C           CI    - THE RESULTANT VALUE CI(X)                           SICI 140
C           X     - THE ARGUMENT OF SI(X) AND CI(X)                     SICI 150
C                                                                       SICI 160
C        REMARKS                                                        SICI 170
C           THE ARGUMENT VALUE REMAINS UNCHANGED                        SICI 180
C                                                                       SICI 190
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SICI 200
C           NONE                                                        SICI 210
C                                                                       SICI 220
C        METHOD                                                         SICI 230
C           DEFINITION                                                  SICI 240
C           SI(X)=INTEGRAL(SIN(T)/T)                                    SICI 250
C           CI(X)=INTEGRAL(COS(T)/T)                                    SICI 260
C           EVALUATION                                                  SICI 270
C           REDUCTION OF RANGE USING SYMMETRY.                          SICI 280
C           DIFFERENT APPROXIMATIONS ARE USED FOR ABS(X) GREATER        SICI 290
C           THAN 4 AND FOR ABS(X) LESS THAN 4.                          SICI 300
C           REFERENCE                                                   SICI 310
C           LUKE AND WIPP, 'POLYNOMIAL APPROXIMATIONS TO INTEGRAL       SICI 320
C           TRANSFORMS', MATHEMATICAL TABLES AND OTHER AIDS TO          SICI 330
C           COMPUTATION, VOL. 15, 1961, ISSUE 74, PP. 174-178.          SICI 340
C                                                                       SICI 350
C     .................................................................SICI 360
      SUBROUTINE SICI(SI,CI,X)                                          SICI 370
      Z=ABS(X)                                                          SICI 380
      IF(Z-4.)1,1,4                                                     SICI 390
    1 Y=(4.-Z)*(4.+Z)                                                   SICI 400
      SI=-1.53C757EC                                                    SICI 410
      IF(Z)3,2,3                                                        SICI 420
    2 CI=-1.E75                                                         SICI 430
      RETURN                                                            SICI 440
    3 SI=X*(((((1.753141E-9*Y+1.568588EE-7)*Y+1.274166E-5)*Y+6.939889E-4)SICI 450
     1*Y+1.564E62E-2)*Y+4.3555C9E-1+SI/X)                               SICI 460
      CI=(((5.772156E-1+ALOG(Z))/Z-Z*(((((1.386E5E5E-1C*Y+1.5E4996E-8)*Y SICI 470
     1+1.725752E-6)*Y+1.1E5559E-4)*Y+4.594052CE-3)*Y+1.3153C8E-11)*Z    SICI 480
      RETURN                                                            SICI 490
    4 SI=SIN(Z)                                                         SICI 500
      Y=COS(Z)                                                          SICI 510
      Z=4./Z                                                            SICI 520
      U=(((((((((4.C48C65E-3*Z-2.279143E-2)*Z+5.515070E-2)*Z-7.261642E-2)SICI 530
     1*Z+4.5E7716E-2)*Z-3.332519E-3)*Z-2.314617E-2)*Z-1.134958E-5)*Z    SICI 540
     2+6.250C11E-2)*Z+2.5E3G85E-1C                                      SICI 550
      V=((((((((((-5.1C6E65E-3*Z+2.815179E-2)*Z-6.5372E3E-2)*Z          SICI 560
     1+7.9G2C34E-2)*Z-4.4CC41EE-2)*Z-7.945556E-3)*Z+2.601293E-2)*Z      SICI 570
     2-3.764CCCE-4)*Z-3.122418E-2)*Z-6.646441E-7)*Z+2.5GCCCOE-1         SICI 580
      CI=Z*(SI*V-Y*U)                                                   SICI 590
      SI=-Z*(SI*U+Y*V)                                                  SICI 600
      IF(X)5,6,6                                                        SICI 610
    5 SI=3.1415926C-SI                                                  SICI 620
    6 RETURN                                                            SICI 630
      END                                                               SICI 640
                                                                        SICI 650
```

Subroutine CS

This subroutine computes the Fresnel integrals for a given value of the argument x.

The Fresnel integrals are defined as:

$$C(x) = \frac{1}{\sqrt{2\pi}} \int_0^x \frac{\cos(t)}{\sqrt{t}}\, dt = \int_0^{\sqrt{\frac{2}{\pi}x}} \cos(\tfrac{\pi}{2}u^2)du$$

and

$$S(x) = \frac{1}{\sqrt{2\pi}} \int_0^x \frac{\sin(t)}{\sqrt{t}}\, dt = \int_0^{\sqrt{\frac{2}{\pi}x}} \sin(\tfrac{\pi}{2}u^2)du$$

The subroutine CS calculates both C(x) and S(x) simultaneously.

If x is negative, $|x|$ is used in CS.

For $0 \leq x \leq 4$ and $t = 16 - x^2$:

$$C(x)/\sqrt{x} = 1.840962E\text{-}1 + 1.102544E\text{-}2 \cdot t + 1.020418E\text{-}3 \cdot t^2 + 3.273308E\text{-}5 \cdot t^3 + 5.451182E\text{-}7 \cdot t^4 + 5.244297E\text{-}9 \cdot t^5 + 5.100785E\text{-}11 \cdot t^6 + \epsilon$$

with $|\epsilon| < 8.5E\text{-}9$

$$S(x)/\sqrt{x^3} = 8.026490E\text{-}2 + 6.121300E\text{-}3 \cdot t + 2.441816E\text{-}4 \cdot t^2 + 5.051141E\text{-}6 \cdot t^3 + 5.883158E\text{-}8 \cdot t^4 + 6.677681E\text{-}10 \cdot t^5 + \epsilon$$

with $|\epsilon| < 3.5E\text{-}8$.

For $x > 4$ and $t = 4/x$:

$$C(x) = \frac{1}{2} + \sqrt{\frac{4}{x}}\,(\sin(x) \cdot P(x) + \cos(x) \cdot Q(x)) + \epsilon$$

$$S(x) = \frac{1}{2} + \sqrt{\frac{4}{x}}\,(-\cos(x) \cdot P(x) + \sin(x) \cdot Q(x)) + \epsilon$$

where $|\epsilon| < 1.3E\text{-}8$ and

$$P(x) = 1.994712E\text{-}1 - 1.207998E\text{-}6 \cdot t - 9.314911E\text{-}3 \cdot t^2 - 4.027145E\text{-}4 \cdot t^3 + 7.428246E\text{-}3 \cdot t^4 - 7.271690E\text{-}3 \cdot t^5 + 3.401409E\text{-}3 \cdot t^6 - 6.633926E\text{-}4 \cdot t^7$$

and

$$Q(x) = 4.444091E\text{-}9 - 2.493322E\text{-}2 \cdot t - 1.606428E\text{-}5 \cdot t^2 + 5.972151E\text{-}3 \cdot t^3 - 3.095341E\text{-}4 \cdot t^4 - 6.792801E\text{-}3 \cdot t^5 + 7.970943E\text{-}3 \cdot t^6 - 4.169289E\text{-}3 \cdot t^7 + 8.768258E\text{-}4 \cdot t^8$$

```
C                                                                       CS    10
C   ....................................................................CS    20
C                                                                       CS    30
C     SUBROUTINE CS                                                     CS    40
C                                                                       CS    50
C     PURPOSE                                                           CS    60
C        COMPUTES THE FRESNEL INTEGRALS.                                CS    70
C                                                                       CS    80
C     USAGE                                                             CS    90
C        CALL CS (C,S,X)                                                CS   100
C                                                                       CS   110
C     DESCRIPTION OF PARAMETERS                                         CS   120
C        C     - THE RESULTANT VALUE C(X).                              CS   130
C        S     - THE RESULTANT VALUE S(X).                              CS   140
C        X     - THE ARGUMENT OF FRESNEL INTEGRALS                      CS   150
C                IF X IS NEGATIVE, THE ABSOLUTE VALUE IS USED.          CS   160
C                                                                       CS   170
C     REMARKS                                                           CS   180
C        THE ARGUMENT VALUE X REMAINS UNCHANGED.                        CS   190
C                                                                       CS   200
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     CS   210
C        NONE                                                           CS   220
C                                                                       CS   230
C     METHOD                                                            CS   240
C        DEFINITION                                                     CS   250
C        C(X)=INTEGRAL(COS(T)/SQRT(2*PI*T) SUMMED OVER T FROM 0 TO X)CS   260
C        S(X)=INTEGRAL(SIN(T)/SQRT(2*PI*T) SUMMED OVER T FROM 0 TO X)CS   270
C        EVALUATION                                                     CS   280
C        USING DIFFERENT APPROXIMATIONS FOR X LESS THAN 4 AND X         CS   290
C        GREATER THAN 4.                                                CS   300
C        REFERENCE                                                      CS   310
C        'COMPUTATION OF FRESNEL INTEGRALS' BY BOERSMA,                 CS   320
C        MATHEMATICAL TABLES AND OTHER AIDS TO COMPUTATION, VOL. 14,    CS   330
C        1960, NO. 72, P. 380.                                          CS   340
C                                                                       CS   350
C   ....................................................................CS   360
      SUBROUTINE CS(C,S,X)                                              CS   370
      Z=ABS(X)                                                          CS   380
      IF(Z-4.)1,1,2                                                     CS   390
    1 C=SQRT(Z)                                                         CS   400
      S=Z*C                                                             CS   410
      Z=(4.-Z)*(4.+Z)                                                   CS   420
      C=C*((((((5.1CC785E-11*Z+5.244297E-9)*Z+5.451182E-7)*Z            CS   430
     1+3.2733CEE-5)*Z+1.02C41EE-3)*Z+1.102544E-2)*Z+1.84C565E-1)        CS   440
      S=S*((((((6.677681E-1C*Z+5.883158E-8)*Z+5.C51141E-6)*Z            CS   450
     1+2.441816E-4)*Z+6.12132CE-3)*Z+8.C264S0E-2)                       CS   460
      RETURN                                                            CS   470
    2 C=CCS(Z)                                                          CS   480
      S=SIN(Z)                                                          CS   490
      Z=4./Z                                                            CS   500
      A=((((((((E.76825EE-4*Z-4.1652E5E-3)*Z+7.57C543E-3)*Z-6.7928C1E-3)CS   510
     1*Z-3.C552341E-4)*Z+5.572151E-3)*Z-1.6CE42EE-5)*Z-2.453322E-2)*Z   CS   520
     2-4.444C51E-5                                                      CS   530
      B=((((((-6.633526E-4*Z+3.4014C5E-3)*Z-7.2811E90E-3)*Z+7.428246E-3)CS   540
     1*Z-4.C27345E-4)*Z-9.314910E-3)*Z-1.2C7598E-6)*Z+1.9547111E-1      CS   550
      Z=SQRT(Z)                                                         CS   560
      C=C.5+Z*(C0A*S0B)                                                 CS   570
      S=C.5+Z*(S0A-C0B)                                                 CS   580
      RETURN                                                            CS   590
      END                                                               CS   600
                                                                        CS   610
```

Subroutines CEL1 and DCEL1

These subroutines compute the complete elliptic integral of the first kind. This is defined as:

$$K(k) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-k^2 \sin^2 t}}, \quad 0 \le k < 1$$

An equivalent definition is:

$$K(k) = \int_0^{\infty} \frac{dx}{\sqrt{(1+x^2)(1+k_c^2 x^2)}}$$

where k_c is the complementary modulus:

$$k_c^2 + k^2 = 1, \quad 0 < k_c^2 \le 1$$

The subroutines CEL1, DCEL1 calculate K(k) for given modulus k. The calculation of RES = K(k) is based on the process of the arithmetic-geometric mean.

Starting with the pair of numbers:

$$a_0 = 2, \quad g_0 = 2 \cdot k_c$$

the sequences of numbers (a_n), (g_n) are generated using the definition:

$$a_n = (a_{n-1} + g_{n-1}), \quad g_n = 2\sqrt{a_{n-1} \cdot g_{n-1}}$$

This iterative process is stopped at the N^{th} step, when $a_N = g_N$.

If D is the number of decimal digits in the mantissa of floating-point numbers, then the equality $a_N = g_N$ must be interpreted as $|a_N - g_N|$ is less than $a_N \cdot 10^{-D}$.

Since the sequences $(2^{-(n+1)} a_n)$, $(2^{-(n+1)} g_n)$ converge quadratically to the same limit (arithmetic-geometric mean) the test for the end of iteration may be replaced by comparing $|a_{N-1} - g_{N-1}|$ against $a_{N-1} \cdot 10^{-D/2}$, thus saving one calculation of the geometric mean.

The value of $K(k) = \frac{2^N \pi}{a_N}$.

```
C                                                                       CEL1  10
C     ..................................................................CEL1  20
C                                                                       CEL1  30
C        SUBROUTINE CEL1                                                CEL1  40
C                                                                       CEL1  50
C        PURPOSE                                                        CEL1  60
C           CALCULATE COMPLETE ELLIPTIC INTEGRAL OF FIRST KIND          CEL1  70
C                                                                       CEL1  80
C        USAGE                                                          CEL1  90
C           CALL CEL1(RES,AK,IER)                                       CEL1 100
C                                                                       CEL1 110
C        DESCRIPTION OF PARAMETERS                                      CEL1 120
C           RES   - RESULT VALUE                                        CEL1 130
C           AK    - MODULUS (INPUT)                                     CEL1 140
C           IER   - RESULTANT ERROR CODE WHERE                          CEL1 150
C                     IER=0  NO ERROR                                   CEL1 160
C                     IER=1  AK NOT IN RANGE -1 TO +1                   CEL1 170
C                                                                       CEL1 180
C        REMARKS                                                        CEL1 190
C           THE RESULT IS SET TO 1.E75 IF ABS(AK) GE 1                  CEL1 200
C           FOR MODULUS AK AND COMPLEMENTARY MODULUS CK,                CEL1 210
C           EQUATION AK**2+CK**2=1.0 IS USED.                           CEL1 220
C           AK MUST BE IN THE RANGE -1 TO +1                            CEL1 230
C                                                                       CEL1 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CEL1 250
C           NONE                                                        CEL1 260
C                                                                       CEL1 270
C        METHOD                                                         CEL1 280
C           DEFINITION                                                  CEL1 290
C           CEL1(AK)=INTEGRAL(1/SQRT((1+T**2)*(1+(CK*T)**2)), SUMMED    CEL1 300
C           OVER T FROM 0 TO INFINITY).                                 CEL1 310
C           EQUIVALENT ARE THE DEFINITIONS                              CEL1 320
C           CEL1(AK)=INTEGRAL(1/(COS(T)SQRT(1+(CK*TAN(T))**2)),SUMMED   CEL1 330
C           OVER T FROM 0 TO PI/2),                                     CEL1 340
C           CEL1(AK)=INTEGRAL(1/SQRT(1-(AK*SIN(T))**2),SUMMED OVER T    CEL1 350
C           FROM 0 TO PI/2), WHERE K=SQRT(1.-CK**2).                    CEL1 360
C           EVALUATION                                                  CEL1 370
C           LANDENS TRANSFORMATION IS USED FOR CALCULATION.             CEL1 380
C           REFERENCE                                                   CEL1 390
C           R.ZELLISCH, 'NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS    CEL1 400
C           AND ELLIPTIC FUNCTIONS', HANDBOOK SERIES SPECIAL FUNCTIONS, CEL1 410
C           NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 76-90.              CEL1 420
C                                                                       CEL1 430
C     ..................................................................CEL1 440
      SUBROUTINE CEL1(RES,AK,IER)                                       CEL1 450
      IER=0                                                             CEL1 460
      ARI=2.                                                            CEL1 470
      CEC=(0.5-AK)+0.5                                                  CEL1 480
      CEC=CEC+CEC*AK                                                    CEL1 490
      RES=0.5                                                           CEL1 500
      IF(CEC)1,2,4                                                      CEL1 510
    1 IER=1                                                             CEL1 520
    2 RES=1.E75                                                         CEL1 530
      RETURN                                                            CEL1 540
    3 CEC=CEC*AARI                                                      CEL1 550
    4 CEC=SQRT(CEC)                                                     CEL1 560
      CEC=CEC+CEC                                                       CEL1 570
      AARI=ARI                                                          CEL1 580
      ARI=ARI+CEC                                                       CEL1 590
      RES=RES*RES                                                       CEL1 600
      IF(CEC/AARI-0.5999)3,5,5                                          CEL1 610
    5 RES=RES/ARI*6.28318530                                            CEL1 620
      RETURN                                                            CEL1 630
      END                                                               CEL1 640
                                                                        CEL1 650
C                                                                       DCE1  10
C     ..................................................................DCE1  20
C                                                                       DCE1  30
C        SUBROUTINE DCEL1                                               DCE1  40
C                                                                       DCE1  50
C        PURPOSE                                                        DCE1  60
C           CALCULATE COMPLETE ELLIPTIC INTEGRAL OF FIRST KIND          DCE1  70
C                                                                       DCE1  80
C        USAGE                                                          DCE1  90
C           CALL DCEL1(RES,AK,IER)                                      DCE1 100
C                                                                       DCE1 110
C        DESCRIPTION OF PARAMETERS                                      DCE1 120
C           RES   - RESULT VALUE IN DOUBLE PRECISION                    DCE1 130
C           AK    - MODULUS (INPUT) IN DOUBLE PRECISION                 DCE1 140
C           IER   - RESULTANT ERROR CODE WHERE                          DCE1 150
C                     IER=0  NO ERROR                                   DCE1 160
C                     IER=1  AK NOT IN RANGE -1 TO +1                   DCE1 170
C                                                                       DCE1 180
C        REMARKS                                                        DCE1 190
C           THE RESULT IS SET TO 1.E75 IF ABS(AK) GE 1                  DCE1 200
C           FOR MODULUS AK AND COMPLEMENTARY MODULUS CK,                DCE1 210
C           EQUATION AK**2+CK**2=1.0D0 IS USED.                         DCE1 220
C           AK MUST BE IN THE RANGE -1 TO +1                            DCE1 230
C                                                                       DCE1 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DCE1 250
C           NONE                                                        DCE1 260
C                                                                       DCE1 270
C        METHOD                                                         DCE1 280
C           DEFINITION                                                  DCE1 290
C           CEL1(AK)=INTEGRAL(1/SQRT((1+T**2)*(1+(CK*T)**2)), SUMMED    DCE1 300
C           OVER T FROM 0 TO INFINITY).                                 DCE1 310
C           EQUIVALENT ARE THE DEFINITIONS                              DCE1 320
C           CEL1(AK)=INTEGRAL(1/(COS(T)SQRT(1+(CK*TAN(T))**2)),SUMMED   DCE1 330
C           OVER T FROM 0 TO PI/2),                                     DCE1 340
C           CEL1(AK)=INTEGRAL(1/SQRT(1-(AK*SIN(T))**2),SUMMED OVER T    DCE1 350
C           FROM 0 TO PI/2), WHERE K=SQRT(1.-CK**2).                    DCE1 360
C           EVALUATION                                                  DCE1 370
C           LANDENS TRANSFORMATION IS USED FOR CALCULATION.             DCE1 380
C           REFERENCE                                                   DCE1 390
C           R.ZELLISCH, 'NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS    DCE1 400
C           AND ELLIPTIC FUNCTIONS', HANDBOOK SERIES SPECIAL FUNCTIONS, DCE1 410
C           NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 76-90.              DCE1 420
C                                                                       DCE1 430
C     ..................................................................DCE1 440
      SUBROUTINE DCEL1(RES,AK,IER)                                      DCE1 450
      DOUBLE PRECISION RES,AK,CEC,ARI,AARI                              DCE1 460
      IER=0                                                             DCE1 470
      ARI=2.0D0                                                         DCE1 480
      CEC=(0.5D0-AK)+0.5D0                                              DCE1 490
      CEC=CEC+CEC*AK                                                    DCE1 500
      RES=0.5D0                                                         DCE1 510
      IF(CEC)1,2,4                                                      DCE1 520
    1 IER=1                                                             DCE1 530
    2 RES=1.E75                                                         DCE1 540
      RETURN                                                            DCE1 550
    3 CEC=CEC*AARI                                                      DCE1 560
    4 CEC=DSQRT(CEC)                                                    DCE1 570
      CEC=CEC+CEC                                                       DCE1 580
      AARI=ARI                                                          DCE1 590
      ARI=ARI+CEC                                                       DCE1 600
      RES=RES*RES                                                       DCE1 610
      IF(CEC/AARI-0.5999999999D0)3,5,5                                  DCE1 620
    5 RES=RES/ARI*6.2831853071795864D0                                  DCE1 630
      RETURN                                                            DCE1 640
      END                                                               DCE1 650
```

Subroutines CEL2 and DCEL 2

These subroutines compute the generalized complete elliptic integral of the second kind. This is defined as:

$$\text{cel 2 } (k;\ A,\ B) = \int_0^{\pi/2} \frac{A + (B - A)\sin^2 t}{\sqrt{1 - k^2 \sin^2 t}}\,dt$$

Equivalent is the definition:

$$\text{cel 2 } (k;\ A,\ B) = \int_0^{\infty} \frac{A + Bx^2}{(1 + x^2)\sqrt{(1 + x^2)(1 + k_c^2 x^2)}}\,dx$$

where k_c is the complementary modulus:

$$k_c^2 + k^2 = 1,\quad 0 < k_c^2 \leq 1$$

The subroutines CEL2, DCEL2 calculate cel 2 (k; A, B) for given modulus k and constants A, B. The calculation of RES = cel 2 (k; A, B) is based on the process of the arithmetic-geometric mean.

Starting with the pair of numbers:

$$a_0 = 2,\quad g_0 = 2 \cdot k_c$$

the sequences of numbers (a_n), (g_n) are generated using for definition:

$$a_n = (a_{n-1} + g_{n-1}),\quad g_n = 2\sqrt{a_{n-1}\, g_{n-1}}$$

This iteration process is stopped at the N^{th} step when $a_N = g_N$.

Further needed are the sequences (A_i), (B_i), defined by means of:

$$A_0 = A,\quad B_0 = B$$

$$A_n = B_{n-1}/a_{n-1} + A_{n-1}$$

$$B_n = 2(B_{n-1} + g_{n-1} \cdot A_{n-1})$$

If D is the number of decimal digits in the mantissa of floating-point numbers, the iteration process is stopped as soon as $(a_{N-1} - g_{N-1})$ is less than $a_{N-1} \cdot 10^{-D/2}$.

Since $(2^{-(n+1)}a_n)$, $(2^{-(n+1)}g_n)$ converge quadratically to the same limit (arithmetic-geometric mean), this implies that $(a_N - g_N)$ is less than $a_N \cdot 10^{-D}$.

The value of cel 2 (k, A, B) $= \frac{\pi}{4} \cdot \frac{A_N + 1}{a_N}$

```
C                                                                       CEL2  10
C     ..................................................................CEL2  20
C                                                                       CEL2  30
C        SUBROUTINE CEL2                                                CEL2  40
C                                                                       CEL2  50
C        PURPOSE                                                        CEL2  60
C           COMPUTES THE GENERALIZED COMPLETE ELLIPTIC INTEGRAL OF      CEL2  70
C           SECOND KIND.                                                CEL2  80
C                                                                       CEL2  90
C        USAGE                                                          CEL2 100
C           CALL CEL2(RES,AK,A,B,IER)                                   CEL2 110
C                                                                       CEL2 120
C        DESCRIPTION OF PARAMETERS                                      CEL2 130
C           RES   - RESULT VALUE                                        CEL2 140
C           AK    - MODULUS (INPUT)                                     CEL2 150
C           A     - CONSTANT TERM IN NUMERATOR                          CEL2 160
C           B     - FACTOR OF QUADRATIC TERM IN NUMERATOR               CEL2 170
C           IER   - RESULTANT ERROR CODE WHERE                          CEL2 180
C                   IER=0  NO ERROR                                     CEL2 190
C                   IER=1  AK NOT IN RANGE -1 TO +1                     CEL2 200
C                                                                       CEL2 210
C        REMARKS                                                        CEL2 220
C           FOR ABS(AK) OF 1 THE RESULT IS SET TO 1.E75 IF B IS         CEL2 230
C           POSITIVE, TO -1.E75 IF B IS NEGATIVE.                       CEL2 240
C           SPECIAL CASES ARE                                           CEL2 250
C           K(K) OBTAINED WITH A = 1, B = 1                             CEL2 260
C           E(K) OBTAINED WITH A = 1, B = CK*CK WHERE CK IS             CEL2 270
C           COMPLEMENTARY MODULUS.                                      CEL2 280
C           B(K) OBTAINED WITH A = 1, B = C                             CEL2 290
C           D(K) OBTAINED WITH A = C, B = 1                             CEL2 300
C           WHERE K, E, B, D DEFINE SPECIAL CASES OF THE GENERALIZED    CEL2 310
C           COMPLETE ELLIPTIC INTEGRAL OF SECOND KIND IN THE USUAL      CEL2 320
C           NOTATION, AND THE ARGUMENT K OF THESE FUNCTIONS MEANS       CEL2 330
C           THE MODULUS.                                                CEL2 340
C                                                                       CEL2 350
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  CEL2 360
C           NONE                                                        CEL2 370
C                                                                       CEL2 380
C        METHOD                                                         CEL2 390
C           DEFINITION                                                  CEL2 400
C           RES=INTEGRAL((A+B*T*T)/(SQRT((1+T*T)*(1+(CK*T)**2))*(1+T*T))CEL2 410
C           SUMMED OVER T FROM 0 TO INFINITY).                          CEL2 420
C           EVALUATION                                                  CEL2 430
C           LANDENS TRANSFORMATION IS USED FOR CALCULATION.             CEL2 440
C           REFERENCE                                                   CEL2 450
C           R.BULIRSCH, 'NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS    CEL2 460
C           AND ELLIPTIC FUNCTIONS', HANDBOOK SERIES SPECIAL FUNCTIONS, CEL2 470
C           NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.              CEL2 480
C                                                                       CEL2 490
C     ..................................................................CEL2 500
C                                                                       CEL2 510
      SUBROUTINE CEL2(RES,AK,A,B,IER)                                   CEL2 520
      IER=0                                                             CEL2 530
      ARI=2.                                                            CEL2 540
      CEC=(0.5-AK)+0.5                                                  CEL2 550
      CEC=CEC+CEC*AK                                                    CEL2 560
      RES=A                                                             CEL2 570
      A1=A+B                                                            CEL2 580
      EC=B+B                                                            CEL2 590
      IF(CEC)1,2,6                                                      CEL2 600
    1 IER=1                                                             CEL2 610
    2 IF(B)3,6,4                                                        CEL2 620
    3 RES=-1.E75                                                        CEL2 630
      RETURN                                                            CEL2 640
    4 RES=1.E75                                                         CEL2 650
      RETURN                                                            CEL2 660
    5 CEC=CEC+ARI                                                       CEL2 670
    6 CEC=SQRT(CEC)                                                     CEL2 680
      CEC=CEC+CEC                                                       CEL2 690
      ARI=ARI                                                           CEL2 700
      ARI=ARI+CEC                                                       CEL2 710
      EC=EC+RES*CEC                                                     CEL2 720
      RES=A1                                                            CEL2 730
      EC=EC+EC                                                          CEL2 740
      A1=EC/ARI+A1                                                      CEL2 750
      IF(CEC/ARI-0.5555)5,7,7                                           CEL2 760
    7 RES=A1/ARI                                                        CEL2 770
      RES=RES+0.57079632*RES                                            CEL2 780
    8 RETURN                                                            CEL2 790
      END                                                               CEL2 800
```

```
C                                                                       DCE2  10
C     ***************************************************************** DCE2  20
C                                                                       DCE2  30
C        SUBROUTINE CCEL2                                               DCE2  40
C                                                                       DCE2  50
C        PURPOSE                                                        DCE2  60
C           COMPUTES THE GENERALIZED COMPLETE ELLIPTIC INTEGRAL OF      DCE2  70
C           SECOND KIND.                                                DCE2  80
C                                                                       DCE2  90
C        USAGE                                                          DCE2 100
C           CALL CCEL2(RES,AK,A,B,IER)                                  DCE2 110
C                                                                       DCE2 120
C        DESCRIPTION OF PARAMETERS                                      DCE2 130
C           RES   - RESULT VALUE IN DOUBLE PRECISION                    DCE2 140
C           AK    - MODULUS (INPUT) IN DOUBLE PRECISION                 DCE2 150
C           A     - DOUBLE PRECISION CONSTANT TERM IN NUMERATOR         DCE2 160
C           B     - DOUBLE PRECISION FACTOR OF QUADRATIC TERM           DCE2 170
C                   IN NUMERATOR                                        DCE2 180
C           IER   - RESULTANT ERROR CODE WHERE                          DCE2 190
C                   IER=0  NO ERROR                                     DCE2 200
C                   IER=1  AK NOT IN RANGE -1 TO +1                     DCE2 210
C                                                                       DCE2 220
C                                                                       DCE2 230
C        REMARKS                                                        DCE2 240
C           FOR ABS(AK) GE 1 THE RESULT IS SET TO 1.E75 IF B IS         DCE2 250
C           POSITIVE, TO -1.E75 IF B IS NEGATIVE.                       DCE2 260
C           SPECIAL CASES ARE                                           DCE2 270
C           K(K) OBTAINED WITH A = 1, B = 1                             DCE2 280
C           E(K) OBTAINED WITH A = 1, B = CK*CK WHERE CK IS             DCE2 290
C           COMPLEMENTARY MODULUS.                                      DCE2 300
C           B(K) OBTAINED WITH A = 1, B = C                             DCE2 310
C           D(K) OBTAINED WITH A = C, B = 1                             DCE2 320
C           WHERE K, E, B, D DEFINE SPECIAL CASES OF THE GENERALIZED    DCE2 330
C           COMPLETE ELLIPTIC INTEGRAL OF SECOND KIND IN THE USUAL      DCE2 340
C           NOTATION, AND THE ARGUMENT K OF THESE FUNCTIONS MEANS       DCE2 350
C           THE MODULUS.                                                DCE2 360
C                                                                       DCE2 370
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DCE2 380
C           NONE                                                        DCE2 390
C                                                                       DCE2 400
C        METHOD                                                         DCE2 410
C           DEFINITION                                                  DCE2 420
C           RES=INTEGRAL((A+B*T*T)/(SQRT((1+T*T)*(1+(CK*T)**2))*(1+T*T))DCE2 430
C           SWEEP OVER T FROM 0 TO INFINITY).                           DCE2 440
C           EVALUATION                                                  DCE2 450
C           LANDENS TRANSFORMATION IS USED FOR CALCULATION.             DCE2 460
C           REFERENCE                                                   DCE2 470
C           R.BULIRSCH, 'NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS    DCE2 480
C           AND ELLIPTIC FUNCTIONS', HANDBOOK SERIES SPECIAL FUNCTIONS, DCE2 490
C           NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.              DCE2 500
C                                                                       DCE2 510
C     ***************************************************************** DCE2 520
C                                                                       DCE2 530
      SUBROUTINE CCEL2(RES,AK,A,B,IER)                                  DCE2 540
      DOUBLE PRECISION RES,AK,A,B,CEC,AR1,AAR1,B0,A1                    DCE2 550
      IER=0                                                             DCE2 560
      AR1=2.D0                                                          DCE2 570
      CEC=(1.D0-AK)*0.5D0                                               DCE2 580
      CEC=CEC+CEC*AK                                                    DCE2 590
      RES=A                                                             DCE2 600
      A1=A+B                                                            DCE2 610
      EC=B+B                                                            DCE2 620
      IF(CEC)1,2,6                                                      DCE2 630
    1 IER=1                                                             DCE2 640
    2 IF(B)3,6,4                                                        DCE2 650
    3 RES=-1.D75                                                        DCE2 660
      RETURN                                                            DCE2 670
    4 RES=1.D75                                                         DCE2 680
      RETURN                                                            DCE2 690
    5 CEC=CEC*AAR1                                                      DCE2 700
    6 CEC=DSQRT(CEC)                                                    DCE2 710
      CEC=CEC*CEC                                                       DCE2 720
      AAR1=AR1                                                          DCE2 730
      AR1=AR1+CEC                                                       DCE2 740
      EC=EC+RES*CEC                                                     DCE2 750
      RES=A1                                                            DCE2 760
      EC=EC+EC                                                          DCE2 770
      A1=EC/AR1+A1                                                      DCE2 780
      IF(CEC/AAR1-0.555555555CD15,7,7                                   DCE2 790
    7 RES=A1/AR1                                                        DCE2 800
      RES=RES+C.57C796326754856620C*RES                                 DCE2 810
    8 RETURN                                                            DCE2 820
      END
```

Subroutines ELI1 and DELI1

These subroutines compute the elliptic integral of the first kind, where:

$$\text{eli 1 } (x,\ ck) = \int_0^x \frac{dt}{\sqrt{(1 + t^2)\ (1 + ck^2 t^2)}}$$

Equivalent definitions are:

$$\text{eli 1 } (x,\ ck) = \int_0^{\arctan x} \frac{dt}{\cos t \sqrt{1 + ck^2 \tan^2 t}}$$

$$= \int_0^{\arctan x} \frac{dt}{\sqrt{1 - k^2 \sin^2 t}}$$

where k is the modulus and ck the complementary modulus.

For reason of numerical stability, ck is chosen as input parameter instead of modulus k:

$$0 \leqq ck^2 < \infty \quad \text{and} \quad k^2 + ck^2 = 1.$$

This allows k to be any pure imaginary or real number such that $k^2 \leqq 1$. In standard notation:

$$F\ (\varphi,\ k) = \text{eli 1 } (\tan \varphi,\ ck)$$

Computation is based on the process of the arithmetic-geometric mean together with Landen's transformation:

$$\text{eli 1 } (x,\ ck) = \frac{1}{1 + ck}\ \text{eli 1 } (x_1,\ ck_1)$$

where:

$$ck_1 = \frac{2\sqrt{ck}}{1 + ck}$$

$$x_1 = \frac{(1 + ck)\ x}{1 - ck \cdot x^2}$$

$$\phi_1 = \arctan x_1$$

$$\sin\phi_1 = \frac{x_1}{\sqrt{1 + x_1^2}}$$

The iteration process begins with $ari_0 = 1$, $geo_0 = |ck|$, and the sequences (ari_n), (geo_n) are generated using for definition:

$$ari_{n+1} = ari_n + geo_n$$

$$geo_{n+1} = 2\sqrt{ari_n \cdot geo_n}$$

The iteration process is stopped at the N^{th} step when $ari_N = geo_N$.

Further needed is an iteration scheme for transformation of the argument x.

Setting $ang_i = \dfrac{ari_i}{x_i}$

then $ang_0 = 1/|x|$

$$ang_{n+1} = ang_n - \frac{ari_n \cdot geo_n}{ang_n}$$

Doing the iteration up to the N^{th} step (characterized by $ari_N = geo_N$):

$$\text{eli 1 } (x,\ ck) = \frac{ari_0}{ari_N}\ \text{eli 1 } (x_N,\ ck_N)$$

with $$\sin\phi_N = \frac{ari_N}{\pm\sqrt{ang_N^2 + ari_N^2}}$$

The sign determination of $\sin\phi_N$ must be done so that $\phi_i = \arctan x_i$ is continuously increasing with index i.

With $ari_N = geo_N$, then $ck_N = 1$, $k_N = 0$ and therefore:

$$\text{eli 1 } (x_N,\ ck_N) = \int_0^{\phi_N} dt = \phi_N$$

and the final result is:

$$\text{eli 1 } (x,\ ck) = \frac{\phi_N}{ari_N}$$

Degenerate cases of argument and modulus:

$x = 0$ gives result eli 1 = 0

$ck = 0$ gives result eli 1 = $\text{sgn } x \ln (|x| + \sqrt{1 + x^2})$

```
C                                                                       ELI1  10
C     ...................................................................ELI1  20
C                                                                       ELI1  30
C        SUBROUTINE ELI1                                                ELI1  40
C                                                                       ELI1  50
C        PURPOSE                                                        ELI1  60
C           COMPUTES THE ELLIPTIC INTEGRAL OF FIRST KIND                ELI1  70
C                                                                       ELI1  80
C        USAGE                                                          ELI1  90
C           CALL ELI1(RES,X,CK)                                         ELI1 100
C                                                                       ELI1 110
C        DESCRIPTION OF PARAMETERS                                      ELI1 120
C           RES   - RESULT VALUE                                        ELI1 130
C           X     - UPPER INTEGRATION BOUND (ARGUMENT OF ELLIPTIC       ELI1 140
C                   INTEGRAL OF FIRST KIND)                             ELI1 150
C           CK    - COMPLEMENTARY MODULUS                               ELI1 160
C                                                                       ELI1 170
C        REMARKS                                                        ELI1 180
C           MODULUS K = SQRT(1.-CK*CK).                                 ELI1 190
C                                                                       ELI1 200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ELI1 210
C           NONE                                                        ELI1 220
C                                                                       ELI1 230
C        METHOD                                                         ELI1 240
C           DEFINITION                                                  ELI1 250
C           RES=INTEGRAL(1/SQRT((1+T*T)*(1+(CK*T)**2)), SUMMED          ELI1 260
C           OVER T FROM 0 TO X).                                        ELI1 270
C           EQUIVALENT ARE THE DEFINITIONS                              ELI1 280
C           RES=INTEGRAL(1/(COS(T)*SQRT(1+(CK*TAN(T))**2)), SUMMED      ELI1 290
C           OVER T FROM 0 TO ATAN(X)),                                  ELI1 300
C           RES=INTEGRAL(1/SQRT(1-(K*SIN(T))**2), SUMMED OVER           ELI1 310
C           T FROM 0 TO ATAN(X)).                                       ELI1 320
C           EVALUATION                                                  ELI1 330
C           LANDENS TRANSFORMATION IS USED FOR CALCULATION.             ELI1 340
C           REFERENCE                                                   ELI1 350
C           R. BULIRSCH, NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS ANDELI1 360
C                 ELLIPTIC FUNCTIONS.                                   ELI1 370
C                 HANDBOOK SERIES OF SPECIAL FUNCTIONS                  ELI1 380
C                 NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.        ELI1 390
C                                                                       ELI1 400
C     ...................................................................ELI1 410
C                                                                       ELI1 420
      SUBROUTINE ELI1(RES,X,CK)                                         ELI1 430
C                                                                       ELI1 440
      IF(X)2,1,2                                                        ELI1 450
    1 RES=0.                                                            ELI1 460
      RETURN                                                            ELI1 470
    2 IF(CK)4,3,4                                                       ELI1 480
    3 RES=ALOG(ABS(X)+SQRT(1.+X*X))                                     ELI1 490
      GOTO 13                                                           ELI1 500
    4 ANGLE=ABS(1./X)                                                   ELI1 510
      GEO=ABS(CK)                                                       ELI1 520
      ARI=1.                                                            ELI1 530
      PIM=0.                                                            ELI1 540
    5 SQGEO=ARI*GEO                                                     ELI1 550
      AARI=ARI                                                          ELI1 560
      ARI=GEO+ARI                                                       ELI1 570
      ANGLE=-SQGEO/ANGLE+ANGLE                                          ELI1 580
      SQGEO=SQRT(SQGEO)                                                 ELI1 590
      IF(ANGLE)7,6,7                                                    ELI1 600
C     REPLACE 0 BY SMALL VALUE                                          ELI1 610
    6 ANGLE=SQGEO*1.E-8                                                 ELI1 620
    7 TEST=AARI*1.E-4                                                   ELI1 630
      IF(ABS(AARI-GEO)-TEST)10,10,8                                     ELI1 640
    8 GEO=SQGEO+SQGEO                                                   ELI1 650
      PIM=PIM+PIM                                                       ELI1 660
      IF(ANGLE)9,5,5                                                    ELI1 670
    9 PIM=PIM+3.1415927                                                 ELI1 680
      GOTO 5                                                            ELI1 690
   10 IF(ANGLE)11,12,12                                                 ELI1 700
   11 PIM=PIM+3.1415927                                                 ELI1 710
   12 RES=(ATAN(ARI/ANGLE)+PIM)/ARI                                     ELI1 720
   13 IF(X)14,15,15                                                     ELI1 730
   14 RES=-RES                                                          ELI1 740
   15 RETURN                                                            ELI1 750
      END                                                               ELI1 760
```

```
C                                                                       DEL1  10
C     ...................................................................DEL1  20
C                                                                       DEL1  30
C        SUBROUTINE DELI1                                               DEL1  40
C                                                                       DEL1  50
C        PURPOSE                                                        DEL1  60
C           COMPUTES THE ELLIPTIC INTEGRAL OF FIRST KIND                DEL1  70
C                                                                       DEL1  80
C        USAGE                                                          DEL1  90
C           CALL DELI1(RES,X,CK)                                        DEL1 100
C                                                                       DEL1 110
C        DESCRIPTION OF PARAMETERS                                      DEL1 120
C           RES   - RESULT VALUE IN DOUBLE PRECISION                    DEL1 130
C           X     - UPPER INTEGRATION BOUND (ARGUMENT OF ELLIPTIC       DEL1 140
C                   INTEGRAL OF FIRST KIND) IN DOUBLE PRECISION         DEL1 150
C           CK    - COMPLEMENTARY MODULUS IN DOUBLE PRECISION           DEL1 160
C                                                                       DEL1 170
C        REMARKS                                                        DEL1 180
C           DOUBLE PRECISION MODULUS K = DSQRT(1.D0-CK*CK).             DEL1 190
C                                                                       DEL1 200
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DEL1 210
C           NONE                                                        DEL1 220
C                                                                       DEL1 230
C        METHOD                                                         DEL1 240
C           DEFINITION                                                  DEL1 250
C           RES=INTEGRAL(1/SQRT((1+T*T)*(1+(CK*T)**2)), SUMMED          DEL1 260
C           OVER T FROM 0 TO X).                                        DEL1 270
C           EQUIVALENT ARE THE DEFINITIONS                              DEL1 280
C           RES=INTEGRAL(1/(COS(T)*SQRT(1+(CK*TAN(T))**2)), SUMMED      DEL1 290
C           OVER T FROM 0 TO ATAN(X)),                                  DEL1 300
C           RES=INTEGRAL(1/SQRT(1-(K*SIN(T))**2), SUMMED OVER           DEL1 310
C           T FROM 0 TO ATAN(X)).                                       DEL1 320
C           EVALUATION                                                  DEL1 330
C           LANDENS TRANSFORMATION IS USED FOR CALCULATION.             DEL1 340
C           REFERENCE                                                   DEL1 350
C           R. BULIRSCH, NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS ANDDEL1 360
C                 ELLIPTIC FUNCTIONS.                                   DEL1 370
C                 HANDBOOK SERIES OF SPECIAL FUNCTIONS                  DEL1 380
C                 NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.        DEL1 390
C                                                                       DEL1 400
C     ...................................................................DEL1 410
C                                                                       DEL1 420
      SUBROUTINE DELI1(RES,X,CK)                                        DEL1 430
C                                                                       DEL1 440
      DOUBLE PRECISION RES,X,CK,ANGLE,GEO,ARI,PIM,SQGEO,AARI,TEST       DEL1 450
C                                                                       DEL1 460
      IF(X)2,1,2                                                        DEL1 470
    1 RES=0.D0                                                          DEL1 480
      RETURN                                                            DEL1 490
C                                                                       DEL1 500
    2 IF(CK)4,3,4                                                       DEL1 510
    3 RES=DLOG(DABS(X)+DSQRT(1.D0+X*X))                                 DEL1 520
      GOTO 13                                                           DEL1 530
C                                                                       DEL1 540
    4 ANGLE=DABS(1.D0/X)                                                DEL1 550
      GEO=DABS(CK)                                                      DEL1 560
      ARI=1.D0                                                          DEL1 570
      PIM=0.D0                                                          DEL1 580
    5 SQGEO=ARI*GEO                                                     DEL1 590
      AARI=ARI                                                          DEL1 600
      ARI=GEO+ARI                                                       DEL1 610
      ANGLE=-SQGEO/ANGLE+ANGLE                                          DEL1 620
      SQGEO=DSQRT(SQGEO)                                                DEL1 630
      IF(ANGLE)7,6,7                                                    DEL1 640
C                                                                       DEL1 650
C        REPLACE 0 BY SMALL VALUE                                       DEL1 660
C                                                                       DEL1 670
    6 ANGLE=SQGEO*1.D-17                                                DEL1 680
    7 TEST=AARI*1.D-9                                                   DEL1 690
      IF(DABS(AARI-GEO)-TEST)10,10,8                                    DEL1 700
    8 GEO=SQGEO+SQGEO                                                   DEL1 710
      PIM=PIM+PIM                                                       DEL1 720
      IF(ANGLE)9,5,5                                                    DEL1 730
    9 PIM=PIM+3.1415926535897932                                        DEL1 740
      GOTO 5                                                            DEL1 750
   10 IF(ANGLE)11,12,12                                                 DEL1 760
   11 PIM=PIM+3.1415926535897932                                        DEL1 770
   12 RES=(DATAN(ARI/ANGLE)+PIM)/ARI                                    DEL1 780
   13 IF(X)14,15,15                                                     DEL1 790
   14 RES=-RES                                                          DEL1 800
   15 RETURN                                                            DEL1 810
      END                                                               DEL1 820
```

Subroutines ELI2 and DELI2

These subroutines compute the generalized elliptic integral of the second kind, where:

$$\text{eli 2 } (x,\ ck,\ a,\ b) = \int_0^x \frac{(a + bt^2)\,dt}{(1 + t^2)\sqrt{(1 + t^2)(1 + ck^2 t^2)}}$$

Equivalent are the definitions:

$$\text{eli 2 } (x,\ ck,\ a,\ b) = \int_0^{\arctan x} \frac{(a + b\tan^2 t)\,dt}{\sqrt{(1+\tan^2 t)(1+ck^2\tan^2 t)}}$$

$$= \int_0^{\arctan x} \frac{(a + (b-a)\sin^2 t)\,dt}{\sqrt{1 - k^2\sin^2 t}}$$

where k is the modulus and ck the complementary modulus.

For reasons of numerical stability, ck is chosen as input parameter instead of modulus k:

$$0 \leqq ck^2 < \infty \text{ and } k^2 + ck^2 = 1$$

This allows k to be any pure imaginary or real number such that $k^2 \leqq 1$.

In standard notation:

$$E(\varphi, k) = \text{eli 2 } (\tan\varphi,\ ck,\ 1,\ ck^2)$$
$$F(\varphi, k) = \text{eli 2 } (\tan\varphi,\ ck,\ 1,\ 1)$$

Computation is based on the process of the arithmetic-geometric mean together with Landen's transformation:

$$\text{eli 2 } (x, ck, a, b) = \frac{1}{1 + ck}\left(\text{eli 2 } (x_1,\ ck_1,\ a_1,\ b_1) + \frac{1}{2}(a - b)\frac{x_1}{\sqrt{1 + x_1^2}}\right)$$

where:

$$a_1 = \frac{1}{2}(a + b)$$

$$b_1 = \frac{1}{1 + ck}(b + a \cdot ck)$$

$$ck_1 = \frac{2\sqrt{ck}}{1 + ck}$$

$$a_1 - b_1 = \frac{1}{2}(a - b)\frac{1 - ck}{1 + ck}$$

$$x_1 = \frac{(1 + ck)x}{1 - ck \cdot x^2}$$

$$k_1 = \frac{1 - ck}{1 + ck}$$

$$\varphi_1 = \arctan x_1$$

$$\sin\varphi_1 = \frac{x_1}{\sqrt{1 + x_1^2}}$$

The iteration process begins with $ari_0 = 1$, $geo_0 = |ck|$, and the sequences (ari_n), (geo_n) are generated, using for definition:

$$ari_{n+1} = ari_n + geo_n$$

$$geo_{n+1} = 2\sqrt{ari_n \cdot geo_n}$$

The iteration process is stopped at the N^{th} step when $ari_N = geo_N$.

Further needed are the sequences (A_i), (B_i), defined by means of:

$A_i = a_i$, $B_i = b_i \cdot ari_i$; that is, by the iteration scheme

$$A_0 = a,\ B_0 = b$$

$$A_{n+1} = \frac{1}{2}\left(A_n + \frac{B_n}{ari_n}\right)$$

$$B_{n+1} = B_n + geo_n \cdot A_n$$

Finally an iteration scheme is needed for transformation of the argument x.

Setting $ang_i = \dfrac{ari_i}{x_i}$

gives $ang_0 = 1/|x|$

$$ang_{n+1} = ang_n - \frac{ari_n \cdot geo_n}{ang_n}$$

Doing the iteration scheme up to the N^{th} step (characterized by $ari_N = geo_N$):

$$eli\,2\,(x, ck, a, b) = \frac{ari_0}{ari_N}\, eli\,2\,(x_N, ck_N, a_N, b_N) + SUM$$

where

$$SUM = \frac{a-b}{2}\left(\frac{1}{ari_1}\sin\phi_1 + \frac{1}{ari_2}\,\frac{ari_0 - geo_0}{ari_1}\,\frac{\sin\phi_2}{2}\right.$$

$$\left. + \ldots + \frac{1}{ari_N}\cdot\frac{ari_0 - geo_0}{ari_1}\cdots\frac{ari_{N-2} - geo_{N-2}}{ari_{N-1}}\cdot\frac{\sin\phi_N}{2^{N-1}}\right)$$

with

$$\sin\phi_n = \frac{ari_n}{\pm\sqrt{ang_n^2 + ari_n^2}}$$

The sign determination of $\sin\phi_n$ must be done so that $\phi_i = \arctan x_i$ is continuously increasing with index i.

With $ari_N = geo_N$, then $ck_N = 1$, $k_N = 0$, and therefore

$$eli\,2\,(x_N, ck_N, a_N, b_N) = \int_0^{\phi_n}\left[a_N + (b_N - a_N)\sin^2 t\right]dt$$

$$= \frac{a_N + b_N}{2}\phi_N - \frac{1}{2}(b_N - a_N)\sin\phi_N\cos\phi_N$$

The final result is:

$$eli\,2\,(x, ck, a, b) = \frac{A_{N+1}}{ari_N}\cdot \arctan\frac{ari_N}{ang_N} + SUM +$$

$$\frac{1}{ari_N}\left(\frac{a_N - b_N}{2}\right)\sin\phi_N\cos\phi_N$$

Degenerate cases of argument and modulus:

x = 0 gives result eli 2 = 0

ck = 0 gives result

$$eli\,2 = \left[b\cdot\ln\left(|x| + \sqrt{1+x^2}\right) + (a-b)\frac{|x|}{\sqrt{1+x^2}}\right]\operatorname{sgn} x$$

```
C                                                                       ELI2  10
C     ...............................................................   ELI2  20
C                                                                       ELI2  30
C       SUBROUTINE ELI2                                                 ELI2  40
C                                                                       ELI2  50
C       PURPOSE                                                         ELI2  60
C          COMPUTES THE GENERALIZED ELLIPTIC INTEGRAL OF SECOND KIND    ELI2  70
C                                                                       ELI2  80
C       USAGE                                                           ELI2  90
C          CALL ELI2(R,X,CK,A,B)                                        ELI2 100
C                                                                       ELI2 110
C       DESCRIPTION OF PARAMETERS                                       ELI2 120
C          R      - RESULT VALUE                                        ELI2 130
C          X      - UPPER INTEGRATION BOUND (ARGUMENT OF ELLIPTIC       ELI2 140
C                   INTEGRAL OF SECOND KIND)                           ELI2 150
C          CK     - COMPLEMENTARY MODULUS                               ELI2 160
C          A      - CONSTANT TERM IN NUMERATOR                          ELI2 170
C          B      - QUADRATIC TERM IN NUMERATOR                         ELI2 180
C                                                                       ELI2 190
C       REMARKS                                                         ELI2 200
C          MODULUS K = SQRT(1.-CK*CK).                                  ELI2 210
C          SPECIAL CASES OF THE GENERALIZED ELLIPTIC INTEGRAL OF        ELI2 220
C          SECOND KIND ARE                                              ELI2 230
C          F(ATAN(X),K) OBTAINED WITH A=1., B=1.                        ELI2 240
C          E(ATAN(X),K) OBTAINED WITH A=1., B=CK*CK.                    ELI2 250
C          B(ATAN(X),K) OBTAINED WITH A=1., B=0.                        ELI2 260
C          D(ATAN(X),K) OBTAINED WITH A=0., B=1.                        ELI2 270
C                                                                       ELI2 280
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   ELI2 290
C          NONE                                                         ELI2 300
C                                                                       ELI2 310
C       METHOD                                                          ELI2 320
C          DEFINITION                                                   ELI2 330
C          R=INTEGRAL((A+B*T*T)/(SQRT((1+T*T)*(1+(CK*T)**2))*(1+T*T)),  ELI2 340
C                SUMMED OVER T FROM 0 TO X).                            ELI2 350
C          EQUIVALENT IS THE DEFINITION                                 ELI2 360
C          R=INTEGRAL((A+(B-A)*(SIN(T))**2)/SQRT(1-(K*SIN(T))**2),      ELI2 370
C                SUMMED OVER T FROM 0 TO ATAN(X)).                      ELI2 380
C          EVALUATION                                                   ELI2 390
C          LANDENS TRANSFORMATION IS USED FOR CALCULATION.              ELI2 400
C          REFERENCE                                                    ELI2 410
C          R. BULIRSCH, NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS ANDELI2 420
C                ELLIPTIC FUNCTIONS                                     ELI2 430
C                HANDBOOK SERIES OF SPECIAL FUNCTIONS                   ELI2 440
C                NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.         ELI2 450
C                                                                       ELI2 460
C     ...............................................................   ELI2 470
C                                                                       ELI2 480
      SUBROUTINE ELI2(R,X,CK,A,B)                                       ELI2 490
C        TEST ARGUMENT                                                  ELI2 500
      IF(X)2,1,2                                                        ELI2 510
    1 R=0.                                                              ELI2 520
      RETURN                                                            ELI2 530
C        TEST MODULUS                                                   ELI2 540
    2 C=0.                                                              ELI2 550
      D=0.5                                                             ELI2 560
      IF(CK)7,3,7                                                       ELI2 570
    3 R=SQRT(1.+X*X)                                                    ELI2 580
      R=(A-B)*ABS(X)/R+B*ALOG(ABS(X)+R)                                 ELI2 590
C        TEST SIGN OF ARGUMENT                                          ELI2 600
    4 R=R+C*(A-B)                                                       ELI2 610
      IF(X)5,6,6                                                        ELI2 620
    5 R=-R                                                              ELI2 630
    6 RETURN                                                            ELI2 640
C        INITIALIZATION                                                 ELI2 650
    7 AN=(B+A)*0.5                                                      ELI2 660
      AA=A                                                              ELI2 670
      R=B                                                               ELI2 680
      ANG=ABS(1./X)                                                     ELI2 690
      PIM=0.                                                            ELI2 700
      ISI=0                                                             ELI2 710
      ARI=1.                                                            ELI2 720
      GEO=ABS(CK)                                                       ELI2 730
C        LANDEN TRANSFORMATION                                          ELI2 740
    8 R=AA*GEO+R                                                        ELI2 750
      SGEO=ARI*GEO                                                      ELI2 760
      AA=AN                                                             ELI2 770
      AARI=ARI                                                          ELI2 780
C        ARITHMETIC MEAN                                                ELI2 790
      ARI=GEO+ARI                                                       ELI2 800
C        SUM OF SINE VALUES                                             ELI2 810
      AN=(R/ARI+AA)*0.5                                                 ELI2 820
      AANG=ABS(ANG)                                                     ELI2 830
      ANG=-SGEO/ANG+ANG                                                 ELI2 840
      PIMA=PIM                                                          ELI2 850
      IF(ANG)10,9,11                                                    ELI2 860
    9 ANG=-1.E-8*AANG                                                   ELI2 870
   10 PIM=PIM+3.1415927                                                 ELI2 880
      ISI=ISI+1                                                         ELI2 890
   11 AANG=ARI*ARI+ANG*ANG                                              ELI2 900
      P=D/SQRT(AANG)                                                    ELI2 910
      IF(ISI-4)13,12,12                                                 ELI2 920
   12 ISI=ISI-4                                                         ELI2 930
   13 IF(ISI-2)15,14,14                                                 ELI2 940
   14 P=-P                                                              ELI2 950
   15 C=C+P                                                             ELI2 960
      D=D*(AARI-GEO)*0.5/ARI                                            ELI2 970
      IF(ABS(AARI-GEO)-1.E-4*AARI)17,17,16                              ELI2 980
   16 SGEO=SQRT(SGEO)                                                   ELI2 990
C        GEOMETRIC MEAN                                                 ELI21000
      GEO=SGEO*SGEO                                                     ELI21010
      PIM=PIM+PIMA                                                      ELI21020
      ISI=ISI+ISI                                                       ELI21030
      GOTO 8                                                            ELI21040
C        ACCURACY WAS SUFFICIENT                                        ELI21050
   17 R=(ATAN(ARI/ANG)+PIM)*AN/ARI                                      ELI21060
      C=C+D*ANG/AANG                                                    ELI21070
      GOTO 4                                                            ELI21080
      END                                                               ELI21090
```

the final result is the iteration scheme:

$$c_{N+1} = ari_{N+1} \cot(y \cdot ari_{N+1})$$

$$d_{N+1} = 1$$

$$c_n = d_{n+1} \cdot c_{n+1}$$

$$d_n = \frac{c_{n+1}^2 / ari_{n+2} + geo_{n+1}}{c_{n+1}^2 / ari_{n+2} + ari_{n+1}}$$

for $n = N, N-1, \ldots, 1.$

Then $c_1 = \cot\varphi$, and:

$$sn(x, k) = \frac{1}{\sqrt{1 + c_1^2}} = \frac{1}{\sqrt{1 + \cot^2\varphi}} = \sin\varphi$$

$$cn(x, k) = sn \cdot c_1 = \sin\varphi \cdot \cot\varphi = \cos\varphi$$

$$dn(x, k) = d_1 = \sqrt{1 - k^2 \sin^2\varphi}$$

```
C                                                                       JELF  10
C     ...............................................................   JELF  20
C                                                                       JELF  30
C        SUBROUTINE JELF                                                JELF  40
C                                                                       JELF  50
C        PURPOSE                                                        JELF  60
C           COMPUTES THE THREE JACOBIAN ELLIPTIC FUNCTIONS SN, CN, DN.  JELF  70
C                                                                       JELF  80
C        USAGE                                                          JELF  90
C           CALL JELF(SN,CN,DN,X,SCK)                                   JELF 100
C                                                                       JELF 110
C        DESCRIPTION OF PARAMETERS                                      JELF 120
C           SN    - RESULT VALUE SN(X)                                  JELF 130
C           CN    - RESULT VALUE CN(X)                                  JELF 140
C           DN    - RESULT VALUE DN(X)                                  JELF 150
C           X     - ARGUMENT OF JACOBIAN ELLIPTIC FUNCTIONS             JELF 160
C           SCK   - SQUARE OF COMPLEMENTARY MODULUS                     JELF 170
C                                                                       JELF 180
C        REMARKS                                                        JELF 190
C           NONE                                                        JELF 200
C                                                                       JELF 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  JELF 220
C           NONE                                                        JELF 230
C                                                                       JELF 240
C        METHOD                                                         JELF 250
C           DEFINITION                                                  JELF 260
C           X=INTEGRAL(1/SQRT((1-T*T)*(1-(K*T)**2)), SUMMED OVER        JELF 270
C           T FROM 0 TO SN), WHERE K=SQRT(1-SCK).                       JELF 280
C           SN**SN + CN**CN = 1                                         JELF 290
C           (K*SN)**2 + DN**2 = 1.                                      JELF 300
C           EVALUATION                                                  JELF 310
C           CALCULATION IS DONE USING THE PROCESS OF THE ARITHMETIC     JELF 320
C           GEOMETRIC MEAN TOGETHER WITH GAUSS DESCENDING TRANSFORMATIONJELF 330
C           BEFORE INVERSION OF THE INTEGRAL TAKES PLACE.               JELF 340
C           REFERENCE                                                   JELF 350
C           R. BULIRSCH, NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS ANDJELF 360
C                 ELLIPTIC FUNCTIONS.                                   JELF 370
C                 HANDBOOK SERIES OF SPECIAL FUNCTIONS                  JELF 380
C                 NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.        JELF 390
C                                                                       JELF 400
C     ...............................................................   JELF 410
C                                                                       JELF 420
      SUBROUTINE JELF(SN,CN,DN,X,SCK)                                   JELF 430
C                                                                       JELF 440
C                                                                       JELF 450
      DIMENSION ARI(12),GEO(12)                                         JELF 460
C     TEST MODULUS                                                      JELF 470
      CM=SCK                                                            JELF 480
      Y=X                                                               JELF 490
      IF(SCK)3,1,4                                                      JELF 500
    1 D=EXP(X)                                                          JELF 510
      A=1./D                                                            JELF 520
      B=A+D                                                             JELF 530
      CN=2./B                                                           JELF 540
      DN=CN                                                             JELF 550
      SN=TANH(X)                                                        JELF 560
C        DEGENERATE CASE SCK=0 GIVES RESULTS                            JELF 570
C           CN X = DN X = 1/COSH X                                      JELF 580
C           SN X = TANH X                                               JELF 590
    2 RETURN                                                            JELF 600
C        JACOBIS MODULUS TRANSFORMATION                                 JELF 610
    3 D=1.-SCK                                                          JELF 620
      CM=-SCK/D                                                         JELF 630
      D=SQRT(D)                                                         JELF 640
      Y=D*X                                                             JELF 650
    4 A=1.                                                              JELF 660
      DN=1.                                                             JELF 670
      DO 6 I=1,12                                                       JELF 680
      L=I                                                               JELF 690
      ARI(I)=A                                                          JELF 700
      CM=SQRT(CM)                                                       JELF 710
      GEO(I)=CM                                                         JELF 720
      C=(A+CM)*.5                                                       JELF 730
      IF(ABS(A-CM)-1.E-4*A)7,7,5                                        JELF 740
    5 CM=A*CM                                                           JELF 750
    6 A=C                                                               JELF 760
C                                                                       JELF 770
C        START BACKWARD RECURSION                                       JELF 780
    7 Y=C*Y                                                             JELF 790
      SN=SIN(Y)                                                         JELF 800
      CN=COS(Y)                                                         JELF 810
      IF(SN)8,13,8                                                      JELF 820
    8 A=CN/SN                                                           JELF 830
      C=A*C                                                             JELF 840
      DO 9 I=1,L                                                        JELF 850
      K=L-I+1                                                           JELF 860
      B=ARI(K)                                                          JELF 870
      A=C*A                                                             JELF 880
      C=DN*C                                                            JELF 890
      DN=(GEO(K)+A)/(B+A)                                               JELF 900
    9 A=C/B                                                             JELF 910
      A=1./SQRT(C*C+1.)                                                 JELF 920
      IF(SN)10,11,11                                                    JELF 930
   10 SN=-A                                                             JELF 940
      GOTO 12                                                           JELF 950
   11 SN=A                                                              JELF 960
   12 CN=C*SN                                                           JELF 970
   13 IF(SCK)14,2,2                                                     JELF 980
   14 A=DN                                                              JELF 990
      DN=CN                                                             JELF1000
      CN=A                                                              JELF1010
      SN=SN/D                                                           JELF1020
      RETURN                                                            JELF1030
      END                                                               JELF1040
```

```
C                                                                       DJEL  10
C     ...............................................................   DJEL  20
C                                                                       DJEL  30
C        SUBROUTINE DJELF                                               DJEL  40
C                                                                       DJEL  50
C        PURPOSE                                                        DJEL  60
C           COMPUTES THE THREE JACOBIAN ELLIPTIC FUNCTIONS SN, CN, DN.  DJEL  70
C                                                                       DJEL  80
C        USAGE                                                          DJEL  90
C           CALL DJELF(SN,CN,DN,X,SCK)                                  DJEL 100
C                                                                       DJEL 110
C        DESCRIPTION OF PARAMETERS                                      DJEL 120
C           SN    - RESULT VALUE SN(X) IN DOUBLE PRECISION              DJEL 130
C           CN    - RESULT VALUE CN(X) IN DOUBLE PRECISION              DJEL 140
C           DN    - RESULT VALUE DN(X) IN DOUBLE PRECISION              DJEL 150
C           X     - DOUBLE PRECISION ARGUMENT OF JACOBIAN ELLIPTIC      DJEL 160
C                   FUNCTIONS                                           DJEL 170
C           SCK   - SQUARE OF COMPLEMENTARY MODULUS IN DOUBLE PRECISION DJEL 180
C                                                                       DJEL 190
C        REMARKS                                                        DJEL 200
C           NONE                                                        DJEL 210
C                                                                       DJEL 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DJEL 230
C           NONE                                                        DJEL 240
C                                                                       DJEL 250
C        METHOD                                                         DJEL 260
C           DEFINITION                                                  DJEL 270
C           X=INTEGRAL(1/SQRT((1-T*T)*(1-(K*T)**2)), SUMMED OVER        DJEL 280
C           T FROM 0 TO SN), WHERE K=SQRT(1-SCK).                       DJEL 290
C           SN**SN + CN**CN = 1                                         DJEL 300
C           (K*SN)**2 + DN**2 = 1.                                      DJEL 310
C           EVALUATION                                                  DJEL 320
C           CALCULATION IS DONE USING THE PROCESS OF THE ARITHMETIC     DJEL 330
C           GEOMETRIC MEAN TOGETHER WITH GAUSS DESCENDING TRANSFORMATIONDJEL 340
C           BEFORE INVERSION OF THE INTEGRAL TAKES PLACE.               DJEL 350
C           REFERENCE                                                   DJEL 360
C           R. BULIRSCH, NUMERICAL CALCULATION OF ELLIPTIC INTEGRALS ANDDJEL 370
C                 ELLIPTIC FUNCTIONS.                                   DJEL 380
C                 HANDBOOK SERIES OF SPECIAL FUNCTIONS                  DJEL 390
C                 NUMERISCHE MATHEMATIK VOL. 7, 1965, PP. 78-90.        DJEL 400
C                                                                       DJEL 410
C     ...............................................................   DJEL 420
C                                                                       DJEL 430
      SUBROUTINE DJELF(SN,CN,DN,X,SCK)                                  DJEL 440
C                                                                       DJEL 450
      DIMENSION ARI(12),GEO(12)                                         DJEL 460
      DOUBLE PRECISION SN,CN,DN,X,SCK,ARI,GEO,CM,Y,A,B,C,D              DJEL 470
C                                                                       DJEL 480
C        TEST MODULUS                                                   DJEL 490
C                                                                       DJEL 500
      CM=SCK                                                            DJEL 510
      Y=X                                                               DJEL 520
      IF(SCK)3,1,4                                                      DJEL 530
    1 D=DEXP(X)                                                         DJEL 540
      A=1.D0/D                                                          DJEL 550
      B=A+D                                                             DJEL 560
      CN=2.D0/B                                                         DJEL 570
      DN=CN                                                             DJEL 580
      A=(D-A)/2.D0                                                      DJEL 590
      SN=A*CN                                                           DJEL 600
C        DEGENERATE CASE SCK=0 GIVES RESULTS                            DJEL 610
C           CN X = DN X = 1/COSH X                                      DJEL 620
C           SN X = TANH X                                               DJEL 630
    2 RETURN                                                            DJEL 640
C                                                                       DJEL 650
C        JACOBIS MODULUS TRANSFORMATION                                 DJEL 660
C                                                                       DJEL 670
    3 D=1.D0-SCK                                                        DJEL 680
      CM=-SCK/D                                                         DJEL 690
      D=DSQRT(D)                                                        DJEL 700
      Y=D*X                                                             DJEL 710
```

```
    4 A=1.D0                                                          DJEL 720
      DN=1.D0                                                         DJEL 730
      DO 6 I=1,12                                                     DJEL 740
      L=I                                                             DJEL 750
      ARI(I)=A                                                        DJEL 760
      CM=DSQRT(CM)                                                    DJEL 770
      GEO(I)=CM                                                       DJEL 780
      C=(A+CM)*.5D0                                                   DJEL 790
      IF(DABS(A-CM)-1.D-9*A)7,7,5                                     DJEL 800
    5 CM=A*CM                                                         DJEL 810
    6 A=C                                                             DJEL 820
C                                                                     DJEL 830
C         START BACKWARD RECURSION                                    DJEL 840
C                                                                     DJEL 850
    7 Y=C*Y                                                           DJEL 860
      SN=DSIN(Y)                                                      DJEL 870
      CN=DCOS(Y)                                                      DJEL 880
      IF(SN)8,13,8                                                    DJEL 890
    8 A=CN/SN                                                         DJEL 900
      C=A*C                                                           DJEL 910
      DO 9 I=1,L                                                      DJEL 920
      K=L-I+1                                                         DJEL 930
      B=ARI(K)                                                        DJEL 940
      A=C*A                                                           DJEL 950
      C=DN*C                                                          DJEL 960
      DN=(GEO(K)+A)/(B+A)                                             DJEL 970
    9 A=C/B                                                           DJEL 980
      A=1.D0/DSQRT(C*C+1.D0)                                          DJEL 990
      IF(SN)10,11,11                                                  DJEL1000
   10 SN=-A                                                           DJEL1010
      GOTO 12                                                         DJEL1020
   11 SN=A                                                            DJEL1030
   12 CN=C*SN                                                         DJEL1040
   13 IF(SCK)14,2,2                                                   DJEL1050
   14 A=DN                                                            DJEL1060
      DN=CN                                                           DJEL1070
      CN=A                                                            DJEL1080
      SN=SN/D                                                         DJEL1090
      RETURN                                                          DJEL1100
      END                                                             DJEL1110
```

APPENDIX A: ACCURACY OF SUBROUTINES

The subroutines in SSP can be broken down into three major categories from the standpoint of accuracy. They are (1) subroutines having little or no effect on accuracy, (2) subroutines whose accuracy is dependent on the characteristics of the input data, and (3) subroutines in which definite statements on accuracy can be made.

SUBROUTINES HAVING LITTLE OR NO EFFECT ON ACCURACY

The following subroutines do not materially affect the accuracy of the results, either because of the simple nature of the computation or because they do not modify the data:

ABSNT -- detection of missing data

ARRAY -- vector storage/double-dimensioned conversion

ATSE, DATSE -- table selection out of an equidistant table

ATSG, DATSG -- table selection out of a general table

ATSM, DATSM -- table selection out of a monotonic table

AVDAT -- data storage allocation

BISER -- biserial correlation coefficient

BOUND -- selection of observations within bounds

CADD -- add column of one matrix to column of another matrix

CCPY -- copy column of matrix into vector

CCUT -- partition by column

CHISQ -- χ^2 test for a contingency table

CINT -- interchange two columns

CONVT -- single-precision/double-precision conversion

CSRT -- sort matrix columns

CSUM -- sum the columns of a matrix

CTAB -- tabulate the columns of a matrix

CTIE -- adjoin two matrices by column

DCLA -- replace diagonal with scalar

DCPY -- copy diagonal of matrix into vector

FRAT, DFRAT -- used with ARAT
used with DARAT

GAUSS -- normal random numbers

GMADD -- add two general matrices

GMSUB -- subtract two general matrices

GMTRA -- transpose of a general matrix

KOLM2 -- Kolmogorov - Smirnov two-sample test

KRANK -- Kendall rank correlation

LOC -- location in compressed-stored matrix

MADD -- add two matrices

MCPY -- matrix copy

MFUN -- matrix transformation by a function

MOMEN -- first four moments

MPAIR -- Wilcoxin's signed rank test

MPRC, DMPRC -- permutations of rows or columns of a matrix

MSTR -- storage conversion

MSUB -- subtract two matrices

MTRA -- transpose a matrix

ORDER -- rearrangement of intercorrelations

PADD -- add two polynomials

PADDM -- multiply polynomial by constant and add to another polynomial

PCLA -- replace one polynomial by another

PERM -- inverse of permutation - transposition

PHI -- phi coefficient

PMPY -- multiply two polynomials

PNORM -- normalize coefficient vector of polynomial

PPRCN -- operations with permutations

PSUB -- subtract one polynomial from another

PVSUB -- substitute variable of polynomial by another polynomial

QTEST -- Cochran Q-test

RADD -- add row of one matrix to row of another matrix

RANDU -- uniform random numbers

RANK -- rank observations

RCPY -- copy row of matrix into vector

RCUT -- partition by row

RECP -- reciprocal function for MFUN

RINT -- interchange two rows

RSRT -- sort matrix rows

RSUM -- sum the rows of a matrix

RTAB -- tabulate the rows of a matrix

RTIE -- adjoin two matrices by row

SADD -- add scalar to matrix

SCLA -- matrix clear and add scalar

SCMA -- scalar-multiply column and add to another column

SDIV -- matrix divided by a scalar

SIGNT -- sign test

SMPY -- matrix multiplied by a scalar

SRANK -- Spearman rank correlation

SRATE -- survival rate

SRMA -- scalar-multiply row and add to another row

SSUB -- subtract scalar from a matrix

SUBMX -- build subset matrix

SUBST -- subset selection from observation matrix

TAB1 -- tabulation of data (one variable)

TAB2 -- tabulation of data (two variables)

TIE -- calculation of ties in ranked observations

TRACE -- cumulative percentage of eigenvalues

TTEST -- tests on population means

TWOAV -- Friedman two-way analysis of variance

UTEST -- Mann-Whitney U-test

WTEST -- Kendall coefficient of concordance

XCPY -- copy submatrix from given matrix

SUBROUTINES WHOSE ACCURACY IS DATA-DEPENDENT

The accuracy of the following subroutines cannot be predicted because it is dependent on the characteristics of the input data and on the size of the problem. The programmer using these subroutines must be aware of the limitations dictated by numerical analyses considerations. It cannot be assumed that the results are accurate simply because subroutine execution is completed. Subroutines in this category are:

ACFI, DACFI -- continued fraction interpolation

AHI, DAHI -- Aitken-Hermite interpolation

ALI, DALI -- Aitken-Lagrange interpolation

APCH, DAPCH -- construction of normal equations for a polynomial least-squares fit to a tabulated function

APFS, DAPFS -- solution of normal equations for least-squares fit

APLL, DAPLL -- construction of normal equations for least-squares fit to tabulated function

APMM, DAPMM -- Chebyshev approximation of tabulated functions

ARAT, DARAT -- least-squares rational approximation of tabulated functions

ATEIG -- eigenvalues of a real Hessenberg matrix

AUTO -- autocovariances

AVCAL -- Σ and Δ operation

CANOR -- canonical correlation

CNPS, DCNPS -- value of series expansion in Chebyshev polynomials

CORRE -- means, standard deviations, and correlations

CROSS -- cross covariances

CSPS, DCSPS -- value of series expansion in shifted Chebyshev polynomials

DBAR, DDBAR -- first derivative of a function at the border of the definition interval

DCAR, DDCAR -- first derivative of a function at the center of the definition interval

DET3, DDET3 -- differentiation of equidistantly tabulated functions using three points interpolation

DET5, DDET5 -- differentiation of equidistantly tabulated functions using five points interpolation

DGT3, DDGT3 -- differentiation of tabulated functions using three points interpolation

DISCR -- discriminant functions

DMATX -- means and dispersion matrix

EIGEN -- eigenvalues and eigenvectors of a real, symmetric matrix

EXSMO -- triple exponential smoothing

FACTR -- factorization of a matrix into a product of triangular matrices

FMCG, DFMCG -- unconstrained minimum of a function of several variables--conjugate gradient method

FMFP, DFMFP -- unconstrained minimum of a function of several variables--Davidon method

FORIF -- Fourier analysis of a given function

FORIT -- Fourier analysis of a tabulated function

GDATA -- data generation

GELB, DGELB -- system of general simultaneous linear equations with band-structured coefficients

GELG, DGELG -- system of general simultaneous linear equations by Gauss elimination

GELS, DGELS -- system of general simultaneous linear equations with symmetric coefficients

GMPRD -- product of two general matrices

GTPRD -- transpose product, general matrices

HARM, DHARM -- complex three-dimensional analysis

HEPS, DHEPS -- value of series expansion in Hermite polynomials

HPCG, DHPCG -- solution of general system of first-order ordinary differential equations with given initial values by Hamming's modified predictor-corrector method

HPCL, DHPCL -- solution of linear system of first-order ordinary differential equations with given initial values by Hamming's modified predictor-corrector method

HSBG -- reduction of a real matrix to Hessenberg form

KOLMO -- Kolmogorov-Smirnov one-sample test

LAPS, DLAPS -- value of series expansion in Laguerre

LBVP, DLBVP -- solution of system of linear first-order ordinary differential equations with linear boundary conditions by method of adjoint equations

LEPS, DLEPS -- value of series expansion in Legendre polynomials

LLSQ, DLLSQ -- solution of linear least-squares problems

LOAD -- factor loading

MCHB, DMCHB -- factorization of a symmetric positive definite band matrix

MATA -- transpose product of a matrix

MEANQ -- mean square operation

MFGR, DMFGR -- matrix factorization and rank determination

MFSD, DMFSD -- factorizes a symmetric positive definite matrix (square root method)

MFSS, DMFSS -- rank determination and factorization of symmetric positive semidefinite matrix

MINV -- matrix inversion

MISR -- missing value correlations

MLSS, DMLSS -- solve a system of linear equations with symmetric positive semidefinite matrix

MPRD -- matrix product

MTDS, DMTDS -- division of a matrix by a triangular matrix

MULTR -- multiple regression and correlation

NROOT -- eigenvalues and eigenvectors of a special nonsymmetric matrix

PCLD -- complete linear division

PDER -- derivative of a polynomial

PDIV -- divide polynomials

PECN, DPECN -- economization of a polynomial for symmetric range

PECS, DPECS -- economization of a polynomial for unsymmetric range

PFQB, DPFQB -- determination of a quadratic factor of a polynomial

PGCD -- greatest common divisor of two polynomials

PILD -- evaluate polynomial and its first derivative

PINT -- integral of a polynomial

POINT -- point biserial correlation

POLRT -- real and complex roots of a real polynomial

PQSD -- quadratic synthetic division of a polynomial

PRBM, DPRBM -- roots of a polynomial with real coefficients--Bairstow's method

PROBT -- probit analysis

PRQD, DPRQD -- roots of a real polynomial by QD algorithm with displacement

PVAL -- evaluate polynomial

QA2-QA10, DQA4-DQA32 -- integration of a given function by associated Gaussian-Laguerre quadrature formulas

QATR, DQATR -- integration of a given function by trapezoidal rule together with Romberg's extrapolation method

QG2-QG10, DQG4-DQG32 -- integration of a given function by Gaussian quadrature formulas

QH2 QH10, DQH8-DQH64 -- integration of a given function by Gaussian - Hermite quadrature formulas

QHFE, DQHFE -- integration of equidistantly tabulated function with first derivative by Hermitian formula of first order

QHFG, DQHFG -- integration of monotonically tabulated function with first derivative by Hermitian formula of first order

QHSG, DQHSG -- integration of monotonically tabulated function with first and second derivatives by Hermitian formula of first order

QHSE, DQHSE -- integration of equidistantly tabulated function with first and second derivatives by Hermitian formula of second order

QL2-QL10, DQL4-DQL32 -- integration of a given function by Gaussian-Laguerre quadrature formulas

QSF, DQSF -- integration of equidistantly tabulated function by Simpson's rule

QTFE, DQTFE integration of equidistantly tabulated function by trapezoidal rule

QTFG, DQTFG -- integration of monotonically tabulated function by trapezoidal rule

RHARM, DRHARM -- real one-dimensional analysis

RKI -- solution of first-order differential equation by Runge-Kutta method

RK2 -- tabulated solution of first-order differential equation by Runge-Kutta method

RKGS, DRKGS -- solution of system of first-order ordinary differential equations with given initial values by the Runge-Kutta method

RSLMC -- solution of a system of linear equations

RTMI, DRTMI -- determine root within a range by Mueller's iteration

RTNI, DRTNI -- refine estimate of root by Newton's iteration

RTWI, DRTWI -- refine estimate of root by Wegstein's iteration

SE13, DSE13 -- local least-squares smoothing of equidistantly tabulated functions

SE15, DSE15 local least-squares smoothing of equidistantly tabulated functions

SE35, DSE35 -- local least-squares smoothing of equidistantly tabulated functions

SG13, DSG13 -- local least-squares smoothing of tabulated functions

SIMQ -- solution of simultaneous linear, algebraic equations

SINV, DSINV -- inversion of a symmetric positive definite matrix

SMO -- application of filter coefficients (weights)

STPRG -- stepwise regression

TALLY -- totals, means, standard deviations, minimums, and maximums

TCNP, DTCNP -- transform series expansion in Chebyshev polynomials to a polynomial

TCSP, DTCSP -- transform series expansion in shifted Chebyshev polynomials to a polynomial

TETRA -- tetrachoric correlation

THEP, DTHEP -- transform series expansion in Hermite polynomials to a polynomial

TLAP, DTLAP -- transform series expansion in Laguerre polynomials to a polynomial

TLEP, DTLEP -- transform a series expansion in Legendre polynomials to a polynomial

TPRD -- transpose product

VARMX -- varimax rotation

SUBROUTINES WITH DEFINITE ACCURACY CHARACTERISTICS

The subroutines in this section have accuracy characteristics that can be specified on an individual basis. The mathematical descriptions for many of these subroutines contain information on truncation error of a strictly theoretical nature. The actual implementation of these subroutines on System/360 results in the accuracy noted in Table 1. The standard reference for comparing the accuracy of these subroutines is M. Abramowitz, I. A. Stegun, Handbook of Mathematical Functions, National Bureau of Standards, Washington, D. C., March 1965. However, in certain cases, other tables were used, as noted below. It should be remembered that in System /360 single-precision floating point, there are just over six significant figures.

Maximum differences below are given in terms of number of decimal places (D. P.) and/or number of significant digits (S. D.) which agree. The number of digits tabled should be considered when accuracy statements are viewed; that is, certain tables are given to only five places, whereas the algorithms used may be more accurate. In compiling maximum differences, the maximum was taken over the set of points indicated in the table. The average difference was normally much smaller.

The notation x = a (b) c implies that a, a + b, a + 2b, ... , c were the arguments (x) used.

TABLE 1

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
BDTR	$p=I_x(a,b)$	$I_x^{-1}(a,b)$ Tables by Leon H. Harter: New Tables of the Incomplete Gamma Function Ratio and of Percentage Points of the χ^2 and Beta Distribution, 1964	p=.0001, .0005 a=1 (1) 40 b=5(5) 40 p=.0100, .0500 a= 2 (2) 10 b=5 (5) 30	correct to 5 D. P.
		"t" distribution: $t(x,n)=$ $[1+I_z(c,d)]/2$ where $z=x^2/(x^2+n)$ c= 1/2 d= n/2 Tables: Biometrika vol. 1	x= .01, and x= .5 (.5) 4 for n= 1 (1) 24, and n= 30, 40, 60, 120	.5 in 5th D. P.

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
BESJ J Bessel function Parameter D=1 • E - 6	$J_n(x)$	$J_n(x)$	n=0(1)2 x=0(0.2)17.4 n=3(1)9 x=0(0.2)20 n=10(1)11 x=10(0.2)20 n=0(1)20 20(10)50 100 x=1,2,5,10,50, 100	2 in 5th S.D. 1 in 5th S.D. for $J_n(x) > 1.0$ exact to 5 D.P. for $J_n(x) < 1.0$ (limit of table) 3 in 5th S.D. 2 in 5th S.D.
BESK K Bessel function	$K_n(x)$	$e^X K_n(x)$ $e^X K_n(x)$ $K_n(x)$	n=0(1)2 x=0.2(0.2)20 n=3(1)9 x=0.2(0.2)10 =10(1.0)20 n=0(1)20 x=1,2,5,10 20(10)50 50,100 100	1 in 6th S.D. 1 in 5th S.D. 2 in 5th S.D.
BESY Y Bessel function	$Y_n(x)$	$Y_n(x)$	n=0(1)2 x=0.2(0.2)17.4 n=3(1)9 x=0.2(0.2)20 n=10 x=10(0.2)20 n=0(1)20 20(10)50 100 x=1,2,5,10,50,100	3 in 5th S.D. 1 in 5th S.D. for $Y_n(x) > 1.0$ exact to 5 D.P. for $Y_n(x) < 1.0$ (limit of table) 3 in 5th S.D. 1 in 5th S.D.
CDTR	$y = P_g(x)$ where P is the χ^2 distribution function with para- meter g.	$y = P_g(x)$	x=.001(.001).01; .01(.01)1.0; 1.0(.1)2.0; 2.0(.2)10.0; 10.0(.5)20.0; 20 (1) 40 40 (2) 76 for g=1(1)30	1 in the 5th D.P.

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
CEL1 Complete elliptic 1st integral	K(k)	K(m); $k = \sqrt{m}$	m = .01 (.01) .99	2 in 7th S. D.
		K(α); k = sin α	α = 1(1)73	2 in 7th S. D.
		(α in degrees)	α = 74(1)86	3 in 7th S. D.
DCEL1 Complete elliptic 1st integral	K(k)	K(m); $k = \sqrt{m}$	m = .01(.01).86	1 in 16th S. D.
			m = .87(.01) .96	4 in 16th S. D.
			m = .97(.01).99	11 in 16th S. D.
		K(α); k = sin α	α = 1(1)75	1 in 16th S. D.
		(α in degrees)	α = 76(1)80	2 in 16th S. D.
			α = 81(1)86	11 in 16th S. D.
CEL2 Generalized complete elliptic 2nd integral	K(k) with A = B = 1 E(k) with A = 1 $B = 1 - k^2$	K(m); $k = \sqrt{m}$	m = .01(.01) .99	2 in 7th S. D.
		K(α); k = sin α	α = 1(1) 73	2 in 7th S. D.
		(α in degrees)	α = 74(1)86	3 in 7th S. D.
		E(m); $k = \sqrt{m}$	m = .01(01)	2 in 7th S. D.
		E(α); k = sin α	α = 1(1) 86	2 in 7th S. D.
		K'E + E'K - KK'	m = .01(.01) .99	7 in 7th S. D.
		(Legendre's relation)	α = 1(1) 89	1 in 6th S. D.
DCEL2 Generalized complete elliptic 2nd integral	K(k) with A = B = 1 E(k) with A = 1 $B = 1 - k^2$	K(m); $k = \sqrt{m}$	m = .01(.01).99	2 in 16th S. D.
		K(α); k = sin α	α = 1(1)80	2 in 16th S. D.
		(α in degrees)	α = 81(1)86	11 in 16th S. D.
		E(α); k = sin α	α = 1(1)89	2 in 16th S. D.
		K'E + E'K - KK'	m = .01(.01).99	9 in 16th S. D.
		(Legendre's relation)	α = 1(1)89	9 in 16th S. D.
CNP Chebyshev polynomials	$T_n(x)$	$T_n(x)$ n = 0(1)12	x = .0(.2)1.0	1 in 5th D. P.
		$T_n(x)$ n = 0(1)50	x = .00(.05)1.00	6 in 5th D. P.+

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
DCNP Chebyshev polynomials	$T_n(x)$	$T_n(x)$ $n = 0(1)12$	$x = .0(.2)1.0$	No error in 10th D. P.
CS	$C_2(u)$	$C_2(u)$	$x = .02(.02).78$ $0 < u < 1$	1 in 7th D. P.
Fresnel integrals	$S_2(u)$		$x = .80(.02)1.58$ $1 < u < 4$	6 in 7th S. D.
	with			
	$u = \frac{\pi}{2} x^2$		$x = 1.60(.02)5.00$ $4 < u < 40$	2 in 7th S. D.
		$S_2(u)$	$x = .02(.02).78$ $0 < u < 1$	1 in 7th D. P.
			$x = .80(.02)1.58$ $1 < u < 4$	8 in 7th S. D.
			$x = 1.60(.02)5.00$ $4 < u < 40$	2 in 7th S. D.
CSP Shifted Chebyshev polynomials	$T_n^*(x)$	$T_n^*(x) = T_n(2x - 1)$ $n = 0(1)12$	$x = .5(.1)1.0$	2 in 5th D. P.
		$T_n^*(x)$ $n = 0(1)50$	$x = .00(.05)1.00$	7 in 5th D. P. +
DCSP Shifted Chebyshev polynomials	$T_n^*(x)$	$T_n^*(x) = T_n(2x - 1)$ $n = 0(1)12$	$x = .5(.1)1.0$	No error in 10th D. P.
DLGAM (log of the gamma function)	$\ln \Gamma(x)$	$\ln \Gamma(x)$	$x=1$	6 in 9th D. P.
			$x=1.005(.005)$ 1.025	9 in 8th D. P.
			$x=1.980(.005)$ 1.995	9 in 8th S. D.
			$x=1.03(.01)1.31$	8 in 9th S. D.
			$x=1.32(.01)1.67$	8 in 10th S. D.
			$x=1.68(.01)1.97$	7 in 9th S. D.
			$x=2$	6 in 9th S. D.
		$\log_{10} \Gamma(x)$	$x=3.0(1.0)100.0$	No error in 8 place tables

+Differences between results of single- and double-precision routines

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
ELI1 Incomplete elliptic 1st integral	$F(\zeta/\alpha)$ with $x = \tan\zeta$ $k = \sin\alpha$ $ck = \sqrt{1-k^2}$	$F(\zeta/\alpha)$ (ζ, α in degrees)	$\zeta = 0(5)10$ $\alpha = 0(2)90$	2 in 7th D. P.
			$\zeta = 15(5)35$ $\alpha = 0(2)90$	7 in 7th S. D
			$\zeta = 40(5)50$ $\alpha = 0(2)90$	11 in 7th D. P.
			$\zeta = 55(5)85$ $\alpha = 0(2)90$	3 in 7th S. D.
DELI1 Incomplete elliptic 1st integral	$F(\varphi/\alpha)$ with $x = \tan\varphi$ $k = \sin\alpha$ $ck = \sqrt{1-k^2}$	$F(\varphi/\alpha)$ (φ, α in degrees)	$\varphi = 0(5)85$ $\alpha = 0(2)90$	1 in 9th D. P. (probably due to rounding errors in table)
		$F(\varphi/\alpha) + F(\psi/\alpha)$ $= F\left(\frac{\pi}{2}/\alpha\right)$	$\varphi = 0(5)85$ $\alpha = 0(2)80$	2 in 15th D. P.
		(φ, α, ψ in degrees)	ψ = Arctan f $f = 1/(\cos\alpha \cdot \tan\varphi)$	
ELI2 Generalized incomplete 2nd integral	$F(\zeta/\alpha)$ with A = B = 1 $E(\zeta/\alpha)$ with A = 1 and $B = 1 - k^2$ $x = \tan\zeta$ $k = \sin\alpha$ $ck = \sqrt{1-k^2}$	$F(\zeta/\alpha)$ (ζ, α in degrees)	$\zeta = 0(5)10$ $\alpha = 0(2)90$	2 in 7th D. P.
			$\zeta = 15(5)35$ $\alpha = 0(2)90$	7 in 7th S. D.
			$\zeta = 40(5)50$ $\alpha = 0(2)90$	11 in 7th D. P.
			$\zeta = 55(5)85$ $\alpha = 0(2)90$	3 in 7th S. D.
		$E(\zeta/\alpha)$ (ζ, α in degrees)	$\zeta = 0, 5$ $\alpha = 0(2)90$	2 in 7th D. P.
			$\zeta = 10(5)35$ $\alpha = 0(2)90$	7 in 7th S. D.
			$\zeta = 40(5)55$ $\alpha = 0(2)90$	12 in 7th D. P.
			$\zeta = 60(5)85$ $\alpha = 0(2)90$	36 in 7th D. P.

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
DELI2 Generalized incomplete elliptic 2nd integral	$F(\varphi/\alpha)$ with A = B = 1 $E(\varphi/\alpha)$ with A = 1 $B = 1-k^2$ and $x = \tan\varphi$ $k = \sin\alpha$ $ck = \sqrt{1-k^2}$	$F(\varphi/\alpha)$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)90	1 in 9th D. P. (probably due to rounding errors in table)
		$E(\varphi/\alpha)$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)90	1 in 9th D. P. (probably due to rounding errors in table)
		$E(\varphi/\alpha) + E(\psi/\alpha)$ $= E\left(\frac{\pi}{2}/\alpha\right) + \sin^2\alpha \sin\phi \sin\psi$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)90 ψ = Arctan f f = 1/(cos α · tan φ)	2 in 15th D. P.
		$F(\varphi/\alpha) + F(\psi/\alpha)$ $= F\left(\frac{\pi}{2}/\alpha\right)$ (φ, α in degrees)	φ = 0(5)85 α = 0(2)82 ψ = Arctan f f = 1/(cos α · tan φ)	3 in 15th D. P.
EXPI Exponential integral	$-E_i(-x)$ when $x < 0$ $E_1(x)$ when $x > 0$	$(E_1(x) + \ln x + \gamma)/x$	x = .01(.01).50	1 in 7th S. D.
		$E_1(x)$	x = .50(.01)1.00	4 in 7th S. D.
		$xe^x E_1(x)$	x = 1.00(.01)2.00	7 in 7th S. D.
			x = 2.0(.1)4.0	2 in 4th S. D.
			x = 4.0(.1)10.0	2 in 7th S. D.
		$(-E_i(-x) + \ln\lvert x\rvert + \gamma)/x$	x = -.01(-.01)-.50	1 in 7th S. D.
		$-E_i(-x)$	x = -.50(.01)-1.00	3 in 7th S. D.
			x = -1.00(-.01)-2.00	4 in 7th S. D.
		$-xe^x E_i(-x)$	x = -2.0(-.1)-4.0	4 in 6th S. D.
GMMMA Gamma function	$\tau(x)$	$\tau(x)$	x = 1.0(0.005)2.0 x = 1.0(1.0)57.0	3 in 6th S. D. 6 in 6th S. D.
HEP Hermite polynomials	$H_n(x)$	$H_n(x)$ n = 0(1)12	x = 0.5, 1, 3, 5, 10	Maximum relative error 2.10^{-7}
		$H_n(x)$ n = 0(1)50	x = 0.0(.1)1.0 x = 1(1)10	Maximum relative error 3.10^{-5+}

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
DHEP Hermite polynomials	$H_n(x)$	$H_n(x)$ n = 0(1)12	x = 0.5,1,3,5,10	No error in 11th S.D.
I0	$I_0(x)$		x = [1 (1) 20] (500 random numbers applied per unit interval)	1.2 in 6th D.P.
INUE	$I_n(x)$ n = 1, 2, ..., 10		x = [1 (1) 20] (500 random arguments per unit interval)	5.5 in 6th D.P.
JELF Jacobian elliptic functions	sn u = sin φ cn u = cos φ dn u = $\sqrt{1-k^2 \sin^2\varphi}$ with φ = am u or u = F(φ/α), k = sin α sck = $1-k^2$	sn u = sin φ (φ, α in degrees) cn u = cos φ (φ, α in degrees) dn u = $\sqrt{1-k^2\sin^2\varphi}$ (φ, α in degrees) sn u cn u dn u sn u - sn(2K-u) sn u + sn(2K + u) sn u + sn(4K - u) cn u + cn(2K - u) cn u + cn(2K + u) cn u - cn(4K - u) dn u - dn(2K - u) dn u - dn(2K + u) dn u - dn(4K - u)	φ = 0(1)89 α = 0(5)85 φ = 0(1)89 α = 0(5)85 φ = 0(1)89 α = 0(5)85 k^2 = .00(.05).95 t = 0(1)25 u = t.K(k)/25 k^2 = .00(.05).95 t = 0(1)25 u = t.K(k)/25 k^2 = .00(.05).95 t = 0(1)25 u = t.K(k)/25 k^2 = .00(.05).90 t = 0(1)25 u = t.K(k)/25 k^2 = .00(.05).90 t = 0(1)25 u = t.K(k)/25	1 in 6th D.P.+ 2 in 6th D.P.+ 1 in 6th D.P.+ 1 in 6th D.P.++ 2 in 6th D.P.++ 1 in 6th D.P.++ 6 in 6th D.P. 6 in 6th D.P. 10 in 6th D.P. 4 in 6th D.P. 4 in 6th D.P. 6 in 6th D.P. 3 in 6th D.P. 3 in 6th D.P. 5 in 6th D.P.

+ Calculation of $\mu = f(\varphi/\alpha)$ with double-precision subroutine
++ Difference between result of single- and double-precision routines

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
DJELF	sn u = sin φ	sn u = sin φ (φ, α in degrees)	φ = 5(5)85 α = 0(2)90	2 in 15th D. P. +
Jacobian elliptic functions	cn u = cos φ	cn u = cos φ (φ, α in degrees)	φ = 5(5)85 α = 0(2)90	3 in 15th D. P. +
	dn u = $\sqrt{1 - k^2\alpha}$ ($\alpha = \sin^2\varphi$ with φ = am u, u = F(φ/α), k = sin α, sck = 1 - k^2)	dn u = $\sqrt{1-k^2\sin^2\varphi}$ (φ, α in degrees)	φ = 5(5)85 α = 0(2)90	2 in 15th D. P. +
		sn u - sn(2K - u)	k^2 = .00(.05).90 t = 0(1)25	5 in 15th D. P.
		sn u + sn(2K + u)	u = t. K(k)/25	5 in 15th D. P.
		sn u + sn(4K - u)		12 in 15th D. P.
		cn u + cn(2K - u)	k^2 = .00(.05).90 t = 0(1)25	3 in 15th D. P.
		cn u + cn(2K + u)	u = t. K(k)/25	3 in 15th D. P.
		cn u - cn(4K - u)		7 in 15th D. P.
		dn u - dn(2K - u)	k^2 = .00(.05).90 t = 0(1)25	3 in 15th D. P.
		dn u - dn(2K + u)	u = t. K(k)/25	2 in 15th D. P.
		dn u - dn(4K - u)		6 in 15th D. P.
LAP Laguerre polynomials	$L_n(x)$	$L_n(x)$	x = 0.5, 1, 3	2 in 6th D. P.
		n = 0(1)12	x = 5, 10	1 in 5th S. D.
		$L_n(x)$ n = 0(1)50	x = 0.0(.1)1.0 except arguments with $L_n(x) < 0.1$	Maximum relative error 4.10^{-6} + +
			x = 1(1)10 except arguments with $L_n(x) < 0.1$	Maximum relative error 1.10^{-5} + +
DLAP Laguerre polynomials	$L_n(x)$	$L_n(x)$ n = 0(1)12	x = 0.5, 1, 3, 5, 10	No error in 10th D. P.

+ Calculation of μ = F (φ/α) with double-precision routine
++ Difference between results of single- and double-precision routines

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
LEP Legendre polynomials	$P_n(x)$	$P_n(x)$ $n = 0,1,2,3,9,10$	$x = .00(.05)1.00$	1 in 6th D. P.
		$P_n(x)$ $n = 0(1)50$	$x = .00(.05)1.00$	5 in 6th D. P. +
DLEP Legendre Polynomials	$P_n(x)$	$P_n(x)$ $n = 0,1,2,3,9,10$	$x = .00(.05)1.00$	No error in 8th D. P.
NDTR	$y = P(x)$ P = normal pdf.	$y = P(x)$	$x = -6(.01)6$	7 in 7th D. P.
NDTRI	$x = P^{-1}(y)$ p = normal pdf.	$x = P^{-1}(y)$	$y = .01(.01).99$	5 in 4th D. P.
SICI	$s_i(x)$	$s_i(x)/x$	$x = .01(.01).50$	1 in 7th S. D.
SINE integral and cosine integral	$c_i(x)$	$s_i(x)$	$x = .50(.01)2.00$	1 in 7th S. D.
			$x = 2.0(.1)10.0$	1 in 7th S. D.
			$x = .01(.01).50$	1 in 7th S. D.
		$-(c_i(x) - \ln x - \gamma)/x^2$	$x = .50(.01)1.50$	2 in 7th S. D.
			$x = 1.50(.01)2.00$	1 in 6th S. D.
		$c_i(x)$	$x = 2.0(.1)4.0$	2 in 6th D. P.
			$x = 4.0(.1)10.0$	1 in 7th D. P.

+Difference between results of single-and double-precision routines.

Name	Functions calculated	Functions checked with reference	Range checked with reference	Maximum difference
SMIRN Kolmogorov-Smirnov limiting distribution	L(x)	L (x); Tables by N. Smirnov, reprinted in Annals of Math. Stat. 19, pp. 280-281 (6- and 7- place tables). Double-precision version differences are given in parentheses in the right-hand column.	x = 0(.01) .61	1 in 6^{th} D. P. (1 in 6^{th} D. P.)
			x = .62	3 in 5^{th} D. P. (see program comments) (3 in 5^{th} D. P.)
			x = .63 (.01) 1.04	3 in 6th D. P. (2 in 6th D. P)
			x = 1.05(.01)1.15	6 in 6th D. P. (2 in 6th D. P)
			x =1.16(.01) 1.20	9 in 6th D. P. (2 in 6th D. P)
			x = 1.21 (.01) 1.45	8 in 6th D. P. (3 in 6th D. P)
			x=1.46(.01) 1.65	6 in 6th D. P. (1 in 6th D. P)
			x =1.66(.01) 1.86	2 in 6th D. P. (0 in 6th D. P)
			x =1.87	2 in 5th D. P. (2 in 5th D. P)
			x =1.88 (.01) 2.04	2 in 6th D. P. (1 in 6th D. P)
			x =2.05 (.01) 2.50	1 in 6th D. P. (1 in 6th D. P)
			x =2.51 (.01) 3.5	2 in 7th D. P. (1 in 7th D. P)

APPENDIX B: SAMPLE PROGRAM DESCRIPTIONS

DATA SCREENING

Problem Description

A set of observations is read along with information on propositions to be satisfied and limits on a selected variable. From this input a subset is obtained and a histogram of frequency over given class intervals is plotted for the selected variable. Total, average, standard deviation, minimum, and maximum are calculated for the selected variable. This procedure is repeated until all sets of input data have been processed.

Program

Description

The data screening sample program consists of a main routine, DASCR, and six subroutines; namely, SUBST, TAB1, LOC, BOOL, HIST, and MATIN. Three of these (SUBST, TAB1, LOC) are from the Scientific Subroutine Package. MATIN is a sample input routine. HIST is a program for plotting a histogram. For a description of subroutine BOOL see subroutine SUBST.

Capacity

The maximum size of matrix of observations has been set at 1000 elements, the number of observations at 200, and the number of conditions at 21. All of these can be increased as described under "Program Modification" below.

Input

Control Cards

A parameter card with the following format must precede each matrix of observations:

Columns	Contents	For Sample Problem
1 - 2	Blank	
3 - 6	Up to four-digit identification code (numeric only)	0001
7 - 10	Number of observations	0100
11 - 14	Number of variables	0004

Each matrix of observations must be followed by a card with a 9 punch in column 1. The condition matrix and bounds data are preceded by a card containing the number of conditions and the variable to be selected for analysis:

Columns	Contents	For Sample Problem
1 - 2	Number of conditions	02
3 - 4	Variable to be selected	03

A blank card after the last set of input data terminates the run.

Data Cards

1. For the observation matrix--data cards have seven fields of ten columns each. The decimal point may appear anywhere in a field. If no decimal point is included, it is assumed that the decimal point is to the right of the last digit. The number in each field may be preceded by blanks. All values for an observation are punched consecutively and may continue from card to card. However, a new observation must start in the first field of the next card.
2. For the condition matrix (see description in the subroutine SUBST)--each ten-column field contains a condition to be satisfied. The first two columns contain the variable number (right-justified), the third column the relational code, and the last seven columns of each field a floating-point number. This number may be punched anywhere in the seven-column field but must contain a decimal point. There may be as many as seven conditions per card and a total of three cards or 21 conditions.
3. For the UBO vector (see description in the subroutine TAB1)--the UBO vector is punched in three fields of ten columns each as a floating-point number with decimal point.

Deck Setup

The deck setup is shown in Figure 35.

Sample

A listing of input cards for the sample problem is presented in Figure 36. Card 002 is the parameter card for the matrix of observations. It shows that there are 100 observations and four variables in matrix number 1. Card 003 is the first observation, card 102 the last. Each observation represents an individual with four characteristics (variables). The variables are, in the order shown, (1) age in years, (2) height in inches, (3) weight in pounds, and (4) education in years.

Card 103 signals the end of the matrix of observations.

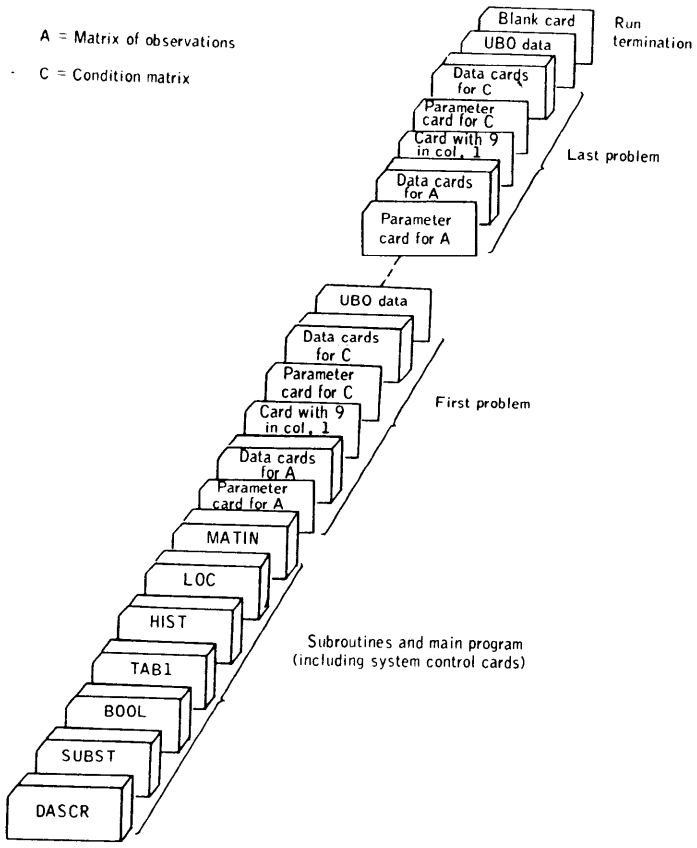


Figure 35. Deck setup (data screening)

Card 104 indicates that there are two conditions to be satisfied and that variable 3 (weight) is selected for analysis. Card 105 shows the condition matrix. The first condition states that variable 1 (age) must be less than or equal to 65, and therefore observations for individuals over 65 will be rejected. The second condition states that variable 4 (education) must be greater than eight years, and consequently observations for individuals with less than eight years of education will be rejected.

Card 106 contains the information on bounds and number of intervals for the selected variable. It shows that the lower bound is 120, the upper bound is 210, and that there are 20 intervals (including one for under lower bound and another for equal to or greater than upper bound).

Card 107 is a blank card for terminating the run.

Output

Description

The output consists of the subset vector showing which observations are rejected (zero) and accepted (nonzero), summary statistics for the selected variable, and a histogram of frequencies versus intervals for that variable.

Sample

The output listing for the sample problem is shown in Figure 37.

Program Modification

The size of the maximum problem to be solved can be increased or decreased by changing the DIMENSION statement in DASCR.

Subroutine BOOL can be replaced if the user wishes to use a different boolean expression (see description in subroutine SUBST). The boolean expression provided in the sample program is for both conditions to be satisfied:

$$T = R(1) * R(2)$$

Operating Instructions

The sample program for data screening is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and logical unit 6 is used for output. Data set 13 is used for intermediate storage.

Error Messages

The following error conditions will result in messages:

1. Reserved storage area is too small for matrix--DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX. GO ON TO NEXT CASE.
2. Number of data cards does not correspond to that required by parameter card--INCORRECT NUMBER OF DATA CARDS FOR MATRIX. EXECUTION TERMINATED.

Error condition 1 allows the computer run to continue. Error condition 2, however, terminates execution and requires another run to process succeeding cases.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 42 seconds.

```
/DATA
  0301010002004
46.       64.       173.      12.
24.       72.       170.       8.
32.       71.       154.      16.
41.       68.       129.      10.
50.       65.       192.       9.
63.       75.       203.      12.
29.       70.       122.      14.
28.       64.       136.      13.
52.       77.       147.      11.
36.       67.       153.      18.
31.       68.       165.       9.
72.       70.       178.      10.
53.       71.       205.      14.
21.       65.       213.      12.
49.       63.       150.       6.
28.       62.       160.      16.
53.       72.       161.      13.
47.       73.       142.      15.
37.       67.       193.      18.
64.       58.       156.      14.
65.       60.       114.      10.
62.       64.       153.      12.
19.       68.       225.       9.
46.       67.       158.      11.
33.       72.       121.       4.
37.       65.       132.      13.
41.       76.       148.      16.
52.       71.       123.      16.
29.       68.       128.      14.
32.       65.       155.      17.
24.       72.       172.      16.
56.       73.       163.      10.
63.       65.       158.      11.
67.       69.       146.       2.
58.       66.       171.       9.
41.       65.       153.      12.
49.       66.       165.      14.
52.       72.       172.      16.
23.       78.       183.      15.
56.       71.       195.      16.
52.       68.       118.       7.
40.       66.       165.      14.
39.       68.       215.      16.
23.       71.       154.      12.
56.       65.       149.      10.
25.       65.       162.      16.
37.       68.       152.      16.
46.       70.       159.      15.
41.       69.       137.      14.
62.       71.       163.      12.
29.       72.       191.       4.
19.       68.       168.      10.
46.       63.       158.      16.
37.       64.       139.      18.
34.       68.       156.      10.
64.       67.       153.      12.
57.       67.       141.      13.
32.       68.       157.      17.
29.       70.       183.      15.
53.       72.       164.      18.
47.       72.       156.      18.
56.       73.       160.      16.
61.       74.       169.      12.
21.       68.       161.      10.
25.       76.       178.      11.
23.       72.       157.      16.
29.       68.       185.      16.
39.       70.       159.      14.
42.       70.       134.      10.
56.       62.       159.      12.
63.       70.       177.      12.
51.       71.       161.       9.
41.       66.       158.      10.
33.       69.       158.      16.
37.       68.       157.      16.
25.       70.       163.      15.
63.       68.       159.      12.
53.       71.       202.       6.
51.       72.       167.      14.
47.       73.       164.      14.
39.       75.       151.      12.
28.       68.       166.      10.
64.       69.       156.      16.
55.       67.       144.      16.
51.       66.       177.      10.
46.       65.       157.      12.
72.       66.       125.      10.
66.       65.       131.      12.
28.       74.       149.      18.
27.       71.       168.      11.
23.       72.       158.      12.
23.       72.       163.      12.
60.       68.       157.       9.
30.       66.       142.      10.
39.       67.       162.      16.
46.       74.       154.      16.
50.       68.       158.      10.
61.       66.       161.      14.
36.       64.       157.      15.
32.       71.       156.      16.
9
0203
 12  65.    46  8.
  120.       20.       210.
```

Figure 36. Input cards sample problem (data screening)

```
DATA SCREENING PROBLEM  1

SUBSET VECTOR

   1   1.
   2   0.0
   3   1.
   4   1.
   5   1.
   6   1.
   7   1.
   8   1.
   9   1.
  10   1.
  11   1.
  12   0.0
  13   1.
  14   1.
  15   0.0
  16   1.
  17   1.
  18   1.
  19   1.
  20   1.
  21   1.
  22   1.
  23   1.
  24   1.
  25   0.0
  26   1.
  27   1.
  28   1.
  29   1.
  30   1.
  31   1.
  32   1.
  33   1.
  34   0.0
  35   1.
  36   1.
  37   1.
  38   1.
  39   1.
  40   1.
  41   0.0
  42   1.
  43   1.
  44   1.
  45   1.
  46   1.
  47   1.
  48   1.
  49   1.
  50   1.
  51   0.0
  52   1.
  53   1.
  54   1.
  55   1.
  56   1.
  57   1.
  58   1.
  59   1.
  60   1.
  61   1.
  62   1.
  63   1.
  64   1.
  65   1.
  66   1.
  67   1.
  68   1.
  69   1.
  70   1.
  71   1.
  72   1.
  73   1.
  74   1.
  75   1.
  76   1.
  77   1.
  78   0.0
  79   1.
  80   1.
  81   1.
  82   1.
  83   1.
  84   1.
  85   1.
  86   1.
  87   0.0
  88   0.0
  89   1.
  90   1.
  91   1.
  92   1.
  93   1.
  94   1.
  95   1.
  96   1.
  97   1.
  98   1.
  99   1.
 100   1.
```

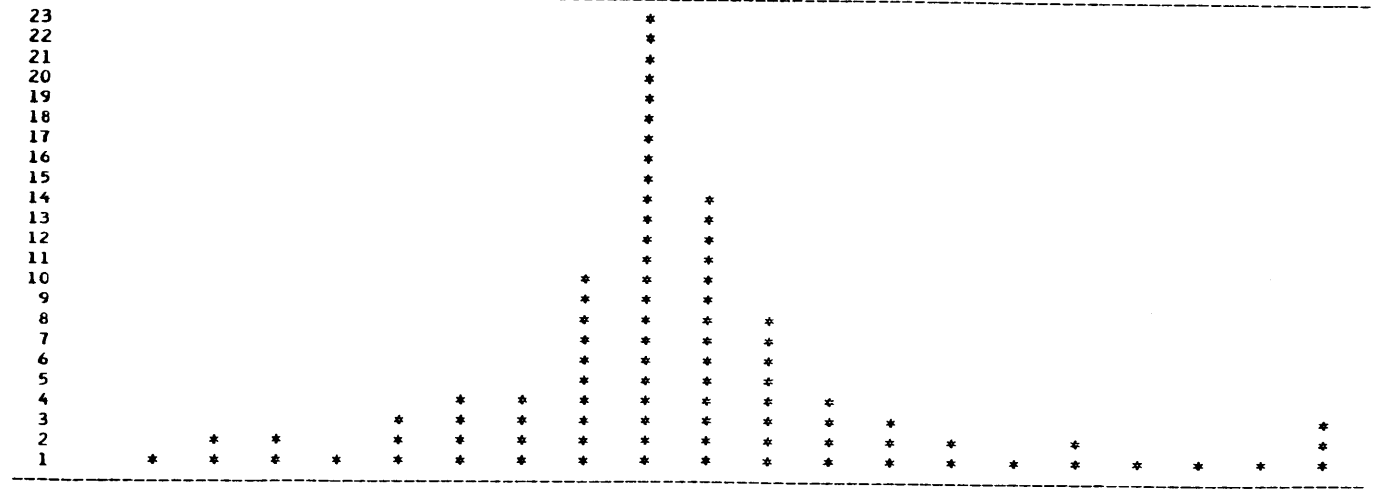
Figure 37. Output listing (data screening)

```
SUMMARY STATISTICS FOR VARIABLE   3

TOTAL = 14492.000  AVERAGE =   161.022  STANDARD DEVIATION =    19.329  MINIMUM =   114.000  MAXIMUM =   225.000

                                        HISTOGRAM   1

FREQUENCY    1   2   2   1   3   4   4  10  23  14   8   4   3   2   1   2   1   1   1   3
```




```
INTERVAL     1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
CLASS

END OF CASE
```

Figure 37. Output listing (data screening) (Continued)

```
C                                                                       DASC  10
C     ...................................................................DASC  20
C                                                                       DASC  30
C        SAMPLE MAIN PROGRAM FOR DATA SCREENING - DASCR                 DASC  40
C                                                                       DASC  50
C        PURPOSE                                                        DASC  60
C           PERFORM DATA SCREENING CALCULATIONS ON A SET OF OBSERVATIONSDASC  70
C                                                                       DASC  80
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DASC  90
C           SUBST                                                       DASC 100
C           TABL                                                        DASC 110
C           LOC                                                         DASC 120
C           BOOL                                                        DASC 130
C           HIST                                                        DASC 140
C           MATIN                                                       DASC 150
C                                                                       DASC 160
C        METHOD                                                         DASC 170
C           DERIVE A SUBSET OF OBSERVATIONS SATISFYING CERTAIN          DASC 180
C           CONDITIONS ON THE VARIABLES. FOR THIS SUBSET, THE FREQUENCY DASC 190
C           OF A SELECTED VARIABLE OVER GIVEN CLASS INTERVALS IS        DASC 200
C           OBTAINED. THIS IS PLOTTED IN THE FORM OF A HISTOGRAM.       DASC 210
C           TOTAL, AVERAGE, STANDARD DEVIATION, MINIMUM, AND MAXIMUM    DASC 220
C           ARE ALSO CALCULATED.                                        DASC 230
C                                                                       DASC 240
C     ...................................................................DASC 250
C                                                                       DASC 260
      DIMENSION A(1000),C(63),UBO(3),S(200),R(21),FREQ(20),             DASC 270
     1PCT(20),STATS(5)                                                  DASC 280
      EXTERNAL BOOL                                                     DASC 290
   10 FORMAT(1H1,22HDATA SCREENING PROBLEM,I3)                          DASC 300
   11 FORMAT(1H0,44HDIMENSIONED AREA TOO SMALL FOR INPUT MATRIX ,I4)    DASC 310
   12 FORMAT(1H0,20HEXECUTION TERMINATED)                               DASC 320
   13 FORMAT(1H0,42HINCORRECT NUMBER OF DATA CARDS FOR MATRIX ,I4)      DASC 330
   14 FORMAT(1H0,18HGO ON TO NEXT CASE)                                 DASC 340
   15 FORMAT(1H0,11HEND OF CASE)                                        DASC 350
   16 FORMAT(7(F2.0,F1.0,F7.3))                                         DASC 360
   17 FORMAT(3F10.0)                                                    DASC 370
   18 FORMAT(1H0,13HSUBSET VECTOR,///)                                  DASC 380
   19 FORMAT(1H ,I3,F5.0)                                               DASC 390
   20 FORMAT(1H1,32HSUMMARY STATISTICS FOR VARIABLE ,I3)                DASC 400
   21 FORMAT(1H0,7HTOTAL =,F10.3,2X,9HAVERAGE =,F10.3,2X,2HSTANDARD DEVDASC 410
     1IATION =,F10.3,2X,9HMINIMUM =,F10.3,2X,9HMAXIMUM =,F10.3)         DASC 420
   22 FORMAT(2F2)                                                       DASC 430
C                                                                       DASC 440
      KC=0                                                              DASC 450
   24 KC=KC+1                                                           DASC 460
      CALL MATIN(ICOD,A,1000,NO,NV,MS,IER)                              DASC 470
      IF(NO) 25,50,25                                                   DASC 480
   25 IF(IER-1) 40,30,35                                                DASC 490
   30 WRITE(6,11) ICOD                                                  DASC 500
      WRITE(6,14)                                                       DASC 510
      GO TO 24                                                          DASC 520
   35 WRITE(6,13)                                                       DASC 530
      WRITE(6,12)                                                       DASC 540
      GO TO 50                                                          DASC 550
   40 READ(5,22)NC,NOVAR                                                DASC 560
      JC=NC*3                                                           DASC 570
      READ(5,16)(C(I),I=1,JC)                                           DASC 580
      READ(5,17)(UBO(I),I=1,3)                                          DASC 590
      CALL SUBST(A,C,R,BOOL,S,NO,NV,NC)                                 DASC 600
      WRITE(6,10)KC                                                     DASC 610
      WRITE(6,18)                                                       DASC 620
      WRITE(6,19) (I,S(I),I=1,NO)                                       DASC 630
      CALL TABL(A,S,NOVAR,UBO,FREQ,PCT,STATS,NO,NV)                     DASC 640
      WRITE(6,20) NOVAR                                                 DASC 650
      WRITE(6,21)(STATS(I),I=1,5)                                       DASC 660
      JZ=UBO(2)                                                         DASC 670
      CALL HIST(KC,FREQ,JZ)                                             DASC 680
      WRITE(6,15)                                                       DASC 690
      GO TO 24                                                          DASC 700
   50 RETURN                                                            DASC 710
      END                                                               DASC 720
```

MULTIPLE LINEAR REGRESSION

Problem Description

Multiple linear regression analysis is performed for a set of independent variables and a dependent variable. Selection of different sets of independent variables and designation of a dependent variable can be made as many times as desired.

The sample problem for multiple linear regression consists of 30 observations with six variables as presented in Table 4. The first five variables are independent variables (predictors), and the last variable is the dependent variable (criteria). All five independent variables are used to predict the dependent variable in the first analysis, and only the second, third, and fifth variables are used to predict the dependent variable in the second analysis.

Table 4. Sample Data for Multiple Linear Regression

	Variables					
Observation	X_1	X_2	X_3	X_4	X_5	X_6
1	29	289	216	85	14	1
2	30	391	244	92	16	2
3	30	424	246	90	18	2
4	30	313	239	91	10	0
5	35	243	275	95	30	2
6	35	365	219	95	21	2
7	43	396	267	100	39	3
8	43	356	274	79	19	2
9	44	346	255	126	56	3
10	44	156	258	95	28	0
11	44	278	249	110	42	4
12	44	349	252	88	21	1
13	44	141	236	129	56	1
14	44	245	236	97	24	1
15	45	297	256	111	45	3
16	45	310	262	94	20	2
17	45	151	339	96	35	3
18	45	370	357	88	15	4
19	45	379	198	147	64	4
20	45	463	206	105	31	3
21	45	316	245	132	60	4
22	45	280	225	108	36	4
23	44	395	215	101	27	1
24	49	139	220	136	59	0
25	49	245	205	113	37	4
26	49	373	215	88	25	1
27	51	224	215	118	54	3
28	51	677	210	116	33	4
29	51	424	210	140	59	4
30	51	150	210	105	30	0

Program

Description

The multiple linear regression program consists of the main routine named REGRE, a special input subroutine named DATA, and four subroutines from the Scientific Subroutine Package: CORRE, ORDER, MINV, and MULTR.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 40 variables, including both independent and dependent variables
2. Up to 99,999 observations, if observations are read into the computer one at a time by the special input subroutine named DATA. If all data are to be stored in core prior to the calculation of correlation coefficients, the limitation on the number of observations depends on the size of core storage available for input data
3. (12F6.0) format for input data cards.

Therefore, if a problem satisfies the above conditions, the sample program need not be modified. However, if there are more than 40 variables, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format in the input subroutine, DATA, must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, REGRE. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE
7 - 11	Number of observations	00030
12 - 13	Number of variables	06
14 - 15	Number of selection cards (see below)	02

Leading zeros are not required to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 4 is keypunched on a separate card using the format (12F6.0). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card.

Selection Card

The selection card is used to specify a dependent variable and a set of independent variables in a multiple linear regression analysis. Any variable in the set of original variables can be designated as a dependent variable, and any number of variables can be specified as independent variables. Selection of a dependent variable and a set of independent variables can be performed over and over again using the same set of original variables.

The selection card is prepared as follows:

Columns	Contents	For Sample Problem Selection 1	Selection 2
1 - 2	Option code for table of residuals: 00 if it is not desired 01 if it is desired	01	01
3 - 4	Dependent variable designated for the forthcoming regression	06	06
5 - 6	Number of independent variables included in the forthcoming regression (the subscript numbers of individual variables are specified below)	05	03
7 - 8	1st independent variable included	01	02
9 - 10	2nd independent variable included	02	03
11 - 12	3rd independent variable included	03	05
13 - 14	4th independent variable included	04	
15 - 16 etc.	5th independent variable included	05	

The input format of (36I2) is used for the selection card.

Deck Setup

The deck setup is shown in Figure 38.

Sample

The listing of input cards for the sample problem is presented in Figure 39.

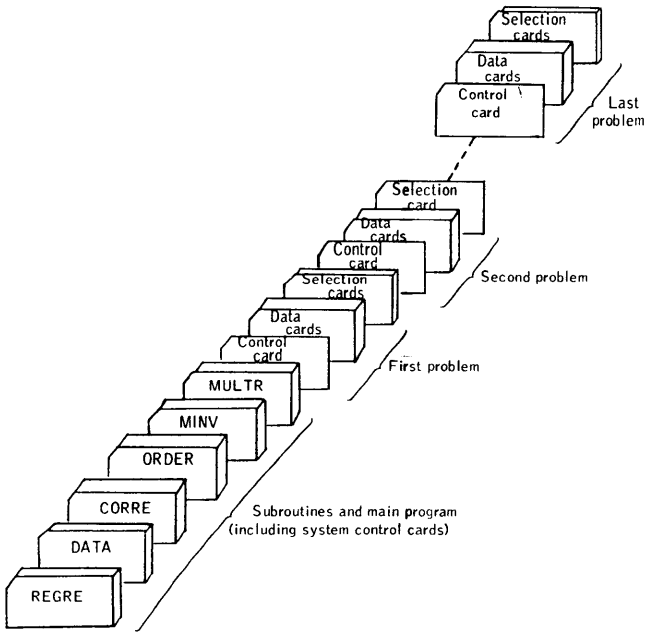


Figure 38. Deck setup (multiple linear regression)

Output

Description

The output of the sample program for multiple linear regression includes:

1. Means
2. Standard deviations
3. Correlation coefficients between the independent variables and the dependent variable
4. Regression coefficients
5. Standard errors of regression coefficients
6. Computed t-values
7. Intercept
8. Multiple correlation coefficients
9. Standard error of estimate
10. Analysis of variance for the multiple regression
11. Table of residuals (optional)

Sample

The output listing for the sample problem is shown in Figure 40.

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize

```
/DATA                                                                  10
SAMPLE000300602                                                        20
    29   289   216    95    14    1                                    30
    30   391   244    92    16    2                                    40
    30   424   246    90    18    2                                    50
    30   313   239    91    10    0                                    60
    35   243   275    95    30    2                                    70
    35   365   219    95    21    2                                    80
    43   396   267   100    39    3                                    90
    43   356   274    79    19    2                                   100
    44   346   255   126    56    3                                   110
    44   156   258    95    28    0                                   120
    44   278   249   110    42    4                                   130
    44   349   252    88    21    1                                   140
    44   141   236   129    56    1                                   150
    44   245   236    97    24    1                                   160
    45   297   256   111    45    3                                   170
    45   310   262    94    20    2                                   180
    45   151   339    96    35    3                                   190
    45   370   357    88    15    4                                   200
    45   379   198   147    64    4                                   210
    45   463   206   105    31    3                                   220
    45   316   245   132    60    4                                   230
    45   280   225   108    36    4                                   240
    44   395   215   101    27    1                                   250
    49   139   220   136    59    0                                   260
    49   245   205   113    37    4                                   270
    49   373   215    88    25    1                                   280
    51   224   215   118    54    3                                   290
    51   677   210   116    33    4                                   300
    51   424   210   140    59    4                                   310
    51   150   210   105    30    0                                   320
010605C102030405                                                       330
010603020305                                                           340
```

Figure 39. Input listing (multiple regression)

the user with the program modification, the following general rules are supplied in terms of the sample problem:

1. Changes in the dimension statements of the main program, REGRE
   a. The dimension of arrays XBAR, STD, D, RY, ISAVE, B, SB, T, and W must be greater than or equal to the number of variables, m. Since there are six variables in the sample problem, the value of m is 6.
   b. The dimension of array RX must be greater than or equal to the product of m x m. For the sample problem this product is 36 = 6 x 6.
   c. The dimension of array R must be greater than or equal to (m + 1)m/2. For the sample problem this number is 21 = (6 + 1)6/2.

2. Changes in the input format statement of the special input subroutine, DATA:

   Only the format statement for input data may be changed. Since sample data are either one-, two-, or three-digit numbers, rather than using six-column fields as in the sample problem, each row of data may be keypunched in six 3-column fields, and, if so, the format is changed to (6F3.0).

   The special input subroutine, DATA, is normally written by the user to handle different formats for different problems. The user may modify this subroutine to perform testing of input data, transformation of data, and so on.

```
MULTIPLE REGRESSION.....SAMPLE

     SELECTION..... 1


VARIABLE      MEAN        STANDARD      CORRELATION     REGRESSION     STD. ERROR      COMPUTED
  NO.                     DEVIATION      X VS Y        COEFFICIENT    OF REG.COEF.     T VALUE
   1        43.13333        6.52176      0.28422        0.01242        0.03635         0.34171
   2       316.16656      114.42590      0.42189        0.00739        0.00186         3.96545
   3       241.79995       36.43074      0.11500        0.01504        0.00635         2.36881
   4       165.66666       17.85640      0.37822        0.00151        0.00379         0.04100
   5        34.13333       15.97571      0.39412        0.04919        0.04141         1.18782
DEPENDENT
   6         2.26667        1.41259


INTERCEPT                   -6.07928

MULTIPLE CORRELATION         0.73575

STD. ERROR OF ESTIMATE       1.05162


                ANALYSIS OF VARIANCE FOR THE REGRESSION

    SOURCE OF VARIATION      DEGREES      SUM OF        MEAN          F VALUE
                             OF FREEDOM   SQUARES       SQUARES
ATTRIBUTABLE TO REGRESSION       5        31.32506      6.26501       5.66508
DEVIATION FROM REGRESSION       24        26.54161      1.10590
     TOTAL                      29        57.86667


MULTIPLE REGRESSION.....SAMPLE

     SELECTION..... 1


                TABLE OF RESIDUALS

CASE NO.    Y VALUE     Y ESTIMATE      RESIDUAL
    1       1.00000       0.48051        0.51949
    2       2.00000       1.77670        0.22330
    3       2.00000       2.14586       -0.14586
    4       0.0           0.82880       -0.82880
    5       2.00000       1.50522        0.49478
    6       2.00000       1.52125        0.47875
    7       3.00000       3.46447       -0.46447
    8       2.00000       2.25887       -0.25887
    9       3.00000       3.80259       -0.80259
   10       0.0           1.02042       -1.02042
   11       4.00000       2.49735        1.50265
   12       1.00000       2.00066       -1.00066
   13       1.00000       2.00735       -1.00735
   14       1.00000       1.15308       -0.15308
   15       3.00000       2.90446        0.09554
   16       2.00000       1.83532        0.16468
   17       3.00000       2.56004        0.43996
   18       4.00000       3.45229        0.54771
   19       4.00000       3.62661        0.37339
   20       3.00000       2.68068        0.31932
   21       4.00000       3.64885        0.35115
   22       4.00000       1.86542        2.13458
   23       1.00000       2.09863       -1.09863
   24       0.0           1.97217       -1.97217
   25       4.00000       1.41253        2.58747
   26       1.00000       1.88027       -0.88027
   27       3.00000       2.27646        0.72354
   28       4.00000       4.51080       -0.51080
   29       4.00000       3.95745        0.04255
   30       0.0           0.45456       -0.45456
```

Figure 40. Output listing (multiple regression)

Operating Instructions

The sample program for multiple linear regression is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output. A scratch tape (data set 13) is used as intermediate storage.

Error Messages

The following error conditions will result in messages:

1. The number of selection cards is not specified on the control card--NUMBER OF SELECTIONS NOT SPECIFIED. JOB TERMINATED.
2. The matrix of correlation coefficients is singular--THE MATRIX IS SINGULAR. THIS SELECTION IS SKIPPED.

Error condition 2 allows the computer run to continue; however, error condition 1 terminates execution of the job.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 42 seconds.

```
C                                                                       REGR  10
C     ..................................................................REGR  20
C                                                                       REGR  30
C        SAMPLE MAIN PROGRAM FOR MULTIPLE REGRESSION - REGRE            REGR  40
C                                                                       REGR  50
C        PURPOSE                                                        REGR  60
C           (1) READ THE PROBLEM PARAMETER CARD FOR A MULTIPLE REGRES-  REGR  70
C           SION, (2) READ SUBSET SELECTION CARDS, (3) CALL THE SUB-    REGR  80
C           ROUTINES TO CALCULATE MEANS, STANDARD DEVIATIONS, SIMPLE    REGR  90
C           AND MULTIPLE CORRELATION COEFFICIENTS, REGRESSION COEFFI-   REGR 100
C           CIENTS, T-VALUES, AND ANALYSIS OF VARIANCE FOR MULTIPLE     REGR 110
C           REGRESSION, AND (4) PRINT THE RESULTS.                      REGR 120
C                                                                       REGR 130
C        REMARKS                                                        REGR 140
C           THE NUMBER OF OBSERVATIONS, N, MUST BE GREATER THAN M+1,    REGR 150
C           WHERE M IS THE NUMBER OF VARIABLES.  IF SUBSET SELECTION    REGR 160
C           CARDS ARE NOT PRESENT, THE PROGRAM CAN NOT PERFORM MULTIPLE REGR 170
C           REGRESSION.                                                 REGR 180
C           AFTER RETURNING FROM SUBROUTINE MINV, THE VALUE OF DETER-   REGR 190
C           MINANT (DET) IS TESTED TO CHECK WHETHER THE CORRELATION     REGR 200
C           MATRIX IS SINGULAR.  IF DET IS COMPARED AGAINST A SMALL     REGR 210
C           CONSTANT, THIS TEST MAY ALSO BE USED TO CHECK NEAR-         REGR 220
C           SINGULARITY.                                                REGR 230
C                                                                       REGR 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  REGR 250
C           CORRE  (WHICH, IN TURN, CALLS THE SUBROUTINE NAMED DATA)    REGR 260
C           ORDER                                                       REGR 270
C           MINV                                                        REGR 280
C           MULTR                                                       REGR 290
C                                                                       REGR 300
C        METHOD                                                         REGR 310
C           REFER TO B. 3STLE, 'STATISTICS IN RESEARCH', THE IOWA STATE REGR 320
C           COLLEGE PRESS', 1954, CHAPTER 8.                            REGR 330
C                                                                       REGR 340
C     ..................................................................REGR 350
C                                                                       REGR 360
C     THE FOLLOWING  DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE    REGR 370
C     NUMBER OF VARIABLES, M..                                          REGR 380
C                                                                       REGR 390
      DIMENSION XBAR(40),STD(40),D(40),RY(40),ISAVE(40),B(40),          REGR 400
     1          SB(40),T(40),W(40)                                      REGR 410
C                                                                       REGR 420
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      REGR 430
C     PRODUCT OF M*M..                                                  REGR 440
C                                                                       REGR 450
      DIMENSION RX(1600)                                                REGR 460
C                                                                       REGR 470
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO          REGR 480
C     (M+1)*M/2..                                                       REGR 490
C                                                                       REGR 500
      DIMENSION R(820)                                                  REGR 510
C                                                                       REGR 520
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 10..     REGR 530
C                                                                       REGR 540
      DIMENSION ANS(10)                                                 REGR 550
C                                                                       REGR 560
C     ..................................................................REGR 570
C                                                                       REGR 580
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  REGR 590
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      REGR 600
C        STATEMENT WHICH FOLLOWS.                                       REGR 610
C                                                                       REGR 620
C     DOUBLE PRECISION XBAR,STD,RX,R,D,B,T,RY,DET,SB,ANS,SUM            REGR 630
C                                                                       REGR 640
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    REGR 650
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      REGR 660
C        ROUTINE.                                                       REGR 670
C                                                                       REGR 680
C        ..............................................................REGR 690
C                                                                       REGR 700
    1 FORMAT(A4,A2,I5,2I2)                                              REGR 710
    2 FORMAT(25H1MULTIPLE REGRESSION.....A4,A2//6X,14HSELECTION.....I2//REGR 720
     1)                                                                 REGR 730
    3 FORMAT(9HOVARIABLE,5X,4HMEAN,6X,8HSTANDARD,6X,11HCORRELATION,4X,10REGR 740
     1HREGRESSION,4X,10HSTD. ERROR,5X,8HCOMPUTED/6H   NO.,18X,9HDEVIATIOREGR 750
     2N,7X,6HX VS Y,7X,11HCOEFFICIENT,3X,12HOF REG.COEF.,3X,7HT VALUE)  REGR 760
    4 FORMAT(1H ,I4,6F14.5)                                             REGR 770
    5 FORMAT(10H DEPENDENT)                                             REGR 780
    6 FORMAT(1HO/10H INTERCEPT,10X,F16.5//23H MULTIPLE CORRELATION  ,F13REGR 790
     1.5//23H STD. ERROR OF ESTIMATE,F13.5//)                           REGR 800
    7 FORMAT(1HO,21X,39HANALYSIS OF VARIANCE FOR THE REGRESSION//5X,19HSREGR 810
     1OURCE OF VARIATION,7X,7HDEGREES,7X,6HSUM OF,10X,4HMEAN,12X,7HF VALREGR 820
     2UE/30X,10HOF FREEDOM,4X,7HSQUARES,9X,7HSQUARES)                   REGR 830
    8 FORMAT(30H ATTRIBUTABLE TO REGRESSION   ,I6,3F16.5/30H DEVIATION FREGR 840
     1ROM REGRESSION    ,I6,2F16.5)                                     REGR 850
    9 FORMAT(1H ,5X,5HTOTAL,19X,I6,F16.5)                               REGR 860
   10 FORMAT(36I2)                                                      REGR 870
   11 FORMAT(1H ,15X,18HTABLE OF RESIDUALS//9H CASE NO.,5X,7HY VALUE,5X,REGR 880
     1 10HY ESTIMATE,6X,8HRESIDUAL)                                     REGR 890
   12 FORMAT(1H ,I6,F15.5,2F14.5)                                       REGR 900
   13 FORMAT(53H1NUMBER OF SELECTIONS NOT SPECIFIED.  JOB TERMINATED.)  REGR 910
   14 FORMAT(52HOTHE MATRIX IS SINGULAR.  THIS SELECTION IS SKIPPED.)   REGR 920
                                                                        REGR 930
C    ..................................................................REGR 940
C                                                                       REGR 950
C    READ PROBLEM PARAMETER CARD                                        REGR 960
C                                                                       REGR 970
  100 READ (5,1) PR,PR1,N,M,NS                                          REGR 980
C        PR........PROBLEM NUMBER (MAY BE ALPHAMERIC)                   REGR 990
C        PR1.......PROBLEM NUMBER (CONTINUED)                          REGR1000
C        N.........NUMBER OF OBSERVATIONS                               REGR1010
C        M.........NUMBER OF VARIABLES                                  REGR1020
C        NS........NUMBER OF SELECTIONS                                 REGR1030
C                                                                       REGR1040
C    LOGICAL TAPE 13 IS USED AS INTERMEDIATE STORAGE TO HOLD INPUT      REGR1050
C    DATA.  THE INPUT DATA ARE WRITTEN ON LOGICAL TAPE 13 BY THE        REGR1060
C    SPECIAL INPUT SUBROUTINE NAMED DATA.  THE STORED DATA MAY BE USED REGR1070
C    FOR RESIDUAL ANALYSIS.                                             REGR1080
C                                                                       REGR1090
      REWIND 13                                                         REGR1100
C                                                                       REGR1110
      IO=0                                                              REGR1120
      X=0.0                                                             REGR1130
C                                                                       REGR1140
      CALL CORRE (N,M,IO,X,XBAR,STD,RX,R,D,B,T)                         REGR1150
C                                                                       REGR1160
      REWIND 13                                                         REGR1170
C                                                                       REGR1180
C     TEST NUMBER OF SELECTIONS                                         REGR1190
C                                                                       REGR1200
      IF(NS) 108, 108, 109                                              REGR1210
  108 WRITE (6,13)                                                      REGR1220
      GO TO 300                                                         REGR1230
C                                                                       REGR1240
  109 DO 200 I=1,NS                                                     REGR1250
      WRITE (6,2) PR,PR1,I                                              REGR1260
C                                                                       REGR1270
C     READ SUBSET SELECTION CARD                                        REGR1280
C                                                                       REGR1290
      READ (5,10) NRESI,NDEP,K,(ISAVE(J),J=1,K)                         REGR1300
C        NRESI.....OPTION CODE FOR TABLE OF RESIDUALS                   REGR1310
C                  0  IF IT IS NOT DESIRED.                            REGR1320
C                  1  IF IT IS DESIRED.                                REGR1330
C        NDEP......DEPENDENT VARIABLE                                   REGR1340
C        K.........NUMBER OF INDEPENDENT VARIABLES INCLUDED             REGR1350
C        ISAVE.....A VECTOR CONTAINING THE INDEPENDENT VARIABLES        REGR1360
C                  INCLUDED                                             REGR1370
C                                                                       REGR1380
      CALL ORDER (M,R,NDEP,K,ISAVE,RX,RY)                               REGR1390
C                                                                       REGR1400
      CALL MINV (RX,K,DET,B,T)                                          REGR1410
C                                                                       REGR1420
C     TEST SINGULARITY OF THE MATRIX INVERTED                           REGR1430
C                                                                       REGR1440
      IF(DET) 112, 110, 112                                             REGR1450
  110 WRITE (6,14)                                                      REGR1460
      GO TO 200                                                         REGR1470
C                                                                       REGR1480
  112 CALL MULTR (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,ANS)                REGR1490
C                                                                       REGR1500
C     PRINT MEANS, STANDARD DEVIATIONS, INTERCORRELATIONS BETWEEN       REGR1510
C     X AND Y, REGRESSION COEFFICIENTS, STANDARD DEVIATIONS OF          REGR1520
C     REGRESSION COEFFICIENTS, AND COMPUTED T-VALUES                    REGR1530
C                                                                       REGR1540
      MM=K+1                                                            REGR1550
      WRITE (6,3)                                                       REGR1560
      DO 115 J=1,K                                                      REGR1570
      L=ISAVE(J)                                                        REGR1580
  115 WRITE (6,4) L,XBAR(L),STD(L),RY(J),B(J),SB(J),T(J)                REGR1590
      WRITE (6,5)                                                       REGR1600
      L=ISAVE(MM)                                                       REGR1610
      WRITE (6,4) L,XBAR(L),STD(L)                                      REGR1620
C                                                                       REGR1630
C     PRINT INTERCEPT, MULTIPLE CORRELATION COEFFICIENT, AND STANDARD   REGR1640
C     ERROR OF ESTIMATE                                                 REGR1650
C                                                                       REGR1660
      WRITE (6,6) ANS(1),ANS(2),ANS(3)                                  REGR1670
C                                                                       REGR1680
C     PRINT ANALYSIS OF VARIANCE FOR THE REGRESSION                     REGR1690
C                                                                       REGR1700
      WRITE (6,7)                                                       REGR1710
      L=ANS(9)                                                          REGR1720
      WRITE (6,8) K,ANS(4),ANS(6),ANS(10),L,ANS(7),ANS(9)               REGR1730
      L=N-1                                                             REGR1740
      SUM=ANS(4)+ANS(7)                                                 REGR1750
      WRITE (6,9) L,SUM                                                 REGR1760
      IF(NRESI) 200, 200, 120                                           REGR1770
C                                                                       REGR1780
C     PRINT TABLE OF RESIDUALS                                          REGR1790
C                                                                       REGR1800
  120 WRITE (6,2) PR,PR1,I                                              REGR1810
      WRITE (6,11)                                                      REGR1820
      MM=ISAVE(K+1)                                                     REGR1830
      DO 140 II=1,N                                                     REGR1840
      READ (13) (W(J),J=1,M)                                            REGR1850
      SUM=ANS(1)                                                        REGR1860
      DO 130 J=1,K                                                      REGR1870
      L=ISAVE(J)                                                        REGR1880
  130 SUM=SUM+W(L)*B(J)                                                 REGR1890
      RESI=W(MM)-SUM                                                    REGR1900
  140 WRITE (6,12) II,W(MM),SUM,RESI                                    REGR1910
      REWIND 13                                                         REGR1920
  200 CONTINUE                                                          REGR1930
      GO TO 100                                                         REGR1940
  300 CONTINUE                                                          REGR1950
      END                                                               REGR1960
```

POLYNOMIAL REGRESSION

Problem Description

Powers of an independent variable are generated to calculate polynomials of successively increasing degrees. If there is no reduction in the residual sum of squares between two successive degrees of polynomials, the program terminates the problem before completing the analysis for the highest degree polynomial specified.

The sample problem for polynomial regression consists of 15 observations, as presented in Table 5. The highest degree polynomial specified for this problem is 4.

Program

Description

The polynomial regression program consists of the main routine named POLRG, a special plot subroutine named PLOT, and four subroutines from the Scientific Subroutine Package: GDATA, ORDER, MINV, and MULTR.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 100 observations
2. Up to 10^{th} degree polynomial
3. (2F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than 100 observations or if greater than 10^{th} degree polynomial is desired, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format in the sample main program must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, POLRG. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE
7 - 11	Number of observations	00015
12 - 13	Highest degree polynomial to be fitted	04
14	Option code for plotting Y values and Y estimates: 0 if it is not desired 1 if it is desired	1

Leading zeros are not required to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each pair of X and Y data in Table 5 is keypunched in that order on a separate card using the format (2F6.0).

Table 5. Sample Data for Polynomial Regression

X	Y
1	10
2	16
3	20
4	23
5	25
6	26
7	30
8	36
9	48
10	62
11	78
12	94
13	107
14	118
15	127

Deck Setup

The deck setup is shown in Figure 41.

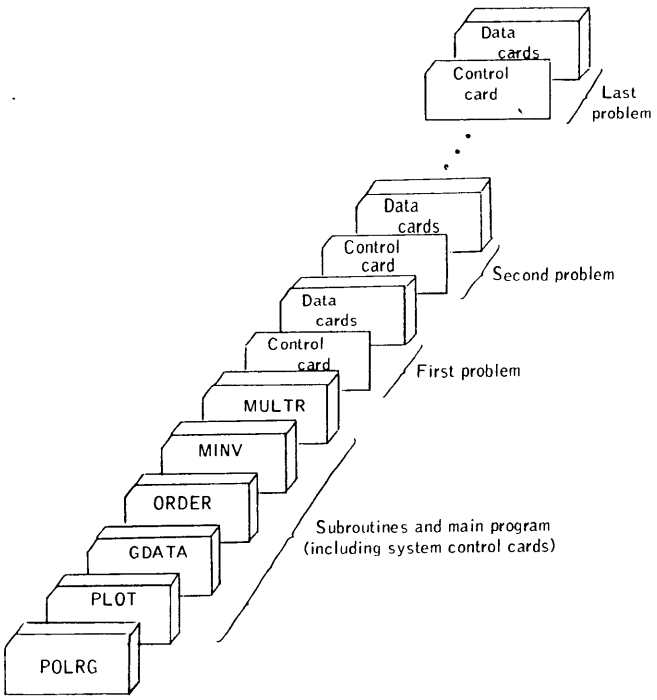


Figure 41. Deck setup (polynomial regression)

Sample

The listing of input cards for the sample problem is presented in Figure 42.

Output

Description

The output of the sample program for polynomial regression includes:

1. Regression coefficients for successive degree polynomials
2. Analysis-of-variance table for successive degree polynomials
3. Table of residuals for the final degree polynomial (optional)
4. Plot of Y values and Y estimates (optional)

```
/DATA
SAMPLE00015041                                                  10
     1    10                                                    20
     2    16                                                    30
     3    20                                                    40
     4    23                                                    50
     5    25                                                    60
     6    26                                                    70
     7    30                                                    80
     8    36                                                    90
     9    48                                                   100
    10    62                                                   110
    11    78                                                   120
    12    94                                                   130
    13   107                                                   140
    14   118                                                   150
    15   127                                                   160
                                                               170
```

Figure 42. Input card listing (polynomial regression)

Sample

The output listing for the sample problem is shown in Figure 43.

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

1. Changes in the dimension statements of the main program, POLRG:
   a. The dimension of array X must be greater than or equal to the product of n (m + 1), where n is the number of observations and m is the highest degree polynomial to be fitted. Since there are 15 observations and the highest degree polynomial specified is 4, the product is 75 = 15 (4 + 1).
   b. The dimension of array DI must be greater than or equal to the product of m x m. For the sample problem this product is 16 = 4 x 4.
   c. The dimension of array D must be greater than or equal to (m + 2) (m + 1)/2. For the sample problem this number is 15 = (4 + 2) (4 + 1)/2.
   d. The dimension of arrays B, E, SB, and T must be greater than or equal to the highest degree polynomial to be fitted, m. For the sample problem the value of m is 4.
   e. The dimension of arrays XBAR, STD, COE, SUMSQ, and ISAVE must be greater than or equal to (m + 1). For the sample problem this value is 5 = (4 + 1).
   f. The dimension of array P must be greater than or equal to 3(n). For the sample problem this value is 45 = 3(15). The array P is used when a plot of Y values and Y estimates is desired.

2. Changes in the input format statement of the main program, POLRG:

   Only the format statement for input data may be changed. Since sample data are either one-, two-, or three-digit numbers, rather than using six-column fields as in the sample problem, each row of data may be keypunched in two 3-column fields, and if so the format is changed to (2F3.0).

```
POLYNOMIAL REGRESSION.....SAMPLE

NUMBER OF OBSERVATIONS    15

POLYNOMIAL REGRESSION OF DEGREE  1

  INTERCEPT       -13.87613

  REGRESSION COEFFICIENTS
    8.56785

                    ANALYSIS OF VARIANCE FOR   1  DEGREE POLYNOMIAL

     SOURCE OF VARIATION        DEGREE OF FREEDOM      SUM OF SQUARES        MEAN SQUARE          F VALUE        IMPROVEMENT IN TERMS OF SUM OF SQUARES

  DUE TO REGRESSION                    1          20554.26172          20554.26172          135.56577              20554.26172
  DEVIATION ABOUT REGRESSION          13           1971.03906            151.61838
       TOTAL                          14          22525.30078


POLYNOMIAL REGRESSION OF DEGREE  2

  INTERCEPT        15.07547

  REGRESSION COEFFICIENTS
   -1.64957       0.63856

                    ANALYSIS OF VARIANCE FOR   2  DEGREE POLYNOMIAL

     SOURCE OF VARIATION        DEGREE OF FREEDOM      SUM OF SQUARES        MEAN SQUARE          F VALUE        IMPROVEMENT IN TERMS OF SUM OF SQUARES

  DUE TO REGRESSION                    2          22235.39062          11117.69531          460.18506              1681.12891
  DEVIATION ABOUT REGRESSION          12            289.91016              24.15918
       TOTAL                          14          22525.30078


POLYNOMIAL REGRESSION OF DEGREE  3

  INTERCEPT        18.49422

  REGRESSION COEFFICIENTS
   -3.88107       0.97684      -0.01409

                    ANALYSIS OF VARIANCE FOR   3  DEGREE POLYNOMIAL

     SOURCE OF VARIATION        DEGREE OF FREEDOM      SUM OF SQUARES        MEAN SQUARE          F VALUE        IMPROVEMENT IN TERMS OF SUM OF SQUARES

  DUE TO REGRESSION                    3          22256.32812          7418.77344           303.40063              20.93750
  DEVIATION ABOUT REGRESSION          11            268.97266             24.45206
       TOTAL                          14          22525.30078


POLYNOMIAL REGRESSION OF DEGREE  4

  NO IMPROVEMENT


POLYNOMIAL REGRESSION.....SAMPLE

POLYNOMIAL REGRESSION OF DEGREE  3

                    TABLE OF RESIDUALS

OBSERVATION NO.      X VALUE          Y VALUE          Y ESTIMATE          RESIDUAL

        1            1.00000          10.00000           15.57588           -5.57588
        2            2.00000          16.00000           14.52666            1.47334
        3            3.00000          20.00000           15.26197            4.73803
        4            4.00000          23.00000           17.69725            5.30275
        5            5.00000          25.00000           21.74792            3.25208
        6            6.00000          26.00000           27.32945           -1.32945
        7            7.00000          30.00000           34.35724           -4.35724
        8            8.00000          36.00000           42.74675           -6.74675
        9            9.00000          48.00000           52.41338           -4.41338
       10           10.00000          62.00000           63.27257           -1.27257
       11           11.00000          78.00000           75.23978            2.76022
       12           12.00000          94.00000           88.23039            5.76961
       13           13.00000         107.00000          102.15990            4.84010
       14           14.00000         118.00000          116.94366            1.05634
       15           15.00000         127.00000          132.49719           -5.49719
```

Figure 43. Output listing (polynomial regression)

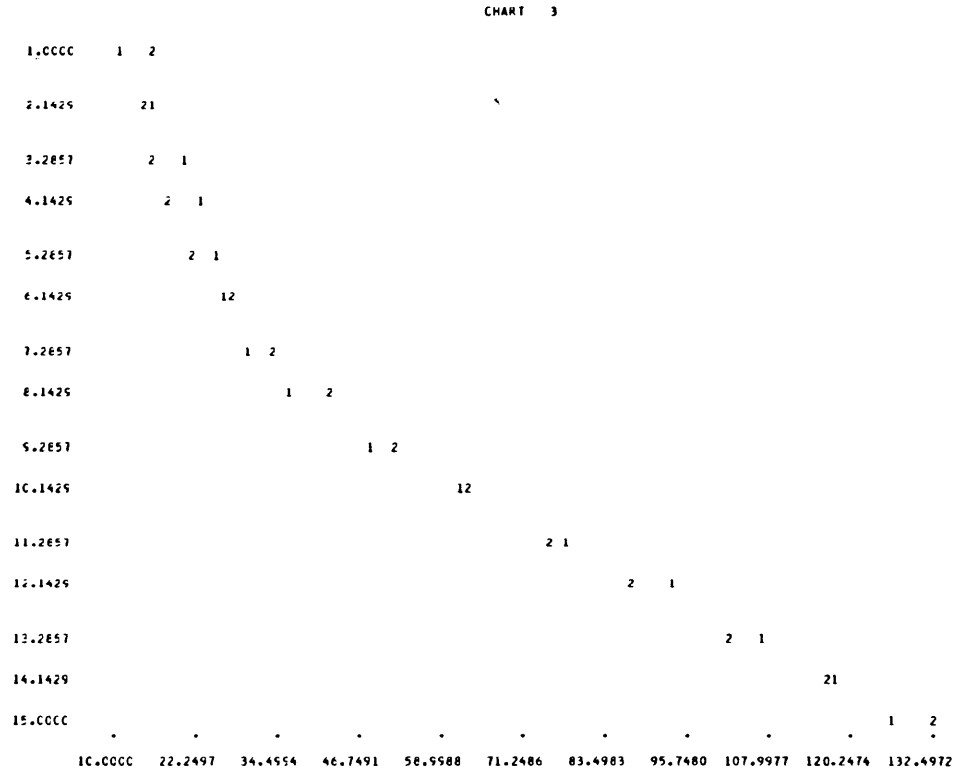


Figure 43. Output listing (polynomial regression) (Continued)

Operating Instructions

The sample program for polynomial regression is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output. A scratch tape (data set 13) is used as intermediate storage when Y values and Y estimates are plotted.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 35 seconds.

```
C                                                                       PLRG  10
C     ..................................................................PLRG  20
C                                                                       PLRG  30
C        SAMPLE MAIN PROGRAM FOR POLYNOMIAL REGRESSION - POLRG          PLRG  40
C                                                                       PLRG  50
C        PURPOSE                                                        PLRG  60
C           (1) READ THE PROBLEM PARAMETER CARD FOR A POLYNOMIAL REGRES-PLRG  70
C           SION, (2) CALL SUBROUTINES TO PERFORM THE ANALYSIS, (3)     PLRG  80
C           PRINT THE REGRESSION COEFFICIENTS AND ANALYSIS OF VARIANCE  PLRG  90
C           TABLE FOR POLYNOMIALS OF SUCCESSIVELY INCREASING DEGREES,   PLRG 100
C           AND (4) OPTIONALLY PRINT THE TABLE OF RESIDUALS AND A PLOT  PLRG 110
C           OF Y VALUES AND Y ESTIMATES.                                PLRG 120
C                                                                       PLRG 130
C        REMARKS                                                        PLRG 140
C           THE NUMBER OF OBSERVATIONS, N, MUST BE GREATER THAN M+1,    PLRG 150
C           WHERE M IS THE HIGHEST DEGREE POLYNOMIAL SPECIFIED.         PLRG 160
C           IF THERE IS NO REDUCTION IN THE RESIDUAL SUM OF SQUARES     PLRG 170
C           BETWEEN TWO SUCCESSIVE DEGREES OF THE POLYNOMIALS, THE      PLRG 180
C           PROGRAM TERMINATES THE PROBLEM BEFORE COMPLETING THE ANALY- PLRG 190
C           SIS FOR THE HIGHEST DEGREE POLYNOMIAL SPECIFIED.            PLRG 200
C                                                                       PLRG 210
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PLRG 220
C           GDATA                                                       PLRG 230
C           ORDER                                                       PLRG 240
C           MINV                                                        PLRG 250
C           MULTR                                                       PLRG 260
C           PLOT  (A SPECIAL PLOT SUBROUTINE PROVIDED FOR THE SAMPLE    PLRG 270
C                 PROGRAM.)                                             PLRG 280
C                                                                       PLRG 290
C        METHOD                                                         PLRG 300
C           REFER TO A. OSTLE, 'STATISTICS IN RESEARCH', THE IOWA STATE PLRG 310
C           COLLEGE PRESS', 1954, CHAPTER 6.                            PLRG 320
C                                                                       PLRG 330
C     ..................................................................PLRG 340
```

```
C                                                                       PLRG 350
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      PLRG 360
C     PRODUCT OF N*(M+1), WHERE N IS THE NUMBER OF OBSERVATIONS AND M   PLRG 370
C     IS THE HIGHEST DEGREE POLYNOMIAL SPECIFIED..                      PLRG 380
C                                                                       PLRG 390
      DIMENSION X(1100)                                                 PLRG 400
C                                                                       PLRG 410
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      PLRG 420
C     PRODUCT OF M*M..                                                  PLRG 430
C                                                                       PLRG 440
      DIMENSION DI(100)                                                 PLRG 450
C                                                                       PLRG 460
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO          PLRG 470
C     (M+2)*(M+1)/2..                                                   PLRG 480
C                                                                       PLRG 490
      DIMENSION D(66)                                                   PLRG 500
C                                                                       PLRG 510
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO M..     PLRG 520
C                                                                       PLRG 530
      DIMENSION B(10),E(10),SB(10),T(10)                                PLRG 540
C                                                                       PLRG 550
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO (M+1).. PLRG 560
C                                                                       PLRG 570
      DIMENSION XBAR(11),STD(11),COE(11),SUMSQ(11),ISAVE(11)            PLRG 580
C                                                                       PLRG 590
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 10..     PLRG 600
C                                                                       PLRG 610
      DIMENSION ANS(10)                                                 PLRG 620
C                                                                       PLRG 630
C     THE FOLLOWING DIMENSION WILL BE USED IF THE PLOT OF OBSERVED DATA PLRG 640
C     AND ESTIMATES IS DESIRED.  THE SIZE OF THE DIMENSION, IN THIS     PLRG 650
C     CASE, MUST BE GREATER THAN OR EQUAL TO N*3.  OTHERWISE, THE SIZE  PLRG 660
C     OF DIMENSION MAY BE SET TO 1.                                     PLRG 670
C                                                                       PLRG 680
      DIMENSION P(300)                                                  PLRG 690
C     ..................................................................PLRG 700
C                                                                       PLRG 710
C     IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE     PLRG 720
C     C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION         PLRG 730
C     STATEMENT WHICH FOLLOWS.                                          PLRG 740
C                                                                       PLRG 750
C     DOUBLE PRECISION X,XBAR,STD,D,SUMSQ,DI,E,B,SB,T,ANS,DET,COE       PLRG 760
C                                                                       PLRG 770
C     THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS       PLRG 780
C     APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS         PLRG 790
C     ROUTINE.                                                          PLRG 800
C                                                                       PLRG 810
C     ..................................................................PLRG 820
C                                                                       PLRG 830
    1 FORMAT(A4,A2,I5,I2,I1)                                            PLRG 840
    2 FORMAT(2F6.0)                                                     PLRG 850
    3 FORMAT(27H1POLYNOMIAL REGRESSION.....,A4,A2/)                     PLRG 860
    4 FORMAT(23HONUMBER OF OBSERVATIONS,I6//)                           PLRG 870
    5 FORMAT(32HOPOLYNOMIAL REGRESSION OF DEGREE,I3)                    PLRG 880
    6 FORMAT(12HO  INTERCEPT,E20.7)                                     PLRG 890
    7 FORMAT(26HO  REGRESSION COEFFICIENTS/(6E20.7))                    PLRG 900
    8 FORMAT(1HO/24X,24HANALYSIS OF VARIANCE FOR,I4,19H  DEGREE POLYNOMIPLRG 910
     1AL/)                                                              PLRG 920
    9 FORMAT(1HO,5X,19HSOURCE OF VARIATION,7X,9HDEGREE OF,7X,6HSUM OF,9XPLRG 930
     1,4HMEAN,10X,1HF,9X,20HIMPROVEMENT IN TERMS/33X,7HFREEDOM,8X,7HSQUAPLRG 940
     2RES.,7X,6HSQUARE,7X,5HVALUE,8X,17HOF SUM OF SQUARES)              PLRG 950
   10 FORMAT(22HO  DUE TO REGRESSION,12X,I6,F17.5,F14.5,F13.5,F20.5)    PLRG 960
   11 FORMAT(32H   DEVIATION ABOUT REGRESSION    ,I6,F17.5,F14.5)      PLRG 970
   12 FORMAT(8X,5HTOTAL,19X,I6,F17.5///)                                PLRG 980
   13 FORMAT(17HO  NO IMPROVEMENT)                                      PLRG 990
   14 FORMAT(1HC//27X,18HTABLE OF RESIDUALS//16H OBSERVATION NO.,5X,7HX PLRG1000
     1VALUE,7X,7HY VALUE,7X,10HY ESTIMATE,7X,8HRESIDUAL/)               PLRG1010
   15 FORMAT(1HO,3X,I6,F18.5,F14.5,F17.5,F15.5)                         PLRG1020
C                                                                       PLRG1030
C     ..................................................................PLRG1040
C                                                                       PLRG1050
C     READ PROBLEM PARAMETER CARD                                       PLRG1060
C                                                                       PLRG1070
  100 READ (5,1) PR,PR1,N,M,NPLOT                                       PLRG1080
C                                                                       PLRG1090
C        PR....PROBLEM NUMBER (MAY BE ALPHAMERIC)                       PLRG1100
C        PR1...PROBLEM NUMBER (CONTINUED)                               PLRG1110
C        N.....NUMBER OF OBSERVATIONS                                   PLRG1120
C        M.....HIGHEST DEGREE POLYNOMIAL SPECIFIED                      PLRG1130
C        NPLOT.OPTION CODE FOR PLOTTING                                 PLRG1140
C              0  IF PLOT IS NOT DESIRED.                               PLRG1150
C              1  IF PLOT IS DESIRED.                                   PLRG1160
C                                                                       PLRG1170
C     PRINT PROBLEM NUMBER AND N.                                       PLRG1180
C                                                                       PLRG1190
      WRITE (6,3) PR,PR1                                                PLRG1200
      WRITE (6,4) N                                                     PLRG1210
C                                                                       PLRG1220
C     READ INPUT DATA                                                   PLRG1230
C                                                                       PLRG1240
      L=N*M                                                             PLRG1250
      DO 110 I=1,N                                                      PLRG1260
      J=L+I                                                             PLRG1270
C                                                                       PLRG1280
C        X(I) IS THE INDEPENDENT VARIABLE, AND X(J) IS THE DEPENDENT    PLRG1290
C        VARIABLE.                                                      PLRG1300
C                                                                       PLRG1310
  110 READ (5,2) X(I),X(J)                                              PLRG1320
C                                                                       PLRG1330
      CALL GDATA (N,M,X,XBAR,STD,D,SUMSQ)                               PLRG1340
C                                                                       PLRG1350
      MM=M+1                                                            PLRG1360
      SUM=0.0                                                           PLRG1370
      NT=N-1                                                            PLRG1380
C                                                                       PLRG1390
      DO 200 I=1,M                                                      PLRG1400
      ISAVE(I)=I                                                        PLRG1410
C                                                                       PLRG1420
C     FORM SUBSET OF CORRELATION COEFFICIENT MATRIX                     PLRG1430
C                                                                       PLRG1440
      CALL ORDER (MM,D,MM,I,ISAVE,DI,E)                                 PLRG1450
C                                                                       PLRG1460
C     INVERT THE SUBMATRIX OF CORRELATION COEFFICIENTS                  PLRG1470
C                                                                       PLRG1480
      CALL MINV (DI,I,DET,B,T)                                          PLRG1490
C                                                                       PLRG1500
      CALL MULTR (N,I,XBAR,STD,SUMSQ,DI,E,ISAVE,B,SB,T,ANS)             PLRG1510
C                                                                       PLRG1520
C     PRINT THE RESULT OF CALCULATION                                   PLRG1530
C                                                                       PLRG1540
      WRITE (6,5) I                                                     PLRG1550
      IF(ANS(7)) 140,130,130                                            PLRG1560
  130 SUMIP=ANS(4)-SUM                                                  PLRG1570
      IF(SUMIP) 140, 140, 150                                           PLRG1580
  140 WRITE (6,13)                                                      PLRG1590
      GO TO 210                                                         PLRG1600
  150 WRITE (6,6) ANS(1)                                                PLRG1610
      WRITE (6,7) (B(J),J=1,I)                                          PLRG1620
      WRITE (6,8) I                                                     PLRG1630
      WRITE (6,9)                                                       PLRG1640
      SUM=ANS(4)                                                        PLRG1650
      WRITE (6,10) I,ANS(4),ANS(6),ANS(10),SUMIP                        PLRG1660
      NI=ANS(8)                                                         PLRG1670
      WRITE (6,11) NI,ANS(7),ANS(9)                                     PLRG1680
      WRITE (6,12) NT,SUMSQ(MM)                                         PLRG1690
C                                                                       PLRG1700
C     SAVE COEFFICIENTS FOR CALCULATION OF Y ESTIMATES                  PLRG1710
C                                                                       PLRG1720
      COE(1)=ANS(1)                                                     PLRG1730
      DO 160 J=1,I                                                      PLRG1740
  160 COE(J+1)=B(J)                                                     PLRG1750
      LA=I                                                              PLRG1760
  200 CONTINUE                                                          PLRG1770
C                                                                       PLRG1780
C     TEST WHETHER PLOT IS DESIRED                                      PLRG1790
C                                                                       PLRG1800
  210 IF(NPLOT) 100, 100, 220                                           PLRG1810
C                                                                       PLRG1820
C        CALCULATE ESTIMATES                                            PLRG1830
C                                                                       PLRG1840
  220 NP3=N+N                                                           PLRG1850
      DO 230 I=1,N                                                      PLRG1860
      NP3=NP3+1                                                         PLRG1870
      P(NP3)=COE(1)                                                     PLRG1880
      L=I                                                               PLRG1890
      DO 230 J=1,LA                                                     PLRG1900
      P(NP3)=P(NP3)+X(L)*COE(J+1)                                       PLRG1910
  230 L=L+N                                                             PLRG1920
C                                                                       PLRG1930
C        COPY OBSERVED DATA                                             PLRG1940
C                                                                       PLRG1950
      N2=N                                                              PLRG1960
      L=N*M                                                             PLRG1970
      DO 240 I=1,N                                                      PLRG1980
      P(I)=X(I)                                                         PLRG1990
      N2=N2+1                                                           PLRG2000
      L=L+1                                                             PLRG2010
  240 P(N2)=X(L)                                                        PLRG2020
C                                                                       PLRG2030
C     PRINT TABLE OF RESIDUALS                                          PLRG2040
C                                                                       PLRG2050
      WRITE (6,3) PR,PR1                                                PLRG2060
      WRITE (6,5) LA                                                    PLRG2070
      WRITE (6,14)                                                      PLRG2080
      NP2=N                                                             PLRG2090
      NP3=N+N                                                           PLRG2100
      DO 250 I=1,N                                                      PLRG2110
      NP2=NP2+1                                                         PLRG2120
      NP3=NP3+1                                                         PLRG2130
      RESID=P(NP2)-P(NP3)                                               PLRG2140
  250 WRITE (6,15) I,P(I),P(NP2),P(NP3),RESID                           PLRG2150
C                                                                       PLRG2160
      CALL PLOT (LA,P,N,3,0,1)                                          PLRG2170
C                                                                       PLRG2180
      GO TO 100                                                         PLRG2190
      END                                                               PLRG2200
                                                                        PLRG2210
```

STEPWISE MULTIPLE REGRESSION

Problem Description

Stepwise multiple regression is a statistical technique for analyzing a relationship between a dependent variable (y) and a set of independent variables ($x_1, x_2, \ldots, x_m$) and for selecting the independent variables in the order of their importance. The criterion of importance is based on the reduction of sums of squares, and the independent variable most important in this reduction in a given step is entered in the regression. Any variable in the original set can be named as the dependent variable. A set of variables can be forced to enter in the regression, and another set of variables can be deleted.

The sample problem for stepwise multiple regression consists of 30 observations on six variables as presented in Table 4. The first five variables are independent variables (predictors), and the last variable is the dependent variable (criterion). All five independent variables are available for selection in the first analysis. In the second analysis, the third variable is forced to enter in the regression, the fourth variable is deleted, and the remaining three independent variables are available for selection. Note that the same sample problem has been used for multiple linear regression and that the results of these two programs may be compared.

Program

Description

The stepwise multiple regression program consists of the main routine named STEPR, a special input subroutine named DATA, a special output subroutine named STOUT, and four subroutines from the Scientific Subroutine Package: CORRE, MSTR, LOC, and STPRG.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 35 variables, including both dependent and independent variables
2. Up to 99,999 observations, if observations are read into the computer one at a time by the special input subroutine named DATA. If all data are to be stored in core prior to the calculation of correlation coefficients, the limitation on the number of observations depends on the size of core storage available for input data.
3. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions, it is not necessary to modify the sample program. However, if there are more than 35 variables, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the format in the input subroutine, DATA, must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, STEPR. This card is prepared as follows:

Columns	Contents	For Sample Problem
1-6	Problem code (may be alphameric)	SAMPLE
7-11	Number of observations	00030
12-13	Number of variables	06
14-15	Number of selection cards (see below)	02
16-21	This constant is the proportion of the sum of squares which will be used to limit the entering of variables into the regression. Unless the proportion of the sum of squares attributable to an entering variable is greater than this value, the variable will not be entered. The keypunched value should have a decimal point.*	0.0
22	Option code for table of residuals 0--if it is not desired 1--if it is desired	1

*The choice of value depends upon the purpose of analysis. A suggested trial value is 0.01 (one percent). If all variables are to be included in the regression, use 0.0.

Leading zeros are not required to be keypunched.

Data Cards

Since input data can be read into the computer one observation at a time, each row of data in Table 4 is keypunched on a separate card using the format (12F6.0). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card.

Selection Card

The selection card is used to specify a dependent variable, independent variables to be forced to enter in the regression, variables to be deleted, and independent variables to be chosen by the program to enter in the regression. Any one variable in the set of original variables can be designated as a dependent variable, and any number of variables can be specified as forcing variables, deleting variables, and unrestricted variables to be chosen by the program. The specification of the variables can be performed over and over again using the same set of original variables.

In a selection card, each variable is specified using one of the following codes:

Code	Specification
0 or blank	Independent variable to be chosen by the program to enter in the regression
1	Independent variable forced by the user to enter in the regression
2	Variable to be deleted
3	Dependent variable

The selection card itself is prepared as follows:

Columns	Contents	For Sample Problem Selections 1	2
1	Code for 1st variable	0	0
2	Code for 2nd variable	0	0
3	Code for 3rd variable	0	1
4	Code for 4th variable	0	2
5	Code for 5th variable	0	0
6	Code for 6th variable	3	3
etc.			

The input format of (72I1) is used for the selection card.

Deck Setup

The deck setup is shown in Figure 44.

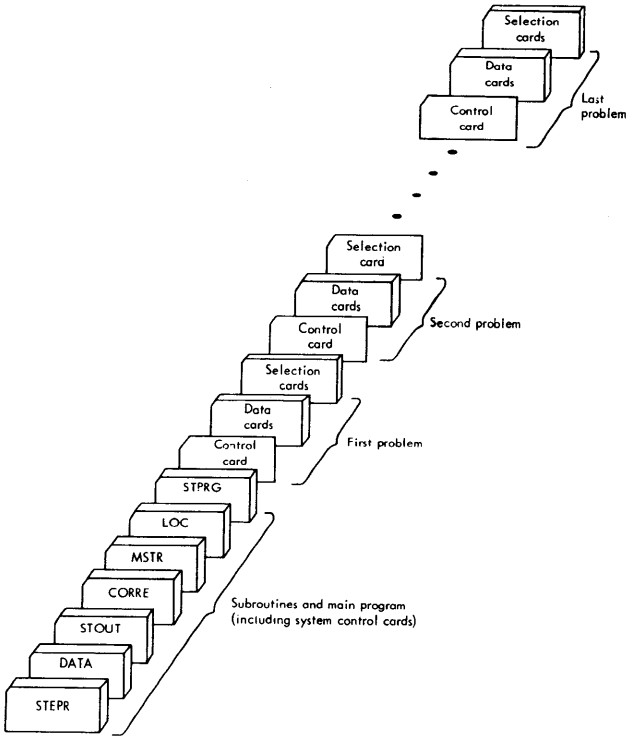


Figure 44. Deck setup (stepwise multiple regression)

Sample

The listing of input cards for the sample problem is presented in Figure 45.

```
/DATA
SAMPLE    30 6 2  C.001
    29   289   216    85    14     1
    30   391   244    92    16     2
    30   424   246    90    18     2
    30   313   239    91    10     0
    35   243   275    95    30     2
    35   365   219    95    21     2
    43   396   267   100    39     3
    43   356   274    79    19     2
    44   346   255   126    56     3
    44   156   258    95    28     0
    44   278   249   110    42     4
    44   349   252    88    21     1
    44   141   236   129    56     1
    44   245   236    97    24     1
    45   297   256   111    45     3
    45   310   262    94    20     2
    45   151   339    96    35     3
    45   370   357    88    15     4
    45   379   198   147    64     4
    45   463   206   105    31     3
    45   316   245   132    60     4
    45   280   225   108    36     4
    44   395   215   101    27     1
    49   139   220   136    59     0
    49   245   205   113    37     4
    49   373   215    88    25     1
    51   224   215   118    54     3
    51   677   210   116    33     4
    51   424   210   140    59     4
    51   150   210   105    30     0
000003
001203
```

Figure 45.

Output

Description

The output of the sample program for stepwise multiple regression includes:

1. For all variables --
   a. Means
   b. Standard deviations
   c. Correlation coefficient matrix
2. For each step of multiple regression --
   a. Sum of squares reduced
   b. Proportion reduced
   c. Cumulative sum of squares reduced
   d. Cumulative proportion reduced
   e. Multiple correlation coefficient (adjusted and unadj.)
   f. F-value for analysis of variance
   g. Standard error of estimate (adjusted and unadj.)
   h. Regression coefficients
   i. Standard errors of regression coefficients
   j. Computed t-values
3. Tables of residuals (optional)

Sample

The output listing for the sample problem is shown in Figure 46.

```
STEP-WISE MULTIPLE REGRESSION.....SAMPLE

NUMBER OF OBSERVATIONS   30
NUMBER OF VARIABLES       6
NUMBER OF SELECTIONS      2

CONSTANT TO LIMIT VARIABLES  0.0

VARIABLE      MEAN      STANDARD
  NO.                   DEVIATION
    1      43.13333      6.52176
    2     316.16650    114.42990
    3     241.79999     36.43074
    4     105.66666     17.85640
    5      34.13333     15.97571
    6       2.26667      1.41259

CORRELATION MATRIX

ROW  1
   1.00000    -0.06721    -0.13689     0.49755     0.55849     0.28422

ROW  2
  -0.06721     1.00000    -0.17857    -0.05227    -0.18381     0.42189

ROW  3
  -0.13689    -0.17857     1.00000    -0.40874    -0.26319     0.11900

ROW  4
   0.49755    -0.05227    -0.40874     1.00000     0.93552     0.37822

ROW  5
   0.55849    -0.18381    -0.26319     0.93552     1.00000     0.39412

ROW  6
   0.28422     0.42189     0.11900     0.37822     0.39412     1.00000



SELECTION..... 1

DEPENDENT VARIABLE..... 6
NUMBER OF VARIABLES FORCED.... 0
NUMBER OF VARIABLES DELETED... 0



STEP  1

VARIABLE ENTERED..... 2

SUM OF SQUARES REDUCED IN THIS STEP....      10.300
PROPORTION REDUCED IN THIS STEP.....          0.178

CUMULATIVE SUM OF SQUARES REDUCED.....       10.300
CUMULATIVE PROPORTION REDUCED.....            0.178  OF      57.867

FOR  1 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...        0.422
      (ADJUSTED FOR D.F.)...........         0.422
  F-VALUE FOR ANALYSIS OF VARIANCE...        6.063
  STANDARD ERROR OF ESTIMATE.....            1.303
      (ADJUSTED FOR D.F.)...........         1.303

  VARIABLE     REGRESSION     STD. ERROR OF     COMPUTED
   NUMBER      COEFFICIENT     REG. COEFF.      T-VALUE
      2          0.00521         0.00212         2.462
  INTERCEPT      0.62005



STEP  2

VARIABLE ENTERED..... 5

SUM OF SQUARES REDUCED IN THIS STEP....      13.324
PROPORTION REDUCED IN THIS STEP.....          0.230

CUMULATIVE SUM OF SQUARES REDUCED.....       23.624
CUMULATIVE PROPORTION REDUCED.....            0.408  OF      57.867

FOR  2 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...        0.639
      (ADJUSTED FOR D.F.)...........         0.622
  F-VALUE FOR ANALYSIS OF VARIANCE...        9.314
  STANDARD ERROR OF ESTIMATE.....            1.126
      (ADJUSTED FOR D.F.)...........         1.146

  VARIABLE     REGRESSION     STD. ERROR OF     COMPUTED
   NUMBER      COEFFICIENT     REG. COEFF.      T-VALUE
      2          0.00632         0.00186         3.397
      5          0.04316         0.01332         3.241
  INTERCEPT     -1.20349



STEP  3

VARIABLE ENTERED..... 3

SUM OF SQUARES REDUCED IN THIS STEP....       7.572
PROPORTION REDUCED IN THIS STEP.....          0.131

CUMULATIVE SUM OF SQUARES REDUCED.....       31.196
CUMULATIVE PROPORTION REDUCED.....            0.539  OF      57.867

FOR  3 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...        0.734
      (ADJUSTED FOR D.F.)...........         0.711
  F-VALUE FOR ANALYSIS OF VARIANCE...       10.137
  STANDARD ERROR OF ESTIMATE.....            1.013
      (ADJUSTED FOR D.F.)...........         1.050

  VARIABLE     REGRESSION     STD. ERROR OF     COMPUTED
   NUMBER      COEFFICIENT     REG. COEFF.      T-VALUE
      2          0.00744         0.00172         4.318
      5          0.05363         0.01258         4.263
      3          0.01497         0.00551         2.717
  INTERCEPT     -5.53529



STEP  4

VARIABLE ENTERED..... 1

SUM OF SQUARES REDUCED IN THIS STEP....       0.127
PROPORTION REDUCED IN THIS STEP.....          0.002

CUMULATIVE SUM OF SQUARES REDUCED.....       31.323
CUMULATIVE PROPORTION REDUCED.....            0.541  OF      57.867

FOR  4 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...        0.736
      (ADJUSTED FOR D.F.)...........         0.699
  F-VALUE FOR ANALYSIS OF VARIANCE...        7.375
  STANDARD ERROR OF ESTIMATE.....            1.030
      (ADJUSTED FOR D.F.)...........         1.088

  VARIABLE     REGRESSION     STD. ERROR OF     COMPUTED
   NUMBER      COEFFICIENT     REG. COEFF.      T-VALUE
      2          0.00741         0.00175         4.222
      5          0.05076         0.01524         3.332
      3          0.01493         0.00561         2.662
      1          0.01226         0.03541         0.346
  INTERCEPT     -5.94617



STEP  5

VARIABLE ENTERED..... 4

SUM OF SQUARES REDUCED IN THIS STEP....       0.002
PROPORTION REDUCED IN THIS STEP.....          0.000

CUMULATIVE SUM OF SQUARES REDUCED.....       31.325
CUMULATIVE PROPORTION REDUCED.....            0.541  OF      57.867

FOR  5 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...        0.736
      (ADJUSTED FOR D.F.)...........         0.684
  F-VALUE FOR ANALYSIS OF VARIANCE...        5.665
  STANDARD ERROR OF ESTIMATE.....            1.052
      (ADJUSTED FOR D.F.)...........         1.133

  VARIABLE     REGRESSION     STD. ERROR OF     COMPUTED
   NUMBER      COEFFICIENT     REG. COEFF.      T-VALUE
      2          0.00739         0.00186         3.965
      5          0.04919         0.04141         1.188
      3          0.01504         0.00635         2.369
      1          0.01242         0.03635         0.342
      4          0.00151         0.03679         0.041
  INTERCEPT     -6.07929
```

Figure 46.

Figure 46. (Continued)

```
SELECTION..... 1

                TABLE OF RESIDUALS

 CASE NO.     Y VALUE     Y ESTIMATE      RESIDUAL
      1      1.00000       0.48090       0.51910
      2      2.00000       1.77670       0.22330
      3      2.00000       2.14586      -0.14586
      4      0.0           0.82880      -0.82880
      5      2.00000       1.90522       0.09478
      6      2.00000       1.52125       0.47875
      7      3.00000       3.46447      -0.46447
      8      2.00000       2.25887      -0.25887
      9      3.00000       3.80259      -0.80259
     10      0.0           1.02042      -1.02042
     11      4.00000       2.49735       1.50265
     12      1.00000       2.00065      -1.00065
     13      1.00000       2.00736      -1.00736
     14      1.00000       1.15308      -0.15308
     15      3.00000       2.90446       0.09554
     16      2.00000       1.83531       0.16469
     17      3.00000       2.56004       0.43996
     18      4.00000       3.45228       0.54772
     19      4.00000       3.62661       0.37339
     20      3.00000       2.68068       0.31932
     21      4.00000       3.64886       0.35114
     22      4.00000       1.86541       2.13459
     23      1.00000       2.09863      -1.09863
     24      0.0           1.97217      -1.97217
     25      4.00000       1.41254       2.58746
     26      1.00000       1.88027      -0.88027
     27      3.00000       2.27646       0.72354
     28      4.00000       4.51080      -0.51080
     29      4.00000       3.95746       0.04254
     30      0.0           0.45458      -0.45458


SELECTION..... 2

DEPENDENT VARIABLE..... 6
NUMBER OF VARIABLES FORCED.... 1
NUMBER OF VARIABLES DELETED... 1


STEP  1

VARIABLE ENTERED..... 3
  (FORCED VARIABLE)

SUM OF SQUARES REDUCED IN THIS STEP....        0.819
PROPORTION REDUCED IN THIS STEP.......         0.014

CUMULATIVE SUM OF SQUARES REDUCED.....         0.819
CUMULATIVE PROPORTION REDUCED.........         0.014  OF       57.867

FOR  1 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...    0.119
      (ADJUSTED FOR D.F.)...........     0.119
  F-VALUE FOR ANALYSIS OF VARIANCE...    0.402
  STANDARD ERROR OF ESTIMATE.......      1.427
      (ADJUSTED FOR D.F.)...........     1.427

  VARIABLE     REGRESSION      STD. ERROR OF      COMPUTED
   NUMBER      COEFFICIENT      REG. COEFF.       T-VALUE
      3          0.00461          0.00728          0.634
 INTERCEPT       1.15093


STEP  2

VARIABLE ENTERED..... 2

SUM OF SQUARES REDUCED IN THIS STEP....       11.738
PROPORTION REDUCED IN THIS STEP.......         0.203

CUMULATIVE SUM OF SQUARES REDUCED.....        12.557
CUMULATIVE PROPORTION REDUCED.........         0.217  OF       57.867

FOR  2 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...    0.466
      (ADJUSTED FOR D.F.)...........     0.435
  F-VALUE FOR ANALYSIS OF VARIANCE...    3.741
  STANDARD ERROR OF ESTIMATE.......      1.295
      (ADJUSTED FOR D.F.)...........     1.318

  VARIABLE     REGRESSION      STD. ERROR OF      COMPUTED
   NUMBER      COEFFICIENT      REG. COEFF.       T-VALUE
      3          0.00778          0.00671          1.160
      2          0.00565          0.00214          2.645
 INTERCEPT       -1.40194


STEP  3

VARIABLE ENTERED..... 5

SUM OF SQUARES REDUCED IN THIS STEP....       18.639
PROPORTION REDUCED IN THIS STEP.......         0.322

CUMULATIVE SUM OF SQUARES REDUCED.....        31.196
CUMULATIVE PROPORTION REDUCED.........         0.539  OF       57.867

FOR  3 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...    0.734
      (ADJUSTED FOR D.F.)...........     0.711
  F-VALUE FOR ANALYSIS OF VARIANCE...   10.137
  STANDARD ERROR OF ESTIMATE.......      1.013
      (ADJUSTED FOR D.F.)...........     1.050

  VARIABLE     REGRESSION      STD. ERROR OF      COMPUTED
   NUMBER      COEFFICIENT      REG. COEFF.       T-VALUE
      3          0.01497          0.00551          2.717
      2          0.00744          0.00172          4.318
      5          0.05363          0.01258          4.263
 INTERCEPT       -5.53528
```

Figure 46. (Continued)

```
STEP  4

VARIABLE ENTERED..... 1

SUM OF SQUARES REDUCED IN THIS STEP....        0.127
PROPORTION REDUCED IN THIS STEP.......         0.002

CUMULATIVE SUM OF SQUARES REDUCED.....        31.323
CUMULATIVE PROPORTION REDUCED.........         0.541  OF       57.867

FOR  4 VARIABLES ENTERED
  MULTIPLE CORRELATION COEFFICIENT...    0.736
      (ADJUSTED FOR D.F.)...........     0.699
  F-VALUE FOR ANALYSIS OF VARIANCE...    7.375
  STANDARD ERROR OF ESTIMATE.......      1.030
      (ADJUSTED FOR D.F.)...........     1.098

  VARIABLE     REGRESSION      STD. ERROR OF      COMPUTED
   NUMBER      COEFFICIENT      REG. COEFF.       T-VALUE
      3          0.01493          0.00561          2.662
      2          0.00741          0.00175          4.222
      5          0.05076          0.01524          3.332
      1          0.01226          0.03541          0.346
 INTERCEPT       -5.94617


SELECTION..... 2

                TABLE OF RESIDUALS

 CASE NO.     Y VALUE     Y ESTIMATE      RESIDUAL
      1      1.00000       0.48498       0.51502
      2      2.00000       1.77220       0.22780
      3      2.00000       2.14799      -0.14799
      4      0.0           0.81528      -0.81528
      5      2.00000       1.91082       0.08918
      6      2.00000       1.52156       0.47844
      7      3.00000       3.47954      -0.47954
      8      2.00000       2.27251      -0.27251
      9      3.00000       3.80533      -0.80533
     10      0.0           1.02152      -1.02152
     11      4.00000       2.50144       1.49856
     12      1.00000       2.00604      -1.00604
     13      1.00000       2.00340      -1.00340
     14      1.00000       1.14922      -0.14922
     15      3.00000       2.91121       0.08879
     16      2.00000       1.82797       0.17203
     17      3.00000       2.56125       0.43875
     18      4.00000       3.43668       0.56332
     19      4.00000       3.61723       0.38277
     20      3.00000       2.68358       0.31642
     21      4.00000       3.64918       0.35082
     22      4.00000       1.86566       2.13434
     23      1.00000       2.09898      -1.09898
     24      0.0           1.96334      -1.96334
     25      4.00000       1.40769       2.59231
     26      1.00000       1.89582      -0.89582
     27      3.00000       2.28895       0.71105
     28      4.00000       4.50336      -0.50336
     29      4.00000       3.94940       0.05060
     30      0.0           0.44790      -0.44790
```

Figure 46. (Continued)

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a different format statement. If the user encounters problems with large or small numbers in his output, he may wish to change output format statements from F to E notation. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

1. Changes in the dimension statements of the main program, STEPR:

a. The dimension of arrays XBAR, STD, D, B, T, IDX, and L must each be greater than or equal to the number of variables, m. Since there are six variables in the sample problem, the value of m is 6.

b. The dimension of array RX must be greater than or equal to the product of m x m. For the sample problem this product is 36 = 6 x 6.

c. The dimension of array R must be greater than or equal to (m+1)m/2. For the sample problem this number is 21 = (6+1)6/2.

2. Changes in the input format statement of the special input subroutine, DATA:

Only the format statement for input data may be changed. If sample data are either one-, two-, or three-digit numbers, each row of data may be keypunched in six 3-column fields rather than using six-column fields as in the sample problem; in such case the format is changed to (6F3.0).

The special input subroutine, DATA, is normally written by the user to handle different formats for different problems. The user may modify this subroutine to perform testing of input data, transformation of data, and so on.

Operating Instructions

The sample program for stepwise multiple regression is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output. A scratch tape (data set 13) written in binary mode is used as intermediate storage.

Error Messages

The following error conditions will result in messages:

1. The number of selection cards is not specified on the control card--NUMBER OF SELECTIONS NOT SPECIFIED. JOB TERMINATED. This error terminates execution of the job.

2. More than one dependent variable is specified on a selection card--SELECTION CARD (N) DOES NOT NAME ONE AND ONLY ONE DEPENDENT VARIABLE. SELECTION IGNORED.

3. A control digit is not 0, 1, 2, or 3 on a selection card--COLUMN (K) OF SELECTION CARD (N) IS IN ERROR. IT IS POSSIBLE THAT COLUMNS SUCCEEDING THAT COLUMN ARE ALSO INCORRECT. THE SELECTION IS IGNORED.

4. There are too few observations for estimation to take place--(N) OBSERVATIONS ARE TOO FEW TO ALLOW PARAMETER ESTIMATION FOR (M) VARIABLES. JOB TERMINATED.

5. The correlation matrix is singular or badly conditioned--EITHER THE MATRIX IS SINGULAR, OR THE RESIDUAL SUM OF SQUARES IS NEGATIVE IMPLYING EXTREME ILL-CONDITION. SELECTION IGNORED.

Two other error types are not detected:

1. If the number of observations is incorrect, the job deck will be such that results on that selection and on succeeding jobs will be incorrect. The user should take care in preparing his job deck according to instructions given above.

2. If some variable is constant over all observations, a zero standard deviation will occur, and results for that selection will be incorrect or not forthcoming.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 45 seconds.

```
C                                                                       STEP  10
C     ...................................................................STEP  20
C                                                                       STEP  30
C        SAMPLE MAIN PROGRAM FOR STEP-WISE MULTIPLE REGRESSION - STEPR  STEP  40
C                                                                       STEP  50
C        PURPOSE                                                        STEP  60
C           (1) READ THE PROBLEM PARAMETER CARD FOR A STEP-WISE MULTIPLESTEP  70
C           REGRESSION, (2) READ SUBSET SELECTION CARDS, (3) CALL THE   STEP  80
C           SUBROUTINE TO CALCULATE MEANS, STANDARD DEVIATIONS, SIMPLE  STEP  90
C           CORRELATION COEFFICIENTS, AND (4) CALL THE SUBROUTINE TO    STEP 100
C           PERFORM EACH STEP OF REGRESSION ANALYSIS.                   STEP 110
C                                                                       STEP 120
C        REMARKS                                                        STEP 130
C            THE NUMBER OF OBSERVATIONS, N, MUST BE GREATER THAN M+2,   STEP 140
C           WHERE M IS THE NUMBER OF VARIABLES.  IF SELECTION CARDS ARE STEP 150
C           NOT PRESENT, THIS PROGRAM CAN NOT PERFORM STEP-WISE MULTIPLESTEP 160
C           REGRESSION.                                                 STEP 170
C                                                                       STEP 180
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  STEP 190
C           CORRE (WHICH, IN TURN, CALLS THE SUBROUTINE DATA)           STEP 200
C           MSTR  (WHICH, IN TURN, CALLS THE SUBROUTINE LOC)            STEP 210
C           STPRG (WHICH, IN TURN, CALLS THE SUBROUTINE STOUT)          STEP 220
C                                                                       STEP 230
C        METHOD                                                         STEP 240
C           REFER TO C. A. BENNETT AND N. L. FRANKLIN, 'STATISTICAL     STEP 250
C           ANALYSIS IN CHEMISTRY AND THE CHEMICAL INDUSTRY', JOHN WILEYSTEP 260
C           AND SONS, 1954, APPENDIX 6A.                                STEP 270
C                                                                       STEP 280
C     ...................................................................STEP 290
C                                                                       STEP 300
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE     STEP 310
C     NUMBER OF VARIABLES, M..                                          STEP 320
C                                                                       STEP 330
C        DIMENSION XBAR(35),STD(35),D(35),B(35),T(35),IDX(35),L(35)     STEP 340
C                                                                       STEP 350
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      STEP 360
C     PRODUCT OF M*M..                                                  STEP 370
C                                                                       STEP 380
C        DIMENSION RX(1225)                                             STEP 390
C                                                                       STEP 400
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      STEP 410
C     (M+1)*M/2..                                                       STEP 420
C                                                                       STEP 430
C        DIMENSION R(630)                                               STEP 440
C                                                                       STEP 450
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 5..      STEP 460
C                                                                       STEP 470
C        DIMENSION NSTEP(5)                                             STEP 480
C                                                                       STEP 490
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 11..     STEP 500
C                                                                       STEP 510
C        DIMENSION ANS(11)                                              STEP 520
C                                                                       STEP 530
C     ...................................................................STEP 540
C                                                                       STEP 550
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  STEP 560
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      STEP 570
C        STATEMENT WHICH FOLLOWS.                                       STEP 580
C                                                                       STEP 590
C     DOUBLE PRECISION XBAR,STD,RX,R,B,T,ANS,YEST                       STEP 600
C                                                                       STEP 610
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    STEP 620
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      STEP 630
C        ROUTINE.                                                       STEP 640
C                                                                       STEP 650
C     ...................................................................STEP 660
C                                                                       STEP 670
      1 FORMAT(A4,A2,I5,2I2,F6.0,I1)                                    STEP 680
      2 FORMAT(53HONUMBER OF SELECTIONS NOT SPECIFIED.  JOB TERMINATED.)STEP 690
      3 FORMAT(35H1STEP-WISE MULTIPLE REGRESSION.....A4,A2)             STEP 700
      4 FORMAT(31HOVARIABLE      MEAN      STANDARD/4X,3HNO.16X,9HDEVIATION)STEP 710
      5 FORMAT(4X,I2,F14.5,F12.5)                                       STEP 720
      6 FORMAT(19H1CORRELATION MATRIX)                                  STEP 730
      7 FORMAT(4HOROW13/(10F12.5))                                      STEP 740
      8 FORMAT(72I1)                                                    STEP 750
      9 FORMAT(23HONUMBER OF OBSERVATIONS15)                            STEP 760
     10 FORMAT(20H NUMBER OF VARIABLES3X,I5)                            STEP 770
     11 FORMAT(21H NUMBER OF SELECTIONS2X,I5)                           STEP 780
     12 FORMAT(28HOCONSTANT TO LIMIT VARIABLES9.5)                      STEP 790
     13 FORMAT(/15H1SELECTION.....I2)                                   STEP 800
     14 FORMAT(16X,18HTABLE OF RESIDUALS//9H CASE NO.5X,7HY VALUE5X,10HY ESTEP 810
       1STIMATE6X,8HRESIDUAL)                                           STEP 820
     15 FORMAT(I7,F15.5,2F14.5)                                         STEP 830
     16 FORMAT(1H )                                                     STEP 840
     17 FORMAT(1H1)                                                     STEP 850
     18 FORMAT(1HO,'****COLUMN',I4,' OF SELECTION CARD',I5,' IS IN ERROR. STEP 860
       1 IT IS POSSIBLE THAT COLUMNS SUCCEEDING THAT COLUMN ARE ALSO'   STEP 870
       2/' INCORRECT.  THE SELECTION IS IGNORED.****')                  STEP 880
     19 FORMAT(1HO,'****SELECTION CARD',I5,' DOES NOT NAME ONE AND ONLY ONESTEP 890
       1E DEPENDENT VARIABLE.  SELECTION IGNORED.****')                 STEP 900
     20 FORMAT(1HO,'****EITHER THE MATRIX IS SINGULAR, OR THE RESIDUAL SUMSTEP 910
       1 OF SQUARES IS NEGATIVE IMPLYING EXTREME ILL CONDITION.',/,' SELECSTEP 920
       2TION IGNORED.****')                                             STEP 930
     21 FORMAT(1HO,'****',I6,' OBSERVATIONS ARE TOO FEW TO ALLOW PARAMETERSTEP 940
       1 ESTIMATION FOR',I5,' VARIABLES.  JOB TERMINATED.****')         STEP 950
C                                                                       STEP 960
C        READ PROBLEM PARAMETER CARD                                    STEP 970
C                                                                       STEP 980
  100 READ (5,1) PR1,PR2,N,M,NS,PCT,NR                                  STEP 990
C        PR1.....PROBLEM CODE (MAY BE ALPHAMERIC)                       STEP1000
C        PR2.....PROBLEM CODE (CONTINUED)                               STEP1010
C        N ......NUMBER OF OBSERVATIONS                                 STEP1020
C        M ......NUMBER OF VARIABLES                                    STEP1030
C        NS......NUMBER OF SELECTIONS                                   STEP1040
C        PCT.....A CONSTANT VALUE OF PROPORTION OF SUM OF SQUARES THAT  STEP1050
C                WILL BE USED TO LIMIT VARIABLES ENTERING IN THE REGRES-STEP1060
C                SION                                                   STEP1070
C        NR......OPTION CODE FOR TABLE OF RESIDUALS                     STEP1080
```

```
C                0 - IF IT IS NOT DESIRED                                    STEP1090
C                1 - IF IT IS DESIRED                                        STEP1100
C                                                                            STEP1110
      WRITE (6,3) PR1,PR2                                                    STEP1120
      WRITE (6,9) N                                                          STEP1130
      WRITE (6,10) M                                                         STEP1140
      IF(N-M-2) 101,101,102                                                  STEP1150
  101 WRITE(6,21) N,M                                                        STEP1160
      STOP                                                                   STEP1170
  102 WRITE (6,11) NS                                                        STEP1180
      WRITE (6,12) PCT                                                       STEP1190
C                                                                            STEP1200
C     LOGICAL TAPE 13 IS USED AS INTERMEDIATE STORAGE TO HOLD INPUT          STEP1210
C     DATA.  THE INPUT DATA ARE WRITTEN ON LOGICAL TAPE 13 BY THE            STEP1220
C     SPECIAL INPUT SUBROUTINE NAMED DATA.  THE STORED DATA MAY BE USED      STEP1230
C     FOR RESIDUAL ANALYSIS.                                                 STEP1240
C                                                                            STEP1250
      REWIND 13                                                              STEP1260
C                                                                            STEP1270
      IO=0                                                                   STEP1280
      X=0.0                                                                  STEP1290
C                                                                            STEP1300
      CALL CORRE (N,M,IO,X,XBAR,STD,RX,R,B,D,T)                              STEP1310
C                                                                            STEP1320
      REWIND 13                                                              STEP1330
C                                                                            STEP1340
C        PRINT MEANS AND STANDARD DEVIATION                                  STEP1350
C                                                                            STEP1360
      WRITE (6,4)                                                            STEP1370
      DO 105 I=1,M                                                           STEP1380
  105 WRITE (6,5) I,XBAR(I),STD(I)                                           STEP1390
C                                                                            STEP1400
C        PRINT CORRELATION MATRIX                                            STEP1410
C                                                                            STEP1420
      WRITE (6,6)                                                            STEP1430
      DO 130 I=1,M                                                           STEP1440
      DO 125 J=1,M                                                           STEP1450
      IF(I-J) 110, 120, 120                                                  STEP1460
  110 K=I+(J*J-J)/2                                                          STEP1470
      GO TO 125                                                              STEP1480
  120 K=J+(I*I-I)/2                                                          STEP1490
  125 T(J)=R(K)                                                              STEP1500
  130 WRITE (6,7) I,(T(J),J=1,M)                                             STEP1510
C                                                                            STEP1520
C        TEST NUMBER OF SELECTIONS                                           STEP1530
C                                                                            STEP1540
      IF(NS) 135, 135, 140                                                   STEP1550
  135 WRITE (6,2)                                                            STEP1560
      GO TO 200                                                              STEP1570
C                                                                            STEP1580
C        SAVE THE MATRIX OF SUMS OF CROSS-PRODUCTS OF DEVIATIONS             STEP1590
C                                                                            STEP1600
  140 CALL MSTR (RX,R,M,0,1)                                                 STEP1610
C                                                                            STEP1620
      NSEL=1                                                                 STEP1630
      GO TO 150                                                              STEP1640
C                                                                            STEP1650
C        COPY THE MATRIX OF SUMS OF CROSS-PRODUCTS OF DEVIATIONS             STEP1660
C                                                                            STEP1670
  145 CALL MSTR (B,RX,M,1,0)                                                 STEP1680
C                                                                            STEP1690
C        READ A SELECTION CARD                                               STEP1700
C                                                                            STEP1710
  150 WRITE (6,13) NSEL                                                      STEP1720
      READ (5,8) (IDX(J),J=1,M)                                              STEP1730
C                                                                            STEP1740
C        IN EACH POSITION OF IDX, ONE OF THE FOLLOWING CODES MUST BE         STEP1750
C        SPECIFIED..                                                         STEP1760
C          0 OR BLANK - INDEPENDENT VARIABLE AVAILABLE FOR SELECTION          STEP1770
C          1          - INDEPENDENT VARIABLE TO BE FORCED IN REGRESSION       STEP1780
C          2          - VARIABLE TO BE DELETED                                STEP1790
C          3          - DEPENDENT VARIABLE                                    STEP1800
C                                                                            STEP1810
      N35=0                                                                  STEP1820
      DO 155 K=1,M                                                           STEP1830
      IF (IDX(K)) 152,153,153                                                STEP1840
  152 WRITE (6,18) K,NSEL                                                    STEP1850
      GO TO 185                                                              STEP1860
  153 IF (IDX(K)-3) 155,154,152                                              STEP1870
  154 N35=N35+1                                                              STEP1880
  155 CONTINUE                                                               STEP1890
      IF (N35-1) 156,157,156                                                 STEP1900
  156 WRITE (6,19) NSEL                                                      STEP1910
      GO TO 185                                                              STEP1920
C        CALL THE SUBROUTINE TO PERFORM A STEP-WISE REGRESSION ANALYSIS      STEP1930
C                                                                            STEP1940
  157 CALL STPRG (M,N,RX,XBAR,IDX,PCT,NSTEP,ANS,L,B,STD,1,D,IER)             STEP1950
      IF (IER) 159,159,158                                                   STEP1960
  158 WRITE (6,20)                                                           STEP1970
      GO TO 185                                                              STEP1980
C                                                                            STEP1990
C        FIND WHETHER TO PRINT THE TABLE OF RESIDUALS                        STEP2000
C                                                                            STEP2010
  159 IF(NP) 185, 185, 160                                                   STEP2020
C                                                                            STEP2030
C        PRINT THE TABLE OF RESIDUALS                                        STEP2040
C                                                                            STEP2050
C                                                                            STEP2060
  160 WRITE (6,13) NSEL                                                      STEP2070
      WRITE (6,16)                                                           STEP2080
      WRITE (6,14)                                                           STEP2090
      MM=NSTEP(1)                                                            STEP2100
      DO 180 I=1,N                                                           STEP2110
      READ (13) (D(J),J=1,M)                                                 STEP2120
      YEST=ANS(9)                                                            STEP2130
      K=NSTEP(4)                                                             STEP2140
      DO 170 J=1,K                                                           STEP2150
      KK=L(J)                                                                STEP2160
  170 YEST=YEST+B(J)*D(KK)                                                   STEP2170
      RESI=D(MM)-YEST                                                        STEP2180
  180 WRITE (6,15) I,D(MM),YEST,RESI                                         STEP2190
      REWIND 13                                                              STEP2200
C                                                                            STEP2210
C        TEST TO SEE WHETHER ALL SELECTIONS ARE COMPLETED                    STEP2220
C                                                                            STEP2230
  185 IF(NSEL-NS) 190, 100, 100                                              STEP2240
  190 NSEL=NSEL+1                                                            STEP2250
      WRITE (6,17)                                                           STEP2260
      GO TO 145                                                              STEP2270
C                                                                            STEP2280
  200 CONTINUE                                                               STEP2290
      END                                                                    STEP2300
```

CANONICAL CORRELATION

Problem Description

An analysis of the interrelations between two sets of variables measured on the same subjects is performed by this program. These variables are predictors in one set and criteria in the other set, but it is irrelevant whether the variables in the first set or in the second set are considered as the prediction variables. The canonical correlation, which gives the maximum correlation between linear functions of the two sets of variables, is calculated. χ^2 is also computed to test the significance of canonical correlation.

The sample problem for canonical correlation consists of four variables in the first set (left-hand side) and three variables in the second set (right-hand side) as presented in Table 6. These two sets of measurements have been made on 23 subjects.

Table 6. Sample Data for Canonical Correlation

	First set				Second set		
Observation	X_1	X_2	X_3	X_4	Y_1	Y_2	Y_3
1	191	155	65	19	179	145	70
2	195	149	70	20	201	152	69
3	181	148	71	19	185	149	75
4	183	153	82	18	188	149	86
5	176	144	67	18	171	142	71
6	208	157	81	22	192	152	77
7	189	150	75	21	190	149	72
8	197	159	90	20	189	152	82
9	188	152	76	19	197	159	84
10	192	150	78	20	187	151	72
11	179	158	99	18	186	148	89
12	183	147	65	18	174	147	70
13	174	150	71	19	185	152	65
14	190	159	91	19	195	157	99
15	188	151	98	20	187	158	87
16	163	137	59	18	161	130	63
17	195	155	85	20	183	158	81
18	196	153	80	21	173	148	74
19	181	145	77	20	182	146	70
20	175	140	70	19	165	137	81
21	192	154	69	20	185	152	63
22	174	143	79	20	178	147	73
23	176	139	70	20	176	143	69

Program

Description

The canonical correlation program consists of the main routine named MCANO, a special input subroutine named DATA, and five subroutines from the Scientific Subroutine Package: CORRE, CANOR, MINV, NROOT, and EIGEN.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 20 variables, including both the first set of variables (that is, left-hand variables) and the second set of variables (that is, right-hand variables) The number of variables in the first set must be greater than or equal to the number of variables in the second set.
2. Up to 99,999 observations
3. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than 20 variables, dimension statements in the sample main program must be modified to handle the particular problem. Similarly, if input data cards are prepared using a different format, the input format in the input subroutine, DATA, must be modified. The general rules for program modification are desc ibed later.

Input

Control Card

One control card is required for each problem and is read by the main program, MCANO. This card is prepared as follows:

Columns	Contents	For Sample Problem
1 - 6	Problem number (may be alphameric)	SAMPLE
7 - 11	Number of observations	00023
12 - 13	Number of variables in the first set (that is, left-hand variables)*	04
14 - 15	Number of variables in the second set (that is, right-hand variables)	03

*The number of variables in the first set must be greater than or equal to the number of variables in the second set.

Leading zeros are not required to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 6 is keypunched on a separate card using the format (12F6.0). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second card until the last data point is keypunched. However, each row of data must begin on a new card.

Deck Setup

The deck setup is shown in Figure 47.

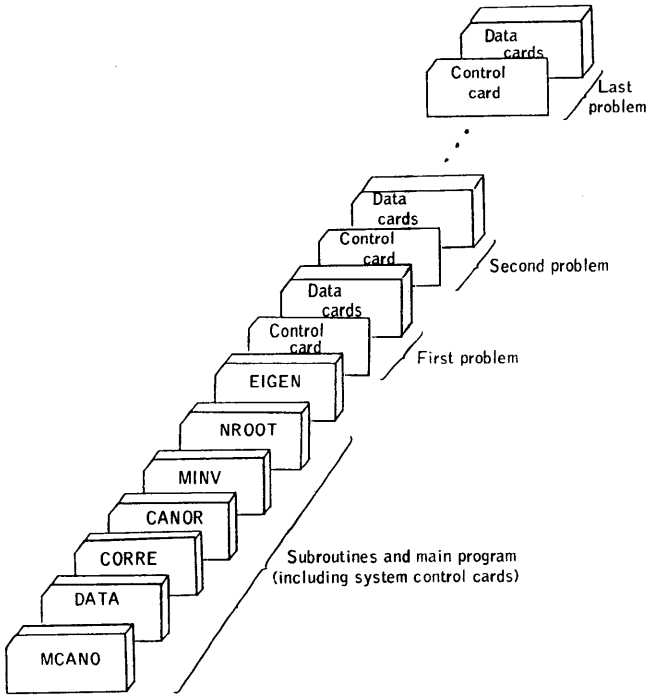


Figure 47. Deck setup (canonical correlation)

Sample

The listing of input cards for the sample problem is presented in Figure 48.

Output

Description

The output of the sample program for canonical correlation includes:

1. Means
2. Standard deviations
3. Correlation coefficients
4. Eigenvalues and corresponding canonical correlation
5. Lambda
6. Chi-square and degrees of freedom
7. Coefficients for left- and right-hand variables

Sample

The output listing for the sample problem is shown in Figure 49 of this sample problem.

```
/DATA
SAMPLE0090230403                                                        10
   191   155    65    19   179   145    70                             20
   195   149    70    20   201   152    69                             30
   181   148    71    19   185   149    75                             40
   183   153    82    18   188   149    86                             50
   176   144    67    18   171   142    71                             60
   208   157    81    22   192   152    77                             70
   189   150    75    21   190   149    72                             80
   197   159    90    20   189   152    82                             90
   188   152    76    19   197   159    84                            100
   192   150    78    20   187   151    72                            110
   179   158    99    18   186   148    89                            120
   183   147    65    18   174   147    70                            130
   174   150    71    19   185   152    65                            140
   190   159    91    19   195   157    99                            150
   188   151    98    20   187   158    87                            160
   163   137    59    18   161   130    63                            170
   195   155    85    20   183   158    81                            180
   196   153    80    21   173   148    74                            190
   181   145    77    20   182   146    70                            200
   175   140    70    19   165   137    81                            210
   192   154    69    20   185   152    63                            220
   174   143    79    20   178   147    73                            230
   176   139    70    20   176   143    69                            240
                                                                       250
```

Figure 48. Input card listing (canonical correlation)

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

1. Changes in the dimension statements of the main program, MCANO:
   a. The dimension of arrays XBAR, STD, CANR, CHISQ, and NDF must be greater than or equal to the total number of variables m (m = p + q, where p is the number of left-hand variables and q is the number of right-hand variables). Since there are seven variables, four on left and three on right, the value of m is 7.

```
CANONICAL CORRELATION.....SAMPLE

  NO. OF OBSERVATIONS          23
  NO. OF LEFT HAND VARIABLES    4
  NO. OF RIGHT HAND VARIABLES   3

MEANS
      185.47826      149.91304      76.86955      19.47826      183.00000      148.82608      75.73912

STANDARD DEVIATIONS
       10.10342       6.31673      10.46338       1.08165       9.84424       6.73965       9.05647

CORRELATION COEFFICIENTS

ROW  1
     1.00000    0.74852    0.37082    0.66441    0.62291    0.66080    0.24683

ROW  2
     0.74852    1.00000    0.63252    0.22590    0.66811    0.72780    0.53194

ROW  3
     0.37082    0.63252    1.00000    0.20657    0.47394    0.60169    0.79684

ROW  4
     0.66441    0.22590    0.20657    1.00000    0.32870    0.34863   -0.10733

ROW  5
     0.62291    0.66811    0.47394    0.32870    1.00000    0.82555    0.39258

ROW  6
     0.66080    0.72780    0.60169    0.34863    0.82555    1.00000    0.47657

ROW  7
     0.24683    0.53194    0.79684   -0.10733    0.39258    0.47657    1.00000

 NUMBER OF      LARGEST        CORRESPONDING                                  DEGREES
 EIGENVALUES    EIGENVALUE     CANONICAL                LAMBDA    CHI-SQUARE    OF
 REMOVED        REMAINING      CORRELATION                                    FREEDOM

     0            0.79880        0.89376              0.11598     40.93277       12
     1            0.41910        0.64738              0.57644     10.46676        6
     2            0.00767        0.08760              0.99233      0.14636        2

CANONICAL CORRELATION      0.89376

  COEFFICIENTS FOR LEFT HAND VARIABLES
       0.66310        -0.16059         1.05822        -0.56651

  COEFFICIENTS FOR RIGHT HAND VARIABLES
      -0.02133         0.44090         0.89730

CANONICAL CORRELATION      0.64738

  COEFFICIENTS FOR LEFT HAND VARIABLES
       0.09454        -0.83915         0.66309        -0.64892

  COEFFICIENTS FOR RIGHT HAND VARIABLES
      -0.43841        -0.55503         0.70692

CANONICAL CORRELATION      0.08760

  COEFFICIENTS FOR LEFT HAND VARIABLES
       0.02681         0.36055        -0.28827        -0.32496

  COEFFICIENTS FOR RIGHT HAND VARIABLES
       0.70325        -0.70384         0.10028

1E00031217
```

Figure 49. Output listing (canonical correlation)

b. The dimension of array RX must be greater than or equal to the product of m x m. For the sample problem this product is 49 = 7 x 7.

c. The dimension of array R must be greater than or equal to (m + 1) m/2. For the sample problem this number is 28 = (7 + 1)7/2.

d. The dimension of array COEFL must be greater than or equal to the product of p x q. For the sample problem this product is 12 = 4 x 3.

e. The dimension of array COEFR must be greater than or equal to the product of q x q. For the sample problem this product is 9 = 3 x 3.

2. Changes in the input format statement of the special input subroutine, DATA:

Only the format statement for input data may be changed. Since sample data are either two- or three-digit numbers, rather than using six-column fields as in the sample problem, each row of data may be keypunched in seven 3-column fields, and, if so, the format is changed to (7F3.0).

The special input subroutine, DATA, is normally written by the user to handle different formats for different problems. The user may modify this subroutine to perform testing of input data, transformation of data, and so on.

Operating Instructions

The sample program for canonical correlation is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 19 seconds.

```
C                                                                       MCAN  10
C     ..................................................................MCAN  20
C                                                                       MCAN  30
C        SAMPLE MAIN PROGRAM FOR CANONICAL CORRELATION - MCANO          MCAN  40
C                                                                       MCAN  50
C        PURPOSE                                                        MCAN  60
C           (1) READ THE PROBLEM PARAMETER CARD FOR A CANONICAL         MCAN  70
C           CORRELATION, (2) CALL TWO SUBROUTINES TO CALCULATE SIMPLE   MCAN  80
C           CORRELATIONS, CANONICAL CORRELATIONS, CHI-SQUARES, DEGREES  MCAN  90
C           OF FREEDOM FOR CHI-SQUARES, AND COEFFICIENTS FOR LEFT AND   MCAN 100
C           RIGHT HAND VARIABLES, NAMELY CANONICAL VARIATES, AND (3)    MCAN 110
C           PRINT THE RESULTS.                                          MCAN 120
C                                                                       MCAN 130
C        REMARKS                                                        MCAN 140
C           THE NUMBER OF LEFT HAND VARIABLES MUST BE GREATER THAN      MCAN 150
C           OR EQUAL TO THE NUMBER OF RIGHT HAND VARIABLES.             MCAN 160
C                                                                       MCAN 170
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MCAN 180
C           CORRE  (WHICH, IN TURN, CALLS THE INPUT SUBROUTINE NAMED    MCAN 190
C                  DATA.)                                               MCAN 200
C           CANOR  (WHICH, IN TURN, CALLS THE SUBROUTINES MINV AND      MCAN 210
C                  NROOT.  NROOT, IN TURN, CALLS THE SUBROUTINE EIGEN.) MCAN 220
C                                                                       MCAN 230
C        METHOD                                                         MCAN 240
C           REFER TO W. W. COOLEY AND P. R. LOHNES, 'MULTIVARIATE PRO-  MCAN 250
C           CEDURES FOR THE BEHAVIORAL SCIENCES', JOHN WILEY AND SONS,  MCAN 260
C           1962, CHAPTER 3.                                            MCAN 270
C                                                                       MCAN 280
C     ..................................................................MCAN 290
C                                                                       MCAN 300
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE     MCAN 310
C     TOTAL NUMBER OF VARIABLES M (M=MP+MQ, WHERE MP IS THE NUMBER OF   MCAN 320
C     LEFT HAND VARIABLES, AND MQ IS THE NUMBER OF RIGHT HAND VARI-     MCAN 330
C     ABLES)..                                                          MCAN 340
C                                                                       MCAN 350
      DIMENSION XBAR(20),STD(20),CANR(20),CHISQ(20),NDF(20)             MCAN 360
C                                                                       MCAN 370
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MCAN 380
C     PRODUCT OF M*M..                                                  MCAN 390
C                                                                       MCAN 400
      DIMENSION RX(400)                                                 MCAN 410
C                                                                       MCAN 420
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO          MCAN 430
C     (M+1)*M/2..                                                       MCAN 440
C                                                                       MCAN 450
      DIMENSION R(210)                                                  MCAN 460
C                                                                       MCAN 470
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MCAN 480
C     PRODUCT OF MP*MQ..                                                MCAN 490
C                                                                       MCAN 500
      DIMENSION COEFL(400)                                              MCAN 510
C                                                                       MCAN 520
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MCAN 530
C     PRODUCT OF MQ*MQ..                                                MCAN 540
C                                                                       MCAN 550
      DIMENSION COEFR(400)                                              MCAN 560
C                                                                       MCAN 570
C     ..................................................................MCAN 580
C                                                                       MCAN 590
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  MCAN 600
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      MCAN 610
C        STATEMENT WHICH FOLLOWS.                                       MCAN 620
C                                                                       MCAN 630
C     DOUBLE PRECISION XBAR,STD,RX,R,CANR,CHISQ,COEFL,COEFR             MCAN 640
C                                                                       MCAN 650
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    MCAN 660
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      MCAN 670
C        ROUTINE.                                                       MCAN 680
C                                                                       MCAN 690
C        ..............................................................MCAN 700
C                                                                       MCAN 710
    1 FORMAT(A4,A2,I5,2I2)                                              MCAN 720
    2 FORMAT(27HICANONICAL CORRELATION.....,A4,A2//22H   NO. OF OBSERVATMCAN 730
     1IONS,8X,I4/29H   NO. OF LEFT HAND VARIABLES,I5/30H   NO. OF RIGHT MCAN 740
     3HAND VARIABLES,I4/)                                               MCAN 750
    3 FORMAT(6HOMEANS/(8F15.5))                                         MCAN 760
    4 FORMAT(20HOSTANDARD DEVIATIONS/(8F15.5))                          MCAN 770
    5 FORMAT(25HOCORRELATION COEFFICIENTS)                              MCAN 780
    6 FORMAT(4HOROW,I3/(10F12.5))                                       MCAN 790
    7 FORMAT(1HC//12H   NUMBER OF,7X,7HLARGEST,7X,13HCORRESPONDING,31X,7MCAN 800
     1HDEGREES/13H   EIGENVALUES,5X,10HEIGENVALUE,7X,9HCANONICAL,7X,6HLAMMCAN 810
     2BDA,5X,10HCHI-SQUARE,7X,2HOF/4X,7HREMOVED,7X,9HREMAINING,7X,11HCORMCAN 820
     3RELATION,32X,7HFREEDOM/)                                          MCAN 830
    8 FORMAT(1H ,I7,F19.5,F16.5,2F14.5,5X,I5)                           MCAN 840
    9 FORMAT(1HO/22H CANONICAL CORRELATION,F12.5)                       MCAN 850
   10 FORMAT(39HO  COEFFICIENTS FOR LEFT HAND VARIABLES/(8F15.5))       MCAN 860
   11 FORMAT(40HO  COEFFICIENTS FOR RIGHT HAND VARIABLES/(8F15.5))      MCAN 870
C                                                                       MCAN 880
C     ..................................................................MCAN 890
C                                                                       MCAN 900
C     READ PROBLEM PARAMETER CARD                                       MCAN 910
C                                                                       MCAN 920
  100 READ (5,1) PR,PR1,N,MP,MQ                                        MCAN 930
C        PR.......PROBLEM NUMBER (MAY BE ALPHAMERIC)                    MCAN 940
C        PR1......PROBLEM NUMBER (CONTINUED)                            MCAN 950
C        N........NUMBER OF OBSERVATIONS                                MCAN 960
C        MP.......NUMBER OF LEFT HAND VARIABLES                         MCAN 970
C        MQ.......NUMBER OF RIGHT HAND VARIABLES                        MCAN 980
C                                                                       MCAN 990
      WRITE (6,2) PR,PR1,N,MP,MQ                                       MCAN1000
C                                                                      MCAN1010
      M=MP+MQ                                                          MCAN1020
      IO=0                                                             MCAN1030
      X=0.0                                                            MCAN1040
C                                                                      MCAN1050
      CALL CORRE (N,M,IO,X,XBAR,STD,RX,R,CANR,CHISQ,COEFL)             MCAN1060
C                                                                      MCAN1070
C     PRINT MEANS, STANDARD DEVIATIONS, AND CORRELATION                MCAN1080
C     COEFFICIENTS OF ALL VARIABLES                                    MCAN1090
C                                                                      MCAN1100
      WRITE (6,3) (XBAR(I),I=1,M)                                      MCAN1110
      WRITE (6,4) (STD(I),I=1,M)                                       MCAN1120
      WRITE (6,5)                                                      MCAN1130
      DO 160 I=1,M                                                     MCAN1140
      DO 150 J=1,M                                                     MCAN1150
      IF(I-J) 120, 130, 130                                            MCAN1160
  120 L=I+(J*J-J)/2                                                    MCAN1170
      GO TO 140                                                        MCAN1180
  130 L=J+(I*I-I)/2                                                    MCAN1190
  140 CANR(J)=R(L)                                                     MCAN1200
  150 CONTINUE                                                         MCAN1210
  160 WRITE (6,6) I,(CANR(J),J=1,M)                                    MCAN1220
C                                                                      MCAN1230
      CALL CANOR (N,MP,MQ,R,XBAR,STD,CANR,CHISQ,NDF,COEFR,COEFL,RX)    MCAN1240
C                                                                      MCAN1250
C     PRINT EIGENVALUES, CANONICAL CORRELATIONS, LAMBDA, CHI-SQUARES,  MCAN1260
C     DEGREES OF FREEDOMS                                              MCAN1270
C                                                                      MCAN1280
      WRITE (6,7)                                                      MCAN1290
      DO 170 I=1,MQ                                                    MCAN1300
      N1=I-1                                                           MCAN1310
C                                                                      MCAN1320
C        TEST WHETHER EIGENVALUE IS GREATER THAN ZERO                  MCAN1330
C                                                                      MCAN1340
      IF(XBAR(I)) 165, 165, 170                                        MCAN1350
  165 MM=N1                                                            MCAN1360
      GO TO 175                                                        MCAN1370
  170 WRITE (6,8) N1,XBAR(I),CANR(I),STD(I),CHISQ(I),NDF(I)            MCAN1380
      MM=MQ                                                            MCAN1390
C                                                                      MCAN1400
C     PRINT CANONICAL COEFFICIENTS                                     MCAN1410
C                                                                      MCAN1420
  175 N1=0                                                             MCAN1430
      N2=0                                                             MCAN1440
      DO 200 I=1,MM                                                    MCAN1450
      WRITE (6,9) CANR(I)                                              MCAN1460
      DO 180 J=1,MP                                                    MCAN1470
      N1=N1+1                                                          MCAN1480
  180 XBAR(J)=COEFL(N1)                                                MCAN1490
      WRITE (6,10) (XBAR(J),J=1,MP)                                    MCAN1500
      DO 190 J=1,MQ                                                    MCAN1510
      N2=N2+1                                                          MCAN1520
  190 XBAR(J)=COEFR(N2)                                                MCAN1530
      WRITE (6,11) (XBAR(J),J=1,MQ)                                    MCAN1540
  200 CONTINUE                                                         MCAN1550
      GO TO 100                                                        MCAN1560
      END                                                              MCAN1570
```

ANALYSIS OF VARIANCE

Problem Description

An analysis of variance is performed for a factorial design by use of three special operators suggested by H. O. Hartley.* The analysis of many other designs can be derived by reducing them first to factorial designs, and then pooling certain components of the analysis-of-variance table.

Consider a three-factor factorial experiment in a randomized complete block design as presented in Table 7. In this experiment, factor A has four levels, factors B and C have three levels, and the entire experiment is replicated twice. The replicates are completely unrelated and do not constitute a factor. Nevertheless, for the purpose of this program a four-factor experiment (with factors A, B, C, and R) is assumed. Thus, each element of the data in Table 5 may be represented in the form:

x_{abcr} where $a = 1, 2, 3, 4$; $b = 1, 2, 3$; $c = 1, 2, 3$; $r = 1, 2$

The general principle of the analysis-of-variance procedure used in the program is first to perform a formal factorial analysis and then to pool certain components in accordance with summary instructions that specifically apply to the particular design. The summary instructions for four different designs are presented in the output section.

Program

Description

The analysis-of-variance program consists of the main routine named ANOVA, and three subroutines from the Scientific Subroutine Package: AVDAT, AVCAL, and MEANQ.

*H. O. Hartley, "Analysis of Variance", Mathematical Methods for Digital Computers, edited by A. Ralston and H. Wilf, John Wiley and Sons, 1962, Chapter 20.

Table 7. Sample Data for Analysis of Variance

Replicate (Block)		b_1				b_2				b_3			
		a_1	a_2	a_3	a_4	a_1	a_2	a_3	a_4	a_1	a_2	a_3	a_4
r_1	c_1	3	10	9	8	24	8	9	3	2	8	9	8
	c_2	4	12	3	9	22	7	16	2	2	2	7	2
	c_3	5	10	5	8	23	9	17	3	2	8	6	3
r_2	c_1	2	14	9	13	29	16	11	3	2	7	5	3
	c_2	7	11	5	8	28	18	10	6	6	6	5	9
	c_3	9	10	27	8	28	16	11	7	8	9	8	15

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to six-factor factorial experiment
2. Up to a total of 3000 data points. The total number of data points in a problem is calculated by the formula:

$$T = \prod_{i=1}^{k} (LEVEL_i + 1)$$

where $LEVEL_i$ = number of levels of i^{th} factor
k = number of factors
Π = notation for cumulative multiplication

3. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than six factors or if the total number of data points is more than 3000, dimension statements in the sample main program must be modified. Similarly, if input data cards are prepared using a different format, the input format statement in the sample main program must be modified. The general rules for program modifications are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, ANOVA. This card is prepared as follows:

Columns	Contents	For Sample Problem
1- 6	Problem number (may be alphameric)	SAMPLE
7- 8	Number of factors	04
9-15	Blank	
16	Label for the first factor	A
17-20	Number of levels of the first factor	0004
21	Label for the second factor	B
22-25	Number of levels of the second factor	0003
26	Label for the third factor	C
27-30	Number of levels of the third factor	0003
31	Label for the fourth factor	R
32-35	Number of levels of the fourth factor	0002
.		
.		
.		
66	Label for the eleventh factor (if present)	
67-70	Number of levels of the eleventh factor	

If there are more than eleven factors, continue to the second card in the same manner.

Columns	Contents
1	Label for the twelfth factor
2 - 5	Number of levels of the twelfth factor
.	
.	
.	
etc.	

Leading zeros are not required to be keypunched.

Data Cards

Data are keypunched in the following order: X_{1111}, X_{2111}, X_{3111}, X_{4111}, X_{1211}, X_{2211}, X_{3211}, ..., X_{4332}. In other words, the innermost subscript is changed first -- namely, the first factor -- and then the second, third, and fourth subscripts. In the sample problem, the first subscript corresponds to factor A, and the second, third, and fourth subscripts to factors B, C, and R. Since the number of data fields per card is twelve, implied by the format (12F6.0), each row in Table 7 is keypunched on a separate card.

Deck Setup

The deck setup is shown in Figure 50.

Sample

The listing of input cards for the sample problem is presented in Figure 51.

Output

Description

The output of the sample analysis-of-variance program includes the numbers of levels of factors as input, the mean of all data, and the table of analysis of variance. In order to complete the analysis of variance properly, however, certain components in the table may need to be pooled. This is accomplished by means of summary instructions that specifically apply to the particular experiment. These are presented in Table 8.

As mentioned earlier, the sample problem is a randomized complete block design with three factors replicated twice. Therefore, it is necessary to pool certain components in the table of analysis of variance shown in Figure 52. Specifically, the components AR, BR, ABR, CR, ACR, BCR, and ABCR are combined into one value called the error term. The result is indicated in Figure 52. Since these data are purely hypothetical, interpretations of the various effects are not made.

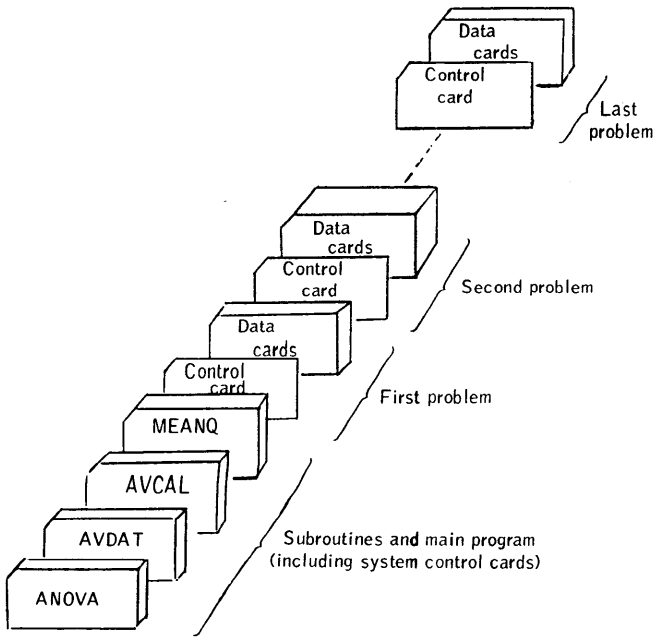


Figure 50. Deck setup (analysis of variance)

Table 8. Instructions to Summarize Components of Analysis of Variance

	Single Classification with Replicates	Two-way Classification with Cell Replicates	Randomized Complete Block with Two Factors	Split Plot
(Input)				
Factor No. 1	Groups = A	Rows = A	Factor 1 = A	Main treatment = A
2	Replicates = R	Columns = B	Factor 2 = B	Subtreatment = B
3		Replicates = R	Blocks = R	Blocks = R
(Output)				
Sums of squares	A	A	A	A
	R	B	B	B
	AR	AB	AB	AB
		R	R	R
		AR	AR	AR
		BR	BR	BR
		ABR	ABR	ABR
Summary instruction	Error = R + (AR)	Error = R + (AR) +(BR)+(ABR)	Error = (AR)+(BR) +(ABR)	Error = (BR)+(ABR) (b)
Analysis of variance	Groups A	Rows A	Factor 1 A	Main treatment A
	Error	Columns B	Factor 2 B	Blocks R
		Interaction AB	Interaction AB	Error (a) AR
		Error	Blocks R	Subtreatment B
			Error	Interaction AB
				Error (b)

```
ANALYSIS OF VARIANCE.....SAMPLE

LEVELS OF FACTORS
A          4
B          3
C          3
R          2

GRAND MEAN                    9.40278

SOURCE OF VARIATION        SUMS OF SQUARES    DEGREES OF FREEDOM    MEAN SQUARES
A                              229.04166              3              76.34721
B                              722.69434              2             361.34717
AB                            1382.08325              6             230.34720
C                               55.11110              2              27.55554
AC                              42.00000              6               7.00000
BC                              13.13889              4               3.28472
ABC                            140.75000             12              11.72917
R          (Block)             141.68054              1             141.68054
AR                              18.81944              3               6.27315
BR                               6.02778              2               3.01389
ABR                            176.97221             6              29.49536
CR         (Error)*  (506.81940)*          2   (35)*  20.38889   (14.48054)*
ACR                             40.77777              6               8.42592
BCR                             50.55554              4              15.65972
ABCR                            62.63889             12              12.58565
TOTAL                          151.02777             71
                              3233.31763

*summarized after the computer output is obtained.
```

Figure 52. Output listing (analysis of variance)

Sample

The output listing for the sample problem is shown in Figure 52.

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

1. Changes in the dimension statements of the main program, ANOVA:
   a. The dimension of array X must be greater than or equal to the total number of data points as calculated by the formula in the program capacity section above. For the sample problem, the total number of data points is 240 = (4+1)(3+1)(3+1)(2+1).
   b. The dimension of arrays HEAD, LEVEL, ISTEP, KOUNT, and LASTS must be greater than or equal to the number of factors, k. Since there are four factors in the sample problem (4 = 3 original factors + 1 pseudo factor), the value of k is 4.
   c. The dimension of arrays SUMSQ, NDF, and SMEAN must be greater than or equal to $n = 2^k-1$, where k is the number of factors. For the sample problem, the value of n is $15 = 2^4-1$.
2. Change in the input format statement of the main program, ANOVA:
   Only the format statement for input data may be changed. Since sample data are either one- or two-digit numbers, rather than using six-column fields as in the sample problem, each data may be keypunched in a two-column field, and, if so, the format is changed to (12F2.0). This format assumes twelve 2-column fields per card, beginning in column 1.

```
/DATA
SAMPLE04        A0004B0003C0003R0002                                        10
   3  10   9   8  24   8   9   3   2   8   9   8                           20
   4  12   3   9  22   7  16   2   2   2   7   2                           30
   5  10   5   8  23   9  17   3   2   8   6   3                           40
   2  14   9  13  29  16  11   3   2   7   5   3                           50
   7  11   5   8  28  18  10   6   6   6   5   9                           60
   9  10  27   8  28  16  11   7   8   9   8  15                           70
                                                                           80
```

Figure 51. Input listing (analysis of variance)

Operating Instructions

The sample analysis-of-variance program is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 11 seconds.

```
C                                                                       ANOV  10
C     ...................................................................ANOV  20
C                                                                       ANOV  30
C        SAMPLE MAIN PROGRAM FOR ANALYSIS OF VARIANCE - ANOVA           ANOV  40
C                                                                       ANOV  50
C        PURPOSE                                                        ANOV  60
C           (1) READ THE PROBLEM PARAMETER CARD FOR ANALYSIS OF VARI-   ANOV  70
C           ANCE, (2) CALL THE SUBROUTINES FOR THE CALCULATION OF SUMS  ANOV  80
C           OF SQUARES, DEGREES OF FREEDOM AND MEAN SQUARE, AND         ANOV  90
C           (3) PRINT FACTOR LEVELS, GRAND MEAN AND ANALYSIS OF VARI-   ANOV 100
C           ANCE TABLE.                                                 ANOV 110
C                                                                       ANOV 120
C        REMARKS                                                        ANOV 130
C           THE PROGRAM HANDLES ONLY COMPLETE FACTORIAL DESIGNS.  THERE-ANOV 140
C           FORE, OTHER EXPERIMENTAL DESIGN MUST BE REDUCED TO THIS FORMANOV 150
C           PRIOR TO THE USE OF THE PROGRAM.                            ANOV 160
C                                                                       ANOV 170
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  ANOV 180
C           AVDAT                                                       ANOV 190
C           AVCAL                                                       ANOV 200
C           MEANQ                                                       ANOV 210
C                                                                       ANOV 220
C        METHOD                                                         ANOV 230
C           THE METHOD IS BASED ON THE TECHNIQUE DISCUSSED BY H. O.     ANOV 240
C           HARTLEY IN 'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS',    ANOV 250
C           EDITED BY A. RALSTON AND H. WILF, JOHN WILEY AND SONS,      ANOV 260
C           1962, CHAPTER 20.                                           ANOV 270
C                                                                       ANOV 280
C     ...................................................................ANOV 290
C                                                                       ANOV 300
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      ANOV 310
C     CUMULATIVE PRODUCT OF EACH FACTOR LEVEL PLUS ONE (LEVEL(I)+1)     ANOV 320
C     FOR I=1 TO K, WHERE K IS THE NUMBER OF FACTORS..                  ANOV 330
C                                                                       ANOV 340
      DIMENSION X(3000)                                                 ANOV 350
C                                                                       ANOV 360
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE     ANOV 370
C     NUMBER OF FACTORS..                                               ANOV 380
C                                                                       ANOV 390
      DIMENSION HEAD(6),LEVEL(6),ISTEP(6),KOUNT(6),LASTS(6)             ANOV 400
C                                                                       ANOV 410
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO 2 TO    ANOV 420
C     THE K-TH POWER MINUS 1, ((2**K)-1)..                              ANOV 430
C                                                                       ANOV 440
      DIMENSION SUMSQ(63),NDF(63),SMEAN(63)                             ANOV 450
C                                                                       ANOV 460
C     THE FOLLOWING DIMENSION IS USED TO PRINT FACTOR LABELS IN ANALYSISANOV 470
C     OF VARIANCE TABLE AND IS FIXED..                                  ANOV 480
C                                                                       ANOV 490
      DIMENSION FMT(15)                                                 ANOV 500
C     ...................................................................ANOV 510
C                                                                       ANOV 520
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  ANOV 530
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      ANOV 540
C        STATEMENT WHICH FOLLOWS.                                       ANOV 550
C                                                                       ANOV 560
C     DOUBLE PRECISION X,GMEAN,SUMSQ,SMEAN,SUM                          ANOV 570
C                                                                       ANOV 580
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    ANOV 590
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      ANOV 600
C        ROUTINE.                                                       ANOV 610
C                                                                       ANOV 620
C     ...................................................................ANOV 630
C                                                                       ANOV 640
    1 FORMAT(A4,A2,I2,A4,3X,11(A1,I4)/(A1,I4,A1,I4,A1,I4,A1,I4,A1,I4)) ANOV 650
    2 FORMAT(2H1ANALYSIS OF VARIANCE.....A4,A2//)                       ANOV 660
    3 FORMAT(18HOLEVELS OF FACTORS/(3X,A1,7X,I4))                       ANOV 670
    4 FORMAT(1HO//11H GRAND MEANF20.5////)                              ANOV 680
    5 FORMAT(10HOSOURCE OF10X,7HSUMS OF10X,10HDEGREES OF9X,4HMEAN/10H VAANOV 690
   1ATION18X,7HSQUARES11X,7HFREEDOM10X,7HSQUARES/)                      ANOV 700
    6 FORMAT(1H 15A1,F20.5,10X,I6,F20.5)                                ANOV 710
    7 FORMAT(6H TOTAL10X,F20.5,10X,I6)                                  ANOV 720
    8 FORMAT(12F6.0)                                                    ANOV 730
C                                                                       ANOV 740
C     ...................................................................ANOV 750
C                                                                       ANOV 760
C     READ PROBLEM PARAMETER CARD                                       ANOV 770
C                                                                       ANOV 780
  100 READ (5,1) PR,PR1,K,BLANK,(HEAD(I),LEVEL(I),I=1,K)                ANOV 790
C        PR.....PROBLEM NUMBER (MAY BE ALPHAMERIC)                      ANOV 800
C        PR1....PROBLEM NUMBER (CONTINUED)                              ANOV 810
C        K......NUMBER OF FACTORS                                       ANOV 820
C        BLANK..BLANK FIELD                                             ANOV 830
C        HEAD...FACTOR LABELS                                           ANOV 840
C        LEVEL..LEVELS OF FACTORS                                       ANOV 850
C                                                                       ANOV 860
C     PRINT PROBLEM NUMBER AND LEVELS OF FACTORS                        ANOV 870
C                                                                       ANOV 880
      WRITE (6,2) PR,PR1                                                ANOV 890
      WRITE (6,3) (HEAD(I),LEVEL(I),I=1,K)                             ANOV 900
C                                                                       ANOV 910
C     CALCULATE TOTAL NUMBER OF DATA                                    ANOV 920
C                                                                       ANOV 930
      N=LEVEL(1)                                                        ANOV 940
      DO 102 I=2,K                                                      ANOV 950
  102 N=N*LEVEL(I)                                                      ANOV 960
C                                                                       ANOV 970
C     READ ALL INPUT DATA                                               ANOV 980
C                                                                       ANOV 990
      READ (5,8) (X(I),I=1,N)                                           ANOV1000
C                                                                       ANOV1010
      CALL AVDAT (K,LEVEL,N,X,L,ISTEP,KOUNT)                            ANOV1020
      CALL AVCAL (K,LEVEL,X,L,ISTEP,LASTS)                              ANOV1030
      CALL MEANQ (K,LEVEL,X,GMEAN,SUMSQ,NDF,SMEAN,ISTEP,KOUNT,LASTS)   ANOV1040
C                                                                       ANOV1050
C     PRINT GRAND MEAN                                                  ANOV1060
C                                                                       ANOV1070
      WRITE (6,4) GMEAN                                                 ANOV1080
C                                                                       ANOV1090
C     PRINT ANALYSIS OF VARIANCE TABLE                                  ANOV1100
C                                                                       ANOV1110
      WRITE (6,5)                                                       ANOV1120
      LL=(2**K)-1                                                       ANOV1130
      ISTEP(1)=1                                                        ANOV1140
      DO 105 I=2,K                                                      ANOV1150
  105 ISTEP(I)=0                                                        ANOV1160
      DO 110 I=1,15                                                     ANOV1170
  110 FMT(I)=BLANK                                                      ANOV1180
      NN=0                                                              ANOV1190
      SUM=0.0                                                           ANOV1200
  120 NN=NN+1                                                           ANOV1210
      L=0                                                               ANOV1220
      DO 140 I=1,K                                                      ANOV1230
      FMT(I)=BLANK                                                      ANOV1240
      IF(ISTEP(I)) 130, 140, 130                                        ANOV1250
  130 L=L+1                                                             ANOV1260
      FMT(L)=HEAD(I)                                                    ANOV1270
  140 CONTINUE                                                          ANOV1280
      WRITE (6,6) (FMT(I),I=1,15),SUMSQ(NN),NDF(NN),SMEAN(NN)           ANOV1290
      SUM=SUM+SUMSQ(NN)                                                 ANOV1300
      IF(NN-LL) 145, 170, 170                                           ANOV1310
  145 DO 160 I=1,K                                                      ANOV1320
      IF(ISTEP(I)) 147, 150, 147                                        ANOV1330
  147 ISTEP(I)=0                                                        ANOV1340
      GO TO 160                                                         ANOV1350
  150 ISTEP(I)=1                                                        ANOV1360
      GO TO 120                                                         ANOV1370
  160 CONTINUE                                                          ANOV1380
  170 N=N-1                                                             ANOV1390
      WRITE (6,7) SUM,N                                                 ANOV1400
      GO TO 100                                                         ANOV1410
      END                                                               ANOV1420
```

DISCRIMINANT ANALYSIS

Problem Description

A set of linear functions is calculated from data on many groups for the purpose of classifying new individuals into one of several groups. The classification of an individual into a group is performed by evaluating each of the calculated linear functions, then finding the group for which the value is the largest.

The sample problem for discriminant analysis consists of four groups of observations as presented in Table 9. The number of observations in the first group is eight; the second group, seven; the third group, seven; and the fourth group, eight. The number of variables is six in all groups.

Program

Description

The discriminant analysis program consists of the main routine named MDISC, and three subroutines from the Scientific Subroutine Package: DMATX, MINV, and DISCR.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to five groups
2. Up to ten variables
3. Up to a total number of 250 observations in all groups combined
4. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than five groups, more than ten variables, or more than 250 observations, dimension statements in the sample

Table 9. Sample Data for Discriminant Analysis

	Observation	X_1	X_2	X_3	X_4	X_5	X_6
Group 1	1	3	10	9	8	24	8
	2	4	12	3	8	22	7
	3	9	3	2	8	9	8
	4	16	2	2	2	7	2
	5	5	10	5	8	23	9
	6	17	3	2	8	6	3
	7	2	10	9	8	29	16
	8	7	10	5	8	28	18
Group 2	1	9	10	27	8	28	16
	2	11	7	8	9	8	15
	3	8	10	2	8	27	16
	4	1	6	8	14	14	13
	5	7	8	9	6	18	2
	6	7	9	8	2	19	9
	7	7	10	5	8	27	17
Group 3	1	3	11	9	15	20	10
	2	9	4	10	7	9	9
	3	4	13	10	7	21	15
	4	8	5	16	16	16	7
	5	6	9	10	5	23	11
	6	8	10	5	8	27	16
	7	17	3	2	7	6	3
Group 4	1	3	10	8	8	23	8
	2	4	12	3	8	23	7
	3	9	3	2	8	21	7
	4	15	2	2	2	7	2
	5	9	10	26	8	27	16
	6	8	9	2	8	26	16
	7	7	8	6	9	18	2
	8	7	10	5	8	26	16

main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format statement in the sample main program must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, MDISC. This card is prepared as follows:

Columns	Contents	For Sample Problem
1- 6	Problem number (may be alphameric)	SAMPLE
7- 8	Number of groups	04
9-10	Number of variables	06
11-15	Number of observations in first group	00008
16-20	Number of observations in second group	00007
21-25	Number of observations in third group	00007
26-30	Number of observations in fourth group	00008
⋮		
65-70	Number of observations in twelfth group (if present)	

If there are more than twelve groups in the problem, continue to the second card in the same manner.

Columns	Contents
1- 5	Number of observations in thirteenth group
6-10	Number of observations in fourteenth group

Leading zeros are not required to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 9 is keypunched on a separate card using the format (12F6.0). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card.

Deck Setup

The deck setup is shown in Figure 53.

Sample

The listing of input cards for the sample problem is presented in Figure 54.

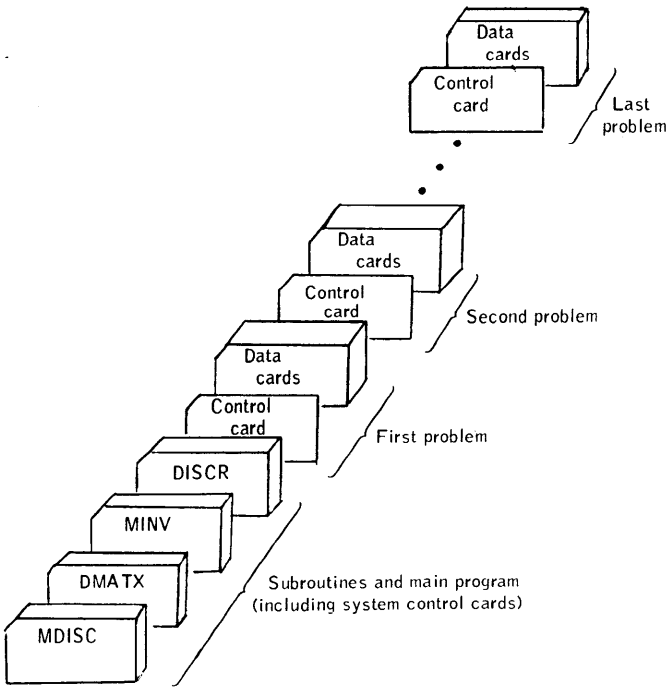


Figure 53. Deck setup (discriminant analysis)

Output

Description

The output of the sample program for discriminant analysis includes:

1. Means of variables in each group
2. Pooled dispersion matrix
3. Common means
4. Generalized Mahalanobis D-square
5. Constant and coefficients of each discriminant function
6. Probability associated with the largest discriminant function evaluated for each observation.

```
/DATA
SAMPLEC4060C0080000C70C90700008
     3    10     9     8    24     8
     4    12     3     8    22     7
     9     3     2     8     9     6
    16     2     2     2     7     2
     5    10     5     8    23     9
    17     3     2     8     6     3
     2    10     9     8    29    16
     7    10     5     8    28    18
     9    10    27     8    28    16
    11     7     8     9     8    15
     8    10     2     8    27    16
     1     6     8    14    14    13
     7     8     9     6    18     2
     7     9     8     2    19     9
     7    10     5     6    27    17
     3    11     9    15    20    10
     9     4    10     7     9     9
     4    13    10     7    21    15
     8     5    16    16    16     7
     6     9    10     5    23    11
     8    10     5     8    27    16
    17     3     2     7     6     3
     3    10     8     8    23     8
     4    12     3     8    23     7
     9     3     2     8    21     7
    15     2     2     2     7     2
     9    10    26     8    27    16
     8     9     2     8    26    16
     7     8     6     9    18     2
     7    10     5     8    26    16
```

```
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
```

Figure 54. Input listing (discriminant analysis)

Sample

The output listing for the sample problem is shown in Figure 55.

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

1. Changes in the dimension statements of the main program, MDISC:
   a. The dimension of array N must be greater than or equal to the number of groups, k. Since there are four groups in the sample problem, the value of k is 4.
   b. The dimension of array CMEAN must be greater than or equal to the number of variables, m. Since there are six variables in the sample problem, the value of m is 6.
   c. The dimension of array XBAR must be greater than or equal to the product of m times k. For the sample problem this product is 24 = 6 x 4.
   d. The dimension of array C must be greater than or equal to the product of (m+1)k. For the sample problem this product is 28 = (6+1)4.
   e. The dimension of array D must be greater than or equal to the product of m times m. For the sample problem this product is 36 = 6 x 6.
   f. The dimension of arrays P and LG must be greater than or equal to the total number of observations in all groups combined, t. For the sample problem this total is 30 = 8 + 7 + 7 + 8.

```
DISCRIMINANT ANALYSIS.....SAMPLE

 NUMBER OF GROUPS          4
 NUMBER OF VARIABLES       6
 SAMPLE SIZES..
        GROUP
          1          8
          2          7
          3          7
          4          8

GROUP  1  MEANS
        7.87500      7.50000      4.62500      7.25000     18.50000      8.87500

GROUP  2  MEANS
        7.14286      8.57143      9.57143      7.85714     20.14285     12.57143

GROUP  3  MEANS
        7.85714      7.85714      8.85714      9.28571     17.42856     10.14286

GROUP  4  MEANS
        7.75000      8.00000      6.75000      7.37500     21.37500      9.25000
```

Figure 55. Output listing (discriminant analysis)

```
POOLED DISPERSION MATRIX

ROW  1
      19.61876      -11.16208      -5.21497      -6.09890      -22.74855      -9.54052

ROW  2
     -11.16208       11.94505       5.61813       1.91758       22.60982      10.66757

ROW  3
      -5.21497        5.61813      35.45938       3.93681       16.23486       9.34546

ROW  4
      -6.09890        1.91758       3.93681       9.83310        4.62156       3.83791

ROW  5
     -22.74855       22.60982      16.23486       4.62156       62.78633      30.18262

ROW  6
      -9.54052       10.66757       9.34546       3.83791       30.18262      29.57480


COMMON MEANS
       7.66667        7.96667       7.33333       7.90000       19.39998      10.13332
GENERALIZED MAHALANOBIS D-SQUARE         12.78063


DISCRIMINANT FUNCTION  1
     CONSTANT     *   COEFFICIENTS
     -28.49431    *         2.63870       2.12205      -0.17167       1.91198       0.58476      -0.40477
DISCRIMINANT FUNCTION  2
     CONSTANT     *   COEFFICIENTS
     -29.21017    *         2.61930       2.25230      -0.04816       1.88319       0.43732      -0.21784
DISCRIMINANT FUNCTION  3
     CONSTANT     *   COEFFICIENTS
     -31.86435    *         2.74450       2.39588      -0.06457       2.13260       0.42619      -0.32718
DISCRIMINANT FUNCTION  4
     CONSTANT     *   COEFFICIENTS
     -30.82028    *         2.71860       2.63937      -0.13352       1.94539       0.71677      -0.48760


EVALUATION OF CLASSIFICATION FUNCTIONS FOR EACH OBSERVATION

GROUP  1
 OBSERVATION   PROBABILITY ASSOCIATED WITH LARGEST DISCRIMINANT FUNCTION   LARGEST FUNCTION NO.
      1                    0.38065                                          4
      2                    0.37045                                          1
      3                    0.36261                                          1
      4                    0.44190                                          1
      5                    0.34454                                          1
      6                    0.44215                                          3
      7                    0.31787                                          2
      8                    0.29274                                          2

GROUP  2
 OBSERVATION   PROBABILITY ASSOCIATED WITH LARGEST DISCRIMINANT FUNCTION   LARGEST FUNCTION NO.
      1                    0.51029                                          2
      2                    0.50060                                          3
      3                    0.34760                                          4
      4                    0.43130                                          3
      5                    0.44282                                          4
      6                    0.36467                                          2
      7                    0.28515                                          2

GROUP  3
 OBSERVATION   PROBABILITY ASSOCIATED WITH LARGEST DISCRIMINANT FUNCTION   LARGEST FUNCTION NO.
      1                    0.47611                                          3
      2                    0.44629                                          2
      3                    0.54636                                          2
      4                    0.46688                                          3
      5                    0.30600                                          2
      6                    0.33043                                          4
      7                    0.39005                                          3

GROUP  4
 OBSERVATION   PROBABILITY ASSOCIATED WITH LARGEST DISCRIMINANT FUNCTION   LARGEST FUNCTION NO.
      1                    0.33727                                          4
      2                    0.37475                                          1
      3                    0.42340                                          4
      4                    0.45697                                          1
      5                    0.52175                                          2
      6                    0.34061                                          4
      7                    0.43135                                          4
      8                    0.27849                                          1
```

Figure 55. Output listing (discriminant analysis) (Continued)

g. The dimension of array X must be greater than or equal to the total number of data points that is equal to the product of t times m. For the sample this product is 180 = 30 x 6.

2. Changes in the input format statement of the main program, MDISC:

Only the format statement for input data may be changed. Since sample data are either one- or two-digit numbers, rather than using six-column fields as in the sample problem, each row of data may be keypunched in two-column fields, and, if so, the format is changed to (6F2.0). This format assumes six 2-column fields per card, beginning in column 1.

Operating Instructions

The sample program for discriminant analysis is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 30 seconds.

```
C                                                                       MDIS  10
C     ..................................................................MDIS  20
C                                                                       MDIS  30
C        SAMPLE MAIN PROGRAM FOR DISCRIMINANT ANALYSIS - MDISC          MDIS  40
C                                                                       MDIS  50
C        PURPOSE                                                        MDIS  60
C           (1) READ THE PROBLEM PARAMETER CARD AND DATA FOR DISCRIMI-  MDIS  70
C           NANT ANALYSIS, (2) CALL THREE SUBROUTINES TO CALCULATE VARI-MDIS  80
C           ABLE MEANS IN EACH GROUP, POOLED DISPERSION MATRIX, COMMON  MDIS  90
C           MEANS OF VARIABLES, GENERALIZED MAHALANOBIS D SQUARE,       MDIS 100
C           COEFFICIENTS OF DISCRIMINANT FUNCTIONS, AND PROBABILITY     MDIS 110
C           ASSOCIATED WITH LARGEST DISCRIMINANT FUNCTION OF EACH       MDIS 120
C           CASE IN EACH GROUP, AND (3) PRINT THE RESULTS.              MDIS 130
C                                                                       MDIS 140
C        REMARKS                                                        MDIS 150
C           THE NUMBER OF VARIABLES MUST BE GREATER THAN OR EQUAL TO    MDIS 160
C           THE NUMBER OF GROUPS.                                       MDIS 170
C                                                                       MDIS 180
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MDIS 190
C           DMATX                                                       MDIS 200
C           MINV                                                        MDIS 210
C           DISCR                                                       MDIS 220
C                                                                       MDIS 230
C        METHOD                                                         MDIS 240
C           REFER TO '360 COMPUTER PROGRAMS MANUAL', EDITED BY W. J.    MDIS 250
C           DIXON, UCLA, 1964, AND T. W. ANDERSON, 'INTRODUCTION TO     MDIS 260
C           MULTIVARIATE STATISTICAL ANALYSIS', JOHN WILEY AND SONS,    MDIS 270
C           1958, SECTION 6.6-6.8.                                      MDIS 280
C                                                                       MDIS 290
C     ..................................................................MDIS 300
C                                                                       MDIS 310
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MDIS 320
C     NUMBER OF GROUPS, K..                                             MDIS 330
C                                                                       MDIS 340
      DIMENSION N(5)                                                    MDIS 350
C                                                                       MDIS 360
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MDIS 370
C     NUMBER OF VARIABLES, M..                                          MDIS 380
C                                                                       MDIS 390
      DIMENSION GMEAN(10)                                               MDIS 400
C                                                                       MDIS 410
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MDIS 420
C     PRODUCT OF M*K..                                                  MDIS 430
C                                                                       MDIS 440
      DIMENSION XBAR(50)                                                MDIS 450
C                                                                       MDIS 460
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MDIS 470
C     PRODUCT OF (M+1)*K..                                              MDIS 480
C                                                                       MDIS 490
      DIMENSION C(55)                                                   MDIS 500
C                                                                       MDIS 510
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MDIS 520
C     PRODUCT OF M*M..                                                  MDIS 530
C                                                                       MDIS 540
      DIMENSION D(100)                                                  MDIS 550
C                                                                       MDIS 560
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE     MDIS 570
C     TOTAL OF SAMPLE SIZES OF K GROUPS COMBINED, T (T = N(1)+N(2)+...  MDIS 580
C     +N(K))..                                                          MDIS 590
C                                                                       MDIS 600
      DIMENSION P(250),LG(250)                                          MDIS 610
C                                                                       MDIS 620
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      MDIS 630
C     TOTAL DATA POINTS WHICH IS EQUAL TO THE PRODUCT OF T*M..          MDIS 640
C                                                                       MDIS 650
      DIMENSION X(2500)                                                 MDIS 660
C                                                                       MDIS 670
C     ..................................................................MDIS 680
C                                                                       MDIS 690
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  MDIS 700
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      MDIS 710
C        STATEMENT WHICH FOLLOWS.                                       MDIS 720
C                                                                       MDIS 730
C     DOUBLE PRECISION GMEAN,XBAR,D,DET,C,V,P                           MDIS 740
C                                                                       MDIS 750
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    MDIS 760
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      MDIS 770
C        ROUTINE.                                                       MDIS 780
C                                                                       MDIS 790
C        ...............................................................MDIS 800
C                                                                       MDIS 810
    1 FORMAT(A4,A2,2I2,12I5/(14I5))                                     MDIS 820
    2 FORMAT(27H1DISCRIMINANT ANALYSIS.....,A4,A2/19H0  NUMBER OF GROUPSMDIS 830
     1,7X,I3/22H   NUMBER OF VARIABLES,I7/17H   SAMPLE SIZES../12X,5HGROMDIS 840
     2UP)                                                               MDIS 850
    3 FORMAT(12X,I3,8X,I4)                                              MDIS 860
    4 FORMAT(1H0)                                                       MDIS 870
    5 FORMAT(12F6.0)                                                    MDIS 880
    6 FORMAT(6H0GROUP,I3,7H  MEANS/(8F15.5))                            MDIS 890
    7 FORMAT(1H0/25H POOLED DISPERSION MATRIX)                          MDIS 900
    8 FORMAT(4HOROW,I3/(8F15.5))                                        MDIS 910
    9 FORMAT(1H0//13H COMMON MEANS/(8F15.5))                            MDIS 920
   10 FORMAT(1H///33H GENERALIZED MAHALANOBIS D-SQUARE,F15.5//)         MDIS 930
   11 FORMAT(22H0DISCRIMINANT FUNCTION,I3/1H ,6X,27HCONSTANT   *  COEFFMDIS 940
     1ICIENTS/1H F14.5,7H   *   ,7F14.5/(22X,7F14.5))                  MDIS 950
   12 FORMAT(1H0//60H EVALUATION OF CLASSIFICATION FUNCTIONS FOR EACH OBMDIS 960
     1SERVATION)                                                        MDIS 970
   13 FORMAT(6H0GROUP,I3/19X,27HPROBABILITY ASSOCIATED WITH,11X,7HLARGESMDIS 980
     1T/13H  OBSERVATION,5X,29HLARGEST DISCRIMINANT FUNCTION,8X,12HFUNCTMDIS 990
     2ION NO.)                                                          MDIS1000
   14 FORMAT(1H ,I7,20X,F8.5,20X,I6)                                    MDIS1010
C                                                                       MDIS1020
C     ..................................................................MDIS1030
C                                                                       MDIS1040
C     READ PROBLEM PARAMETER CARD                                       MDIS1050
C                                                                       MDIS1060
  100 READ (5,1) PR,PRL,K,M,(N(I),I=1,K)                                MDIS1070
C        PR.......PROBLEM NUMBER (MAY BE ALPHAMERIC)                    MDIS1080
C        PRL.....PROBLEM NUMBER (CONTINUED)                             MDIS1090
C        K........NUMBER OF GROUPS                                      MDIS1100
```

```
C        M.....NUMBER OF VARIABLES                                      MDIS1110
C        N.....VECTOR OF LENGTH < CONTAINING SAMPLE SIZES               MDIS1120
C                                                                       MDIS1130
      WRITE (6,2) PR,PRI,K,M                                            MDIS1140
      DO 110 I=1,K                                                      MDIS1150
  110 WRITE (6,3) I,N(I)                                                MDIS1160
      WRITE (6,4)                                                       MDIS1170
C                                                                       MDIS1180
C     READ DATA                                                         MDIS1190
C                                                                       MDIS1200
      L=0                                                               MDIS1210
      DO 130 I=1,K                                                      MDIS1220
      N1=N(I)                                                           MDIS1230
      DO 120 J=1,N1                                                     MDIS1240
      READ (5,5) (CMEAN(IJ),IJ=1,M)                                     MDIS1250
      L=L+1                                                             MDIS1260
      N2=L-N1                                                           MDIS1270
      DO 120 IJ=1,M                                                     MDIS1280
      N2=N2+N1                                                          MDIS1290
  120 X(N2)=CMEAN(IJ)                                                   MDIS1300
  130 L=N2                                                              MDIS1310
C                                                                       MDIS1320
      CALL DMATX (K,M,N,X,XBAR,D,CMEAN)                                 MDIS1330
C                                                                       MDIS1340
C     PRINT MEANS AND POOLED DISPERSION MATRIX                          MDIS1350
C                                                                       MDIS1360
      L=0                                                               MDIS1370
      DO 150 I=1,K                                                      MDIS1380
      DO 140 J=1,M                                                      MDIS1390
      L=L+1                                                             MDIS1400
  140 CMEAN(J)=XBAR(L)                                                  MDIS1410
  150 WRITE (6,6) I,(CMEAN(J),J=1,M)                                    MDIS1420
      WRITE (6,7)                                                       MDIS1430
      DO 170 I=1,M                                                      MDIS1440
      L=I-M                                                             MDIS1450
      DO 160 J=1,M                                                      MDIS1460
      L=L+M                                                             MDIS1470
  160 CMEAN(J)=D(L)                                                     MDIS1480
  170 WRITE (6,8) I,(CMEAN(J),J=1,M)                                    MDIS1490
C                                                                       MDIS1500
      CALL MINV (D,M,DET,CMEAN,C)                                       MDIS1510
C                                                                       MDIS1520
      CALL DISCR (K,M,N,X,XBAR,D,CMEAN,V,C,P,LG)                        MDIS1530
C                                                                       MDIS1540
C     PRINT COMMON MEANS                                                MDIS1550
C                                                                       MDIS1560
      WRITE (6,9) (CMEAN(I),I=1,M)                                      MDIS1570
C                                                                       MDIS1580
C     PRINT GENERALIZED MAHALANOBIS D-SQUARE                            MDIS1590
C                                                                       MDIS1600
      WRITE (6,10) V                                                    MDIS1610
C                                                                       MDIS1620
C     PRINT CONSTANTS AND COEFFICIENTS OF DISCRIMINANT FUNCTIONS        MDIS1630
C                                                                       MDIS1640
      N1=1                                                              MDIS1650
      N2=M+1                                                            MDIS1660
      DO 180 I=1,K                                                      MDIS1670
      WRITE (6,11) I,(C(J),J=N1,N2)                                     MDIS1680
      N1=N1+(M+1)                                                       MDIS1690
  180 N2=N2+(M+1)                                                       MDIS1700
C                                                                       MDIS1710
C     PRINT EVALUATION OF CLASSIFICATION FUNCTIONS FOR EACH OBSERVATION MDIS1720
C                                                                       MDIS1730
      WRITE (6,12)                                                      MDIS1740
      N1=1                                                              MDIS1750
      N2=N(1)                                                           MDIS1760
      DO 210 I=1,K                                                      MDIS1770
      WRITE (6,13) I                                                    MDIS1780
      L=0                                                               MDIS1790
      DO 190 J=N1,N2                                                    MDIS1800
      L=L+1                                                             MDIS1810
  190 WRITE (6,14) L,P(J),LG(J)                                         MDIS1820
      IF(I-K) 200, 100, 100                                             MDIS1830
  200 N1=N1+N(I)                                                        MDIS1840
      N2=N2+N(I+1)                                                      MDIS1850
  210 CONTINUE                                                          MDIS1860
      END                                                               MDIS1870
```

FACTOR ANALYSIS

Problem Description

A principal component solution and the varimax rotation of the factor matrix are performed. Principal component analysis is used to determine the minimum number of independent dimensions needed to account for most of the variance in the original set of variables. The varimax rotation is used to simplify columns (factors) rather than rows (variables) of the factor matrix.

The sample problem for factor analysis consists of 23 observations with nine variables as presented in Table 10. In order to keep the number of independent dimensions as small as possible, only those eigenvalues (of correlation coefficients) greater than or equal to 1.0 are retained in the analysis.

Table 10. Sample Data for Factor Analysis

Observation	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9
1	7	7	9	7	15	36	60	15	24
2	13	18	25	15	13	35	61	18	30
3	9	18	24	23	12	43	62	14	31
4	7	13	25	36	11	12	63	26	32
5	6	8	20	7	15	46	18	28	15
6	10	12	30	11	10	42	27	12	17
7	7	6	11	7	15	35	60	20	25
8	16	19	25	16	13	30	64	20	30
9	9	22	26	24	13	40	66	15	32
10	8	15	26	30	13	10	66	25	34
11	8	10	20	8	17	40	20	30	18
12	9	12	28	11	8	45	30	15	19
13	11	17	21	30	10	45	60	17	30
14	9	16	26	27	14	31	59	19	17
15	10	15	24	18	12	29	48	18	26
16	11	11	30	19	19	26	57	20	30
17	16	9	16	20	18	31	60	21	17
18	9	8	19	14	16	33	67	9	19
19	7	18	22	9	15	37	62	11	20
20	8	11	23	18	9	36	61	22	24
21	6	6	27	23	7	40	55	24	31
22	10	9	26	26	10	37	57	27	29
23	8	10	26	15	11	42	59	20	28

Program

Description

The factor analysis program consists of the main routine named FACTO, a special input subroutine named DATA, and five subroutines from the Scientific Subroutine Package: CORRE, EIGEN, TRACE, LOAD, and VARMX.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 35 variables
2. Up to 99,999 observations
3. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions it is not necessary to modify the sample program. However, if there are more than 35 variables, dimension statements in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format statement in the input subroutine, DATA, must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, FACTO. This card is prepared as follows:

Columns	Contents	For Sample Problem
1- 6	Problem number (may be alphameric)	SAMPLE
7-11	Number of observations	00023
12-13	Number of variables	09
14-19	Value used to limit the number of eigenvalues of correlation coefficients. Only those eigenvalues greater than or equal to this value are retained in the analysis. (A decimal point must be specified.)	0001.0

Leading zeros are not required to be keypunched.

Data Cards

Since input data are read into the computer one observation at a time, each row of data in Table 10 is keypunched on a separate card using the format (12F6.0). This format assumes twelve 6-column fields per card.

If there are more than twelve variables in a problem, each row of data is continued on the second and third cards until the last data point is keypunched. However, each row of data must begin on a new card.

Deck Setup

The deck setup is shown in Figure 56.

Sample

The listing of input cards for the sample problem is presented in Figure 57.

Output

Description

The output of the sample program for factor analysis includes:

1. Means
2. Standard deviations
3. Correlation coefficients
4. Eigenvalues
5. Cumulative percentage of eigenvalues
6. Eigenvectors
7. Factor matrix
8. Variance of the factor matrix for each iteration cycle

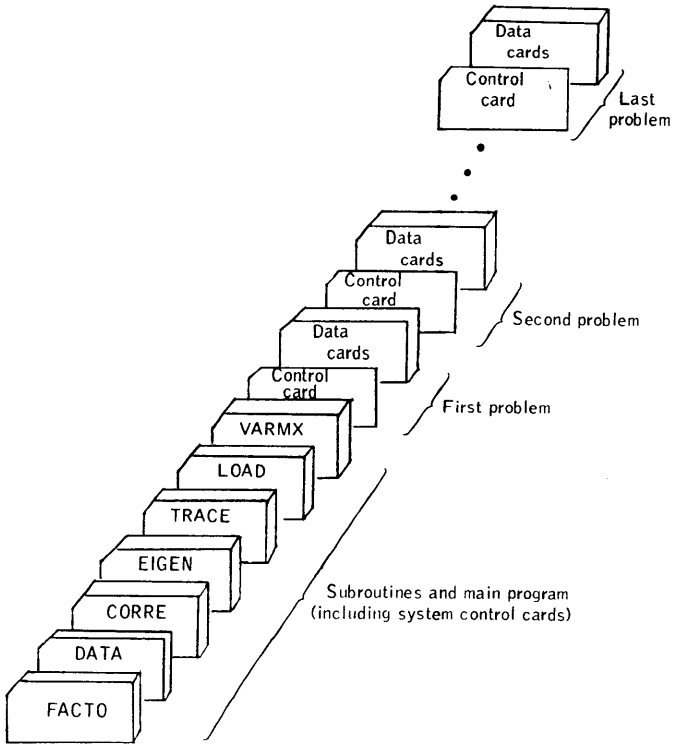


Figure 56. Deck setup (factor analysis)

9. Rotated factor matrix
10. Check on communalities

Sample

The output listing for the sample problem is shown in Figure 58.

Program Modification

Program capacity can be increased or decreased by making changes in dimension statements. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the

```
/DATA                                                                  10
SAMPLEC0G23090001.0                                                    20
   7   7   9   7  15  36  60  15  24                                   30
  13  18  25  15  13  35  61  18  30                                   40
   9  18  24  23  12  43  62  14  31                                   50
   7  13  25  36  11  12  63  26  32                                   60
   6   8  20   7  15  46  18  28  15                                   70
  10  12  30  11  10  42  27  12  17                                   80
   7   6  11   7  15  35  60  20  25                                   90
  16  19  25  16  13  30  64  20  30                                  100
   9  22  26  24  13  40  66  15  32                                  110
   8  15  26  30  13  10  66  25  34                                  120
   9  10  20   8  17  40  20  30  18                                  130
   9  12  28  11   8  45  30  15  19                                  140
  11  17  21  30  10  45  60  17  30                                  150
   9  16  26  27  14  31  59  19  17                                  160
  10  15  24  18  12  29  48  18  26                                  170
  11  11  30  19  19  26  57  20  30                                  180
  16   9  16  20  18  31  60  21  17                                  190
   9   8  19  14  16  33  67   9  19                                  200
   7  18  22   9  15  37  62  11  20                                  210
   8  11  23  18   9  36  61  22  24                                  220
   6   6  27  23   7  40  55  24  31                                  230
  10   9  26  26  10  37  57  27  29                                  240
   8  10  26  15  11  42  59  20  28                                  250
```

Figure 57. Input listing (factor analysis)

```
FACTOR ANALYSIS.....SAMPLE

  NO. OF CASES        73
  NO. OF VARIABLES     9

MEANS
      9.30435      12.60870      73.00000      14.00000      12.86957      34.82609      44.00000      13.
     25.13043

STANDARD DEVIATIONS
      2.70417       4.59978       5.33427       8.33333       3.13741       9.29149      14.87824      7.
      6.09249

CORRELATION COEFFICIENTS

ROW  1
    1.00000     0.34987     0.11975     0.12102     0.21917    -0.09549     0.20901    -0.12908     0.05818

ROW  2
    0.34987     1.00000     0.41311     0.35572    -0.08243    -0.09100     0.29622    -0.32044     0.35387

ROW  3
    0.11975     0.41311     1.00000     0.41512    -0.43179    -0.08346    -0.10252     0.03215     0.27833

ROW  4
    0.12102     0.35572     0.41512     1.00000    -0.31288    -0.50365     0.49856     0.22539     0.59890

ROW  5
    0.21917    -0.08243    -0.43179    -0.31288     1.00000    -0.23000     0.03310    -0.00475    -0.30341

ROW  6
   -0.09549    -0.09100    -0.08346    -0.50365    -0.23000     1.00000    -0.44520    -0.25441    -0.37456

ROW  7
    0.20901     0.29622    -0.10252     0.49856     0.03310    -0.44520     1.00000    -0.28050     0.60124

ROW  8
   -0.12908    -0.32044     0.03215     0.22539    -0.00475    -0.25441    -0.28050     1.00000     0.13516

ROW  9
    0.05818     0.35387     0.27833     0.59890    -0.30341    -0.37456     0.60124     0.13516     1.00000

EIGENVALUES
    2.94988     1.64368     1.55514     1.06579

CUMULATIVE PERCENTAGE OF EIGENVALUES
    0.32776     0.51040     0.68319     0.80161

EIGENVECTORS

VECTOR  1
    0.16437     0.34836     0.28797     0.49661    -0.16806    -0.32922     0.39935     0.01287     0.47518

VECTOR  2
    0.34837     0.06552    -0.44647    -0.11893     0.61210    -0.26428     0.38860    -0.24845    -0.06014

VECTOR  3
   -0.29899    -0.46825    -0.23534     0.17377     0.14468    -0.43545     0.01881     0.61587     0.12470

VECTOR  4
    0.54441     0.16909     0.38288     0.04163     0.30537    -0.16163    -0.43410     0.40283    -0.23789

FACTOR MATRIX (  4 FACTORS)

VARIABLE  1
    0.28232     0.44663    -0.37286     0.56203

VARIABLE  2
    0.59831     0.08400    -0.58394     0.17457

VARIABLE  3
    0.49460    -0.57240    -0.29348     0.39528

VARIABLE  4
    0.85293    -0.15248     0.21671     0.04297

VARIABLE  5
   -0.28865     0.78475     0.18043     0.31525

VARIABLE  6
   -0.56544    -0.33482    -0.54303    -0.16686

VARIABLE  7
    0.68590     0.49821     0.02345    -0.44816

VARIABLE  8
    0.02711    -0.31853     0.76802     0.41587

VARIABLE  9
    0.81614    -0.07710     0.15551    -0.24559

ITERATION       VARIANCES
  CYCLE
     0          0.211288
     1          0.336137
     2          0.397022
     3          0.403005
     4          0.405177
     5          0.405528
     6          0.405581
     7          0.405587
     8          0.405588
     9          0.405587
    10          0.405587
    11          0.405587
    12          0.405587

ROTATED FACTOR MATRIX (  4 FACTORS)

VARIABLE  1
    0.05498     0.07183    -0.05578     0.85017

VARIABLE  2
    0.29329    -0.39653    -0.35581     0.60549

VARIABLE  3
    0.05114    -0.82493     0.15068     0.32984

VARIABLE  4
    0.74040    -0.41401     0.24579     0.13972

VARIABLE  5
   -0.09091     0.83662     0.13525     0.39229
```

Figure 58. Output listing (factor analysis)

```
VARIABLE  6
   -0.68286     -0.21579     -0.44983     -0.20503

VARIABLE  7
    0.88997      0.19299     -0.34918      0.08830

VARIABLE  8
    0.03602     -0.05500      0.91375     -0.15962

VARIABLE  9
    0.80511     -0.32759      0.00994     -0.02380

CHECK ON COMMUNALITIES

VARIABLE        ORIGINAL            FINAL          DIFFERENCE
    1            0.73409            0.73408          0.00001
    2            0.73645            0.73647          0.00001
    3            0.81464            0.81463          0.00001
    4            0.79955            0.79954          0.00001
    5            0.83109            0.83108          0.00001
    6            0.75725            0.75724          0.00001
    7            0.92006            0.92005          0.00001
    8            0.86476            0.86475          0.00001
    9            0.75652            0.75651          0.00001

LE0031217
```

Figure 58. Output listing (factor analysis) (Continued)

following general rules are supplied in terms of the sample problem.

1. Changes in the dimension statements of the main program, FACTO:

   a. The dimension of arrays B, D, S, T, and XBAR must be greater than or equal to the number of variables, m. Since there are nine variables in the sample problem, the value of m is 9.

   b. The dimension of array V must be greater than or equal to the product of m times m. For the sample problem this product is 81 = 9 x 9.

   c. The dimension of array R must be greater than $\frac{(m+1)m}{2}$. For the sample problem, this number is $45 = \frac{(9+1)9}{2}$.

2. Changes in the input format statement of the special input subroutine, DATA:

   Only the format statement for input data may be changed. Since sample data are either one- or two-digit numbers, rather than using six-column fields as in the sample problem, each row of data may be keypunched in two-column fields, and, if so, the format is changed to (9F2.0). This format assumes nine 2-column fields per card, beginning in column 1.

   The special input subroutine, DATA, is normally written by the user to handle different formats for different problems. The user may modify this subroutine to perform testing of input data, transformation of data, and so on.

Operating Instructions

The sample program for factor analysis is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Error Messages

If the number of factors to be rotated is one or zero, the following message will be printed:

ONLY____FACTOR RETAINED. NO ROTATION.

The program skips rotation and goes to the next problem if it is present.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 50 seconds.

```
C                                                                       FCTO  10
C     ..................................................................FCTO  20
C                                                                       FCTO  30
C        SAMPLE MAIN PROGRAM FOR FACTOR ANALYSIS - FACTO                FCTO  40
C                                                                       FCTO  50
C        PURPOSE                                                        FCTO  60
C           (1) READ THE PROBLEM PARAMETER CARD, (2) CALL FIVE SUBROU-  FCTO  70
C           TINES TO PERFORM A PRINCIPAL COMPONENT SOLUTION AND THE     FCTO  80
C           VARIMAX ROTATION OF A FACTOR MATRIX, AND (3) PRINT THE      FCTO  90
C           RESULTS.                                                    FCTO 100
C                                                                       FCTO 110
C        REMARKS                                                        FCTO 120
C           NONE                                                        FCTO 130
C                                                                       FCTO 140
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FCTO 150
C           CORRE  (WHICH, IN TURN, CALLS THE SUBROUTINE NAMED DATA.)   FCTO 160
C           EIGEN                                                       FCTO 170
C           TRACE                                                       FCTO 180
C           LOAD                                                        FCTO 190
C           VARMX                                                       FCTO 200
C                                                                       FCTO 210
C        METHOD                                                         FCTO 220
C           REFER TO 'BMD COMPUTER PROGRAMS MANUAL', EDITED BY W. J.    FCTO 230
C           DIXON, UCLA, 1964.                                          FCTO 240
C                                                                       FCTO 250
C     ..................................................................FCTO 260
C                                                                       FCTO 270
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE     FCTO 280
C     NUMBER OF VARIABLES, M..                                          FCTO 290
C                                                                       FCTO 300
      DIMENSION B(35),D(35),S(35),T(35),XBAR(35)                        FCTO 310
C                                                                       FCTO 320
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      FCTO 330
C     PRODUCT OF M*M..                                                  FCTO 340
C                                                                       FCTO 350
      DIMENSION V(1225)                                                 FCTO 360
C                                                                       FCTO 370
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO          FCTO 380
C     (M+1)*M/2..                                                       FCTO 390
C                                                                       FCTO 400
      DIMENSION R(630)                                                  FCTO 410
C                                                                       FCTO 420
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 51..     FCTO 430
C                                                                       FCTO 440
      DIMENSION TV(51)                                                  FCTO 450
C                                                                       FCTO 460
C     ..................................................................FCTO 470
C                                                                       FCTO 480
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  FCTO 490
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      FCTO 500
C        STATEMENT WHICH FOLLOWS.                                       FCTO 510
C                                                                       FCTO 520
C     DOUBLE PRECISION XBAR,S,V,R,D,B,T,TV                              FCTO 530
C                                                                       FCTO 540
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    FCTO 550
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      FCTO 560
C        ROUTINE.                                                       FCTO 570
C                                                                       FCTO 580
C     ..................................................................FCTO 590
C                                                                       FCTO 600
    1 FORMAT(21H1FACTOR ANALYSIS.....A4,A2//3X,12HNO. OF CASES,4X,I6/3X,FCTO 610
     116HNO. OF VARIABLES,I6/)                                          FCTO 620
    2 FORMAT(6HOMEANS/(8F15.5))                                         FCTO 630
    3 FORMAT(2CHOSTANDARD DEVIATIONS/(8F15.5))                          FCTO 640
    4 FORMAT(25HOCORRELATION COEFFICIENTS)                              FCTO 650
    5 FORMAT(4HOROW I3/(10F12.5))                                       FCTO 660
    6 FORMAT(1HO/12H EIGENVALUES/(10F12.5))                             FCTO 670
    7 FORMAT(37HOCUMULATIVE PERCENTAGE OF EIGENVALUES/(10F12.5))        FCTO 680
    8 FORMAT(1HO/13H EIGENVECTORS)                                      FCTO 690
    9 FORMAT(7HOVECTOR I3/(10F12.5))                                    FCTO 700
   10 FORMAT(1HO/16H FACTOR MATRIX (,I3,9H FACTORS))                    FCTO 710
   11 FORMAT(9HOVARIABLE I3/(10F12.5))                                  FCTO 720
   12 FORMAT(1HO/1CH ITERATION,7X,9HVARIANCES/8H   CYCLE)               FCTO 730
   13 FORMAT(I6,F2C.6)                                                  FCTO 740
   14 FORMAT(1HO/24H ROTATED FACTOR MATRIX (I3,9H FACTORS))             FCTO 750
   15 FORMAT(9HOVARIABLE I3/(10F12.5))                                  FCTO 760
   16 FORMAT(1HO/23H CHECK ON COMMUNALITIES//9H VARIABLE,7X,8HORIGINAL,1FCTO 770
     12X,5HFINAL,10X,10HDIFFERENCE)                                     FCTO 780
   17 FORMAT(I6,3F18,5)                                                 FCTO 790
   18 FORMAT(A4,A2,I5,I2,F6.C)                                          FCTO 800
   19 FORMAT(5HOONLY,I2,30H FACTOR RETAINED.  NO ROTATION)              FCTO 810
C                                                                       FCTO 820
C     ..................................................................FCTO 830
C                                                                       FCTO 840
C     READ PROBLEM PARAMETER CARD                                       FCTO 850
C                                                                       FCTO 860
  100 READ (5,18) PR,PR1,N,M,CON                                        FCTO 870
C        PR.........PROBLEM NUMBER (MAY BE ALPHAMERIC)                  FCTO 880
C        PR1........PROBLEM NUMBER (CONTINUED)                          FCTO 890
C        N..........NUMBER OF CASES                                     FCTO 900
C        M..........NUMBER OF VARIABLES                                 FCTO 910
C        CON........CONSTANT USED TO DECIDE HOW MANY EIGENVALUES        FCTO 920
C                   TO RETAIN                                           FCTO 930
C                                                                       FCTO 940
      WRITE (6,1) PR,PR1,N,M                                            FCTO 950
C                                                                       FCTO 960
```

```
      IO=0                                                              FCTO 970
      X=0.0                                                             FCTO 980
C                                                                       FCTO 990
      CALL CORRE (N,M,IO,X,XBAR,S,V,R,D,B,T)                            FCT01000
C                                                                       FCT01010
C     PRINT MEANS                                                       FCT01020
C                                                                       FCT01030
      WRITE (6,2) (XBAR(J),J=1,M)                                       FCT01040
C                                                                       FCT01050
C     PRINT STANDARD DEVIATIONS                                         FCT01060
C                                                                       FCT01070
      WRITE (6,3) (S(J),J=1,M)                                          FCT01080
C                                                                       FCT01090
C     PRINT CORRELATION COEFFICIENTS                                    FCT01100
C                                                                       FCT01110
      WRITE (6,4)                                                       FCT01120
      DO 120 I=1,M                                                      FCT01130
      DO 110 J=1,M                                                      FCT01140
      IF(I-J) 102, 104, 104                                             FCT01150
  102 L=I+(J*J-J)/2                                                     FCT01160
      GO TO 110                                                         FCT01170
  104 L=J+(I*I-I)/2                                                     FCT01180
  110 D(J)=R(L)                                                         FCT01190
  120 WRITE (6,5) I,(D(J),J=1,M)                                        FCT01200
C                                                                       FCT01210
      MV=0                                                              FCT01220
      CALL EIGEN (R,V,M,MV)                                             FCT01230
C                                                                       FCT01240
      CALL TRACE (M,R,CON,K,D)                                          FCT01250
C                                                                       FCT01260
C     PRINT EIGENVALUES                                                 FCT01270
C                                                                       FCT01280
      DO 130 I=1,K                                                      FCT01290
      L=I+(I*I-I)/2                                                     FCT01300
  130 S(I)=R(L)                                                         FCT01310
      WRITE (6,6) (S(J),J=1,K)                                          FCT01320
C                                                                       FCT01330
C     PRINT CUMULATIVE PERCENTAGE OF EIGENVALUES                        FCT01340
C                                                                       FCT01350
      WRITE (6,7) (D(J),J=1,K)                                          FCT01360
C                                                                       FCT01370
C     PRINT EIGENVECTORS                                                FCT01380
C                                                                       FCT01390
      WRITE (6,8)                                                       FCT01400
      L=0                                                               FCT01410
      DO 150 J=1,K                                                      FCT01420
      DO 140 I=1,M                                                      FCT01430
      L=L+1                                                             FCT01440
  140 D(I)=V(L)                                                         FCT01450
  150 WRITE (6,9) J,(D(I),I=1,M)                                        FCT01460
C                                                                       FCT01470
      CALL LOAD (M,K,R,V)                                               FCT01480
C                                                                       FCT01490
C     PRINT FACTOR MATRIX                                               FCT01500
C                                                                       FCT01510
      WRITE (6,10) K                                                    FCT01520
      DO 180 I=1,M                                                      FCT01530
      DO 170 J=1,K                                                      FCT01540
      L=M*(J-1)+I                                                       FCT01550
  170 D(J)=V(L)                                                         FCT01560
  180 WRITE (6,11) I,(D(J),J=1,K)                                       FCT01570
C                                                                       FCT01580
      IF(K-1) 185, 185, 188                                             FCT01590
  185 WRITE (6,19) K                                                    FCT01600
      GO TO 100                                                         FCT01610
C                                                                       FCT01620
  188 CALL VARMX (M,K,V,NC,TV,B,T,D)                                    FCT01630
C                                                                       FCT01640
C     PRINT VARIANCES                                                   FCT01650
C                                                                       FCT01660
      NV=NC+1                                                           FCT01670
      WRITE (6,12)                                                      FCT01680
      DO 190 I=1,NV                                                     FCT01690
      NC=I-1                                                            FCT01700
  190 WRITE (6,13) NC,TV(I)                                             FCT01710
C                                                                       FCT01720
C     PRINT ROTATED FACTOR MATRIX                                       FCT01730
C                                                                       FCT01740
      WRITE (6,14) K                                                    FCT01750
      DO 220 I=1,M                                                      FCT01760
      DO 210 J=1,K                                                      FCT01770
      L=M*(J-1)+I                                                       FCT01780
  210 S(J)=V(L)                                                         FCT01790
  220 WRITE (6,15) I,(S(J),J=1,K)                                       FCT01800
C                                                                       FCT01810
C     PRINT COMMUNALITIES                                               FCT01820
C                                                                       FCT01830
      WRITE (6,16)                                                      FCT01840
      DO 230 I=1,M                                                      FCT01850
  230 WRITE (6,17) I,B(I),T(I),D(I)                                     FCT01860
      GO TO 100                                                         FCT01870
      END                                                               FCT01880
```

KOLMOGOROV - SMIRNOV TEST

Problem Description

This program is concerned with the problem of determining (a) from what probability density function a particular sample is drawn, or (b) whether two different samples were drawn from the same population. In other words, in the one sample case, the actual distribution function of the sample is compared with one or more theoretical distribution functions, which may be normal, and/or exponential, and/or Cauchy, and/or uniform, and/or a user-specified distribution. In the two-sample case, the pair of sample (actual) distribution functions are compared with one another.

From the above comparisons, a statistic is derived. In the one sample case, this statistic evaluates the probability that the statistic will be as great as or greater than its current value, if the hypothesis that the actual (sample) and the theoretical distribution functions are equal is correct. In other words, if the probability is determined to be 0.40, for example, rejecting the hypothesis of equality of the distribution functions will be an incorrect action 40 times out of 100. Similarly, in the two-sample case, the hypothesis being tested is the equality of the two actual (sample) distribution functions.

This probability is calculated using asymptotic formulas. This means that the sample sizes involved should be large. Sizes greater than 100 are suggested by the literature. In this connection, the remarks given under the topic "Subroutine SMIRN" should be considered.

Note also that added problems arise when, in the one sample case, the parameters of the continuous distribution in question are estimated from the sample. Lilliefors discusses these problems (see reference given in KOLMO description).

Program

Description

This program consists of the main routine KOLM, and four subroutines from the Scientific Subroutine Package: KOLMO, KOLM2, SMIRN, and NDTR.

Capacity

This program allows up to two samples each with 500 or fewer observations to be examined. If the user desires to modify this program to handle more observations, the instructions given below under "Program Modification" should be followed.

Input

After two initializing cards (1, 2 below) each job consists of two control cards and the data cards (3-5 below).

1. Initializing card (minus signs in cc 1-4)
2. Names of distribution functions (as supplied, these are the normal, exponential, Cauchy, uniform, and user's pdf). These names are punched in the order given, centrally located in 16 digit fields on one card; that is, "normal" is punched in cc 1-16, "exponential" in cc 17-32, and so on.
3. Job control card (minus signs in cc 1-4)
4. Program control card

Each job requires one program control card, defined below:

Columns	Contents	For Sample Problems
1 - 20	Title (alphameric)	Uniform test (Job 1) Uniform-Gauss Test (job 2)
21	1 -- one-sample test	1 (job 1)
	2 -- two-sample test	2 (job 2)
22	Leave blank for one-sample test.	0 (job 1) 1 (job 2)
	0 -- Read both samples (two-sample tests).	
	1 -- Read only one sample and compare it with the first sample read on preceding job.	
23	0 -- Do not print the sample(s).	0 (job 1)
	1 -- Print the sorted sample(s).	1 (job 2)
	(F10.3, ten per line)	
(The rest of this control card pertains to a one-sample test.)		
24	0 -- Do not compare with normal pdf.	1 (job 1)
	1 -- Compare with normal pdf.	
25 - 29	u -- mean of the normal pdf	0.5 (job 1)
30 - 34	s -- standard deviation of the normal pdf	0.5 (job 1)
35	0 -- Do not compare with exponential pdf.	
	1 -- Compare with exponential pdf.	1 (job 1)
36 - 40	u -- mean of the exponential pdf	0.5 (job 1)
41 - 45	s -- standard deviation of the exponential pdf	1.0 (job 1)
46	0 -- Do not compare with Cauchy pdf.	
	1 -- Compare with Cauchy pdf.	1 (job 1)
47 - 51	u -- median of the Cauchy pdf	0.5 (job 1)
52 - 56	s -- u-s is the first quartile of the Cauchy pdf	1.0 (job 1)
57	0 -- Do not compare with uniform pdf.	
	1 -- Compare with uniform pdf.	1 (job 1)
58 - 62	u -- left endpoint of the uniform pdf	0 (job 1)
63 - 67	s -- right endpoint of uniform pdf	1.0 (job 1)
68	0 -- Do not compare with user's pdf.	0 (job 1)
	1 -- Compare with user-specified pdf.	
69 - 73	u } -- Parameters for	0 (job 1)
74 - 78	s } -- user-specified pdf	0 (job 1)
	u and s are described fully in "Description of Parameters" under subroutine KOLMO, and are read using Format F 5.0; decimal points will override the format specification.	

5. Data is read into the computer one sample at a time. The reading of a sample is terminated by a data element of 999999. New samples must begin on a new card. Data elements are punched on cards using format F6.0, which assumes twelve 6-column fields per card; decimal points on the card override the format specification. Since the routines KOLMO and KOLM2 sort the samples, no particular order within a sample is necessary.

Deck Setup

See figure 59.

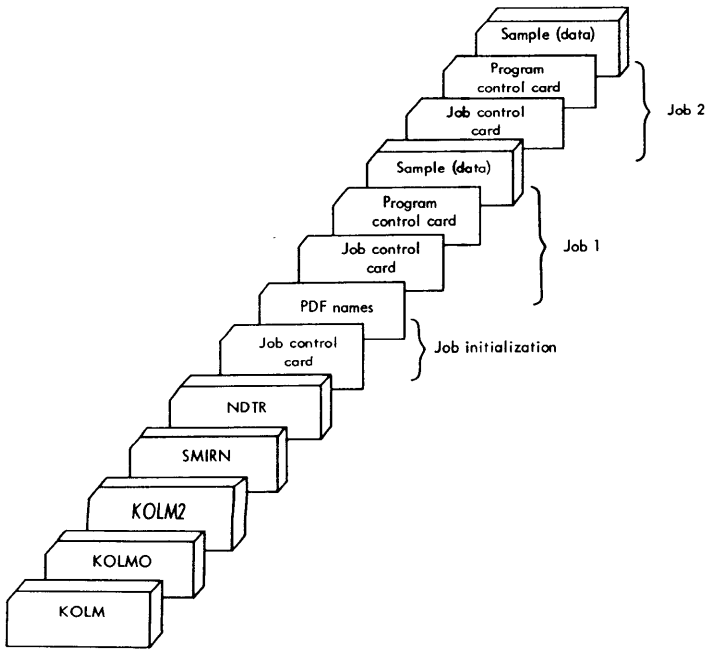


Figure 59. Deck setup (Kolmogorov - Smirnov test)

Sample Data

See Figure 60.

```
/DATA                                                                                                                  10
----                                                                                                                   20
     NORMAL          EXPONENTIAL          CAUCHY          UNIFORM          USER'                                    30
----                                                                                                                   40
UNIFORM TEST          1CC1C00.5C0C.51000.5000C110CC.5000C11000000000001                                                50
 0.377 0.260 0.172 0.688 0.581 0.290 0.514 0.472 0.204 0.976 0.018 0.326                                               60
 0.795 0.837 0.870 0.686 0.288 0.555 0.737 0.427 0.931 0.745 0.092 0.843                                               70
 0.231 0.806 0.753 0.263 0.804 0.458 0.508 0.928 0.994 0.608 0.702 0.743                                               80
 0.005 0.951 0.664 0.425 0.570 0.596 0.444 0.302 0.817 0.183 0.746 0.833                                               90
 0.282 0.201 0.662 0.167 0.043 0.750 0.117 0.953 0.665 0.411 0.477 0.164                                              100
 0.692 0.663 0.867 0.054 0.518 0.624 0.083 0.882 0.540 0.301 0.953 0.006                                              110
 0.458 0.694 0.041 0.995 0.604 0.666 0.561 0.367 0.156 0.630 0.377 0.589                                              120
 0.139 0.536 0.963 0.956 0.068 0.801 0.199 0.985 0.113 0.816 0.880 0.931                                              130
 0.670 0.640 0.805 0.073 0.196 0.516 0.336 0.371 0.197 0.843 0.288 0.139                                              140
 0.242 0.208 0.025 0.349 0.870 0.080 0.652 0.190 0.275 0.939 0.161 0.514                                              150
 0.636 0.190 0.416 0.786 0.973 0.767 0.845 0.168 0.400 0.888 0.726 0.365                                              160
 0.652 0.632 0.923 0.844 0.761 0.969 0.965 0.073 0.751 0.851 0.340 0.383                                              170
 0.243 0.008 0.840 0.093 0.816 0.058 0.006 0.515 0.033 0.565 0.093 0.470                                              180
 0.982 0.666 0.154 0.933 0.215 0.890 0.409 0.441 0.963 0.810 0.195 0.876                                              190
 0.501 0.123 0.228 0.264 0.531 0.810 0.083 0.202 0.469 0.996 0.752 0.545                                              200
 0.503 0.117 0.170 0.972 0.298 0.042 0.574 0.065 0.225 0.766 0.570 0.520                                              210
 0.996 0.292 0.790 0.111 0.556 0.337 0.012 0.042 0.143 0.482 0.607 0.302                                              220
 0.353 0.397 0.206 0.662 0.119 0.756 0.450 0.918 0.453 0.463 0.699 0.022                                              230
 0.842 0.859 0.577 0.725 0.163 0.450 0.232 0.349 0.000 0.864 0.181 0.311                                              240
 0.236 0.622 0.607 0.042 0.787 0.348 0.006 0.904 0.365 0.053 0.037 0.745                                              250
 0.136 0.113 0.455 0.708 0.158 0.572 0.012 0.928 0.455 0.381 0.193 0.728                                              260
 0.629 0.220 0.657 0.962 0.860 0.501 0.268 0.098 0.181 0.203 0.588 0.701                                              270
 0.909 0.148 0.708 0.909 0.088 0.345 0.277 0.556 0.840 0.033 0.639 0.539                                              280
 0.482 0.041 0.907 0.077 0.299 0.097 0.892 0.478 0.835 0.707 0.733 0.029                                              290
 0.581 0.224 0.112 0.659 0.945 0.741 0.940 0.969 0.360 0.434 0.365 0.285                                              300
 0.422 0.967 0.005 0.328 0.924 0.595 0.253 0.157 0.668 0.594 0.554 0.984                                              310
 0.913 0.622 0.516 0.502 0.364 0.667 0.724 0.344 0.546 0.178 0.151 0.302                                              320
 0.457 0.021 0.019 0.923 0.365 0.882 0.010 0.121 0.637 0.734 0.671 0.416                                              330
 0.459 0.009 0.919 0.434 0.331 0.079 0.500 0.284 0.209 0.694 0.283 0.454                                              340
 0.178 0.978 0.272 0.827 0.512 0.634 0.195 0.462 0.019 0.956 0.560 0.761                                              350
 0.524 0.294 0.047 0.634 0.382 0.591 0.103 0.303 0.889 0.607 0.638 0.367                                              360
 0.463 0.471 0.664 0.742 0.476 0.178 0.785 0.113 0.610 0.646 0.390 0.520                                              370
 0.611 0.988 0.431 0.699 0.312 0.580 0.672 0.810 0.814 0.597 0.256 0.164                                              380
 0.679 0.603 0.504 0.595 0.033 0.846 0.783 0.079 0.430 0.868 0.343 0.244                                              390
 0.376 0.062 0.990 0.381 0.371 0.801 0.467 0.592 0.348 0.759 0.422 0.697                                              400
 0.388 0.055 0.836 0.518 0.585 0.842 0.793 0.177 0.926 0.964 0.450 0.022                                              410
 0.085 0.311 0.102 0.816 0.973 0.494 0.208 0.803 0.948 0.462 0.242 0.287                                              420
 0.546 0.698 0.269 0.339 0.607 0.594 0.102 0.266 0.677 0.668 0.913 0.462                                              430
 0.562 0.207 0.188 0.264 0.895 0.991 0.893 0.442 0.615 0.709 0.722 0.950                                              440
 0.208 0.696 0.304 0.557 0.605 0.617 0.256 0.984 0.595 0.715 0.936 0.178                                              450
 0.141 0.153 0.654 0.544 0.376 0.363 0.793 0.492 0.812 0.447 0.376 0.231                                              460
 0.644 0.263 0.785 0.341 0.982 0.829999999                                                                            470
----                                                                                                                   480
UNIFORM-GAUSS TEST  211                                                                                                490
-0.283 0.916 0.776 0.690 0.910 0.506 0.816 0.348 0.659-0.301 0.630-0.397                                               500
 0.515 0.227 1.253 0.421 0.499 0.288 1.189-0.264 0.099 0.051 0.411 0.951                                               510
 0.273 0.154 0.861 0.937 0.446 0.702 1.451 0.035 0.515 0.770 0.559 1.053                                               520
-1.157 0.902 0.533 1.270 0.761 1.110 1.190 0.433 0.573 0.374 1.317 1.255                                              530
 0.547 1.145 0.667-0.077 0.422-0.159-0.037 0.088 0.406 0.849 0.898 0.372                                               540
-0.324 0.025 0.632 0.365 0.375 0.694-0.206 0.126-0.381 1.149 0.983 1.184                                              550
-0.011 0.653 0.266 1.035 0.536 0.936 1.177 1.644 0.782 0.198 0.222 0.445                                              560
 0.714 0.607 0.374 0.341 0.790 0.302 1.075 0.204 0.436 0.887 0.234 0.874                                              570
 0.048 0.938 0.733-0.340-0.012 0.497 0.418 0.840 0.091 0.578 0.606-0.340                                              580
 0.656 0.660 0.584 0.837 0.454 0.695 0.606 0.053-0.276 1.600 1.394-0.038                                              590
 1.173 0.762 0.642 0.185-0.023 0.037 0.508 0.313-0.718-0.249 0.124-0.096                                              600
-0.299 0.196 1.086 0.487 0.317 0.635 0.462 0.559 0.181 1.799 0.287 0.583                                              610
 0.313 0.387 1.067 0.996 0.702 0.068-0.227 0.198 0.305-0.021 0.840 1.063                                              620
 1.049 0.226-0.297 0.930 0.828 0.884 1.217-0.391 0.007-0.004 1.238 0.376                                              630
 0.418 1.075 0.083-0.020 0.362 0.601 0.037 0.634 0.109 0.524 1.356 1.024                                              640
-0.602 0.763 1.261 0.302-0.063 0.704 0.446-0.410 0.401 0.704 1.070-0.023                                              650
-0.064 1.087-0.737-0.476 1.156 0.648 0.624 0.257 0.643 0.147 0.719 0.174                                              660
-0.552-0.183 0.583 0.740 0.592-0.144 0.222 0.388 0.563 0.933 1.108 1.022                                              670
 0.818 0.686 0.683 0.514 0.284-0.280 0.358 1.203-0.643 0.110 0.012 0.399                                              680
 0.899 0.400 0.994 0.880 0.743 0.102 1.120 0.391 0.191 0.196 1.176 0.149                                              690
 0.512 1.132 0.916 0.838 0.445 1.330 0.563 0.610 0.699 0.675 0.310 0.586                                              700
 0.448-0.475 0.317 0.858 0.839-0.297 0.214 0.985 0.484 1.004 1.598 0.494                                              710
 0.467 1.188 0.536 0.381 1.339-0.011 0.064 0.113 0.619 0.604 0.687 0.622                                              720
 0.297 0.203 0.378 1.313 0.829 0.422 0.078 0.057 0.143 0.868-0.302 0.693                                              730
 0.633 1.116 0.118-0.469 0.663 0.708 0.685 0.850 0.566 0.657 1.217 0.394                                              740
 0.643-0.055-0.000 0.881 1.163 0.520 0.787 1.493 1.366 0.801 0.301 1.384                                              750
-0.541 1.176 0.236 0.675 1.119 1.000 0.250 0.457-0.010 0.098 0.975 0.288                                              760
 0.686 0.764 0.007 0.697 0.789 0.259 0.414 0.680 0.852 0.315 0.231 0.203                                              770
 1.394 0.131 0.963 0.699 0.404-0.124 0.583 0.071 1.838-0.313-0.467 0.191                                              780
 0.125 1.670 0.224 0.400 0.658 0.900 1.034 0.005 0.801 0.920-0.188 0.786                                              790
 0.387 1.243 0.875 0.989 0.718-0.152 0.009 1.329 0.562 0.687 0.968 0.490                                              800
 0.160 0.177-0.025 1.125 0.217 1.206 1.221-0.145-0.088 0.629-0.131 0.272                                              810
 0.388 0.772 1.046-0.067 0.760 0.428 0.852 0.867 0.610 0.359 1.352 0.571                                              820
-0.011-0.205 1.084 0.009 0.917 0.438 1.050 0.616 0.884 0.954-0.275 1.295                                              830
 0.346-1.018 1.049 0.417 1.230 1.127 1.435 0.823-0.069 0.464 1.261-0.179                                              840
 0.812 0.537 0.875 0.190 0.707 0.857 0.094 0.176 0.916 0.406 0.204 0.494                                              850
 1.709 0.133 0.460 0.828-0.174 0.457 0.584 0.832-0.026 1.265-0.232-0.373                                              860
-0.172 0.913 0.673 0.303 0.035 1.226-0.072 0.920 1.207-0.003 0.632 0.004                                              870
 0.951 0.307 0.798 1.479 0.196 1.058 0.873 0.060 0.524 0.501 0.373 0.954                                              880
-0.072 0.988 0.351 0.053 0.248 0.430-0.379 0.533 0.688 0.524 0.447 1.376                                              890
-0.263-0.064 0.301 1.486 0.351 0.806-0.374 0.735 0.958-0.262 0.332 0.963                                              900
999999                                                                                                               910
```

Figure 60.

Output

Description

The output from the program KOLM gives the statistics and probability statements described below, and in addition identifies the distribution functions being considered. Sorted samples are printed on option.

The following items are produced as output:

1. Z score, where $z = \sqrt{n}\, D_n$ for the one-sample test; n is the sample size, and D_n is the maximum difference between the empirical distribution function and the theoretical distribution function.

   $z = \sqrt{\frac{mn}{m+n}}\, D_{m,n}$ for the two-sample test, m is the size of the second sample; n is the size of the first sample; $D_{m,n}$ is the maximum difference between the two empirical distribution functions.

2. The probability of incorrectly rejecting the hypothesis of equality of distribution functions.

Sample

See Figure 61.

Program Modification

1. Program capacity may be increased or decreased by making changes in the dimension statements. If this is done, the statements DO 111 I = 1, 50 and DO 117 I = 1, 50 may require modification (under READ SAMPLE comments card in listing of program). This will also be true if data formats require changing. The "read sample" sections of the program use FORMAT statement 3, and the user may wish to change these sections.

2. Any modifications to the subroutine KOLMO in terms of added continuous pdf's should be reflected in the program KOLM. It may be necessary to:

   a. Modify the dimensions of DIST (5, 3), which contains the switches calling on pdf's and also contains the parameters u and s used by KOLMO
   b. Modify the pdf titling card, statement 6 (FORMAT), the READ (5, 6)TIT1 card which reads titles, and the dimension of TIT1 (now 20, to hold five 16-digit titles)
   c. Modify the section of the program from statement 121 through 132 to reflect changes a and b above. These statements call KOLMO to perform tests and output results.

3. List of names in KOLM, and their usage:

D -- Temporary vector used in reading samples
DAS2 -- Initializing card name (----)
DASH -- Job control card name (----)
DIST -- 5 by 3 matrix. The five elements in column 1 are switches that allow the (5) pdf's to be used in one-sample tests. Columns 2 and 3 contain the parameters u and s for the associated test.
IFL -- Error indicator (job deck error)
IER -- Error (in KOLMO, used for skipping the test concerned)
IES -- Error (in KOLMO , used for error message)

```
UNIFORM TEST

A 1 SAMPLE TEST WAS REQUESTED

THE SIZE OF SAMPLE  1 IS 498.

THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)      NORMAL      DISTRIBUTION
 WITH MEAN       0.5000 AND VARIANCE       0.2500
 CAN BE REJECTED WITH PROBABILITY 0.0   OF BEING INCORRECT.  THE STATISTIC Z
 IS  0.3504E 01 FOR THIS SAMPLE.

THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)   EXPONENTIAL    DISTRIBUTION
 WITH MEAN       0.5000 AND VARIANCE       1.0000
 CAN BE REJECTED WITH PROBABILITY 0.0   OF BEING INCORRECT.  THE STATISTIC Z
 IS  0.8803E 01 FOR THIS SAMPLE.

THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)      CAUCHY      DISTRIBUTION
 WITH MEDIAN       0.5000 AND FIRST QUARTILE      -0.5000
 CAN BE REJECTED WITH PROBABILITY 0.0   OF BEING INCORRECT.  THE STATISTIC Z
 IS  0.7887E 01 FOR THIS SAMPLE.

THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N)     UNIFORM      DISTRIBUTION
 IN THE INTERVAL       0.0    TO       1.0000 INCLUSIVE
 CAN BE REJECTED WITH PROBABILITY 0.989 OF BEING INCORRECT.  THE STATISTIC Z
 IS  0.4444E 00 FOR THIS SAMPLE.

THE JOB WITH TITLE UNIFORM TEST          WAS COMPLETED.


UNIFORM-GAUSS TEST

A 2 SAMPLE TEST WAS REQUESTED

THE SIZE OF SAMPLE  2 IS 492.

SORTED SAMPLE ONE FOLLOWS

  0.0     0.005   0.005   0.006   0.006   0.006   0.008   0.009   0.010   0.012
  0.012   0.018   0.019   0.019   0.021   0.022   0.022   0.025   0.029   0.033
  0.033   0.033   0.037   0.041   0.041   0.042   0.042   0.042   0.043   0.047
  0.053   0.054   0.055   0.058   0.062   0.065   0.068   0.073   0.073   0.077
  0.079   0.079   0.080   0.083   0.083   0.085   0.088   0.092   0.093   0.093
  0.097   0.098   0.102   0.102   0.103   0.111   0.112   0.113   0.113   0.113
  0.117   0.117   0.119   0.121   0.123   0.136   0.139   0.139   0.141   0.143
  0.148   0.151   0.153   0.154   0.156   0.157   0.158   0.161   0.163   0.164
  0.164   0.167   0.168   0.170   0.172   0.177   0.178   0.178   0.178   0.178
  0.181   0.181   0.183   0.188   0.190   0.190   0.193   0.195   0.195   0.196
  0.197   0.199   0.200   0.201   0.202   0.203   0.204   0.206   0.207   0.208
  0.208   0.209   0.215   0.220   0.224   0.225   0.228   0.231   0.231   0.232
  0.236   0.242   0.242   0.243   0.244   0.253   0.256   0.256   0.260   0.263
  0.263   0.264   0.264   0.266   0.268   0.269   0.272   0.275   0.277   0.282
  0.283   0.284   0.285   0.287   0.288   0.288   0.290   0.292   0.294   0.298
  0.299   0.301   0.302   0.302   0.302   0.303   0.304   0.311   0.311   0.312
  0.326   0.328   0.331   0.336   0.337   0.339   0.340   0.341   0.343   0.344
  0.345   0.348   0.348   0.349   0.349   0.353   0.360   0.363   0.364   0.365
  0.365   0.365   0.365   0.367   0.367   0.371   0.371   0.376   0.376   0.376
  0.377   0.377   0.381   0.381   0.382   0.383   0.388   0.390   0.397   0.400
  0.409   0.411   0.416   0.416   0.422   0.422   0.425   0.427   0.430   0.431
  0.434   0.434   0.441   0.442   0.444   0.447   0.450   0.450   0.450   0.453
  0.454   0.455   0.455   0.457   0.458   0.458   0.459   0.462   0.462   0.462
  0.463   0.463   0.467   0.469   0.470   0.471   0.472   0.476   0.477   0.478
  0.482   0.482   0.492   0.494   0.500   0.501   0.501   0.502   0.503   0.504
  0.508   0.512   0.514   0.514   0.515   0.516   0.516   0.518   0.518   0.520
  0.520   0.524   0.531   0.536   0.539   0.540   0.544   0.545   0.546   0.546
  0.554   0.555   0.556   0.556   0.557   0.560   0.561   0.562   0.565   0.570
  0.570   0.572   0.574   0.577   0.580   0.581   0.581   0.585   0.588   0.589
  0.591   0.592   0.594   0.594   0.595   0.595   0.595   0.596   0.597   0.603
  0.604   0.605   0.607   0.607   0.607   0.607   0.608   0.610   0.611   0.615
  0.617   0.622   0.622   0.624   0.629   0.630   0.632   0.634   0.634   0.636
  0.637   0.638   0.639   0.640   0.644   0.646   0.652   0.652   0.654   0.657
  0.659   0.662   0.662   0.664   0.664   0.665   0.666   0.666   0.667   0.668
  0.668   0.670   0.671   0.672   0.677   0.679   0.683   0.686   0.688   0.692
  0.694   0.694   0.696   0.697   0.698   0.699   0.699   0.701   0.702   0.707
  0.708   0.708   0.709   0.715   0.722   0.724   0.725   0.726   0.728   0.733
  0.734   0.737   0.741   0.742   0.743   0.745   0.745   0.746   0.750   0.751
  0.752   0.753   0.754   0.759   0.761   0.761   0.766   0.767   0.783   0.785
  0.785   0.786   0.787   0.790   0.793   0.793   0.795   0.801   0.801   0.803
  0.804   0.805   0.806   0.810   0.810   0.810   0.812   0.814   0.816   0.816
  0.816   0.817   0.827   0.829   0.833   0.835   0.836   0.837   0.840   0.842
  0.842   0.843   0.843   0.844   0.845   0.846   0.851   0.859   0.860   0.860
  0.864   0.867   0.868   0.870   0.870   0.876   0.880   0.882   0.882   0.888
  0.889   0.890   0.892   0.893   0.895   0.904   0.907   0.909   0.909   0.913
  0.913   0.918   0.919   0.923   0.923   0.924   0.926   0.928   0.928   0.931
  0.931   0.933   0.936   0.939   0.940   0.945   0.948   0.950   0.951   0.953
  0.953   0.956   0.956   0.962   0.963   0.963   0.964   0.965   0.967   0.969
  0.969   0.972   0.973   0.973   0.976   0.978   0.982   0.982   0.984   0.984
  0.985   0.988   0.990   0.991   0.994   0.995   0.996   0.996
```

Figure 61.

```
SORTED SAMPLE TWO FOLLOWS

-1.157   -1.018   -0.737   -0.718   -0.643   -0.602   -0.552   -0.541   -0.476   -0.475
-0.469   -0.467   -0.410   -0.397   -0.391   -0.381   -0.379   -0.374   -0.373   -0.340
-0.340   -0.324   -0.313   -0.302   -0.301   -0.299   -0.297   -0.297   -0.283   -0.280
-0.276   -0.275   -0.264   -0.263   -0.262   -0.249   -0.232   -0.227   -0.206   -0.205
-0.188   -0.183   -0.179   -0.174   -0.172   -0.159   -0.152   -0.145   -0.144   -0.131
-0.124   -0.096   -0.088   -0.077   -0.072   -0.072   -0.069   -0.067   -0.064   -0.064
-0.063   -0.055   -0.038   -0.037   -0.026   -0.025   -0.023   -0.023   -0.021   -0.020
-0.012   -0.011   -0.011   -0.011   -0.010   -0.004   -0.003    0.0      0.004    0.005
 0.007    0.007    0.009    0.009    0.012    0.025    0.035    0.035    0.037    0.037
 0.048    0.051    0.053    0.053    0.057    0.060    0.064    0.068    0.071    0.078
 0.083    0.088    0.091    0.094    0.098    0.099    0.102    0.109    0.110    0.113
 0.118    0.124    0.125    0.126    0.131    0.133    0.143    0.147    0.149    0.154
 0.160    0.174    0.176    0.177    0.181    0.185    0.190    0.191    0.191    0.196
 0.196    0.196    0.198    0.198    0.203    0.203    0.204    0.204    0.214    0.217
 0.222    0.222    0.224    0.226    0.227    0.231    0.234    0.236    0.248    0.250
 0.257    0.259    0.266    0.272    0.273    0.284    0.287    0.288    0.288    0.297
 0.301    0.301    0.302    0.302    0.303    0.305    0.307    0.310    0.313    0.313
 0.315    0.317    0.317    0.332    0.341    0.346    0.348    0.351    0.351    0.358
 0.359    0.362    0.365    0.372    0.373    0.374    0.374    0.375    0.376    0.378
 0.381    0.387    0.387    0.388    0.388    0.391    0.394    0.399    0.400    0.400
 0.401    0.404    0.406    0.406    0.411    0.414    0.417    0.418    0.418    0.421
 0.422    0.422    0.428    0.430    0.433    0.436    0.438    0.445    0.445    0.446
 0.446    0.447    0.448    0.454    0.457    0.457    0.460    0.462    0.464    0.467
 0.484    0.487    0.490    0.494    0.494    0.497    0.499    0.501    0.506    0.508
 0.512    0.514    0.515    0.515    0.520    0.524    0.524    0.524    0.533    0.533
 0.536    0.536    0.537    0.547    0.559    0.559    0.562    0.563    0.563    0.566
 0.571    0.573    0.578    0.583    0.583    0.583    0.584    0.584    0.586    0.592
 0.601    0.604    0.606    0.606    0.607    0.610    0.610    0.616    0.619    0.622
 0.624    0.629    0.630    0.632    0.632    0.633    0.634    0.635    0.642    0.643
 0.643    0.648    0.653    0.656    0.657    0.658    0.659    0.660    0.663    0.667
 0.673    0.675    0.675    0.680    0.683    0.685    0.686    0.686    0.687    0.687
 0.688    0.690    0.693    0.694    0.695    0.697    0.699    0.699    0.702    0.702
 0.704    0.704    0.707    0.708    0.714    0.718    0.719    0.733    0.735    0.740
 0.743    0.760    0.761    0.762    0.763    0.764    0.770    0.772    0.776    0.782
 0.786    0.787    0.789    0.790    0.798    0.801    0.801    0.806    0.812    0.816
 0.818    0.823    0.828    0.828    0.829    0.832    0.837    0.838    0.839    0.840
 0.849    0.849    0.850    0.852    0.852    0.857    0.858    0.861    0.867    0.868
 0.873    0.874    0.875    0.875    0.880    0.881    0.884    0.884    0.887    0.898
 0.899    0.900    0.902    0.910    0.913    0.916    0.916    0.916    0.917    0.920
 0.920    0.930    0.933    0.936    0.937    0.938    0.951    0.951    0.954    0.954
 0.958    0.963    0.963    0.968    0.975    0.983    0.985    0.988    0.989    0.994
 0.996    1.000    1.004    1.022    1.024    1.034    1.035    1.046    1.049    1.049
 1.050    1.053    1.058    1.063    1.067    1.070    1.075    1.075    1.084    1.086
 1.087    1.108    1.110    1.116    1.119    1.120    1.125    1.127    1.132    1.145
 1.149    1.156    1.163    1.173    1.176    1.176    1.177    1.184    1.188    1.189
 1.190    1.203    1.206    1.207    1.217    1.217    1.221    1.226    1.230    1.238
 1.243    1.253    1.255    1.261    1.261    1.265    1.270    1.295    1.313    1.317
 1.329    1.330    1.339    1.352    1.356    1.366    1.376    1.384    1.394    1.394
 1.435    1.451    1.479    1.486    1.493    1.598    1.600    1.644    1.670    1.709
 1.799    1.838

THE HYPOTHESIS THAT THE TWO SAMPLES ARE FROM THE SAME POPULATION CAN BE REJECTED WITH (ASYMPTOTIC)
PROBABILITY OF BEING INCORRECT OF  0.000.  THE STATISTIC Z IS   0.2590E 01 FOR THESE SAMPLES.

 THE JOB WITH TITLE UNIFORM-GAUSS TEST   WAS COMPLETED.
```

Figure 61. (Continued)

IO -- Switch (used for printing samples)
IR -- Number of samples to be read in current job
IS -- Number of samples to be used in current job (1 or 2)
K -- Counter used to print correct pdf name for pdf used in the test
M -- Size of second sample
N -- Size of first sample
N1 -- 1 or 2, for number of samples tested
P -- Probability of being incorrect if hypothesis is rejected
S2 -- Temporary storage for u and s output
TIT1 -- Current pdf names
TITLE -- Job title
X -- Sample 1
Y -- Sample 2
Z -- Z statistic, from KOLMO or KOLM2

Operating Instructions

This sample program is a standard FORTRAN program and needs no special operating instructions. Data set 5 is used for input, and 6 for output.

Error Messages

The following error conditions will result in messages, followed by the action specified:

1. Neither a one- nor two-sample test is requested, or the size of either sample is larger than 500 -- CC.21, CONTROL CARD, INCORRECT, OR SAMPLE SIZE TOO LARGE. JOB IGNORED. Action: Cards are read until a new job control card is found, or until the hopper is empty.

2. Sample size is less than 100 (not an error) -- NOTE THE REMARKS CONCERNING ASYMPTOTIC RESULTS AND SAMPLE SIZE IN SUBROUTINE SMIRN. Action: None - job continues.

3. The requirement of subroutine KOLMO that certain parameters be nonzero or positive is violated -- AT LEAST ONE (S) ENTRY PARAMETER FOR THE SUBROUTINE KOLMO WAS INCORRECT. THE TEST FOR THE ASSOCIATED CONTINUOUS PDF WAS IGNORED. Action: All tests are made for cases where the parameter s was correct.

4. A case in which an error requires aborting the job, and the succeeding job in the job stack requests a two-sample test where the second sample is to be

compared with a (first) sample which was read on the previous job -- THIS JOB CALLS FOR THE USE OF A PREVIOUSLY READ SAMPLE, AND THE PREVIOUS JOB WAS IGNORED BECAUSE OF ERRORS. JOB IGNORED. Action: Cards are read until a new job control card is found, or until the hopper is empty.

5. The job control card preceding a job is not there or is incorrect -- FIRST CARD IN JOB DECK (JOB CONTROL CARD) IS INCORRECT. Action: Cards are read until a new job control card is found, or until the hopper is empty.

Timing

The execution time of this program on a System/360, Model 40, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 Printer as output, is:

33 seconds for job 1

50 seconds for job 2

```
C                                                                       KOLM  10
C     ..................................................................KOLM  20
C                                                                       KOLM  30
C        SAMPLE MAIN PROGRAM FOR THE KOLMOGOROV-SMIRNOV TEST-KOLM       KOLM  40
C                                                                       KOLM  50
C        PURPOSE                                                        KOLM  60
C           (1) READ THE CONTROL CARD FOR A ONE OR TWO SAMPLE TEST      KOLM  70
C           (2) READ THE SAMPLE DATA AND DETERMINE THE SAMPLE SIZES     KOLM  80
C           (3) PRINT RESULTS                                           KOLM  90
C                                                                       KOLM 100
C        REMARKS                                                        KOLM 110
C           THE USER SHOULD NOTE THE REMARKS GIVEN IN SUBROUTINES       KOLM 120
C           KOLMO, KOLM2, AND SMIRN, AND THE MATHEMATICAL DESCRIPTIONS  KOLM 130
C           FOR THESE SUBROUTINES.                                      KOLM 140
C                                                                       KOLM 150
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  KOLM 160
C           KOLMO                                                       KOLM 170
C           KOLM2                                                       KOLM 180
C           SMIRN                                                       KOLM 190
C           NDTR                                                        KOLM 200
C                                                                       KOLM 210
C        METHOD                                                         KOLM 220
C           REFER TO SUBROUTINES KOLMO, KOLM2, AND SMIRN                KOLM 230
C                                                                       KOLM 240
C     ..................................................................KOLM 250
C                                                                       KOLM 260
C     THE FOLLOWING DIMENSIONS MUST BE GREATER THAN THE NUMBER OF DATA  KOLM 270
C     ELEMENTS IN THE TWO SAMPLES, M AND N                              KOLM 280
C                                                                       KOLM 290
      DIMENSION X(501),Y(501)                                           KOLM 300
C                                                                       KOLM 310
C     ..................................................................KOLM 320
C                                                                       KOLM 330
      DIMENSION TITLE(5),D(12),TITL(20),DIST(5,3)                       KOLM 340
C                                                                       KOLM 350
C     ..................................................................KOLM 360
C                                                                       KOLM 370
    1 FORMAT(5A4,3I1,5(F1.0,2F5.0))                                     KOLM 380
    2 FORMAT(//'CC.21, CONTROL CARD, INCORRECT, OR SAMPLE SIZE IS TOO LAKOLM 390
     1RGE.  JOB IGNORED.')                                              KOLM 400
    3 FORMAT(12F6.0)                                                    KOLM 410
    4 FORMAT(1H1,5A4)                                                   KOLM 420
    5 FORMAT(//2H A,I2,' SAMPLE TEST WAS REQUESTED')                    KOLM 430
    6 FORMAT(20A4)                                                      KOLM 440
    7 FORMAT(//(10F10.3))                                               KOLM 450
    8 FORMAT(//' SORTED SAMPLE ONE FOLLOWS')                            KOLM 460
    9 FORMAT(//' THE HYPOTHESIS THAT THE SAMPLE IS FROM A(N) ',4A4,  ' DKOLM 470
     1ISTRIBUTION')                                                     KOLM 480
   10 FORMAT(//' SORTED SAMPLE TWO FOLLOWS')                            KOLM 490
   11 FORMAT(//' THE HYPOTHESIS THAT THE TWO SAMPLES ARE FROM THE SAME PKOLM 500
     1OPULATION CAN BE REJECTED WITH (ASYMPTOTIC)',/,' PROBABILITY OF BEKOLM 510
     2ING INCORRECT OF ',F6.3,'.  THE STATISTIC Z IS ',E12.4,' FOR THESEKOLM 520
     3 SAMPLES.')                                                       KOLM 530
   12 FORMAT(//,' THE SIZE OF SAMPLE',I3,' IS',I4,'.')                  KOLM 540
   13 FORMAT(//,' NOTE THE REMARKS CONCERNING ASYMPTOTIC RESULTS AND SAMKOLM 550
     1PLE SIZE IN SUBROUTINE SMIRN')                                    KOLM 560
   14 FORMAT(//,' AT LEAST ONE (S) ENTRY PARAMETER FOR THE SUBROUTINE KOKOLM 570
     1LMO WAS INCORRECT.'/' THE TEST FOR THE ASSOCIATED CONTINUOUS PDF WKOLM 580
     2AS IGNORED.')                                                     KOLM 590
   15 FORMAT(A4)                                                        KOLM 600
   16 FORMAT(//,' THIS JOB CALLS FOR THE USE OF A PREVIOUSLY READ SAMPLEKOLM 610
     1, AND THE PREVIOUS JOB WAS IGNORED BECAUSE OF ERRORS.'/ ' JOB IGNOKOLM 620
     2RED.')                                                            KOLM 630
   17 FORMAT(//,' FIRST CARD IN JOB DECK (JOB CONTROL CARD) IS INCORRECTKOLM 640
     1.')                                                               KOLM 650
   18 FORMAT(1H ,' WITH MEAN',F13.4,' AND VARIANCE',F13.4)              KOLM 660
   19 FORMAT(1H ,' WITH MEDIAN',F13.4,' AND FIRST QUARTILE',F13.4)      KOLM 670
   20 FORMAT(1H ,' IN THE INTERVAL',F13.4,' TO',F13.4,' INCLUSIVE')     KOLM 680
   21 FORMAT(1H ,' CAN BE REJECTED WITH PROBABILITY',F6.3,' OF BEING INCKOLM 690
     1ORRECT.  THE STATISTIC Y',/,'  IS',E12.4,' FOR THIS SAMPLE.')     KOLM 700
   22 FORMAT(//,'  THE JOB WITH TITLE ',5A4,' WAS COMPLETED.')           KOLM 710
C                                                                       KOLM 720
C        READ DISTRIBUTION NAMES AND JOB CONTROL CARD                   KOLM 730
C                                                                       KOLM 740
      IFL=0                                                             KOLM 750
      READ(5,15)DASH                                                    KOLM 760
      READ(5,6)TITL                                                     KOLM 770
C                                                                       KOLM 780
C        SELECT PROGRAM CONTROLS                                        KOLM 790
C                                                                       KOLM 800
  100 READ(5,15)DAS2                                                    KOLM 810
      IF(DASH-DAS2)101,102,101                                          KOLM 820
  101 WRITE(6,17)                                                       KOLM 830
      GO TO 107                                                         KOLM 840
  102 READ(5,1)TITLE,IS,IP,IO,((DIST(I,J),J=1,3),I=1,5)                 KOLM 850
      IES=0                                                             KOLM 860
      WRITE(6,4)TITLE                                                   KOLM 870
      WRITE(6,5)IS                                                      KOLM 880
C                                                                       KOLM 890
C        NUMBER OF SAMPLES DECISION                                     KOLM 900
C                                                                       KOLM 910
      IF(IP)103,105,103                                                 KOLM 920
  103 IF(IFL)104,115,104                                                KOLM 930
  104 WRITE(6,16)                                                       KOLM 940
      GO TO 107                                                         KOLM 950
  105 IF(IS-1)106,109,109                                               KOLM 960
C                                                                       KOLM 970
C        NOT ONE OR TWO SAMPLES                                         KOLM 980
C                                                                       KOLM 990
  106 WRITE(6,2)                                                        KOLM1000
  107 READ(5,15)DAS2                                                    KOLM1010
      IF(DASH-DAS2)107,108,107                                          KOLM1020
  108 IFL=1                                                             KOLM1030
      GO TO 102                                                         KOLM1040
C                                                                       KOLM1050
C        READ FIRST SAMPLE                                              KOLM1060
C                                                                       KOLM1070
  109 N=0                                                               KOLM1080
      DO 111 I=1,50                                                     KOLM1090
      READ(5,3)D                                                        KOLM1100
      DO 111 J=1,12                                                     KOLM1110
      IF(D(J)-999999.0)110,112,110                                      KOLM1120
  110 N=N+1                                                             KOLM1130
      IF(N-501)111,106,106                                              KOLM1140
  111 X(N)=D(J)                                                         KOLM1150
  112 N1=1                                                              KOLM1160
      WRITE(6,12)N1,N                                                   KOLM1170
C                                                                       KOLM1180
C        CHECK THE SIZE OF N                                            KOLM1190
C                                                                       KOLM1200
      IF(N-100)113,113,114                                              KOLM1210
  113 WRITE(6,13)                                                       KOLM1220
  114 IF(IS-2)121,115,106                                               KOLM1230
C                                                                       KOLM1240
C        READ SECOND SAMPLE                                             KOLM1250
C                                                                       KOLM1260
  115 M=0                                                               KOLM1270
      DO 117 I=1,50                                                     KOLM1280
      READ(5,3)D                                                        KOLM1290
      DO 117 J=1,12                                                     KOLM1300
      IF(D(J)-999999.0)116,118,116                                      KOLM1310
  116 M=M+1                                                             KOLM1320
      IF(M-501)117,106,106                                              KOLM1330
  117 Y(M)=D(J)                                                         KOLM1340
  118 N1=2                                                              KOLM1350
      WRITE(6,12)N1,M                                                   KOLM1360
C                                                                       KOLM1370
C        CHECK THE SIZE OF M                                            KOLM1380
C                                                                       KOLM1390
      IF(M-100)119,119,120                                              KOLM1400
  119 WRITE(6,13)                                                       KOLM1410
  120 IF(IS-1)121,121,133                                               KOLM1420
C                                                                       KOLM1430
C        ONE SAMPLE TEST USING ALL DISTRIBUTIONS REQUESTED              KOLM1440
C                                                                       KOLM1450
  121 DO 130 I=1,5                                                      KOLM1460
      IF(DIST(I,1))130,130,122                                          KOLM1470
  122 CALL KOLMO(X,N,Z,P,I,DIST(I,2),DIST(I,3),IER)                     KOLM1480
      IES=IER+IES                                                       KOLM1490
      IF(IER)130,124,130                                                KOLM1500
  123 WRITE(6,14)                                                       KOLM1510
      GO TO 136                                                         KOLM1520
C                                                                       KOLM1530
C        OUTPUT RESULTS                                                 KOLM1540
C                                                                       KOLM1550
  124 K=4*I-3                                                           KOLM1560
      WRITE(6,9)TITL(K),TITL(K+1),TITL(K+2),TITL(K+3)                   KOLM1570
      IF(I-3)125,126,127                                                KOLM1580
  125 S2=DIST(I,3)**2                                                   KOLM1590
      WRITE(6,18)DIST(I,2),S2                                           KOLM1600
      GO TO 129                                                         KOLM1610
  126 S2=DIST(I,2)-DIST(I,3)                                            KOLM1620
      WRITE(6,19)DIST(I,2),S2                                           KOLM1630
      GO TO 129                                                         KOLM1640
  127 IF(I-4)128,128,130                                                KOLM1650
  128 WRITE(6,20)DIST(I,2),DIST(I,3)                                    KOLM1660
  129 WRITE(6,21)P,Z                                                    KOLM1670
  130 CONTINUE                                                          KOLM1680
C                                                                       KOLM1690
C        OUTPUT SAMPLE ONE DECISION                                     KOLM1700
C                                                                       KOLM1710
      IF(IO)131,132,131                                                 KOLM1720
  131 WRITE(6,8)                                                        KOLM1730
      WRITE(6,7)(X(J),J=1,N)                                            KOLM1740
  132 IF(IES)123,136,123                                                KOLM1750
C                                                                       KOLM1760
C        TWO SAMPLE TEST                                                KOLM1770
C                                                                       KOLM1780
  133 CALL KOLM2(X,Y,N,M,Z,P)                                           KOLM1790
C                                                                       KOLM1800
C        OUTPUT SAMPLES DECISION                                        KOLM1810
C                                                                       KOLM1820
      IF(IO)134,135,134                                                 KOLM1830
  134 WRITE(6,8)                                                        KOLM1840
      WRITE(6,7)(X(J),J=1,N)                                            KOLM1850
      WRITE(6,10)                                                       KOLM1860
      WRITE(6,7)(Y(J),J=1,M)                                            KOLM1870
  135 WRITE(6,11)P,Z                                                    KOLM1890
  136 IFL=0                                                             KOLM1895
      WRITE(6,22)TITLE                                                  KOLM1900
      GO TO 100                                                         KOLM1910
      END                                                               KOLM1920
```

TRIPLE EXPONENTIAL SMOOTHING

Problem Description

Given a time series X, a smoothing constant, and three coefficients of the prediction equation, this sample program finds the triple exponentially smoothed series S of the time series X.

Program

Description

The sample program for triple exponential smoothing consists of the main program named EXPON, and one subroutine, EXSMO, from the Scientific Subroutine Package.

Capacity

The capacity of the sample program and the format required for data input have been set up as follows:

1. Up to 1000 data points in a given time series
2. (12F6.0) format for input data cards

Therefore, if a problem satisfies the above conditions, the sample program need not be modified. However, if there are more than 1000 data points, the dimension statement in the sample main program must be modified to handle this particular problem. Similarly, if input data cards are prepared using a different format, the input format in the sample main program must be modified. The general rules for program modification are described later.

Input

Control Card

One control card is required for each problem and is read by the main program, EXPON. This card is prepared as follows:

Columns	Contents	For Sample Problem
1- 6	Problem number (may be alphameric)	SAMPLE
7-10	Number of data points in a given time series	0038
11-15	Smoothing constant, α $(0.0 < \alpha < 1.0)$	0.1
16-25	First coefficient (A) of the prediction equation	0.0
26-35	Second coefficient (B) of the prediction equation	0.0
36-45	Third coefficient (C) of the prediction equation	0.0

Smoothing constant and three coefficients must be keypunched with decimal points.

Leading zeros are not required to be keypunched.

Data Card

Time series data are keypunched using the format (12F6.0). This format assumes that each data point is keypunched in a six-column field and twelve fields per card.

Deck Setup

The deck setup is shown in Figure 62.

Sample

The listing of input cards for the sample problem is presented in Figure 63.

Output

Description

The output of the sample program for triple exponential smoothing includes:

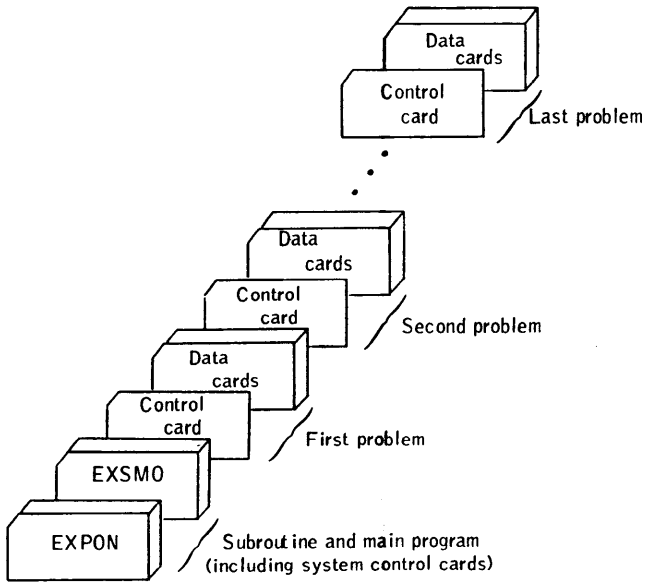


Figure 62. Deck setup (triple exponential smoothing)

```
/DATA                                                                  10
SAMPLE  38  0.1      0.0       0.0       0.0                           20
   430   426   422   419   414   413   412   409   411   417   422   430  30
   438   441   447   455   461   453   448   449   454   463   470   472  40
   476   481   483   487   491   492   485   486   482   479   479   476  50
   472   470                                                            60
```

Figure 63. Input listing (triple exponential smoothing)

1. Original and updated coefficients
2. Time series as input and triple exponentially smoothed time series

Sample

The output listing for the sample problem is shown in Figure 64.

Program Modification

Program capacity can be increased or decreased by making changes in the dimension statement. Input data in a different format can also be handled by providing a specific format statement. In order to familiarize the user with the program modification, the following general rules are supplied in terms of the sample problem.

```
TRIPLE EXPONENTIAL SMOOTHING.....SAMPLE

NUMBER OF DATA POINTS     38
SMOOTHING CONSTANT      0.100

COEFFICIENTS          A              B              C

ORIGINAL            0.0            0.0            0.0

UPDATED         484.80176        1.71309        0.04166

                              SMOOTHED DATA
      INPUT DATA               (FORECAST)
       430.00000                 430.00000
       426.00000                 426.00000
       422.00000                 422.00000
       419.00000                 418.00000
       414.00000                 414.29980
       413.00000                 410.23950
       412.00000                 407.08960
       409.00000                 404.66797
       411.00000                 402.22363
       417.00000                 401.25049
       422.00000                 402.64575
       430.00000                 405.61621
       438.00000                 410.71338
       441.00000                 417.46948
       447.00000                 423.99829
       455.00000                 431.18286
       461.00000                 439.43359
       453.00000                 447.87866
       448.00000                 452.21558
       449.00000                 454.10522
       454.00000                 455.80713
       463.00000                 458.54614
       470.00000                 463.30518
       472.00000                 469.06445
       476.00000                 474.09521
       481.00000                 479.11035
       483.00000                 484.38623
       487.00000                 488.94629
       491.00000                 493.50854
       492.00000                 498.05444
       485.00000                 501.66992
       486.00000                 502.12549
       482.00000                 502.44434
       479.00000                 501.16724
       479.00000                 498.92749
       476.00000                 496.84155
       472.00000                 494.00806
       470.00000                 490.30420
```

Figure 64. Output listing (triple exponential smoothing)

1. Changes in the dimension statement of the main program, EXPON:

The dimension of arrays X and S must be greater than or equal to the number of data points in time series, NX. Since there are 38 data points in the sample problem, the value of NX is 38.

2. Changes in the input format statement of the main program, EXPON:

Only the format statement for input data may be changed. Since sample data are three-digit numbers, rather than using six-column fields as in the sample problem, each data point may be keypunched in a three-column field and 24 fields per card. If so, the format is changed to (24F3.0).

Operating Instructions

The sample program for triple exponential smoothing is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is twelve seconds.

```
C                                                                       EXPO  10
C     ...................................................................EXPO  20
C                                                                       EXPO  30
C        SAMPLE MAIN PROGRAM FOR TRIPLE EXPONENTIAL SMOOTHING - EXPON   EXPO  40
C                                                                       EXPO  50
C        PURPOSE                                                        EXPO  60
C           (1) READ THE PROBLEM PARAMETER CARD AND A TIME SERIES,      EXPO  70
C           (2) CALL THE SUBROUTINE EXSMO TO SMOOTH THE TIME SERIES,    EXPO  80
C           AND (3) PRINT THE RESULT.                                   EXPO  90
C                                                                       EXPO 100
C        REMARKS                                                        EXPO 110
C           A SMOOTHING CONSTANT SPECIFIED IN THE PROBLEM PARAMETER     EXPO 120
C           CARD MUST BE GREATER THAN ZERO BUT LESS THAN ONE IN ORDER   EXPO 130
C           TO OBTAIN REASONABLE RESULTS.                               EXPO 140
C                                                                       EXPO 150
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  EXPO 160
C           EXSMO                                                       EXPO 170
C                                                                       EXPO 180
C        METHOD                                                         EXPO 190
C           REFER TO R. G. BROWN, 'SMOOTHING, FORECASTING AND PREDICTIONEXPO 200
C           OF DISCRETE TIME SERIES', PRENTICE-HALL, N.J., 1963,        EXPO 210
C           PP. 140 TO 144.                                             EXPO 220
C                                                                       EXPO 230
C     ...................................................................EXPO 240
C                                                                       EXPO 250
C     THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE      EXPO 260
C     NUMBER OF DATA POINTS IN A GIVEN TIME SERIES..                    EXPO 270
C                                                                       EXPO 280
      DIMENSION X(1000),S(1000)                                         EXPO 290
C                                                                       EXPO 300
C     ...................................................................EXPO 310
C                                                                       EXPO 320
    1 FORMAT(A4,A2,I4,F5.0,3F10.0)                                      EXPO 330
    2 FORMAT(12F6.0)                                                    EXPO 340
    3 FORMAT(34H1TRIPLE EXPONENTIAL SMOOTHING.....,A4,A2//22H NUMBER OF EXPO 350
     1DATA POINTS,I6/19H SMOOTHING CONSTANT,F9.3/)                      EXPO 360
    4 FORMAT(13HOCOEFFICIENTS,9X,1HA,14X,1HB,14X,1HC)                   EXPO 370
    5 FORMAT(9HOORIGINAL,F19.5,2F15.5)                                  EXPO 380
    6 FORMAT(8HOUPDATED,F20.5,2F15.5/)                                  EXPO 390
    7 FORMAT(1HO,27X,13HSMOOTHED DATA/7X,10HINPUT DATA,12X,10H(FORECAST)EXPO 400
     1)                                                                 EXPO 410
    8 FORMAT(F17.5,8X,F15.5)                                            EXPO 420
C                                                                       EXPO 430
C     ...................................................................EXPO 440
C                                                                       EXPO 450
C     READ PROBLEM PARAMETER CARD                                       EXPO 460
C
  100 READ (5,1) PR,PR1,NX,AL,A,B,C                                     EXPO 470
C        PR......PROBLEM NUMBER (MAY BE ALPHAMERIC)                     EXPO 480
C        PR1.....PROBLEM NUMBER (CONTINUED)                             EXPO 490
C        NX......NUMBER OF DATA POINTS IN TIME SERIES                   EXPO 500
C        AL......SMOOTHING CONSTANT                                     EXPO 510
C        A,B,C...COEFFICIENTS OF THE PREDICTION EQUATION                EXPO 520
C                                                                       EXPO 530
      WRITE (6,3) PR,PR1,NX,AL                                          EXPO 540
C                                                                       EXPO 550
C     PRINT ORIGINAL COEFFICIENTS                                       EXPO 560
C                                                                       EXPO 570
      WRITE (6,4)                                                       EXPO 580
      WRITE (6,5) A,B,C                                                 EXPO 590
                                                                        EXPO 600
```

```
C
C     READ TIME SERIES DATA                                          EXPO 620
C                                                                    EXPO 630
      READ (5,2) (X(I),I=1,NX)                                       EXPO 640
C                                                                    EXPO 650
      CALL EXSMO (X,NX,AL,A,B,C,S)                                   EXPO 660
C                                                                    EXPO 670
C     PRINT UPDATED COEFFICIENTS                                     EXPO 680
C                                                                    EXPO 690
      WRITE (6,6) A,B,C                                              EXPO 700
C                                                                    EXPO 710
C     PRINT INPUT AND SMOOTHED DATA                                  EXPO 720
C                                                                    EXPO 730
      WRITE (6,7)                                                    EXPO 740
      DO 200 I=1,NX                                                  EXPO 750
  200 WRITE (6,8) X(I),S(I)                                          EXPO 760
      GO TO 100                                                      EXPO 770
      END                                                            EXPO 780
```

MATRIX ADDITION

Problem Description

An input matrix is added to another input matrix to form a resultant matrix. Each set of input matrices and the corresponding output matrix is printed. This procedure is repeated until all sets of input matrices have been processed.

Program

Description

The matrix addition program consists of a main routine, ADSAM, and four subroutines, MATIN, MADD, MXOUT, and LOC. MADD and LOC are from the Scientific Subroutine Package. MATIN and MXOUT are sample subroutines for matrix input and output (see program listings).

Capacity

Matrix size has arbitrarily been set at 1000 data elements.

Input

Control Cards

Each input matrix must be preceded by a parameter card with the following format:

Columns	Contents	For Sample Problem
1-2	Blank	
3-6	Up to four-digit identification code	0001
7-10	Number of rows in matrix	0008
11-14	Number of columns in matrix	0011
15-16	Storage mode of matrix 0 for general matrix 1 for symmetric matrix 2 for diagonal matrix	0

Each input matrix must be followed by a card with a 9-punch in column 1.

A blank card after the last pair of input matrices terminates the run.

Data Cards

Data cards are assumed to have seven fields of ten columns each. The decimal point may appear anywhere in a field. If no decimal point is included, it is assumed that the decimal point is to the right of the last digit. The number in each field may be preceded by blanks. Data elements must be punched by row. A row may continue from card to card. However, each new row must start in the first field of the next card. Only the upper triangular portion of a symmetric matrix or the diagonal elements of a diagonal matrix are contained on data cards. The first element of each new row will be the diagonal element for a matrix with symmetric or diagonal storage mode. Columns 71-80 of data cards may be used for identification, sequence numbering, and so on.

Deck Setup

The deck setup is shown in Figure 65.

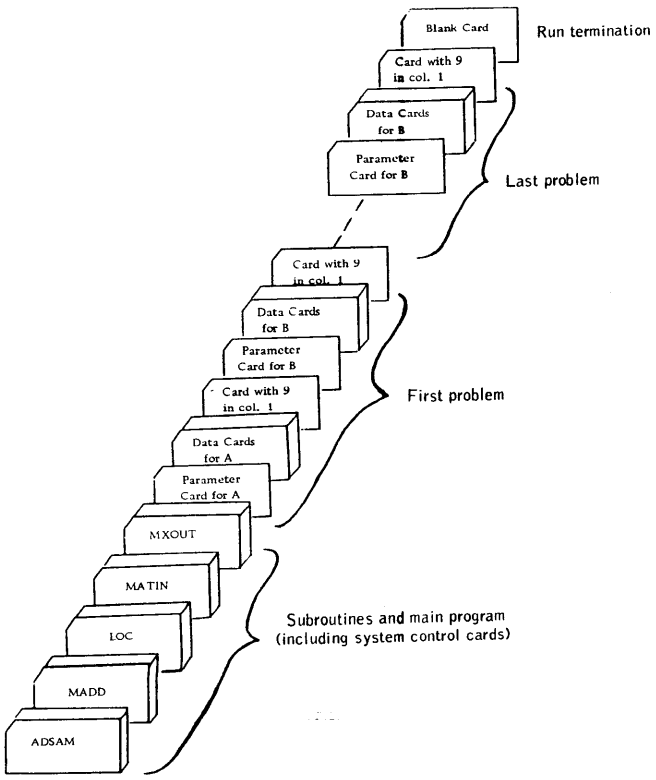


Figure 65. Deck setup (matrix addition)

Sample

A listing of input cards for the sample problem is presented in Figure 66.

```
/DATA
  0001000800110O
 0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
 0.6751766 0.8635910 0.7446845 0.6963269
 0.6544085 1.0000000 0.6271802 0.6194650 0.3547574 0.0027470 0.6010878
 0.5571068 0.7125728 0.6144597 0.5745585
 1.0000000 0.6644085 0.7601008 0.7507505 0.4299425 0.0033291 0.7284786
 0.6373449 0.8152021 0.7029582 0.6573101
 0.6963269 0.5745585 0.6573101 0.6492243 0.3718001 0.0028789 0.6299642
 0.6295047 0.8051740 0.6943108 0.6492243
 0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
 0.3605070 0.4611099 0.3976204 0.3718001
 0.6751766 0.5571068 0.6373449 0.6295047 0.3605070 0.0027915 0.6108296
 0.0027915 0.0035705 0.0030789 0.0028789
 0.0033291 0.0027470 0.0031426 0.0031039 0.0017776 1.0000000 0.0030119
 0.6108296 0.7812874 0.6737132 0.6299642
 0.4299425 0.3547574 0.4058519 0.4038593 1.0000000 0.0017776 0.3889673
 1.0000000 0.7241215 0.6244183 0.5838704
9
  0002000800110O
 0.7507505 0.6194650 0.7086843 1.0000000 0.4008593 0.0031039 0.6792011
 0.7241215 1.0000000 0.7986682 0.7468050
 0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
 0.6244183 0.7986682 1.0000000 0.6439786
 0.8635910 0.7125728 0.8152021 0.8051740 0.4611099 0.0035705 0.7812874
 0.5838704 0.7468050 0.6439786 1.0000000
 0.6963269 0.5745585 0.6573101 0.6492243 0.3718001 0.0028789 0.6299642
 1.0000000 0.6644085 0.7601008 0.7507505 0.4299425 0.0033291 0.7284786
 0.6751766 0.5571068 0.6373449 0.6295047 0.3605070 0.0027915 0.6108296
 0.7284786 0.6010878 0.6876602 0.6792311 0.3889673 0.0030119 1.0000000
 0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132
 0.4299425 0.3547574 0.4058519 0.4008593 1.0000000 0.0017776 0.3889673
 0.8635910 0.7125728 0.8152021 0.8051740 0.4611099 0.0035705 0.7812874
 0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
 0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602
 0.6963269 0.5745585 0.6573101 0.6492243 0.3718001 0.0028789 0.6299642
9
```

Figure 66. Input listing (matrix addition)

Output

Description

The resultant matrix is printed for any size array as a general matrix regardless of the storage mode. Each page is headed with the matrix code number, dimensions, and storage mode. Columns and rows are headed with their respective number. The code number for the output matrix is derived by adding the code numbers for the input matrices.

Sample

The output listing for the sample problem is shown in Figure 67.

Program Modification

Matrix size can be increased or reduced by making the following changes in ADSAM:

1. Modify the DIMENSION statement to reflect the number of elements for A, B, and R.

2. Insert the same number in the third parameter of the two CALL MATIN statements (20 and 45).

```
MATRIX    1       8 ROWS      11 COLUMNS      STORAGE MODE 0      PAGE  1

      COLUMN        1             2             3             4             5             6

 ROW   1  0.7601010E 00  0.6271800E 00  0.1000000E 01  0.7086844E 00  0.4058520E 00  0.3142600E-02
 ROW   2  0.6644408E 00  0.1000000E 01  0.6271800E 00  0.6194650E 00  0.3547570E 00  0.2747000E-02
 ROW   3  0.1000000E 01  0.6644408E 00  0.7601010E 00  0.7507500E 00  0.4299420E 00  0.3329100E-02
 ROW   4  0.6963270E 00  0.5745580E 00  0.6573100E 00  0.6492240E 00  0.3718000E 00  0.2878900E-02
 ROW   5  0.7446844E 00  0.6144600E 00  0.7029580E 00  0.6943110E 00  0.3976200E 00  0.3078900E-02
 ROW   6  0.6751770E 00  0.5571070E 00  0.6373450E 00  0.6295050E 00  0.3605000E 00  0.2791500E-02
 ROW   7  0.3321910E-02  0.2747000E-02  0.3142600E-02  0.3103900E-02  0.1777600E-02  0.1000000E 01
 ROW   8  0.4299420E 00  0.3547570E 00  0.4058520E 00  0.4008590E 00  0.1000000E 01  0.1777600E-02

MATRIX    1       8 ROWS      11 COLUMNS      STORAGE MODE 0      PAGE  2

      COLUMN        7             8             9            10            11

 ROW   1  0.6876660E 00  0.6793010E 00  0.8635910E 00  0.7446840E 00  0.6963270E 00
 ROW   2  0.6010880E 00  0.5571070E 00  0.7125730E 00  0.6144600E 00  0.5745580E 00
 ROW   3  0.7284790E 00  0.6373450E 00  0.8152020E 00  0.7029580E 00  0.6573100E 00
 ROW   4  0.6299640E 00  0.6295050E 00  0.8051740E 00  0.6943110E 00  0.6492240E 00
 ROW   5  0.6737130E 00  0.3605070E 00  0.4611100E 00  0.3976200E 00  0.3718000E 00
 ROW   6  0.6108300E 00  0.2791500E-02  0.3570500E-02  0.3078900E-02  0.2878900E-02
 ROW   7  0.3211900E-02  0.6108300E 00  0.7812870E 00  0.6737130E 00  0.6299640E 00
 ROW   8  0.3889670E 00  0.1000000E 01  0.7241210E 00  0.6244180E 00  0.5838700E 00

MATRIX    2       8 ROWS      11 COLUMNS      STORAGE MODE 0      PAGE  1

      COLUMN        1             2             3             4             5             6

 ROW   1  0.7507500E 00  0.6194650E 00  0.7086844E 00  0.1000000E 01  0.4008590E 00  0.3103900E-02
 ROW   2  0.7446840E 00  0.6144600E 00  0.7029580E 00  0.6943110E 00  0.3976200E 00  0.3078900E-02
 ROW   3  0.8635910E 00  0.7125730E 00  0.8152020E 00  0.8051740E 00  0.4611100E 00  0.3570500E-02
 ROW   4  0.6963270E 00  0.5745580E 00  0.6573100E 00  0.6492240E 00  0.3718000E 00  0.2878900E-02
 ROW   5  0.6751770E 00  0.5571070E 00  0.6373450E 00  0.6295050E 00  0.3605070E 00  0.2791500E-02
 ROW   6  0.7446840E 00  0.6144600E 00  0.7029580E 00  0.6943110E 00  0.3976200E 00  0.3078900E-02
 ROW   7  0.8635910E 00  0.7125730E 00  0.8152020E 00  0.8051740E 00  0.4611100E 00  0.3570500E-02
 ROW   8  0.7601010E 00  0.6271800E 00  0.1000000E 01  0.7086844E 00  0.4058520E 00  0.3142600E-02

MATRIX    2       8 ROWS      11 COLUMNS      STORAGE MODE 0      PAGE  2

      COLUMN        7             8             9            10            11

 ROW   1  0.6792010E 00  0.7241210E 00  0.1000000E 01  0.7986680E 00  0.7468050E 00
 ROW   2  0.6737130E 00  0.6244180E 00  0.7986680E 00  0.1000000E 01  0.6439790E 00
 ROW   3  0.7812870E 00  0.5838700E 00  0.7468050E 00  0.6439790E 00  0.1000000E 01
 ROW   4  0.6299640E 00  0.1000000E 01  0.6644080E 00  0.7601010E 00  0.7507500E 00
 ROW   5  0.6108300E 00  0.7284790E 00  0.6010880E 00  0.6876600E 00  0.6792010E 00
 ROW   6  0.6737130E 00  0.4299420E 00  0.3547570E 00  0.4058520E 00  0.4008590E 00
 ROW   7  0.7812870E 00  0.7601010E 00  0.6271800E 00  0.1000000E 01  0.7086844E 00
 ROW   8  0.6876600E 00  0.6963270E 00  0.5745580E 00  0.6573100E 00  0.6492240E 00

MATRIX    3       8 ROWS      11 COLUMNS      STORAGE MODE 0      PAGE  1

      COLUMN        1             2             3             4             5             6

 ROW   1  0.1510850E 01  0.1246640E 01  0.1708680E 01  0.1708680E 01  0.8067110E 00  0.6244500E-02
 ROW   2  0.1409090E 01  0.1614460E 01  0.1330140E 01  0.1313780E 01  0.7523780E 00  0.5825900E-02
 ROW   3  0.1863590E 01  0.1376980E 01  0.1575300E 01  0.1555920E 01  0.8910520E 00  0.6899600E-02
 ROW   4  0.1392650E 01  0.1149120E 01  0.1314620E 01  0.1298450E 01  0.7436000E 00  0.5757800E-02
 ROW   5  0.1419860E 01  0.1171570E 01  0.1340300E 01  0.1323820E 01  0.7581270E 00  0.5870400E-02
 ROW   6  0.1419860E 01  0.1171570E 01  0.1340300E 01  0.1323820E 01  0.7581270E 00  0.5870400E-02
 ROW   7  0.8669200E 00  0.7153200E 00  0.8183450E 00  0.8082780E 00  0.4628870E 00  0.1003570E 01
 ROW   8  0.1190040E 01  0.9819380E 00  0.1405850E 01  0.1109540E 01  0.1405850E 01  0.4920200E-02

MATRIX    3       8 ROWS      11 COLUMNS      STORAGE MODE 0      PAGE  2

      COLUMN        7             8             9            10            11

 ROW   1  0.1366860E 01  0.1399300E 01  0.1863590E 01  0.1548350E 01  0.1443130E 01
 ROW   2  0.1274800E 01  0.1181520E 01  0.1511240E 01  0.1614460E 01  0.1218540E 01
 ROW   3  0.1509770E 01  0.1221220E 01  0.1562010E 01  0.1346940E 01  0.1657310E 01
 ROW   4  0.1259930E 01  0.1629500E 01  0.1469580E 01  0.1454410E 01  0.1399970E 01
 ROW   5  0.1284540E 01  0.1088990E 01  0.1062200E 01  0.1085280E 01  0.1051000E 01
 ROW   6  0.1284540E 01  0.4327340E 00  0.3583280E 00  0.4089310E 00  0.4037380E 00
 ROW   7  0.7842990E 00  0.1370930E 01  0.1408470E 01  0.1673710E 01  0.1338650E 01
 ROW   8  0.1076630E 01  0.1696330E 01  0.1298680E 01  0.1281730E 01  0.1233090E 01
END OF CASE
```

Figure 67. Output listing (matrix addition)

The output listing is set for 60 print lines per page, 132 print positions across the page, and double spacing. This can be changed by means of the last three parameters in the three-call MXOUT statements in ADSAM (statements 40, 80, 90).

Operating Instructions

The matrix addition sample program is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Error Messages

The following error conditions will result in messages:

1. Reserved storage area is too small for matrix -- DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX (matrix code no.). GO ON TO NEXT CASE.

2. Input matrices do not have the same dimensions -- MATRIX DIMENSIONS NOT CONSISTENT. GO ON TO NEXT CASE.

3. Number of data cards does not correspond to that required by parameter card -- INCORRECT NUMBER OF DATA CARDS FOR MATRIX (matrix code no.). EXECUTION TERMINATED.

Error conditions 1 and 2 allow the computer run to continue. Error condition 3, however, terminates execution and requires another run to process succeeding cases.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 36 seconds.

```
C                                                                       ADSA  10
C    .....................................................................ADSA  20
C                                                                       ADSA  30
C       SAMPLE MAIN PROGRAM FOR MATRIX ADDITION - ADSAM                 ADSA  40
C                                                                       ADSA  50
C       PURPOSE                                                         ADSA  60
C          MATRIX ADDITION SAMPLE PROGRAM                               ADSA  70
C                                                                       ADSA  80
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   ADSA  90
C          MADD                                                         ADSA 100
C          MATIN                                                        ADSA 110
C          MXOUT                                                        ADSA 120
C          LOC                                                          ADSA 130
C                                                                       ADSA 140
C       METHOD                                                          ADSA 150
C          TWO INPUT MATRICES ARE READ FROM THE STANDARD INPUT DEVICE.  ADSA 160
C          THEY ARE ADDED AND THE RESULTANT MATRIX IS LISTED ON         ADSA 170
C          THE STANDARD OUTPUT DEVICE. THIS CAN BE REPEATED FOR ANY     ADSA 180
C          NUMBER OF PAIRS OF MATRICES UNTIL A BLANK CARD IS            ADSA 190
C          ENCOUNTERED                                                  ADSA 200
C                                                                       ADSA 210
C    .....................................................................ADSA 220
C                                                                       ADSA 230
C       MATRICES ARE DIMENSIONED FOR 10CC ELEMENTS. THEREFORE, PRODUCT  ADSA 240
C       OF NUMBER OF ROWS BY NUMBER OF COLUMNS CANNOT EXCEED 1000.      ADSA 250
C                                                                       ADSA 260
      DIMENSION A(1000),B(10000),R(1000)                                ADSA 270
C                                                                       ADSA 280
    1C FORMAT(1H1,15HMATRIX ADDITION)                                   ADSA 290
    11 FORMAT(1HO,44HDIMENSIONED AREA TOO SMALL FOR INPUT MATRIX ,I4)   ADSA 300
    12 FORMAT(1HO,2CHEXECUTION TERMINATED)                              ADSA 310
    13 FORMAT(1HO,32HMATRIX DIMENSIONS NOT CONSISTENT)                  ADSA 320
    14 FORMAT(1HO,42HINCORRECT NUMBER OF DATA CARDS FOR MATRIX ,I4)     ADSA 330
    15 FORMAT(1HO,18HGO ON TO NEXT CASE)                                ADSA 340
    16 FORMAT(1HO,11HEND OF CASE)                                       ADSA 350
C                                                                       ADSA 360
C    .....................................................................ADSA 370
C                                                                       ADSA 380
      WRITE(6,1C)                                                       ADSA 390
    2C CALL MATIN(ICODA,A,1000,NA,MA,MSA,IER)                           ADSA 400
      IF( NA ) 25,95,25                                                 ADSA 410
    25 IF(IER-1) 4J,3C,35                                               ADSA 420
    3C WRITE(6,11) ICODA                                                ADSA 430
      GO TO 45                                                          ADSA 440
    35 WRITE(6,14) ICODA                                                ADSA 450
    37 WRITE(6,12)                                                      ADSA 460
      GO TO 95                                                          ADSA 470
    4C CALL MXOUT(ICODA,A,NA,MA,MSA,60,120,2)                           ADSA 480
    45 CALL MATIN(ICODB,B,1000,NB,MB,MSB,IER)                           ADSA 490
      IF(IER-1) 6C,5C,55                                                ADSA 500
    5C WRITE(6,11) ICODB                                                ADSA 510
      WRITE(6,15)                                                       ADSA 520
      GO TO 2C                                                          ADSA 530
    55 WRITE(6,14) ICODB                                                ADSA 540
      GO TO 37                                                          ADSA 550
    6C IF(NA-NB) 75,7C,75                                               ADSA 560
    7C IF(MA-MB) 75,8C,75                                               ADSA 570
    75 WRITE(6,13)                                                      ADSA 580
      WRITE(6,15)                                                       ADSA 590
      GO TO 2C                                                          ADSA 600
    8C CALL MXOUT(ICODB,B,NB,MB,MSB,60,120,2)                           ADSA 610
      ICODR=ICODA+ICODB                                                 ADSA 620
      CALL MADD(A,B,R,NA,MA,MSA,MSB)                                    ADSA 630
      MSR=MSA                                                           ADSA 640
      IF(MSA-MSB) 9C,9C,85                                              ADSA 650
    85 MSR=MSB                                                          ADSA 660
    9C CALL MXOUT(ICODR,R,NA,MA,MSR,60,120,2)                           ADSA 670
      WRITE(6,16)                                                       ADSA 680
      GO TO 2C                                                          ADSA 690
    95 RETURN                                                           ADSA 700
      END                                                               ADSA 710
```

NUMERICAL QUADRATURE INTEGRATION

Problem Description

The tabulated values of a function for a given spacing are integrated. Multiple sets of tabulated values may be processed.

Program

Description

The numerical quadrature integration program consists of a main routine, QDINT, and one subroutine, QSF, from the Scientific Subroutine Package.

Capacity

Up to 500 tabulated values of a function may be integrated.

Input

Control Cards

Each integration requires a parameter card with the following format:

Columns	Contents	For Sample Problem
1- 5	Up to 5-digit numeric identification code	12345
6-10	Number of tabulated values for this function	0020
11-20	Interval between tabulated values	1.0

The first two parameters consist of up to five digits with no decimal point (FORMAT (2I5)). Note that the second parameter may not exceed 500. The third parameter consists of up to ten digits with decimal point. If no decimal point is included, it is assumed that the decimal point is to the right of the field (FORMAT (F10.0)). A blank card following the last set of data terminates the run.

Data Cards

Data cards are assumed to be seven fields of ten columns each. The decimal point may appear anywhere in the field. The number in each field may be preceded by blanks. Columns 71 through 80 of the data cards may be used for identification, sequence numbering, and so on. If there are more than seven tabulated values, the values should continue from card to card with seven values per card until the number of values specified in the parameter card has been reached.

Deck Setup

The deck setup is shown in Figure 68.

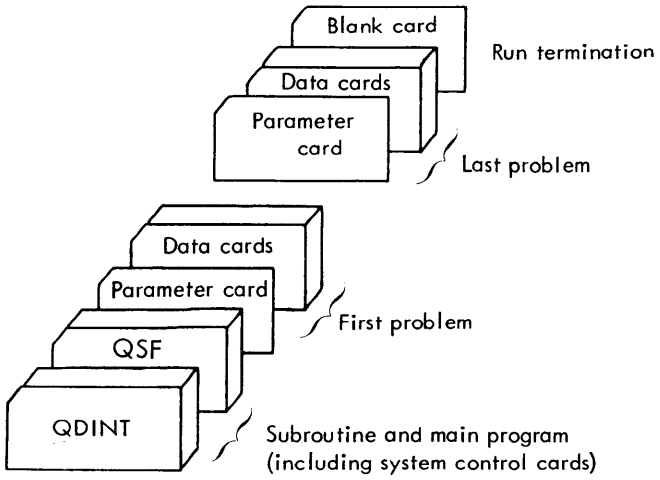


Figure 68 Deck setup (numerical quadrature integration)

Sample

A listing of input cards for the sample program is presented in Figure 69.

```
/DATA
12345   20    1.0                                                        10
        2.0     2.0     2.0     2.0     2.0     2.0     2.0            20
        2.0     2.0     2.0     2.0     2.0     2.0     2.0            30
        2.0     2.0     2.0     2.0     2.0     2.0                    40
  543   10      1.0                                                    50
        1.0     2.0     3.0     4.0     5.0     6.0     7.0            60
        8.0     9.0     10.0                                           70
                                                                       80
                                                                       90
```

Figure 69. Input listing (numerical quadrature integration)

Output

Description

The identification code number, number of tabulated input values, the interval for the tabulated values, and the resultant integral values at each step are printed.

Sample

The output listing for the sample program is shown in Figure 70.

```
INTEGRATION OF TABULATED VALUES FOR DY/DX USING SUBROUTINE QSF

FUNCTION  12345      20 TABULATED VALUES      INTERVAL = 0.10000000E 01

      RESULTANT VALUE OF INTEGRAL AT EACH STEP IS
 0.0           0.19999990E 01 0.39999990E 01 0.59999981E 01 0.79999981E 01 0.99999971E 01
 0.11999697E 02 0.13999996E 02 0.15999996E 02 0.17999985E 02 0.19999985E 02 0.21999969E 02
 0.23999969E 02 0.25999954E 02 0.27999954E 02 0.29999939E 02 0.31999939E 02 0.33999924E 02
 0.35999924E 02 0.37999908E 02

INTEGRATION OF TABULATED VALUES FOR DY/DX USING SUBROUTINE QSF

FUNCTION    543      10 TABULATED VALUES      INTERVAL = 0.10000000E 01

      RESULTANT VALUE OF INTEGRAL AT EACH STEP IS
 0.0           0.14999955E 01 0.39999990E 01 0.74999876E 01 0.11999697E 02 0.17499985E 02
 0.23999985E 02 0.31499969E 02 0.39999969E 02 0.49499954E 02
```

Figure 70. Output listing (numerical quadrature integration)

Program Modification

The maximum number of tabulated values acceptable to the sample program may be changed by modifying the dimension statement in QDINT. The format of the parameter cards and data cards may be changed by modifying statements 10 and 40, respectively, in QDINT.

Operating Instructions

The numerical quadrature integration sample program is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Error Messages

The following conditions will result in error messages:

1. The number of tabulated values specified in the parameter card is less than or equal to one -- ILLEGAL CONDITION. NUMBER OF TABULATED VALUES IS LESS THAN THREE. The program will go on to the next set of data.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is six seconds.

```
C                                                                       QDIN  10
C     .....................................................................QDIN  20
C                                                                       QDIN  30
C        SAMPLE PROGRAM FOR INTEGRATION OF A TABULATED FUNCTION BY      QDIN  40
C        NUMERICAL QUADRATURE - QDINT                                   QDIN  50
C                                                                       QDIN  60
C.       PURPOSE                                                        QDIN  70
C           INTEGRATES A SET OF TABULATED VALUES FOR F(X) GIVEN THE     QDIN  80
C           NUMBER OF VALUES AND THEIR SPACING                          QDIN  90
C                                                                       QDIN 100
C        REMARKS                                                        QDIN 110
C           THE NUMBER OF VALUES MUST BE MORE THAN TWO AND THE SPACING  QDIN 120
C           GREATER THAN ZERO                                           QDIN 130
C                                                                       QDIN 140
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  QDIN 150
C           QSF                                                         QDIN 160
C                                                                       QDIN 170
C        METHOD                                                         QDIN 180
C           READS CONTROL CARD CONTAINING THE CODE NUMBER, NUMBER OF    QDIN 190
C           VALUES, AND THE SPACING OF THE FUNCTION VALUES CONTAINED    QDIN 200
C           ON THE FOLLOWING DATA CARDS. DATA CARDS ARE THEN READ AND   QDIN 210
C           INTEGRATION IS PERFORMED. MORE THAN ONE CONTROL CARD AND    QDIN 220
C           CORRESPONDING DATA CAN BE INTEGRATED IN ONE RUN. EXECUTION  QDIN 230
C           IS TERMINATED BY A BLANK CONTROL CARD.                      QDIN 240
C                                                                       QDIN 250
C     .....................................................................QDIN 260
C                                                                       QDIN 270
C        THE FOLLOWING DIMENSION MUST BE AS LARGE AS THE MAXIMUM NUMBER QDIN 280
C        OF TABULATED VALUES TO BE INTEGRATED                           QDIN 290
C                                                                       QDIN 300
      DIMENSION Z(500)                                                  QDIN 310
C                                                                       QDIN 320
C     .....................................................................QDIN 330
C                                                                       QDIN 340
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  QDIN 350
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      QDIN 360
C        STATEMENT WHICH FOLLOWS.                                       QDIN 370
C                                                                       QDIN 380
C     DOUBLE PRECISION Z,SPACE                                          QDIN 390
C                                                                       QDIN 400
C     .....................................................................QDIN 410
C                                                                       QDIN 420
   10 FORMAT (2I5,F10.0)                                                QDIN 430
   20 FORMAT(1H1,62HINTEGRATION OF TABULATED VALUES FOR DY/DX USING SUBR QDIN 440
     1OUTINE QSF//1H ,10HFUNCTION  ,I5,3X,I5,17H TABULATED VALUES,      QDIN 450
     25X,10HINTERVAL =,E15.8//)                                         QDIN 460
   22 FORMAT(1H ,17HILLEGAL CONDITION/)                                 QDIN 470
   23 FORMAT(1H ,45HNUMBER OF TABULATED VALUES IS LESS THAN THREE)      QDIN 480
   30 FORMAT(1H ,7X,'RESULTANT VALUE OF INTEGRAL AT EACH STEP IS ',     QDIN 490
     1(1H ,6E15.8))                                                     QDIN 500
   32 FORMAT(7F10.0)                                                    QDIN 510
C                                                                       QDIN 520
   35 READ(5,10)ICOD,NUMBR,SPACE                                        QDIN 530
      IF(ICOD+NUMBR)70,70,38                                            QDIN 540
   38 WRITE(6,20)ICOD,NUMBR,SPACE                                       QDIN 550
   50 READ(5,32)(Z(I),I=1,NUMBR)                                        QDIN 560
      IF(NUMBR-3)100,55,55                                              QDIN 570
   55 CALL QSF(SPACE,Z,Z,NUMBR)                                         QDIN 580
   60 WRITE(6,30)(Z(I),I=1,NUMBR)                                       QDIN 590
      GO TO 35                                                          QDIN 600
   70 RETURN                                                            QDIN 610
  100 WRITE(6,22)                                                       QDIN 620
      WRITE (6,23)                                                      QDIN 630
      GO TO 35                                                          QDIN 640
  200 WRITE(6,22)                                                       QDIN 650
      GO TO 35                                                          QDIN 660
      END                                                               QDIN 670
```

RUNGE-KUTTA INTEGRATION

Problem Description

A differential equation of the form:

$$\frac{dy}{dx} = f(x, y)$$

is integrated with initial conditions as specified in a parameter card. The differential equation is defined in the form of a function subprogram that is provided by the user.

Program

Description

The Runge-Kutta integration program consists of a main routine RKINT, one subroutine RK2 from the Scientific Subroutine Package, and one user-supplied function subprogram FUN, which defines the differential equation to be integrated.

Capacity

Up to 500 values of the integral may be tabulated.

Input

Control Cards

Each integration requires a parameter card with the following format:

Columns	Contents	For Sample Problem
1-10	Initial value of $X = X_0$	1.0
11-20	Initial value of $Y = Y(X_0)$	0.0
21-30	Step size	0.01
31-35	Number of steps required between tabulated values	10
36-40	Total number of tabulated values required	30

The first three parameters consist of up to ten digits with decimal point. If no decimal point is included, it is assumed that the decimal point is to the right of the field.

(FORMAT (F10.0))

The last two parameters consist of up to four digits plus a blank with no decimal point.

(FORMAT (15))

Multiple parameter cards may be used. A blank card terminates the run.

Data Cards

None.

Deck Setup

The deck setup is shown in Figure 71.

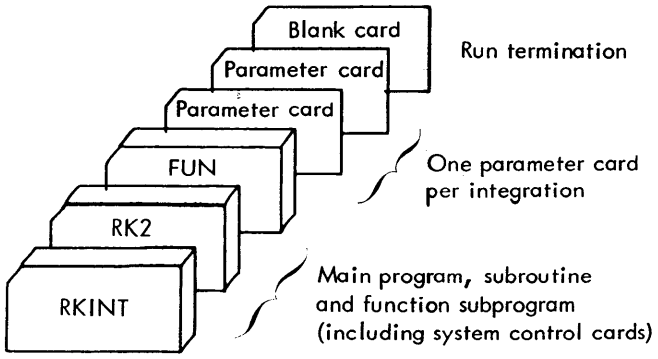


Figure 71. Deck setup (Runge-Kutta integration)

Sample

A listing of the input cards for the sample problem is presented in Figure 72.

```
/DATA
      1.0        0.0        .01    10    30                    10
                                                               20
                                                               30
```

Figure 72. Input listing (Runge-Kutta integration)

Output

Description

The values for the initial conditions and the tabulated values of the integral are printed.

Sample

The output listing for the sample problem is shown in Figure 73.

```
SOLUTION OF DY/DX=FUN(X,Y) BY RK2 SUBROUTINE

  H=  0.010   XO=   1.000   YO=   0.0

    X                    Y(X)


  1.10              0.95310390E-01
  1.20              0.18232232E 00
  1.30              0.26236582E 00
  1.40              0.33647484E 00
  1.50              0.40546888E 00
  1.60              0.47000873E 00
  1.70              0.53063482E 00
  1.80              0.58779466E 00
  1.90              0.64186341E 00
  2.00              0.69315827E 00
  2.10              0.74194998E 00
  2.20              0.78847140E 00
  2.30              0.83292466E 00
  2.40              0.87548572E 00
  2.50              0.91630906E 00
  2.60              0.95553130E 00
  2.70              0.99327296E 00
  2.80              0.10296392E 01
  2.90              0.10647268E 01
  3.00              0.10986242E 01
  3.10              0.11314125E 01
  3.20              0.11631584E 01
  3.30              0.11939259E 01
  3.40              0.12237749E 01
  3.50              0.12527580E 01
  3.60              0.12809258E 01
  3.70              0.13083200E 01
  3.80              0.13349857E 01
  3.90              0.13609591E 01
  4.00              0.13862734E 01
```

Figure 73. Output listing (Runge-Kutta integration)

Program Modification

The function subprogram FUN may be replaced by any function subprogram having the same name and parameter list. In this way, the user may define any desired first-order differential equation. The maximum number of tabulated values may be changed by altering the dimension statement in the sample program RKINT.

Operating Instructions

The sample program for Runge-Kutta integration is a standard FORTRAN program. Special operating instructions are not required. Data set reference 5 is used for input, and data set reference 6 is used for output.

Error Messages

None.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is twelve seconds.

```
C                                                                RKIN  10
C     ...........................................................RKIN  20
C                                                                RKIN  30
C        SAMPLE PROGRAM FOR RUNGE-KUTTA INTEGRATION OF A GIVEN FUNCTION RKIN  40
C        WITH TABULATED OUTPUT - RKINT                           RKIN  50
C                                                                RKIN  60
C        PURPOSE                                                 RKIN  70
C           INTEGRATES THE FUNCTION SUBPROGRAM FUN USING THE INITIAL   RKIN  80
C           CONDITIONS CONTAINED IN CONTROL CARDS.  PRODUCES TABULATED RKIN  90
C           OUTPUT.                                              RKIN 100
C                                                                RKIN 110
C        REMARKS                                                 RKIN 120
C           NONE                                                 RKIN 130
C                                                                RKIN 140
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED           RKIN 150
C           RK2                                                  RKIN 160
C           FUN - USER-SUPPLIED FUNCTION SUBPROGRAM GIVING       RKIN 170
C                 DY/DX=FUN(X,Y)                                 RKIN 180
C                                                                RKIN 190
C        METHOD                                                  RKIN 200
C           READS CONTROL CARD CONTAINING INITIAL VALUES OF X AND Y,   RKIN 210
C           STEP SIZE, NUMBER OF STEPS DESIRED BETWEEN TABULATED VALUES,RKIN 220
C           AND NUMBER OF TABULATED VALUES REQUIRED. PROGRAM THEN ENTERSRKIN 230
C           RK2 TO PERFORM INTEGRATION. MULTIPLE CONTROL CARDS CAN BE   RKIN 240
C           USED ON THE SAME FUNCTION.                           RKIN 250
C                                                                RKIN 260
C     ...........................................................RKIN 270
C                                                                RKIN 280
C        THE FOLLOWING DIMENSION MUST BE AS LARGE AS THE MAXIMUM RKIN 290
C        NUMBER OF TABULATED VALUES DESIRED                      RKIN 300
C                                                                RKIN 310
      DIMENSION A(500)                                           RKIN 320
C                                                                RKIN 330
      EXTERNAL FUN                                               RKIN 340
C                                                                RKIN 350
C     ...........................................................RKIN 360
C                                                                RKIN 370
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE RKIN 380
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION   RKIN 390
C        STATEMENT WHICH FOLLOWS.                                RKIN 400
C                                                                RKIN 410
C     DOUBLE PRECISION H,XO,YO,A,FUN                             RKIN 420
C                                                                RKIN 430
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS RKIN 440
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS   RKIN 450
C        ROUTINE.                                                RKIN 460
C                                                                RKIN 470
C        USER FUNCTION SUBPROGRAM, FUN, MUST BE IN DOUBLE PRECISION. RKIN 480
C                                                                RKIN 490
C        ...........................................................RKIN 500
C                                                                RKIN 510
    1 FORMAT (3F10.0,2I5)                                        RKIN 520
    2 FORMAT(1H1,7X,44HSOLUTION OF DY/DX=FUN(X,Y) BY RK2 SUBROUTINE//  RKIN 530
     11H ,1CX,2HH=,F7.3,2X,3HXO=,F7.3, 2X,3HYO=,F7.3//1H ,12X,1HX,18X,  RKIN 540
     24HY(X)//)                                                  RKIN 550
    3 FORMAT(1H ,1CX,F5.2,10X,E15.8)                             RKIN 560
C                                                                RKIN 570
C        READ CONTROL CARD CONTAINING ITEMS LISTED UNDER METHOD. RKIN 580
C                                                                RKIN 590
   10 READ(5,1)XO,YO,H,JNT,IENT                                  RKIN 600
C                                                                RKIN 610
C        CHECK IF CARD IS BLANK. IF SO, RETURN.                  RKIN 620
C                                                                RKIN 630
      IF(IENT)20,40,20                                           RKIN 640
C                                                                RKIN 650
C        WRITE HEADING INFORMATION.                              RKIN 660
C                                                                RKIN 670
   20 WRITE(6,2)H,XO,YO                                          RKIN 680
C                                                                RKIN 690
C        PERFORM INTEGRATION                                     RKIN 700
C                                                                RKIN 710
      CALL RK2(FUN,H,XO,YO,JNT,IENT,A)                           RKIN 720
C                                                                RKIN 730
C        WRITE OUTPUT                                            RKIN 740
C                                                                RKIN 750
      STEP=FLOAT(JNT)*H                                          RKIN 760
      X=XO                                                       RKIN 770
```

```
      DO 30 I=1,IENT                                                    RKIN 780
      X=X+STEP                                                          RKIN 790
   30 WRITE(6,31)X,A(I)                                                 RKIN 800
C                                                                       RKIN 810
C        GO BACK AND CHECK FOR ADDITIONAL CONTROL CARD.                 RKIN 820
C                                                                       RKIN 830
      GO TO 10                                                          RKIN 840
   40 RETURN                                                            RKIN 850
      END                                                               RKIN 860
```

POLYNOMIAL ROOTS

Problem Description

The real and complex roots are computed for a real polynomial with given coefficients. Multiple sets of coefficients may be processed.

Program

Description

The polynomial roots sample program consists of a main routine, SMPRT, and one subroutine POLRT from the Scientific Subroutine Package.

Capacity

Roots for polynomials of order 36 or less may be computed.

Input

Control Cards

Each set of data requires a control card with the following format:

Columns	Contents	For Sample Problem
1	Blank	
2-5	Up to four-digit identification code	360
6-8	Blank	
9-10	Order of polynomial	9

The first parameter consists of up to four digits without decimal point. The second parameter consists of up to two digits with no decimal point. The order of the polynomial must be less than or equal to 36.

Data Cards

Data cards are assumed to have seven fields of ten columns each. The decimal point may appear anywhere in the field. If no decimal point is included, it is assumed to be to the right of the field. The number in each field may be preceded by blanks. Columns 71 to 80 of the data cards may be used for identification, sequence numbering, and so on. If there are more than seven coefficients, the values should continue from card to card with seven values per card until the number of values has been reached that is one greater than the order of the polynomial.

The first coefficient is for the constant term of the polynomial and the last coefficient for the highest order term. Fields with zero coefficients may be left blank.

Deck Setup

The deck setup is shown in Figure 74.

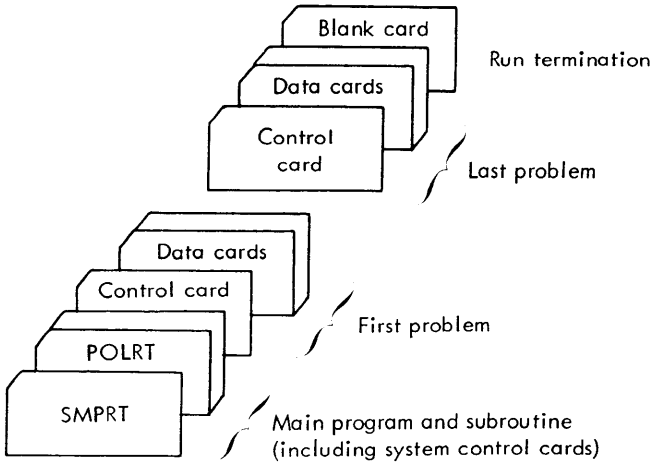


Figure 74. Deck setup (polynomial roots)

Sample

A listing of the input cards for the sample program is shown in Figure 75.

```
/DATA
 360    9
     -1.0
                    1.0                                  1.0
                                                                    10
                                                                    20
                                                                    30
                                                                    40
                                                                    50
```

Figure 75. Input listing (polynomial roots)

Output

Description

The identification code, the polynomial order, the input coefficients, and the real and complex roots are printed.

Sample

The output listing of the sample program is shown in Figure 76.

```
REAL AND COMPLEX ROOTS OF A POLYNOMIAL USING SUBROUTINE POLRT

FOR POLYNOMIAL   360  OF ORDER   9

THE INPUT COEFFICIENTS ARE

-0.10000000E 01   0.0            0.0            0.0            0.0            0.0
 0.10000000E 01   0.0            0.0            0.10000000E 01

     REAL ROOT       COMPLEX ROOT

  0.7206228E 00    0.7609009E 00
  0.7206228E 00   -0.7609009E 00
 -0.1019271E 01   -0.2436270E 00
 -0.1019271E 01    0.2436270E 00
  0.9105257E 00    0.0
 -0.4552628E 00   -0.7885384E 00
 -0.4552628E 00    0.7885384E 00
  0.2986479E 00   -0.1004528E 01
  0.2986479E 00    0.1004528E 01
```

Figure 76. Output listing (polynomial roots)

Program Modification

The maximum order of the polynomial is fixed by the subroutine POLRT. The sample program can accept polynomials up to the maximum of 36th order, which is allowed by the subroutine. The format of the control card and data cards may be changed by modifying statements 10 and 40, respectively, in SMPRT.

Operating Instructions

The polynomial roots sample program is a standard FORTRAN program. Special operating instructions are not required. Data set 5 is used for input, and data set 6 is used for output.

Error Messages

The following conditions will result in error messages:

1. The order of the polynomial specified in the control card is less than one -- ORDER OF POLYNOMIAL LESS THAN ONE.

   The program will go on to the next set of data.

2. The order of the polynomial specified in the control card is greater than 36 -- ORDER OF POLYNOMIAL GREATER THAN 36.

   The program will go on to the next set of data.

3. The subroutine POLRT is unable to determine a root after 500 iterations on eight different starting values -- UNABLE TO DETERMINE ROOT. THOSE ALREADY FOUND ARE....

   The program will print all the roots that were computed and then go on to the next set of data.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is eleven seconds.

```
C                                                                       SMPR  10
C     .................................................................SMPR  20
C                                                                       SMPR  30
C        SAMPLE PROGRAM FOR REAL AND COMPLEX ROOTS OF A REAL POLY-      SMPR  40
C        NOMIAL - SMPRT                                                 SMPR  50
C                                                                       SMPR  60
C        PURPOSE                                                        SMPR  70
C           COMPUTES THE REAL AND COMPLEX ROOTS OF A REAL POLYNOMIAL    SMPR  80
C           WHOSE COEFFICIENTS ARE INPUT.                               SMPR  90
C                                                                       SMPR 100
C        REMARKS                                                        SMPR 110
C           THE ORDER OF THE POLYNOMIAL MUST BE GREATER THAN ONE AND    SMPR 120
C           LESS THAN THIRTY SEVEN                                      SMPR 130
C                                                                       SMPR 140
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SMPR 150
C           POLRT                                                       SMPR 160
C                                                                       SMPR 170
C        METHOD                                                         SMPR 180
C           READS A CONTROL CARD CONTAINING THE IDENTIFICATION CODE AND SMPR 190
C           THE ORDER OF THE POLYNOMIAL WHOSE COEFFICIENTS ARE          SMPR 200
C           CONTAINED ON THE FOLLOWING DATA CARDS. THE COEFFICIENTS     SMPR 210
C           ARE THEN READ AND THE ROOTS ARE COMPUTED.                   SMPR 220
C           MORE THAN ONE CONTROL CARD AND CORRESPONDING DATA CAN BE    SMPR 230
C           PROCESSED. EXECUTION IS TERMINATED BY A BLANK CONTROL CARD. SMPR 240
C                                                                       SMPR 250
C     .................................................................SMPR 260
C                                                                       SMPR 270
      DIMENSION A(37),W(37),ROOTR(37),ROOTI(37)                         SMPR 280
C                                                                       SMPR 290
C     .................................................................SMPR 300
C                                                                       SMPR 310
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  SMPR 320
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      SMPR 330
C        STATEMENT WHICH FOLLOWS.                                       SMPR 340
C                                                                       SMPR 350
C     DOUBLE PRECISION A,W,ROOTR,ROOTI                                  SMPR 360
C                                                                       SMPR 370
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    SMPR 380
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      SMPR 390
C        ROUTINE.                                                       SMPR 400
C                                                                       SMPR 410
C     .................................................................SMPR 420
C                                                                       SMPR 430
    5 READ(5,10)ID,IORD                                                 SMPR 440
   10 FORMAT(1X,I4,3X,I2)                                               SMPR 450
      IF(ID+IORD)100,100,20                                             SMPR 460
   20 WRITE(6,30)ID,IORD                                                SMPR 470
   30 FORMAT(1H1,61HREAL AND COMPLEX ROOTS OF A POLYNOMIAL USING SUBROUTSMPR 480
     1INE POLRT///  17H FOR POLYNOMIAL  ,I4,2X,10HOF ORDER  ,I2//1H ,26HSMPR 490
     2THE INPUT COEFFICIENTS ARE//)                                     SMPR 500
      J=IORD+1                                                          SMPR 510
      READ(5,40)(A(I),I=1,J)                                            SMPR 520
   40 FORMAT(7F10.0)                                                    SMPR 530
      WRITE(6,50)(A(I),I=1,J)                                           SMPR 540
   50 FORMAT(6E16.7)                                                    SMPR 550
      CALL POLRT(A,W,IORD,ROOTR,ROOTI,IER)                              SMPR 560
      IF(IER-1)90,60,70                                                 SMPR 570
   60 WRITE(6,65)                                                       SMPR 580
   65 FORMAT(//1H ,33HORDER OF POLYNOMIAL LESS THAN ONE)                SMPR 590
      GO TO 5                                                           SMPR 600
   70 IF(IER-3)75,80,78                                                 SMPR 610
   75 WRITE(6,77)                                                       SMPR 620
   77 FORMAT(//1H ,35HORDER OF POLYNOMIAL GREATER THAN 36)              SMPR 630
      GO TO 5                                                           SMPR 640
   78 WRITE(6,79)                                                       SMPR 650
   79 FORMAT(//1H ,31H HIGH ORDER COEFFICIENT IS ZERO)                  SMPR 660
      GO TO 5                                                           SMPR 670
   80 WRITE(6,85)                                                       SMPR 680
   85 FORMAT(//1H ,49HUNABLE TO DETERMINE ROOT. THOSE ALREADY FOUND ARE)SMPR 690
   90 WRITE(6,95)                                                       SMPR 700
   95 FORMAT(//1H ,5X,9HREAL ROOT,6X,12HCOMPLEX ROOT//)                 SMPR 710
      DO 96 I=1,IORD                                                    SMPR 720
   96 WRITE(6,97)ROOTR(I),ROOTI(I)                                      SMPR 730
   97 FORMAT(1H ,2E16.7)                                                SMPR 740
      GO TO 5                                                           SMPR 750
  100 RETURN                                                            SMPR 760
      END                                                               SMPR 770
```

SOLUTION OF SIMULTANEOUS EQUATIONS

Problem Description

A solution is obtained for a set of simultaneous equations by the method of elimination using largest pivotal divisor. Both the input data and the solution values are printed. This procedure is repeated until all sets of input data have been processed.

Program

Description

The solution of the simultaneous equations program consists of a main routine, SOLN, and four subroutines, MATIN, SIMQ, MXOUT, and LOC. SIMQ and LOC are from the Scientific Subroutine Package. MATIN and MXOUT are sample subroutines for matrix input and output (see program listings).

Capacity

The program will solve up to 50 equations. This can easily be changed as described under "Program Modification" below.

Input

Control Cards

A parameter card with the following format must precede each matrix of coefficients:

Columns	Contents	For Sample Problem
1-2	Blank	
3-6	Up to four-digit identification code (numeric only)	1
7-10	Number of rows in matrix	10
11-14	Number of columns in matrix (same as number of rows)	10

Each matrix must be followed by a card with a 9-punch in column 1. This, in turn, is followed by the constant vector.

A blank card after the last set of input data terminates the run.

Data Cards

Data Cards are assumed to have seven fields of ten columns each. The decimal point may appear anywhere in a field. If no decimal point is included, it is assumed that the decimal point is to the right of the last digit. The number in each field may be preceded by blanks. Equation coefficients must be punched by row. A row may continue from card to card. However, each new row must start in the first field of the next card. The vector of constants is punched in continuous data fields following the 9 card. Columns 71-80 of data cards may be used for identification, sequence numbering, and so on.

Deck Setup

The deck setup is shown in Figure 77.

Sample

A listing of input cards for the sample problem is presented in Figure 78.

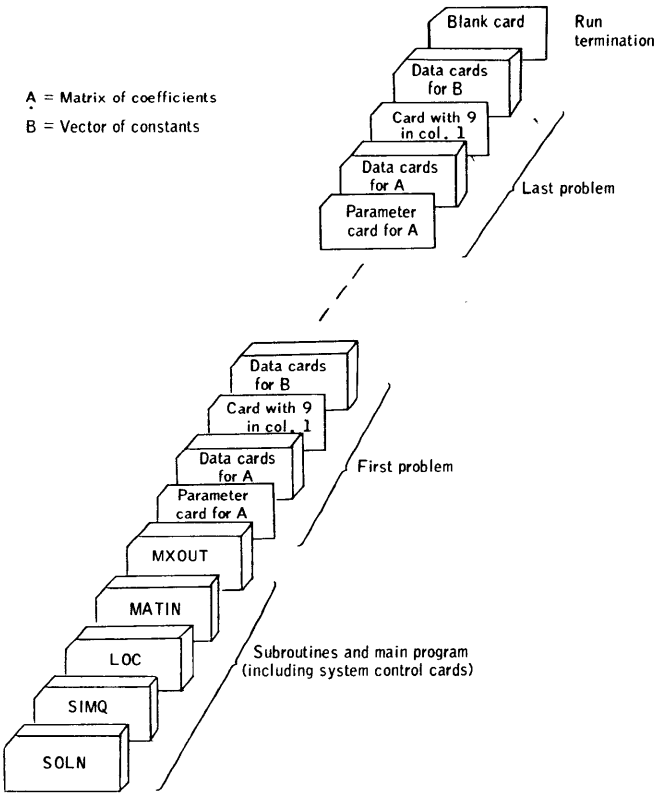


Figure 77. Deck setup (solution of simultaneous equations)

```
/DATA                                                                    10
  000100100010                                                           20
 1.0000000 0.6644085 0.7501008 0.7507505 0.4299425 0.0033291 0.7284786   30
 0.6751766 0.8635910 0.7446845                                           40
 0.6644085 1.0000000 0.6271802 0.6194650 0.3547574 0.0027470 0.6010878   50
 0.5571068 0.7125728 0.6144597                                           60
 0.7601008 0.6271802 1.0000000 0.7086843 0.4058519 0.0031426 0.6876602   70
 0.6373449 0.8152021 0.7029582                                           80
 0.7507505 0.6194650 0.7086843 1.0000000 0.4008593 0.0031039 0.6792011   90
 0.6295047 0.8051740 0.6943108                                          100
 0.4299425 0.3547574 0.4058519 0.4008593 1.0000000 0.0017776 0.3889673  110
 0.3605070 0.4611099 0.3976204                                          120
 0.0033291 0.0027470 0.0031426 0.0031039 0.0017776 1.0000000 0.0030119  130
 0.0027915 0.0035705 0.0030789                                          140
 0.7284786 0.6010878 0.6876602 0.6792011 0.3889673 0.0030119 1.0000000  150
 0.6108296 0.7812874 0.6737132                                          160
 0.6751766 0.5571068 0.6373449 0.6295047 0.3605070 0.0027915 0.6108296  170
 1.0000000 0.7241215 0.6244183                                          180
 0.8635910 0.7125728 0.8152021 0.8051740 0.4611099 0.0035705 0.7812874  190
 0.7241215 1.0000000 0.7986682                                          200
 0.7446845 0.6144597 0.7029582 0.6943108 0.3976204 0.0030789 0.6737132  210
 0.6244183 0.7986682 1.0000000                                          220
9                                                                       230
 110.     -120.      10.      145.     -50.      44.2     -14.          240
  38.5     22.     1650.                                                250
```

Figure 78. Input listing (solution of simultaneous equations)

Output

Description

The original matrix is printed for any size array. Each page is headed with the matrix code number, dimensions, and storage mode (always 0 in this sample program). Columns and rows are headed with their respective number. The original vector of constants is also printed. The solution values are then listed. This output is given for each case to be processed.

Sample

The output listing for the sample problem is shown in Figure 79.

```
MATRIX    1     10 ROWS     10 COLUMNS     STORAGE MODE 0     PAGE  1

          COLUMN      1             2             3             4             5             6
  ROW   1   0.100000E 01   0.664408E 00   0.760101E 00   0.750750E 00   0.429942E 00   0.332910E-02
  ROW   2   0.664408E 00   0.100000E 01   0.627180E 00   0.619465E 00   0.354757E 00   0.274700E-02
  ROW   3   0.760101E 00   0.627180E 00   0.100000E 01   0.708684E 00   0.405852E 00   0.314260E-02
  ROW   4   0.750750E 00   0.619465E 00   0.708684E 00   0.100000E 01   0.400859E 00   0.310390E-02
  ROW   5   0.429942E 00   0.354757E 00   0.405852E 00   0.400859E 00   0.100000E 01   0.177760E-02
  ROW   6   0.332910E-02   0.274700E-02   0.314260E-02   0.310390E-02   0.177760E-02   0.100000E 01
  ROW   7   0.728479E 00   0.601088E 00   0.687660E 00   0.679201E 00   0.388967E 00   0.301190E-02
  ROW   8   0.675177E 00   0.557107E 00   0.637345E 00   0.629505E 00   0.360507E 00   0.279150E-02
  ROW   9   0.863591E 00   0.712573E 00   0.815202E 00   0.805174E 00   0.461110E 00   0.357050E-02
  ROW  10   0.744684E 00   0.614460E 00   0.702958E 00   0.694311E 00   0.397620E 00   0.307890E-02

MATRIX    1     10 ROWS     10 COLUMNS     STORAGE MODE 0     PAGE  2

          COLUMN      7             8             9            10
  ROW   1   0.728479E 00   0.675177E 00   0.863591E 00   0.744684E 00
  ROW   2   0.601088E 00   0.557107E 00   0.712573E 00   0.614460E 00
  ROW   3   0.687666E 00   0.637345E 00   0.815202E 00   0.702958E 00
  ROW   4   0.679201E 00   0.629505E 00   0.805174E 00   0.694311E 00
  ROW   5   0.388967E 00   0.360507E 00   0.461110E 00   0.397620E 00
  ROW   6   0.301190E-02   0.279150E-02   0.357050E-02   0.307890E-02
  ROW   7   0.100000E 01   0.610830E 00   0.781287E 00   0.673713E 00
  ROW   8   0.610830E 00   0.100000E 01   0.724121E 00   0.624418E 00
  ROW   9   0.781287E 00   0.724121E 00   0.100000E 01   0.798668E 00
  ROW  10   0.673713E 00   0.624418E 00   0.798668E 00   0.100000E 01

ORIGINAL B VECTOR

 1          0.110000E 03
 2         -0.120000E 03
 3          0.100000E 02
 4          0.145000E 03
 5         -0.500000E 02
 6          0.442000E 02
 7         -0.140000E 02
 8          0.385000E 02
 9          0.220000E 02
10          0.165000E 04

SOLUTION VALUES

 1         -0.283124E 03
 2         -0.567240E 03
 3         -0.516456E 03
 4         -0.299155E 02
 5         -0.179352E 03
 6          0.435176E 02
 7         -0.479274E 03
 8         -0.230430E 03
 9         -0.210172E 04
10          0.480574E 04

END OF CASE
```

Figure 79. Output listing (solution of simultaneous equations)

Program Modification

The size of the maximum problem to be solved can be increased or decreased by making the following changes in SOLN:

1. Modify the DIMENSION statement to reflect the maximum number of elements for matrix A (= N x N) and the maximum number of equations (N) for B.

2. Insert the dimension size for A in the third argument of the CALL MATIN statement (statement 25).

The matrix listing is set for 60 print lines per page, 120 print positions across the page, and double spacing. This can be changed by means of the last three arguments in the CALL MXOUT statement in SOLN (statement 65). The format of solution values can be altered by changing statement 21 in SOLN.

Operating Instructions

The sample program for the solution of simultaneous equations is a standard FORTRAN program. Special operating instructions are not required. Data set reference 5 is used for input, and data set reference 6 is used for output.

Error Messages

The following error conditions will result in messages:

1. Reserved storage area is too small for matrix -- DIMENSIONED AREA TOO SMALL FOR INPUT MATRIX (matrix code no.). GO ON TO NEXT CASE.
2. Matrix of coefficients is not square -- ROW AND COLUMN DIMENSIONS NOT EQUAL FOR MATRIX (matrix code no.). GO ON TO NEXT CASE.
3. Number of data cards does not correspond to that required by parameter card -- INCORRECT NUMBER OF DATA CARDS FOR MATRIX (matrix code no.). EXECUTION TERMINATED.
4. Singular input matrix -- MATRIX IS SINGULAR. GO ON TO NEXT CASE.

Error conditions 1, 2, and 4 allow the computer run to continue. Error condition 3, however, terminates execution and requires another run to process succeeding cases.

Timing

The execution time of this sample program on a System/360, Model 30, using an IBM 2540 Card Reader as input and an IBM 1403, Model 3 as output, is 21 seconds.

```
C                                                                       SOLN  10
C     ..................................................................SOLN  20
C                                                                       SOLN  30
C        SAMPLE MAIN PROGRAM - SOLN                                     SOLN  40
C                                                                       SOLN  50
C        PURPOSE                                                        SOLN  60
C           SOLUTION OF A SET OF SIMULTANEOUS EQUATIONS                 SOLN  70
C                                                                       SOLN  80
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  SOLN  90
C           SIMQ                                                        SOLN 100
C           MATIN                                                       SOLN 110
C           MXOUT                                                       SOLN 120
C           LOC                                                         SOLN 130
C                                                                       SOLN 140
C        METHOD                                                         SOLN 150
C           A MATRIX OF SIMULTANEOUS EQUATIONS COEFFICIENTS AND A VECTORSOLN 160
C           OF CONSTANTS ARE READ FROM THE STANDARD INPUT DEVICE. THE   SOLN 170
C           SOLUTION IS OBTAINED AND LISTED ON THE STANDARD OUTPUT      SOLN 180
C           DEVICE. THIS PROCEDURE IS REPEATED FOR OTHER SETS OF        SOLN 190
C           EQUATIONS UNTIL A BLANK CARD IS ENCOUNTERED.                SOLN 200
C                                                                       SOLN 210
C     ..................................................................SOLN 220
C                                                                       SOLN 230
C        MATRIX IS DIMENSIONED FOR 2500 ELEMENTS. THEREFORE, NUMBER OF  SOLN 240
C        EQUATIONS TO BE SOLVED CANNOT EXCEED 50 UNLESS DIMENSION       SOLN 250
C        STATEMENT IS CHANGED                                           SOLN 260
C                                                                       SOLN 270
      DIMENSION A(2500),B(50)                                           SOLN 280
C                                                                       SOLN 290
   10 FORMAT(1H1,34HSOLUTION OF SIMULTANEOUS EQUATIONS)                 SOLN 300
   11 FORMAT(1HO,44HDIMENSIONED AREA TOO SMALL FOR INPUT MATRIX ,I4)    SOLN 310
   12 FORMAT(1HO,20HEXECUTION TERMINATED)                               SOLN 320
   13 FORMAT(1HO,47HROW AND COLUMN DIMENSIONS NOT EQUAL FOR MATRIX ,I4) SOLN 330
   14 FORMAT(1HO,42HINCORRECT NUMBER OF DATA CARDS FOR MATRIX ,I4)      SOLN 340
   15 FORMAT(1HO,18HGO ON TO NEXT CASE)                                 SOLN 350
   16 FORMAT(1HO,38HSTRUCTURE CODE IS NOT ZERO FOR MATRIX ,I4)          SOLN 360
   17 FORMAT(1H1,17HORIGINAL B VECTOR,////)                             SOLN 370
   18 FORMAT(1H1,15HSOLUTION VALUES,////)                               SOLN 380
   19 FORMAT(1HO,18HMATRIX IS SINGULAR)                                 SOLN 390
   20 FORMAT(7F10.0)                                                    SOLN 400
   21 FORMAT(I3,10X,E16.6)                                              SOLN 410
   22 FORMAT(1HO,11HEND OF CASE)                                        SOLN 420
C                                                                       SOLN 430
C     ..................................................................SOLN 440
C                                                                       SOLN 450
      WRITE (6,10)                                                      SOLN 460
   25 CALL MATIN(ICOD,A,2500,N,M,MS,IER)                                SOLN 470
      IF(N) 30,95,30                                                    SOLN 480
   30 IF(IER-1) 45,35,40                                                SOLN 490
   35 WRITE(6,11) ICOD                                                  SOLN 500
      GO TO 90                                                          SOLN 510
   40 WRITE(6,14) ICOD                                                  SOLN 520
      GO TO 95                                                          SOLN 530
   45 IF(M-N) 50,55,50                                                  SOLN 540
   50 WRITE(6,13) ICOD                                                  SOLN 550
      GO TO 90                                                          SOLN 560
   55 IF(MS) 60,65,60                                                   SOLN 570
   60 WRITE(6,16) ICOD                                                  SOLN 580
      GO TO 90                                                          SOLN 590
   65 CALL MXOUT(ICOD,A,N,M,MS,60,120,2)                                SOLN 600
      READ(5,20)(B(I),I=1,N)                                            SOLN 610
      WRITE(6,17)                                                       SOLN 620
      DO 70 I=1,N                                                       SOLN 630
   70 WRITE(6,21) I,B(I)                                                SOLN 640
      CALL SIMQ(A,B,N,KS)                                               SOLN 650
      IF(KS-1) 80,75,80                                                 SOLN 660
   75 WRITE(6,19)                                                       SOLN 670
      WRITE(6,15)                                                       SOLN 680
      GO TO 25                                                          SOLN 690
   80 WRITE(6,18)                                                       SOLN 700
      DO 85 I=1,N                                                       SOLN 710
   85 WRITE(6,21) I,B(I)                                                SOLN 720
      WRITE(6,22)                                                       SOLN 730
      GO TO 25                                                          SOLN 740
   90 READ(5,20)(B(I),I=1,N)                                            SOLN 750
      WRITE(6,15)                                                       SOLN 760
      GO TO 25                                                          SOLN 770
   95 WRITE(6,12)                                                       SOLN 780
      RETURN                                                            SOLN 790
      END                                                               SOLN 800
```

SPECIAL SUBROUTINES USED WITH SAMPLE PROGRAMS

```
C                                                                       BOOL  10
C     ..................................................................BOOL  20
C                                                                       BOOL  30
C        USER-SUPPLIED SPECIAL SUBROUTINE - BOOL                        BOOL  40
C                                                                       BOOL  50
C        THIS SPECIAL SUBROUTINE ILLUSTRATES AN EXTERNAL SUBROUTINE     BOOL  60
C        CALLED BY SUBROUTINE SUBST.                                    BOOL  70
C                                                                       BOOL  80
C        IF DIFFERENT PROPOSITIONS ARE USED FOR DIFFERENT PROBLEMS IN   BOOL  90
C        THE SAME RUN, DIFFERENT SUBROUTINES WITH APPROPRIATE PROPOSI-  BOOL 100
C        TIONS MUST BE COMPILED UNDER DIFFERENT NAMES.  IF SO, THESE    BOOL 110
C        SUBROUTINE NAMES MUST BE DEFINED BY AN EXTERNAL STATEMENT      BOOL 120
C        APPEARING IN THE MAIN PROGRAM WHICH CALLS SUBST.  THEN, FOR    BOOL 130
C        EACH PROBLEM, SUBST IS CALLED WITH A PROPER SUBROUTINE NAME    BOOL 140
C        IN ITS ARGUMENT LIST.                                          BOOL 150
C                                                                       BOOL 160
C     ..................................................................BOOL 170
C                                                                       BOOL 180
      SUBROUTINE BOOL(R,T)                                              BOOL 190
      DIMENSION R(1)                                                    BOOL 200
C                                                                       BOOL 210
      T=R(1)*R(2)                                                       BOOL 220
C                                                                       BOOL 230
      RETURN                                                            BOOL 240
      END                                                               BOOL 250
```

```
C                                                                       DATA  10
C     ..................................................................DATA  20
C                                                                       DATA  30
C        SAMPLE INPUT SUBROUTINE - DATA                                 DATA  40
C                                                                       DATA  50
C        PURPOSE                                                        DATA  60
C           READ AN OBSERVATION (M DATA VALUES) FROM INPUT DEVICE.      DATA  70
C           THIS SUBROUTINE IS CALLED BY THE SUBROUTINE CORRE AND MUST  DATA  80
C           BE PROVIDED BY THE USER.  IF SIZE AND LOCATION OF DATA      DATA  90
C           FIELDS ARE DIFFERENT FROM PROBLEM TO PROBLEM, THIS SUB-     DATA 100
C           ROUTINE MUST BE RECOMPILED WITH A PROPER FORMAT STATEMENT.  DATA 110
C                                                                       DATA 120
C        USAGE                                                          DATA 130
C           CALL DATA (M,D)                                             DATA 140
C                                                                       DATA 150
C        DESCRIPTION OF PARAMETERS                                      DATA 160
C           M - THE NUMBER OF VARIABLES IN AN OBSERVATION.              DATA 170
C           D - OUTPUT VECTOR OF LENGTH M CONTAINING THE OBSERVATION    DATA 180
C               DATA.,                                                  DATA 190
C                                                                       DATA 200
C        REMARKS                                                        DATA 210
C           THE TYPE OF CONVERSION SPECIFIED IN THE FORMAT MUST BE      DATA 220
C           EITHER F OR E.                                              DATA 230
C                                                                       DATA 240
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  DATA 250
C           NONE                                                        DATA 260
C     ..................................................................DATA 270
C                                                                       DATA 280
      SUBROUTINE DATA (M,D)                                             DATA 290
C                                                                       DATA 300
      DIMENSION D(1)                                                    DATA 310
C                                                                       DATA 320
    1 FORMAT(12F6.0)                                                    DATA 330
C                                                                       DATA 340
C     READ AN OBSERVATION FROM INPUT DEVICE.                            DATA 350
C                                                                       DATA 360
      READ (5,1) (D(I),I=1,M)                                           DATA 370
C                                                                       DATA 380
C     INPUT DATA ARE WRITTEN ON LOGICAL TAPE 13 FOR THE RESIDUAL ANALY- DATA 390
C     SIS PERFORMED IN THE SAMPLE MULTIPLE REGRESSION PROGRAM.          DATA 400
C                                                                       DATA 410
      WRITE (13) (D(I),I=1,M)                                           DATA 420
      RETURN                                                            DATA 430
      END                                                               DATA 440
```

```
      FUNCTION FUN(X,Y)                                                 FUN   10
C                                                                       FUN   20
      FUN=1./X                                                          FUN   30
      RETURN                                                            FUN   40
      END                                                               FUN   50
```

```
C                                                                       HIST  10
C     ..................................................................HIST  20
C                                                                       HIST  30
C        SUBROUTINE HIST                                                HIST  40
C                                                                       HIST  50
C        PURPOSE                                                        HIST  60
C           PRINT A HISTOGRAM OF FREQUENCIES VERSUS INTERVALS           HIST  70
C                                                                       HIST  80
C        USAGE                                                          HIST  90
C           CALL HIST(NU,FREQ,IN)                                       HIST 100
C                                                                       HIST 110
C        DESCRIPTION OF PARAMETERS                                      HIST 120
C           NU   - HISTOGRAM NUMBER (3 DIGITS MAXIMUM)                  HIST 130
C           FREQ - VECTOR OF FREQUENCIES                                HIST 140
C           IN   - NUMBER OF INTERVALS AND LENGTH OF FREQ (MAX IS 20)   HIST 150
C                  NORMALLY, FREQ(1) CONTAINS THE FREQUENCY SMALLER THANHIST 160
C                  THE LOWER BOUND AND FREQ(IN) CONTAINS THE FREQUENCY  HIST 170
C                  LARGER THAN THE UPPER BOUND                          HIST 180
C                                                                       HIST 190
C        REMARKS                                                        HIST 200
C           FREQUENCIES MUST BE POSITIVE NUMBERS                        HIST 210
C                                                                       HIST 220
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  HIST 230
C           NONE                                                        HIST 240
C                                                                       HIST 250
C        METHOD                                                         HIST 260
C           THE LARGEST FREQUENCY IS DETERMINED AND SCALING IS USED     HIST 270
C           IF REQUIRED                                                 HIST 280
C                                                                       HIST 290
C     ..................................................................HIST 300
      SUBROUTINE HIST(NU,FREQ,IN)                                       HIST 310
      DIMENSION JOUT(20),FREQ(20)                                       HIST 320
C                                                                       HIST 330
    1 FORMAT(6H EACH ,A1,6H EQUALS ,I2,7H POINTS,/)                     HIST 340
    2 FORMAT(I6,4X,20(4X,A1))                                           HIST 350
                                                                        HIST 360
    3 FORMAT(9HOINTERVAL,4X,19(I2,3X),I2)                               HIST 370
    4 FORMAT(1H1,47X,11H HISTOGRAM ,I3)                                 HIST 380
    5 FORMAT(10HOFREQUENCY,20I5)                                        HIST 390
    6 FORMAT(6H CLASS)                                                  HIST 400
    7 FORMAT(113H   ----------------------------------------------------HIST 410
     1----------)                                                       HIST 420
    8 FORMAT(1H )                                                       HIST 430
    9 FORMAT(A1)                                                        HIST 440
   10 FORMAT(1H*)                                                       HIST 450
C                                                                       HIST 460
      REWIND 13                                                         HIST 470
      WRITE(13,10)                                                      HIST 480
      REWIND 13                                                         HIST 490
      READ(13,9) K                                                      HIST 500
      REWIND 13                                                         HIST 510
      WRITE(13,8)                                                       HIST 520
      REWIND 13                                                         HIST 530
      READ(13,9) NOTH                                                   HIST 540
      REWIND 13                                                         HIST 550
C                                                                       HIST 560
C        PRINT TITLE AND FREQUENCY VECTOR                               HIST 570
C                                                                       HIST 580
      WRITE(6,4) NU                                                     HIST 590
      DO 12 I=1,IN                                                      HIST 600
   12 JOUT(I)=FREQ(I)                                                   HIST 610
      WRITE(6,5)(JOUT(I),I=1,IN)                                        HIST 620
      WRITE(6,7)                                                        HIST 630
C                                                                       HIST 640
C        FIND LARGEST FREQUENCY                                         HIST 650
C                                                                       HIST 660
      FMAX=0.0                                                          HIST 670
      DO 20 I=1,IN                                                      HIST 680
      IF(FREQ(I)-FMAX) 20,20,15                                         HIST 690
   15 FMAX=FREQ(I)                                                      HIST 700
   20 CONTINUE                                                          HIST 710
C                                                                       HIST 720
C        SCALE IF NECESSARY                                             HIST 730
C                                                                       HIST 740
      JSCAL=1                                                           HIST 750
      IF(FMAX-50.0) 40,40,30                                            HIST 760
   30 JSCAL=(FMAX+49.0)/50.0                                            HIST 770
      WRITE(6,1)K,JSCAL                                                 HIST 780
C                                                                       HIST 790
C        CLEAR OUTPUT AREA TO BLANKS                                    HIST 800
C                                                                       HIST 810
   40 DO 50 I=1,IN                                                      HIST 820
   50 JOUT(I)=NOTH                                                      HIST 830
C                                                                       HIST 840
C        LOCATE FREQUENCIES IN EACH INTERVAL                            HIST 850
C                                                                       HIST 860
      MAX=FMAX/FLOAT(JSCAL)                                             HIST 870
      DO 80 I=1,MAX                                                     HIST 880
      X=MAX-(I-1)                                                       HIST 890
      DO 70 J=1,IN                                                      HIST 900
      IF(FREQ(J)/FLOAT(JSCAL)-X) 70,60,60                               HIST 910
   60 JOUT(J)=K                                                         HIST 920
   70 CONTINUE                                                          HIST 930
      IX=X*FLOAT(JSCAL)                                                 HIST 940
C                                                                       HIST 950
C        PRINT LINE OF FREQUENCIES                                      HIST 960
C                                                                       HIST 970
   80 WRITE(6,2)IX,(JOUT(J),J=1,IN)                                     HIST 980
C                                                                       HIST 990
C        GENERATE CONSTANTS                                             HIST1000
C                                                                       HIST1010
      DO 90 I=1,IN                                                      HIST1020
   90 JOUT(I)=I                                                         HIST1030
C                                                                       HIST1040
C        PRINT INTERVAL NUMBERS                                         HIST1050
C                                                                       HIST1060
      WRITE(6,7)                                                        HIST1070
      WRITE(6,3)(JOUT(J),J=1,IN)                                        HIST1080
      WRITE(6,6)                                                        HIST1090
      RETURN                                                            HIST1100
      END                                                               HIST1110
```

```
C                                                                       PLOT  10
C     ..................................................................PLOT  20
C                                                                       PLOT  30
C        SUBROUTINE PLOT                                                PLOT  40
C                                                                       PLOT  50
C        PURPOSE                                                        PLOT  60
C           PLOT SEVERAL CROSS-VARIABLES VERSUS A BASE VARIABLE         PLOT  70
C                                                                       PLOT  80
C        USAGE                                                          PLOT  90
C           CALL PLOT (NO,A,N,M,ML,NS)                                  PLOT 100
C                                                                       PLOT 110
C        DESCRIPTION OF PARAMETERS                                      PLOT 120
C           NO - CHART NUMBER (3 DIGITS MAXIMUM)                        PLOT 130
C           A  - MATRIX OF DATA TO BE PLOTTED. FIRST COLUMN REPRESENTS  PLOT 140
C                BASE VARIABLE AND SUCCESSIVE COLUMNS ARE THE CROSS-    PLOT 150
C                VARIABLES (MAXIMUM IS 9).                              PLOT 160
C           N  - NUMBER OF ROWS IN MATRIX A                             PLOT 170
C           M  - NUMBER OF COLUMNS IN MATRIX A (EQUAL TO THE TOTAL      PLOT 180
C                NUMBER OF VARIABLES). MAXIMUM IS 10.                   PLOT 190
C           ML - NUMBER OF LINES IN THE PLOT. IF 0 IS SPECIFIED, 50     PLOT 200
C                LINES ARE USED.                                        PLOT 210
C           NS - CODE FOR SORTING THE BASE VARIABLE DATA IN ASCENDING   PLOT 220
C                ORDER                                                  PLOT 230
C                  0  SORTING IS NOT NECESSARY (ALREADY IN ASCENDING    PLOT 240
C                     ORDER).                                           PLOT 250
C                  1  SORTING IS NECESSARY.                             PLOT 260
C                                                                       PLOT 270
C        REMARKS                                                        PLOT 280
C           NONE                                                        PLOT 290
C                                                                       PLOT 300
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  PLOT 310
C           NONE                                                        PLOT 320
C                                                                       PLOT 330
C     ..................................................................PLOT 340
      SUBROUTINE PLOT(NO,A,N,M,ML,NS)                                   PLOT 350
      DIMENSION OUT(101),YPR(11),ANG(9),A(1)                            PLOT 360
C                                                                       PLOT 370
    1 FORMAT(1H1,60X,7H CHART ,I3,//)                                   PLOT 380
    2 FORMAT(1H ,F11.4,5X,101A1)                                        PLOT 390
    3 FORMAT(1H )                                                       PLOT 400
    4 FORMAT(10H 1234567890)                                            PLOT 410
    5 FORMAT(10A1)                                                      PLOT 420
    7 FORMAT(1H ,16X,1014.                                              PLOT 430
     1    .         .         .         .         .         .          PLOT 440
     1    .         .         .         .         .         .)         PLOT 450
    8 FORMAT(1HO,9X,11F10.4)                                            PLOT 460
C                                                                       PLOT 470
C     ..................................................................PLOT 480
```

```
C                                                                       PLOT 490
      NLL=NL                                                            PLOT 500
C                                                                       PLOT 510
      IF(NS) 16, 16, 10                                                 PLOT 520
C                                                                       PLOT 530
C        SORT BASE VARIABLE DATA IN ASCENDING ORDER                     PLOT 540
C                                                                       PLOT 550
   10 DO 15 I=1,N                                                       PLOT 560
      DO 14 J=I,N                                                       PLOT 570
      IF(A(I)-A(J)) 14, 14, 11                                          PLOT 580
   11 L=I-N                                                             PLOT 590
      LL=J-N                                                            PLOT 600
      DO 12 K=1,M                                                       PLOT 610
      L=L+N                                                             PLOT 620
      LL=LL+N                                                           PLOT 630
      F=A(L)                                                            PLOT 640
      A(L)=A(LL)                                                        PLOT 650
   12 A(LL)=F                                                           PLOT 660
   14 CONTINUE                                                          PLOT 670
   15 CONTINUE                                                          PLOT 680
C                                                                       PLOT 690
C        TEST NLL                                                       PLOT 700
C                                                                       PLOT 710
   16 IF(NLL) 20, 18, 20                                                PLOT 720
   18 NLL=50                                                            PLOT 730
C                                                                       PLOT 740
C        PRINT TITLE                                                    PLOT 750
C                                                                       PLOT 760
   20 WRITE(6,1)NO                                                      PLOT 770
C                                                                       PLOT 780
C        DEVELOP BLANK AND DIGITS FOR PRINTING                          PLOT 790
C                                                                       PLOT 800
      REWIND 13                                                         PLOT 810
      WRITE (13,4)                                                      PLOT 820
      REWIND 13                                                         PLOT 830
      READ (13,5) BLANK,(ANG(I),I=1,9)                                  PLOT 840
      REWIND 13                                                         PLOT 850
C                                                                       PLOT 860
C        FIND SCALE FOR BASE VARIABLE                                   PLOT 870
C                                                                       PLOT 880
      XSCAL=(A(N)-A(1))/(FLOAT(NLL-1))                                  PLOT 890
C                                                                       PLOT 900
C        FIND SCALE FOR CROSS-VARIABLES                                 PLOT 910
C                                                                       PLOT 920
      M1=N+1                                                            PLOT 930
      YMIN=A(M1)                                                        PLOT 940
      YMAX=YMIN                                                         PLOT 950
      M2=M*N                                                            PLOT 960
      DO 40 J=M1,M2                                                     PLOT 970
      IF(A(J)-YMIN) 28,26,26                                            PLOT 980
   26 IF(A(J)-YMAX) 40,40,30                                            PLOT 990
   28 YMIN=A(J)                                                         PLOT1000
      GO TO 40                                                          PLOT1010
   30 YMAX=A(J)                                                         PLOT1020
   40 CONTINUE                                                          PLOT1030
      YSCAL=(YMAX-YMIN)/100.0                                           PLOT1040
C                                                                       PLOT1050
C        FIND BASE VARIABLE PRINT POSITION                              PLOT1060
C                                                                       PLOT1070
      XB=A(1)                                                           PLOT1080
      L=1                                                               PLOT1090
      MY=M-1                                                            PLOT1100
      I=1                                                               PLOT1110
   45 F=I-1                                                             PLOT1120
      XPR=XB+F*XSCAL                                                    PLOT1130
      IF(A(L)-XPR) 50,50,70                                             PLOT1140
C                                                                       PLOT1150
C        FIND CROSS-VARIABLES                                           PLOT1160
C                                                                       PLOT1170
   50 DO 55 IX=1,101                                                    PLOT1180
   55 OUT(IX)=BLANK                                                     PLOT1190
      DO 60 J=1,MY                                                      PLOT1200
      LL=L+J*N                                                          PLOT1210
      JP=((A(LL)-YMIN)/YSCAL)+1.0                                       PLOT1220
      OUT(JP)=ANG(J)                                                    PLOT1230
   60 CONTINUE                                                          PLOT1240
C                                                                       PLOT1250
C        PRINT LINE AND CLEAR, OR SKIP                                  PLOT1260
C                                                                       PLOT1270
      WRITE(6,2)XPR,(OUT(IZ),IZ=1,101)                                  PLOT1280
      L=L+1                                                             PLOT1290
      GO TO 80                                                          PLOT1300
   70 WRITE(6,3)                                                        PLOT1310
   80 I=I+1                                                             PLOT1320
      IF(I-NLL) 45, 84, 86                                              PLOT1330
   84 XPR=A(N)                                                          PLOT1340
      GO TO 50                                                          PLOT1350
C                                                                       PLOT1360
C        PRINT CROSS-VARIABLES NUMBERS                                  PLOT1370
C                                                                       PLOT1380
   86 WRITE(6,7)                                                        PLOT1390
      YPR(1)=YMIN                                                       PLOT1400
      DO 90 KN=1,9                                                      PLOT1410
   90 YPR(KN+1)=YPR(KN)+YSCAL*10.0                                      PLOT1420
      YPR(11)=YMAX                                                      PLOT1430
      WRITE(6,8)(YPR(IP),IP=1,11)                                       PLOT1440
      RETURN                                                            PLOT1450
      END                                                               PLOT1460
```

```
C                                                                       MATI  10
C  ...................................................................  MATI  20
C                                                                       MATI  30
C     SUBROUTINE MATIN                                                  MATI  40
C                                                                       MATI  50
C     PURPOSE                                                           MATI  60
C        READS CONTROL CARD AND MATRIX DATA ELEMENTS FROM LOGICAL       MATI  70
C        UNIT 5                                                         MATI  80
C                                                                       MATI  90
C     USAGE                                                             MATI 100
C        CALL MATIN(ICODE,A,ISIZE,IROW,ICOL,IS,IER)                     MATI 110
C                                                                       MATI 120
C     DESCRIPTION OF PARAMETERS                                         MATI 130
C        ICODE-UPON RETURN, ICODE WILL CONTAIN FOUR DIGIT               MATI 140
C              IDENTIFICATION CODE FROM MATRIX PARAMETER CARD           MATI 150
C        A    -DATA AREA FOR INPUT MATRIX                               MATI 160
C        ISIZE-NUMBER OF ELEMENTS DIMENSIONED BY USER FOR AREA A        MATI 170
C        IROW -UPON RETURN, IROW WILL CONTAIN ROW DIMENSION FROM        MATI 180
C              MATRIX PARAMETER CARD                                    MATI 190
C        ICOL -UPON RETURN, ICOL WILL CONTAIN COLUMN DIMENSION FROM     MATI 200
C              MATRIX PARAMETER CARD                                    MATI 210
C        IS   -UPON RETURN, IS WILL CONTAIN STORAGE MODE CODE FROM      MATI 220
C              MATRIX PARAMETER CARD WHERE                              MATI 230
C              IS=0 GENERAL MATRIX                                      MATI 240
C              IS=1 SYMMETRIC MATRIX                                    MATI 250
C              IS=2 DIAGONAL MATRIX                                     MATI 260
C        IER  -UPON RETURN, IER WILL CONTAIN AN ERROR CODE WHERE        MATI 270
C              IER=0   NO ERROR                                         MATI 280
C              IER=1   ISIZE IS LESS THAN NUMBER OF ELEMENTS IN         MATI 290
C                      INPUT MATRIX                                     MATI 300
C              IER=2   INCORRECT NUMBER OF DATA CARDS                   MATI 310
C                                                                       MATI 320
C     REMARKS                                                           MATI 330
C        NONE                                                           MATI 340
C                                                                       MATI 350
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     MATI 360
C        LOC                                                            MATI 370
C                                                                       MATI 380
C     METHOD                                                            MATI 390
C        SUBROUTINE ASSUMES THAT INPUT MATRIX CONSISTS OF PARAMETER     MATI 400
C        CARD FOLLOWED BY DATA CARDS                                    MATI 410
C        PARAMETER CARD HAS THE FOLLOWING FORMAT                        MATI 420
C          COL. 1- 2 BLANK                                              MATI 430
C          COL. 3- 6 UP TO FOUR DIGIT IDENTIFICATION CODE               MATI 440
C          COL. 7-10 NUMBER OF ROWS IN MATRIX                           MATI 450
C          COL.11-14 NUMBER OF COLUMNS IN MATRIX                        MATI 460
C          COL.15-16 STORAGE MODE OF MATRIX WHERE                       MATI 470
C              0 - GENERAL MATRIX                                       MATI 480
C              1 - SYMMETRIC MATRIX                                     MATI 490
C              2 - DIAGONAL MATRIX                                      MATI 500
C        DATA CARDS ARE ASSUMED TO HAVE SEVEN FIELDS OF TEN COLUMNS     MATI 510
C        EACH.  DECIMAL POINT MAY APPEAR ANYWHERE IN A FIELD.  IF NO    MATI 520
C        DECIMAL POINT IS INCLUDED, IT IS ASSUMED THAT THE DECIMAL      MATI 530
C        POINT IS AT THE END OF THE 10 COLUMN FIELD. NUMBER IN EACH     MATI 540
C        FIELD MAY BE PRECEDED BY BLANKS.  DATA ELEMENTS MUST BE        MATI 550
C        PUNCHED BY ROW.  A ROW MAY CONTINUE FROM CARD TO CARD.         MATI 560
C        HOWEVER EACH NEW ROW MUST START IN THE FIRST FIELD OF THE      MATI 570
C        NEXT CARD.  ONLY THE UPPER TRIANGULAR PORTION OF A SYMMETRIC   MATI 580
C        OR THE DIAGONAL ELEMENTS OF A DIAGONAL MATRIX ARE CONTAINED    MATI 590
C        ON DATA CARDS.  THE FIRST ELEMENT OF EACH NEW ROW WILL BE      MATI 600
C        THE DIAGONAL ELEMENT FOR A MATRIX WITH  SYMMETRIC OR           MATI 610
C        DIAGONAL STORAGE MODE. COLUMNS 71-80 OF DATA CARDS MAY BE      MATI 620
C        USED FOR IDENTIFICATION, SEQUENCE NUMBERING, ETC..             MATI 630
C        THE LAST DATA CARD FOR ANY MATRIX MUST BE FOLLOWED BY A CARD   MATI 640
C        WITH A 9 PUNCH IN COLUMN 1.                                    MATI 650
C                                                                       MATI 660
C  ...................................................................  MATI 670
C                                                                       MATI 680
      SUBROUTINE MATIN(ICODE,   A,ISIZE,IROW,ICOL,IS,IER)               MATI 690
      DIMENSION A(1)                                                    MATI 700
      DIMENSION CARD(8)                                                 MATI 710
    1 FORMAT(7F10.0)                                                    MATI 720
    2 FORMAT(I6,2I4,I2)                                                 MATI 730
C                                                                       MATI 740
      IDC=7                                                             MATI 750
      IER=0                                                             MATI 760
      READ( 5,2)ICODE,IROW,ICOL,IS                                      MATI 770
      CALL LOC(IROW,ICOL,ICNT,IROW,ICOL,IS)                             MATI 780
      IF(ISIZE-ICNT)6,7,7                                               MATI 790
    6 IER=1                                                             MATI 800
    7 IF (ICNT)38,38,8                                                  MATI 810
    8 ICOLT=ICOL                                                        MATI 820
      IROCR=1                                                           MATI 830
C                                                                       MATI 840
C        COMPUTE NUMBER OF CARDS FOR THIS ROW                           MATI 850
C                                                                       MATI 860
   11 IRCDS=(ICOLT-1)/IDC+1                                             MATI 870
      IF(IS-1)15,15,12                                                  MATI 880
   12 IRCDS=1                                                           MATI 890
C                                                                       MATI 900
C        SET UP LOOP FOR NUMBER OF CARDS IN ROW                         MATI 910
C                                                                       MATI 920
   15 DO 31 K=1,IRCDS                                                   MATI 930
      READ(5,1)(CARD(I),I=1,IDC)                                        MATI 940
C                                                                       MATI 950
C        SKIP THROUGH DATA CARDS IF INPUT AREA TOO SMALL                MATI 960
C                                                                       MATI 970
      IF(IER)16,16,31                                                   MATI 980
   16 L=0                                                               MATI 990
C                                                                       MATI1000
C        COMPUTE COLUMN NUMBER FOR FIRST FIELD IN CURRENT CARD          MATI1010
C                                                                       MATI1020
      JS=(K-1)*IDC+ICOL-ICOLT+1                                         MATI1030
      JE=JS+IDC-1                                                       MATI1040
      IF(IS-1)19,19,17                                                  MATI1050
   17 JE=JS                                                             MATI1060
C                                                                       MATI1070
C        SET UP LOOP FOR DATA ELEMENTS  WITHIN CARD                     MATI1080
C                                                                       MATI1090
   19 DO 30 J=JS,JE                                                     MATI1100
      IF(J-ICOL)20,20,31                                                MATI1110
   20 CALL LOC(IROCR ,J,IJ,IROW,ICOL,IS)                                MATI1120
      L=L+1                                                             MATI1130
   30 A(IJ)=CARD(L)                                                     MATI1140
   31 CONTINUE                                                          MATI1150
      IROCR=IROCR+1                                                     MATI1160
      IF(IROW-IROCR) 38,35,35                                           MATI1170
   35 IF(IS-1)37,36,36                                                  MATI1180
   36 ICOLT=ICOLT-1                                                     MATI1190
   37 GO TO 11                                                          MATI1200
   38 READ(5,1) CARD(1)                                                 MATI1210
      IF(CARD(1)-9.E9)39,40,39                                          MATI1220
   39 IER=2                                                             MATI1230
   40 RETURN                                                            MATI1240
      END                                                               MATI1250
```

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C                                                                       MXOU  10
C     ...................................................................MXOU  20
C                                                                       MXOU  30
C        SUBROUTINE MXOUT                                               MXOU  40
C                                                                       MXOU  50
C        PURPOSE                                                        MXOU  60
C           PRODUCES AN OUTPUT LISTING OF ANY SIZED ARRAY ON            MXOU  70
C           LOGICAL UNIT 6                                              MXOU  80
C                                                                       MXOU  90
C        USAGE                                                          MXOU 100
C           CALL MXOUT(ICODE,A,N,M,MS,LINS,IPOS,ISP)                    MXOU 110
C                                                                       MXOU 120
C        DESCRIPTION OF PARAMETERS                                      MXOU 130
C           ICODE- INPUT CODE NUMBER TO BE PRINTED ON EACH OUTPUT PAGE  MXOU 140
C           A-NAME OF OUTPUT MATRIX                                     MXOU 150
C           N-NUMBER OF ROWS IN A                                       MXOU 160
C           M-NUMBER OF COLUMNS IN A                                    MXOU 170
C           MS-STORAGE MODE OF A WHERE MS=                              MXOU 180
C                 0-GENERAL                                             MXOU 190
C                 1-SYMMETRIC                                           MXOU 200
C                 2-DIAGONAL                                            MXOU 210
C           LINS-NUMBER OF PRINT LINES ON THE PAGE (USUALLY 60)         MXOU 220
C           IPOS-NUMBER OF PRINT POSITIONS ACROSS THE PAGE (USUALLY 132)MXOU 230
C           ISP-LINE SPACING CODE, 1 FOR SINGLE SPACE, 2 FOR DOUBLE     MXOU 240
C               SPACE                                                   MXOU 250
C                                                                       MXOU 260
C        REMARKS                                                        MXOU 270
C           NONE                                                        MXOU 280
C                                                                       MXOU 290
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  MXOU 300
C           LOC                                                         MXOU 310
C                                                                       MXOU 320
C        METHOD                                                         MXOU 330
C           THIS SUBROUTINE CREATES A STANDARD OUTPUT LISTING OF ANY    MXOU 340
C           SIZED ARRAY WITH ANY STORAGE MODE. EACH PAGE IS HEADED WITH MXOU 350
C           THE CODE NUMBER,DIMENSIONS AND STORAGE MODE OF THE ARRAY.   MXOU 360
C           EACH COLUMN AND ROW IS ALSO HEADED WITH ITS RESPECTIVE      MXOU 370
C           NUMBER.                                                     MXOU 380
C                                                                       MXOU 390
C     ...................................................................MXOU 400
C                                                                       MXOU 410
      SUBROUTINE MXOUT (ICODE,A,N,M,MS,LINS,IPOS,ISP)                   MXOU 420
      DIMENSION A(1),B(8)                                               MXOU 430
    1 FORMAT(1H1,5X, 7HMATRIX ,I5,6X,I3,5H ROWS,6X,I3,8H COLUMNS,       MXOU 440
     18X,13HSTORAGE MODE ,I1,8X,5HPAGE ,I2,/)                           MXOU 450
    2 FORMAT(12X,8HCOLUMN  ,7(3X,I3,10X))                              MXOU 460
    3 FORMAT(1H )                                                       MXOU 470
    4 FORMAT(1H ,7X,4HROW ,I3,7(E16.6))                                 MXOU 480
    5 FORMAT(1HO,7X,4HROW ,I3,7(E16.6))                                 MXOU 490
C                                                                       MXOU 500
      J=1                                                               MXOU 510
C                                                                       MXOU 520
C        WRITE HEADING                                                  MXOU 530
C                                                                       MXOU 540
      NEND=IPOS/16-1                                                    MXOU 550
      LEND=(LINS/ISP)-2                                                 MXOU 560
      IPAGE=1                                                           MXOU 570
   10 LSTRT=1                                                           MXOU 580
   20 WRITE(6,1)ICODE,N,M,MS,IPAGE                                      MXOU 590
      JNT=J+NEND-1                                                      MXOU 600
      IPAGE=IPAGE+1                                                     MXOU 610
   31 IF(JNT-M)33,33,32                                                 MXOU 620
   32 JNT=M                                                             MXOU 630
   33 CONTINUE                                                          MXOU 640
      WRITE(6,2)(JCOL,JCOL=J,JNT)                                       MXOU 650
      IF(ISP-1) 35,35,40                                                MXOU 660
   35 WRITE(6,3)                                                        MXOU 670
   40 LTEND=LSTRT+LEND-1                                                MXOU 680
      DO 80 L=LSTRT,LTEND                                               MXOU 690
C                                                                       MXOU 700
C        FORM OUTPUT ROW LINE                                           MXOU 710
C                                                                       MXOU 720
      DO 55 K=1,NEND                                                    MXOU 730
      KK=K                                                              MXOU 740
      JT = J+K-1                                                        MXOU 750
      CALL LOC(L,JT,IJNT,N,M,MS)                                        MXOU 760
      B(K)=0.0                                                          MXOU 770
      IF(IJNT)50,50,45                                                  MXOU 780
   45 B(K)=A(IJNT)                                                      MXOU 790
   50 CONTINUE                                                          MXOU 800
C                                                                       MXOU 810
C        CHECK IF LAST COLUMN.  IF YES GO TO 60                         MXOU 820
C                                                                       MXOU 830
      IF(JT-M) 55,60,60                                                 MXOU 840
   55 CONTINUE                                                          MXOU 850
C                                                                       MXOU 860
C        END OF LINE, NOW WRITE                                         MXOU 870
C                                                                       MXOU 880
   60 IF(ISP-1)65,65,70                                                 MXOU 890
   65 WRITE(6,4)L,(B(JW),JW=1,KK)                                       MXOU 900
      GO TO 75                                                          MXOU 910
   70 WRITE(6,5)L,(B(JW),JW=1,KK)                                       MXOU 920
C                                                                       MXOU 930
C        IF END OF ROWS,GO CHECK COLUMNS                                MXOU 940
C                                                                       MXOU 950
   75 IF(N-L)85,85,80                                                   MXOU 960
   80 CONTINUE                                                          MXOU 970
C                                                                       MXOU 980
C        END OF PAGE, NOW CHECK FOR MORE OUTPUT                         MXOU 990
C                                                                       MXOU1000
      LSTRT=LSTRT+LEND                                                  MXOU1010
      GO TO 20                                                          MXOU1020
C                                                                       MXOU1030
C        END OF COLUMNS, THEN RETURN                                    MXOU1040
C                                                                       MXOU1050
   85 IF(JT-M)90,95,95                                                  MXOU1060
   90 J=JT+1                                                            MXOU1070
      GO TO 10                                                          MXOU1080
   95 RETURN                                                            MXOU1090
      END                                                               MXOU1100
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C                                                                       STOU  10
C     ...................................................................STOU  20
C                                                                       STOU  30
C        SAMPLE OUTPUT SUBROUTINE STOUT                                 STOU  40
C                                                                       STOU  50
C        PURPOSE                                                        STOU  60
C           PRINT THE RESULT OF A STEP-WISE MULTIPLE REGRESSION.  THIS  STOU  70
C           SUBROUTINE IS CALLED BY THE SUBROUTINE STPRG.               STOU  80
C                                                                       STOU  90
C        USAGE                                                          STOU 100
C           CALL STOUT (NSTEP,ANS,L,B,S,T,NSTOP)                        STOU 110
C                                                                       STOU 120
C        DESCRIPTION OF PARAMETERS                                      STOU 130
C           NSTEP - INPUT VECTOR OF LENGTH 5 CONTAINING THE FOLLOWING   STOU 140
C                   INFORMATION..                                       STOU 150
C                     NSTEP(1)  DEPENDENT VARIABLE                      STOU 160
C                     NSTEP(2)  NUMBER OF VARIABLES FORCED TO ENTER     STOU 170
C                               IN THE REGRESSION                       STOU 180
C                     NSTEP(3)  NUMBER OF VARIABLES DELETED             STOU 190
C                     NSTEP(4)  THE LAST STEP NUMBER                    STOU 200
C                     NSTEP(5)  THE LAST VARIABLE ENTERED               STOU 210
C              ANS  - INPUT VECTOR OF LENGTH 11 CONTAINING THE FOLLOWING STOU 220
C                     INFORMATION FOR THE LAST STEP..                   STOU 230
C                     ANS(1)  SUM OF SQUARES REDUCED                    STOU 240
C                     ANS(2)  PROPORTION REDUCED                        STOU 250
C                     ANS(3)  CUMULATIVE SUM OF SQUARES REDUCED         STOU 260
C                     ANS(4)  CUMULATIVE PROPORTION REDUCED             STOU 270
C                     ANS(5)  SUM OF SQUARES OF THE DEPENDENT VARIABLE  STOU 280
C                     ANS(6)  MULTIPLE CORRELATION COEFFICIENT          STOU 290
C                     ANS(7)  F-VALUE FOR ANALYSIS VARIANCE (FOR THE    STOU 300
C                             REGRESSION)                               STOU 310
C                     ANS(8)  STANDARD ERROR OF ESTIMATE                STOU 320
C                     ANS(9)  INTERCEPT                                 STOU 330
C                     ANS(10) ADJUSTED MULTIPLE R                       STOU 340
C                     ANS(11) ADJUSTED STANDARD ERROR OF ESTIMATE       STOU 350
C              L    - INPUT VECTOR OF LENGTH K (K=M-NSTEP(3)-1) CONTAIN- STOU 360
C                     ING VARIABLES ENTERED IN THE REGRESSION.  L(1)=FIRSTSTOU 370
C                     VARIABLE ENTERED, L(2)=SECOND VARIABLE ENTERED, ETC.STOU 380
C              B    - INPUT VECTOR OF LENGTH K (K=M-NSTEP(3)-1) CONTAIN- STOU 390
C                     ING REGRESSION COEFFICIENTS CORRESPONDING TO THE  STOU 400
C                     VARIABLES IN VECTOR L                             STOU 410
C              S    - INPUT VECTOR OF LENGTH K (K=M-NSTEP(3)-1) CONTAIN- STOU 420
C                     ING STANDARD ERRORS OF REGRESSION COEFFICIENTS    STOU 430
C                     CORRESPONDING TO THE VARIABLES IN VECTOR L         STOU 440
C              T    - INPUT VECTOR OF LENGTH K (K=M-NSTEP(3)-1) CONTAIN- STOU 450
C                     ING COMPUTED T-VALUES CORRESPONDING TO THE VARIABLESSTOU 460
C                     IN VECTOR L                                       STOU 470
C           NSTOP - OUTPUT OPTION CODE TO STOP THE STEP-WISE REGRESSION STOU 480
C                     1 - IF THE STEP-WISE REGRESSION IS TO BE TERMI-   STOU 490
C                         NATED BY SOME CRITERIA OTHER THAN PROPORTION  STOU 500
C                         OF SUM OF SQUARES, SUCH AS F-TEST AND SO ON,  STOU 510
C                         THIS SUBROUTINE MAY BE MODIFIED TO PERFORM    STOU 520
C                         DESIRED TESTS.  WHEN IT BECOMES NO LONGER     STOU 530
C                         NECESSARY TO CONTINUE THE STEP-WISE REGRES-   STOU 540
C                         SION, SET NSTOP EQUAL TO 1.                   STOU 550
C                     0 - IF THE STEP-WISE REGRESSION IS TO BE CONTINUEDSTOU 560
C                                                                       STOU 570
C        REMARKS                                                        STOU 580
C           THE CONTENTS OF THE VECTORS NSTEP, ANS, L ARE REQUIRED IN   STOU 590
C           SUBSEQUENT STEPS AND MUST NOT BE DESTROYED.                 STOU 600
C                                                                       STOU 610
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  STOU 620
C           NONE                                                        STOU 630
C                                                                       STOU 640
C                                                                       STOU 650
C     ...................................................................STOU 660
C                                                                       STOU 670
      SUBROUTINE STOUT (NSTEP,ANS,L,B,S,T,NSTOP)                        STOU 680
C                                                                       STOU 690
      DIMENSION NSTEP(1),ANS(1),L(1),B(1),S(1),T(1)                     STOU 700
C                                                                       STOU 710
C     ...................................................................STOU 720
C                                                                       STOU 730
C        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  STOU 740
C        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION      STOU 750
C        STATEMENT WHICH FOLLOWS.                                       STOU 760
C                                                                       STOU 770
C     DOUBLE PRECISION ANS,B,S,T                                        STOU 780
C                                                                       STOU 790
C        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS    STOU 800
C        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS      STOU 810
C        ROUTINE.                                                       STOU 820
C                                                                       STOU 830
C     ...................................................................STOU 840
C                                                                       STOU 850
    1 FORMAT(/5H1STEP(3)                                                STOU 860
    2 FORMAT(22HOVARIABLE ENTERED.....(2)                               STOU 870
    3 FORMAT(40HOSUM OF SQUARES REDUCED IN THIS STEP....F13.3)          STOU 880
    4 FORMAT(40H PROPORTION REDUCED IN THIS STEP.......F13.3)           STOU 890
    5 FORMAT(40HOCUMULATIVE SUM OF SQUARES REDUCED.....F13.3)           STOU 900
    6 FORMAT(40H CUMULATIVE PROPORTION REDUCED.........F13.3,4H  OFF13.STOU 910
     13)                                                                STOU 920
    7 FORMAT(4HOFOR13,16H VARIABLES ENTERED)                            STOU 930
    8 FORMAT(38H    MULTIPLE CORRELATION COEFFICIENT...F9.3)            STOU 940
    9 FORMAT(38H    F-VALUE FOR ANALYSIS OF VARIANCE...F9.3)            STOU 950
   10 FORMAT(38H    STANDARD ERROR OF ESTIMATE.....F9.3)                STOU 960
   11 FORMAT(/57H   VARIABLE     REGRESSION     STD. ERROR OF     COMPUTSTOU 970
     LED/56H     NUMBER       COEFFICIENT      REG. COEFF.       T-VALUE)STOU 980
   12 FORMAT(5X,I3,F18.5,F16.5,F14.3)                                   STOU 990
   13 FORMAT(12H    INTERCEPTF14.5)                                     STOU1000
   14 FORMAT(31HODEPENDENT VARIABLE.............I2)                      STOU1010
   15 FORMAT(31H NUMBER OF VARIABLES FORCED....I2)                      STOU1020
   16 FORMAT(31H NUMBER OF VARIABLES DELETED...I2)                      STOU1030
   17 FORMAT(20H    (FORCED VARIABLE))                                  STOU1040
   18 FORMAT(38H         (ADJUSTED FOR D.F.).....F9.3)                  STOU1050
C                                                                       STOU1060
C        TEST WHETHER THIS IS THE FIRST STEP                            STOU1070
C                                                                       STOU1080
      IF(NSTEP(4)-1) 30, 30, 35                                         STOU109C
   30 WRITE (6,14) NSTEP(1)                                             STOU1100
      WRITE (6,15) NSTEP(2)                                             STOU1110
      WRITE (6,16) NSTEP(3)                                             STOU1120
C                                                                       STOU1130
C        PRINT THE RESULT OF A STEP                                     STOU1140
C                                                                       STOU1150
   35 WRITE (6,1) NSTEP(4)                                              STOU1160
      WRITE (6,2) NSTEP(5)                                              STOU1170
      IF(NSTEP(4)-NSTEP(2)) 37, 37, 38                                  STOU1180
   37 WRITE (6,17)                                                      STOU1190
   38 WRITE (6,3) ANS(1)                                                STOU1200
      WRITE (6,4) ANS(2)                                                STOU1210
      WRITE (6,5) ANS(3)                                                STOU1220
      WRITE (6,6) ANS(4), ANS(5)                                        STOU1230
      WRITE (6,7) NSTEP(4)                                              STOU1240
      WRITE (6,8) ANS(6)                                                STOU1250
      WRITE(6,18)ANS(10)                                                STOU1260
      WRITE (6,9) ANS(7)                                                STOU1270
      WRITE (6,10) ANS(8)                                               STOU1280
      WRITE(6,18)ANS(11)                                                STOU1290
      WRITE (6,11)                                                      STOU1300
      N=NSTEP(4)                                                        STOU1310
      DO 40 I=1,N                                                       STOU1320
   40 WRITE (6,12) L(I),B(I),S(I),T(I)                                  STOU1330
      WRITE (6,13) ANS(9)                                               STOU1340
C                                                                       STOU1350
      NSTOP=0                                                           STOU1360
      RETURN                                                            STOU1370
      END                                                               STOU1380
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