NAG Fortran Library Manual
Mark 19

Volume 12

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Chapter H – Operations Research

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
H02BBF	14	Integer LP problem (dense)
H02BFF	16	Interpret MPSX data file defining IP or LP problem, optimize and print solution
H02BUF	16	Convert MPSX data file defining IP or LP problem to format required by H02BBF or E04MFF
H02BVF	16	Print IP or LP solutions with user specified names for rows and columns
H02BZF	15	Integer programming solution, supplies further information on solution obtained by H02BBF
H02CBF	19	Integer QP problem (dense)
H02CCF	19	Read optional parameter values for H02CBF from external file
H02CDF	19	Supply optional parameter values to H02CBF
H02CEF	19	Integer LP or QP problem (sparse)
H02CFF	19	Read optional parameter values for H02CEF from external file
H02CGF	19	Supply optional parameter values to H02CEF
H03ABF	4	Transportation problem, modified 'stepping stone' method
H03ADF	18	Shortest path problem, Dijkstra's algorithm

Chapter H

Operations Research

Contents

1 Scope of the Chapter

This chapter provides routines to solve certain integer programming, transportation and shortest path problems.

2 Background to the Problems

General **linear programming** (LP) problems (see Dantzig [2]) are of the form:

find $x = (x_1, x_2, \ldots, x_n)^T$ to maximize $F(x) = \sum_{j=1}^{n} c_j x_j$

subject to linear constraints which may have the forms:

$$\begin{array}{lll}
\sum_{j=1}^{n} a_{ij}x_j = b_i, & i = 1,2,\ldots,m_1 & \text{(equality)} \\
\sum_{j=1}^{n} a_{ij}x_j \leq b_i, & i = m_1+1,\ldots,m_2 & \text{(inequality)} \\
\sum_{j=1}^{n} a_{ij}x_j \geq b_i, & i = m_2+1,\ldots,m & \text{(inequality)} \\
x_j \geq l_j, & j = 1,2,\ldots,n & \text{(simple bound)} \\
x_j \leq u_j, & j = 1,2,\ldots,n & \text{(simple bound)}
\end{array}$$

This chapter deals with **integer programming** (IP) problems in which some or all the elements of the solution vector x are further constrained to be **integers**. For general LP problems where x takes only real (i.e., non-integer) values, refer to Chapter E04.

IP problems may or may not have a solution, which may or may not be unique.

Consider for example the following problem:

$$\begin{array}{ll}
\text{minimize} & 3x_1 + 2x_2 \\
\text{subject to} & 4x_1 + 2x_2 \geq 5 \\
& 2x_2 \leq 5 \\
& x_1 - x_2 \leq 2 \\
\text{and} & x_1 \geq 0,\ x_2 \geq 0.
\end{array}$$

The hatched area in Figure 1 is the **feasible region**, the region where all the constraints are satisfied, and the points within it which have integer co-ordinates are circled. The lines of hatching are in fact contours of decreasing values of the objective function $3x_1 + 2x_2$, and it is clear from Figure 1 that the optimum IP solution is at the point (1,1). For this problem the solution is unique.

However, there are other possible situations:

(a) there may be more than one solution; e.g., if the objective function in the above problem were changed to $x_1 + x_2$, both (1,1) and (2,0) would be IP solutions.

(b) the feasible region may contain no points with integer co-ordinates, e.g., if an additional constraint

$$3x_1 \leq 2$$

were added to the above problem.

(c) there may be no feasible region, e.g., if an additional constraint

$$x_1 + x_2 \leq 1$$

were added to the above problem.

(d) the objective function may have no finite minimum within the feasible region; this means that the feasible region is unbounded in the direction of decreasing values of the objective function, e.g., if the constraints

$$4x_1 + 2x_2 \geq 5, \quad x_1 \geq 0, \quad x_2 \geq 0,$$

were deleted from the above problem.

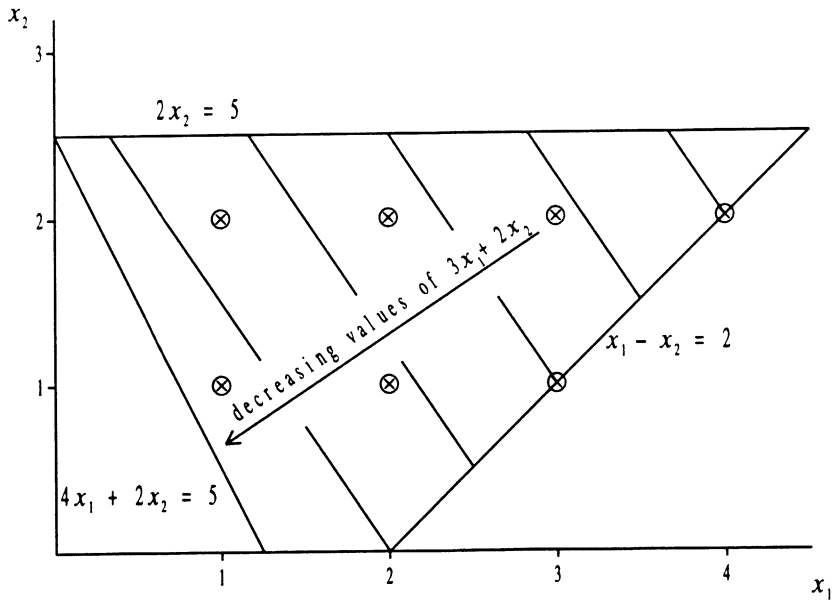

Figure 1

Algorithms for IP problems are usually based on algorithms for general LP problems, together with some procedure for constructing additional constraints which exclude non-integer solutions (see Beale [1]).

The Branch and Bound (B&B) method is a well-known and widely used technique for solving IP problems (see Beale [1] or Mitra [3]). It involves subdividing the optimum solution to the original LP problem into two mutually exclusive sub-problems by branching an integer variable that currently has a fractional optimal value. Each sub-problem can now be solved as an LP problem, using the objective function of the original problem. The process of branching continues until a solution for one of the sub-problems is feasible with respect to the integer problem. In order to prove the optimality of this solution, the rest of the sub-problems in the B&B tree must also be solved. Naturally, if a better integer feasible solution is found for any sub-problem, it should replace the one at hand.

A common method for specifying IP and LP problems in general is the use of the MPSX file format (see [4]). A full description of this file format is provided in the routine documents for H02BUF and E04MZF.

The efficiency in computations is enhanced by discarding inferior sub-problems. These are problems in the B&B search tree whose LP solutions are lower than (in the case of maximization) the best integer solution at hand.

The B&B method may also be applied to convex quadratic programming (QP) problems. Routines have been introduced into this chapter to formally apply the technique to dense general QP problems and to sparse LP or QP problems.

A special type of linear programming problem is the **transportation** problem in which there are $p \times q$ variables y_{kl} which represent quantities of goods to be transported from each of p sources to each of q destinations.

The problem is to minimize

$$\sum_{k=1}^{p}\sum_{l=1}^{q} c_{kl}y_{kl}$$

where c_{kl} is the unit cost of transporting from source k to destination l. The constraints are:

$$\sum_{l=1}^{q} y_{kl} = A_k \quad \text{(availabilities)}$$

$$\sum_{k=1}^{p} y_{kl} = B_l \quad \text{(requirements)}$$

$$y_{kl} \geq 0.$$

Note that the availabilities must equal the requirements:

$$\sum_{k=1}^{p} A_k = \sum_{l=1}^{q} B_l = \sum_{k=1}^{p}\sum_{l=1}^{q} y_{kl}$$

and if all the A_k and B_l are integers, then so are the optimal y_{kl}.

The **shortest path** problem is that of finding a path of minimum length between two distinct vertices n_s and n_e through a network. Suppose the vertices in the network are labelled by the integers $1, 2, \ldots, n$. Let (i, j) denote an ordered pair of vertices in the network (where i is the origin vertex and j the destination vertex of the arc), x_{ij} the amount of flow in arc (i, j) and d_{ij} the length of the arc (i, j). The LP formulation of the problem is thus given as

$$\text{minimize } \sum\sum d_{ij}x_{ij} \text{ subject to } Ax = b,\ 0 \leq x \leq 1, \tag{1}$$

where

$$a_{ij} = \begin{cases} +1 & \text{if arc } j \text{ is directed away from vertex } i, \\ -1 & \text{if arc } j \text{ is directed towards vertex } i, \\ 0 & \text{otherwise} \end{cases}$$

and

$$b_i = \begin{cases} +1 & \text{for } i = n_s, \\ -1 & \text{for } i = n_e, \\ 0 & \text{otherwise.} \end{cases}$$

The above formulation only yields a meaningful solution if $x_{ij} = 0$ or 1; that is, arc (i, j) forms part of the shortest route only if $x_{ij} = 1$. In fact since the optimal LP solution will (in theory) always yield $x_{ij} = 0$ or 1, (1) can also be solved as an IP problem. Note that the problem may also be solved directly (and more efficiently) using a variant of Dijkstra's algorithm (see [6]).

The **travelling salesman** problem is that of finding a minimum distance route round a given set of cities. The salesperson must visit each city only once before returning to his or her city of origin. It can be formulated as an IP problem in a number of ways. One such formulation is described in Williams [5]. There are currently no routines in the Library for solving such problems.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

H02BBF solves dense integer programming problems using a branch and bound method.

H02BFF solves dense integer or linear programming problems defined by a MPSX data file.

H02BUF converts an MPSX data file defining an integer or a linear programming problem to the form required by H02BBF or E04MFF.

H02BVF prints the solution to an integer or a linear programming problem using specified names for rows and columns.

H02BZF supplies further information on the optimum solution obtained by H02BBF.

H02CBF solves dense integer general quadratic programming problems.

H02CCF reads optional parameter values for H02CBF from external file.

H02CDF supplies optional parameter values to H02CBF.

H02CEF solves sparse integer linear programming or quadratic programming problems.

H02CFF reads optional parameter values for H02CEF from external file.

H02CGF supplies optional parameter values to H02CEF.

H03ABF solves transportation problems. It uses integer arithmetic throughout and so produces exact results. On a few machines, however, there is a risk of integer overflow without warning, so the integer values in the data should be kept as small as possible by dividing out any common factors from the coefficients of the constraint or objective functions.

H03ADF solves shortest path problems using Dijkstra's algorithm.

H02BBF, H02BFF and H03ABF treat all matrices as dense and hence are not intended for large sparse problems. For solving large sparse LP problems, use E04NKF or E04UGF.

4 Routines Withdrawn or Scheduled for Withdrawal

Since Mark 13 the following routines have been withdrawn. Advice on replacing calls to these routines is given in the document 'Advice on Replacement Calls for Withdrawn/Superseded Routines'.

H02BAF

5 References

[1] Beale E M (1977) Integer Programming *The State of the Art in Numerical Analysis* (ed D A H Jacobs) Academic Press

[2] Dantzig G B (1963) *Linear Programming and Extensions* Princeton University Press

[3] Mitra G (1973) Investigation of some branch and bound strategies for the solution of mixed integer linear programs *Math. Programming* **4** 155–170

[4] (1971) MPSX - Mathematical programming system *Program Number 5734 XM4* IBM Trade Corporation, New York

[5] Williams H P (1990) *Model Building in Mathematical Programming* (3rd Edition) Wiley

[6] Ahuja R K, Magnanti T L and Orlin J B (1993) *Network Flows: Theory, Algorithms, and Applications* Prentice Hall

H02BBF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

Warning. The specification of the parameters BIGBND and LIWORK changed at Mark 16: the 'default' value of the parameter BIGBND has been increased to 10^{20} and the minimum dimension of the array IWORK has been increased by N + 3.

1 Purpose

H02BBF solves 'zero-one', 'general', 'mixed' or 'all' integer programming problems using a branch and bound method. The routine may also be used to find either the first integer solution or the optimum integer solution. It is not intended for large sparse problems.

2 Specification

```
 SUBROUTINE H02BBF(ITMAX, MSGLVL, N, M, A, LDA, BL, BU, INTVAR,
1                  CVEC, MAXNOD, INTFST, MAXDPT, TOLIV, TOLFES,
2                  BIGBND, X, OBJMIP, IWORK, LIWORK, RWORK, LRWORK,
3                  IFAIL)
 INTEGER           ITMAX, MSGLVL, N, M, LDA, INTVAR(N), MAXNOD,
1                  INTFST, MAXDPT, IWORK(LIWORK), LIWORK, LRWORK,
2                  IFAIL
 real              A(LDA,*), BL(N+M), BU(N+M), CVEC(N), TOLIV,
1                  TOLFES, BIGBND, X(N), OBJMIP, RWORK(LRWORK)
```

3 Description

H02BBF is capable of solving certain types of integer programming (IP) problems using a branch and bound (B&B) method, see Taha [1]. In order to describe these types of integer programs and to briefly state the B&B method, we define the following linear programming (LP) problem:

Minimize

$$F(x) = c_1x_1 + c_2x_2 + \ldots + c_nx_n$$

subject to

$$\sum_{j=1}^{n} a_{ij}x_j \left\{ \begin{array}{c} = \\ \leq \\ \geq \end{array} \right\} b_i, \quad i = 1,2,\ldots,m$$

$$l_j \leq x_j \leq u_j, \quad j = 1,2,\ldots,n \tag{1}$$

If, in (1), it is required that (some or) all the variables take integer values, then the integer program is of type (*mixed* or) *all* general IP problem. If additionally, the integer variables are restricted to take only 0-1 values (i.e., $l_j = 0$ and $u_j = 1$) then the integer program is of type (mixed or all) *zero-one* IP problem.

The B&B method applies directly to these integer programs. The general idea of B&B (for a full description see Dakin [2] or Mitra [3]) is to solve the problem without the integral restrictions as an LP problem (first *node*). If in the optimal solution an integer variable x_k takes a non-integer value x_k^*, two LP sub-problems are created by *branching*, imposing $x_k \leq [x_k^*]$ and $x_k \geq [x_k^*] + 1$ respectively, where $[x_k^*]$ denotes the integer part of x_k^*. This method of branching continues until the first integer solution (*bound*) is obtained. The hanging nodes are then solved and investigated in order to prove the optimality of the solution. At each node, an LP problem is solved using E04MFF.

4 References

[1] Taha H A (1987) *Operations Research: An Introduction* Macmillan, New York

[2] Dakin R J (1965) A tree search algorithm for mixed integer programming problems *Comput. J.* **8** 250–255

[3] Mitra G (1973) Investigation of some branch and bound strategies for the solution of mixed integer linear programs *Math. Programming* **4** 155–170

5 Parameters

1: ITMAX — INTEGER *Input/Output*

On entry: an upper bound on the number of iterations for each LP problem.

On exit: unchanged if on entry ITMAX > 0, else ITMAX $= \max(50, 5\times(N+M))$.

2: MSGLVL — INTEGER *Input*

On entry: the amount of printout produced by H02BBF, as indicated below (see Section 5.1 for a description of the printed output). All output is written to the current advisory message unit (as defined by X04ABF).

Value	**Definition**
0	No output.
1	The final IP solution only.
5	One line of output for each node investigated and the final IP solution.
10	The original LP solution (first node), one line of output for each node investigated and the final IP solution.

3: N — INTEGER *Input*

On entry: n, the number of variables.

Constraint: N > 0.

4: M — INTEGER *Input*

On entry: m, the number of general linear constraints.

Constraint: M ≥ 0.

5: A(LDA,$*$) — ***real*** array *Input*

Note: the second dimension of the array A must be at least N when M > 0, and at least 1 when M $= 0$.

On entry: the ith row of A must contain the coefficients of the ith general constraint, for $i = 1, 2, \ldots, m$.

If M $= 0$ then the array A is not referenced.

6: LDA — INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which H02BBF is called.

Constraint: LDA $\geq \max(1,$M$)$.

7: BL(N+M) — ***real*** array *Input*

8: BU(N+M) — ***real*** array *Input*

On entry: BL must contain the lower bounds and BU the upper bounds, for all the constraints in the following order. The first n elements of each array must contain the bounds on the variables, and the next m elements the bounds for the general linear constraints (if any). To specify a non-existent lower bound (i.e., $l_j = -\infty$), set BL(j) $\leq$ −BIGBND and to specify a non-existent upper bound (i.e., $u_j = +\infty$), set BU(j) $\geq$ BIGBND. To specify the jth constraint as an equality, set BL(j) = BU(j) = β, say, where $|\beta| <$ BIGBND.

Constraints:

BL(j) $\leq$ BU(j), for $j = 1, 2, \ldots,$N + M,
$|\beta| <$ BIGBND when BL(j) = BU(j) = β.

9: INTVAR(N) — INTEGER array *Input*

On entry: indicates which are the integer variables in the problem. For example, if x_j is an integer variable then INTVAR(j) must be set to 1, and 0 otherwise.

Constraints:

INTVAR(j) = 0 or 1 for $j = 1, 2, \ldots,$N, and
INTVAR(j) = 1 for at least one value of j.

10: CVEC(N) — ***real*** array *Input*

On entry: the coefficients c_j of the objective function $F(x) = c_1x_1 + c_2x_2 + \ldots + c_nx_n$. The routine attempts to find a minimum of $F(x)$. If a maximum of $F(x)$ is desired, CVEC(j) should be set to $-c_j$, for $j = 1, 2, \ldots, n$, so that the routine will find a minimum of $-F(x)$.

11: MAXNOD — INTEGER *Input*

On entry: the maximum number of nodes that are to be searched in order to find a solution (optimum integer solution). If MAXNOD $\leq$ 0 and INTFST $\leq$ 0, then the B&B tree search is continued until all the nodes have been investigated.

12: INTFST — INTEGER *Input*

On entry: specifies whether to terminate the B&B tree search after the first integer solution (if any) is obtained. If INTFST > 0 then the B&B tree search is terminated at node k say, which contains the first integer solution. For MAXNOD > 0 this applies only if $k \leq$ MAXNOD.

13: MAXDPT — INTEGER *Input*

On entry: the maximum depth of the B&B tree used for branch and bound.

Suggested value: MAXDPT = 3 × N/2.

Constraint: MAXDPT $\geq$ 2.

14: TOLIV — ***real*** *Input/Output*

On entry: the integer feasibility tolerance; i.e., an integer variable is considered to take an integer value if its violation does not exceed TOLIV. For example, if the integer variable x_j is of order unity then x_j is considered to be integer only if (1−TOLIV) $\leq x_j \leq$ (1+TOLIV).

On exit: unchanged if on entry TOLIV > 0.0, else TOLIV = 10^{-5}.

15: TOLFES — ***real*** *Input/Output*

On entry: the maximum acceptable absolute violation in each constraint at a 'feasible' point (feasibility tolerance); i.e., a constraint is considered satisfied if its violation does not exceed TOLFES.

On exit: unchanged if on entry TOLFES > 0.0, else TOLFES = $\sqrt{\epsilon}$ (where ϵ is the ***machine precision***).

16: BIGBND — ***real*** *Input/Output*

On entry: the 'infinite' bound size in the definition of the problem constraints. More precisely, any upper bound greater than or equal to BIGBND will be regarded as $+\infty$ and any lower bound less than or equal to $-$BIGBND will be regarded as $-\infty$.

On exit: unchanged if on entry BIGBND > 0.0, else BIGBND $= 10^{20}$.

17: X(N) — ***real*** array *Input/Output*

On entry: an initial estimate of the original LP solution.

On exit: with IFAIL = 0, X contains a solution which will be an estimate of either the optimum integer solution or the first integer solution, depending on the value of INTFST. If IFAIL = 9, then X contains a solution which will be an estimate of the best integer solution that was obtained by searching MAXNOD nodes.

18: OBJMIP — ***real*** *Output*

On exit: with IFAIL = 0 or 9, OBJMIP contains the value of the objective function for the IP solution.

19: IWORK(LIWORK) — INTEGER array *Workspace*

20: LIWORK — INTEGER *Input*

On entry: the dimension of the array IWORK as declared in the (sub)program from which H02BBF is called.

Constraint: LIWORK $\geq$ (25+N+M) $\times$ MAXDPT + 5 $\times$ N + M + 4.

21: RWORK(LRWORK) — ***real*** array *Workspace*

22: LRWORK — INTEGER *Input*

On entry: the dimension of the array RWORK as declared in the (sub)program from which H02BBF is called.

Constraint: LRWORK $\geq$ MAXDPT $\times$ (N+1) + 2 $\times$ MIN(N,M+1)^2 + 14 $\times$ N + 12 $\times$ M.

If MSGLVL > 0, the amounts of workspace provided and required (with MAXDPT $= 3 \times$ N/2) are printed. As an alternative to computing MAXDPT, LIWORK and LRWORK from the formulas given above, the user may prefer to obtain appropriate values from the output of a preliminary run with the values of MAXDPT, LIWORK and LRWORK set to 1. If however only LIWORK and LRWORK are set to 1, then the appropriate values of these parameters for the given value of MAXDPT will be computed and printed unless MAXDPT < 2. In both cases H02BBF will then terminate with IFAIL = 6.

23: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error or gives a warning (see Section 6).

For this routine, because the values of output parameters may be useful even if IFAIL $\neq 0$ on exit, users are recommended to set IFAIL to -1 before entry. **It is then essential to test the value of IFAIL on exit**.

5.1 Description of Printed Output

The level of printed output from H02BBF is controlled by the user (see the description of MSGLVL in Section 5).

When MSGLVL > 0, the summary printout at the end of execution of H02BBF includes a listing of the status of every variable and constraint. Note that default names are assigned to all variables and constraints. The following describes the printout for each variable.

Varbl gives the name (**V**) and index j, for $j = 1, 2, \ldots, n$ of the variable.

State gives the state of the variable (**FR** if neither bound is in the working set, **EQ** if a fixed variable, **LL** if on its lower bound, **UL** if on its upper bound, **TF** if temporarily fixed at its current value). If **Value** lies outside the upper or lower bounds by more than the feasibility tolerance, **State** will be **++** or **--** respectively.

Value is the value of the variable at the final iteration.

Lower Bound is the lower bound specified for the variable. (**None** indicates that $\mathrm{BL}(j) \leq -\mathrm{BIGBND}$.) Note that if $\mathrm{INTVAR}(j) = 1$, then the printed value of **Lower Bound** for the jth variable may not be the same as that originally supplied in $\mathrm{BL}(j)$.

Upper Bound is the upper bound specified for the variable. (**None** indicates that $\mathrm{BU}(j) \geq \mathrm{BIGBND}$.) Note that if $\mathrm{INTVAR}(j) = 1$, then the printed value of **Upper Bound** for the jth variable may not be the same as that originally supplied in $\mathrm{BU}(j)$.

Lagr Mult is the value of the Lagrange multiplier for the associated bound constraint. This will be zero if **State** is **FR** or **TF**. If x is optimal, the multiplier should be non-negative if **State** is **LL**, and non-positive if **State** is **UL**.

Residual is the difference between the variable **Value** and the nearer of its bounds $\mathrm{BL}(j)$ and $\mathrm{BU}(j)$.

The meaning of the printout for general constraints is the same as that given above for variables, except that 'variable' is replaced by 'constraint', $\mathrm{BL}(j)$ and $\mathrm{BU}(j)$ are replaced by $\mathrm{BL}(n+j)$ and $\mathrm{BU}(n+j)$ respectively, and with the following change in the heading.

L Con gives the name (**L**) and index j, for $j = 1, 2, \ldots, m$ of the constraint.

When MSGLVL > 1, the summary printout at the end of every node during the execution of H02BBF is a listing of the outcome of forcing an integer variable with a non-integer value to take a value within its specified lower and upper bounds.

Node No is the current node number of the B&B tree being investigated.

Parent Node is the parent node number of the current node.

Obj Value is the final objective function value. If a node does not have a feasible solution then **No Feas Soln** is printed instead of the objective function value. If a node whose optimum solution exceeds the best integer solution so far is encountered (i.e., it does not pay to explore the sub-problem any further), then its objective function value is printed together with a **CO** (Cut Off).

Varbl Chosen is the index of the integer variable chosen for branching.

Value Before is the non-integer value of the integer variable chosen.

Lower Bound is the lower bound value that the integer variable is allowed to take.

Upper Bound is the upper bound value that the integer variable is allowed to take.

Value After is the value of the integer variable after the current optimization.

Depth is the depth of the B&B tree at the current node.

6 Error Indicators and Warnings

If on entry IFAIL $= 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings specified by the routine:

IFAIL = 1

No feasible integer point was found, i.e., it was not possible to satisfy all the integer variables to within the integer feasibility tolerance (determined by TOLIV). Increase TOLIV and rerun H02BBF.

IFAIL = 2

The original LP solution appears to be unbounded. This value of IFAIL implies that a step as large as BIGBND would have to be taken in order to continue the algorithm (see Section 8).

IFAIL = 3

No feasible point was found for the original LP problem, i.e., it was not possible to satisfy all the constraints to within the feasibility tolerance (determined by TOLFES). If the data for the constraints are accurate only to the absolute precision σ, the user should ensure that the value of the feasibility tolerance is greater than σ. For example, if all elements of A are of order unity and are accurate only to three decimal places, the feasibility tolerance should be at least 10^{-3} (see Section 8).

IFAIL = 4

The maximum number of iterations (determined by ITMAX) was reached before normal termination occurred for the original LP problem (see Section 8).

IFAIL = 5

Not used by this routine.

IFAIL = 6

An input parameter is invalid.

IFAIL = 7

The IP solution reported is not the optimum IP solution. In other words, the B&B tree search for at least one of the branches had to be terminated since an LP sub-problem in the branch did not have a solution (see Section 8).

IFAIL = 8

The maximum depth of the B&B tree used for branch and bound (determined by MAXDPT) is too small. Increase MAXDPT (along with LIWORK and/or LRWORK if appropriate) and rerun H02BBF.

IFAIL = 9

The IP solution reported is the best IP solution for the number of nodes (determined by MAXNOD) investigated in the B&B tree.

IFAIL = 10

No feasible integer point was found for the number of nodes (determined by MAXNOD) investigated in the B&B tree.

Overflow

It may be possible to avoid the difficulty by increasing the magnitude of the feasibility tolerance (TOLFES) and rerunning the program. If the message recurs even after this change, see Section 8.

7 Accuracy

The routine implements a numerically stable active set strategy and returns solutions that are as accurate as the condition of the problem warrants on the machine.

8 Further Comments

The original LP problem may not have an optimum solution, i.e., H02BBF terminates with IFAIL = 2,3,4 or overflow may occur. In this case, the user is recommended to relax the integer restrictions of the problem and try to find the optimum LP solution by using E04MFF instead.

In the B&B method, it is possible for an LP sub-problem to terminate without finding a solution. This may occur due to the number of iterations exceeding the maximum allowed. Therefore the B&B tree search for that particular branch cannot be continued. Thus the final IP solution reported is not the optimum IP solution (IFAIL = 7). For the second and unlikely case, a solution could not be found despite a second attempt at an LP solution.

9 Example

To solve the integer programming problem:

maximize

$$F(x) = 3x_1 + 4x_2$$

subject to the bounds

$$\begin{aligned} x_1 &\geq 0 \\ x_2 &\geq 0 \end{aligned}$$

and to the general constraints

$$\begin{aligned} 2x_1 + 5x_2 &\leq 15 \\ 2x_1 - 2x_2 &\leq 5 \\ 3x_1 + 2x_2 &\geq 5 \end{aligned}$$

where x_1 and x_2 are integer variables.

The initial point, which is feasible, is

$$x_0 = (1,1)^T,$$

and $F(x_0) = 7$.

The optimal solution is

$$x^* = (2,2)^T,$$

and $F(x^*) = 14$.

Note that maximizing $F(x)$ is equivalent to minimizing $-F(x)$.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02BBF Example Program Text
*     Mark 16 Revised. NAG Copyright 1993.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX
      PARAMETER        (NMAX=10,MMAX=10)
      INTEGER          LDA
      PARAMETER        (LDA=MMAX)
      INTEGER          LIWORK, LRWORK
      PARAMETER        (LIWORK=1000,LRWORK=1000)
*     .. Local Scalars ..
      real             BIGBND, OBJMIP, TOLFES, TOLIV
      INTEGER          I, IFAIL, INTFST, ITMAX, J, M, MAXDPT, MAXNOD,
     +                 MSGLVL, N
```

```
*     .. Local Arrays ..
      real             A(LDA,NMAX), BL(MMAX+NMAX), BU(MMAX+NMAX),
     +                 CVEC(NMAX), RWORK(LRWORK), X(NMAX)
      INTEGER          INTVAR(NMAX), IWORK(LIWORK)
*     .. External Subroutines ..
      EXTERNAL         H02BBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02BBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, M
      IF (N.LE.NMAX .AND. M.LE.MMAX) THEN
*
*        Read ITMAX, MSGLVL, MAXNOD, INTFST, MAXDPT, TOLFES, TOLIV,
*        CVEC, A, BIGBND, BL, BU, INTVAR and X from data file
*
         READ (NIN,*) ITMAX, MSGLVL
         READ (NIN,*) MAXNOD
         READ (NIN,*) INTFST, MAXDPT
         READ (NIN,*) TOLFES, TOLIV
         READ (NIN,*) (CVEC(I),I=1,N)
         READ (NIN,*) ((A(I,J),J=1,N),I=1,M)
         READ (NIN,*) BIGBND
         READ (NIN,*) (BL(I),I=1,N+M)
         READ (NIN,*) (BU(I),I=1,N+M)
         READ (NIN,*) (INTVAR(I),I=1,N)
         READ (NIN,*) (X(I),I=1,N)
*
*        Solve the IP problem
*
         IFAIL = -1
*
         CALL H02BBF(ITMAX,MSGLVL,N,M,A,LDA,BL,BU,INTVAR,CVEC,MAXNOD,
     +               INTFST,MAXDPT,TOLIV,TOLFES,BIGBND,X,OBJMIP,IWORK,
     +               LIWORK,RWORK,LRWORK,IFAIL)
*
      END IF
      STOP
      END
```

9.2 Program Data

```
H02BBF Example Program Data
  2  3                                              :Values of N and M
  0  10                                             :Values of ITMAX and MSGLVL
  0                                                 :Value of MAXNOD
  0  4                                              :Values of INTFST and MAXDPT
  0.0   0.0                                         :Values of TOLFES and TOLIV
 -3.0  -4.0                                         :End of CVEC
  2.0   5.0
  2.0  -2.0
  3.0   2.0                                         :End of matrix A
  1.0E+20                                           :Value of BIGBND
  0.0      0.0      -1.0E+20  -1.0E+20  5.0        :End of BL
  1.0E+20  1.0E+20  15.0       5.0      1.0E+20    :End of BU
  1     1                                           :End of INTVAR
  1.0   1.0                                         :End of X
```

9.3 Program Results

```
H02BBF Example Program Results

*** H02BBF
*** Start of NAG Library implementation details ***

Implementation title: Generalised Base Version
           Precision: FORTRAN double precision
        Product Code: FLBAS19D
                Mark: 19A

*** End of NAG Library implementation details ***

Parameters
----------

Linear constraints......         3        First integer solution..       OFF
Variables...............         2        Max depth of the tree...         4

Feasibility tolerance...  1.05E-08        Print level.............        10
Infinite bound size.....  1.00E+20        EPS (machine precision).  1.11E-16

Integer feasibility tol.  1.00E-05        Iteration limit.........        50
Max number of nodes.....      NONE

** Workspace provided with MAXDPT =     4: LRWORK =  1000  LIWORK =  1000
** Workspace required with MAXDPT =     4: LRWORK =    84  LIWORK =   137


  *** Optimum LP solution ***   -17.50000


Varbl State     Value     Lower Bound   Upper Bound    Lagr Mult   Residual

V  1    FR    3.92857      0.000000E+00     None        0.0000E+00   3.929
V  2    FR    1.42857      0.000000E+00     None        0.0000E+00   1.429


L Con State     Value     Lower Bound   Upper Bound    Lagr Mult   Residual

L  1    UL    15.0000         None        15.0000     -1.0000      0.0000E+00
L  2    UL    5.00000         None        5.00000     -0.5000     -8.8818E-16
L  3    FR    14.6429       5.00000         None       0.0000E+00   9.643


  *** Start of tree search ***


 Node  Parent    Obj       Varbl  Value      Lower      Upper      Value    Depth
  No    Node    Value      Chosen Before     Bound      Bound      After
   2     1    No Feas Soln    1    3.93       4.00       None       4.00       1
   3     1      -16.2         1    3.93     0.000E+00    3.00       3.00       1
   4     3      -15.5         2    1.80       2.00       None       2.00       2
   5     3      -13.0         2    1.80     0.000E+00    1.00       1.00       2
     *** Integer solution ***
```

```
 Node  Parent    Obj        Varbl  Value      Lower      Upper      Value     Depth
  No    Node     Value      Chosen Before     Bound      Bound      After
   6     4    No Feas Soln    1    2.50       3.00       3.00       3.00        3
   7     4      -14.8         1    2.50     0.000E+00    2.00       2.00        3
   8     7      -12.0      CO 2    2.20       3.00       None       3.00        4
   9     7      -14.0         2    2.20       2.00       2.00       2.00        4
     *** Integer solution ***

    *** End of tree search ***


Total of     9 nodes investigated.

Exit H02BBF - Optimum IP solution found.

Final IP objective value =   -14.00000


Varbl State     Value     Lower Bound   Upper Bound    Lagr Mult   Residual

V  1    UL    2.00000      0.000000E+00   2.00000      -3.000      0.0000E+00
V  2    EQ    2.00000        2.00000      2.00000      -4.000      0.0000E+00


L Con State     Value     Lower Bound   Upper Bound    Lagr Mult   Residual

L  1    FR    14.0000         None        15.0000      0.0000E+00   1.000
L  2    FR   0.000000E+00     None        5.00000      0.0000E+00   5.000
L  3    FR    10.0000       5.00000         None       0.0000E+00   5.000
```

H02BFF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

H02BFF solves linear or integer programming problems specified in MPSX input format. It is not intended for large sparse problems.

2 Specification

```
      SUBROUTINE H02BFF(INFILE, MAXN, MAXM, OPTIM, XBLDEF, XBUDEF,
     1                  MAXDPT, MSGLVL, N, M, X, CRNAME, IWORK, LIWORK,
     2                  RWORK, LRWORK, IFAIL)
      INTEGER           INFILE, MAXN, MAXM, MAXDPT, MSGLVL, N, M,
     1                  IWORK(LIWORK), LIWORK, LRWORK, IFAIL
      real              XBLDEF, XBUDEF, X(MAXN), RWORK(LRWORK)
      CHARACTER*3       OPTIM
      CHARACTER*8       CRNAME(MAXN+MAXM)
```

3 Description

H02BFF solves linear programming (LP) or integer programming (IP) problems specified in MPSX [1] input format. It calls either E04MFF (to solve an LP problem) or H02BBF and H02BZF (to solve an IP problem); these routines are designed to solve problems of the form

$$\underset{x \in R^n}{\text{minimize}}\ c^T x \text{ subject to } l \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u$$

where c is an n element vector and A is an m by n matrix (i.e., there are n variables and m general linear constraints). H02BBF is used if at least one of the variables is restricted to take an integer value at the optimum solution. The document for H02BUF should be consulted for a detailed description of the MPSX format.

In the MPSX data file the first free row, that is, a row defined with the row type N, is taken as the objective row. Similarly, if there are more than one RHS, RANGES or BOUNDS sets, then the first set is used for the optimization. H02BFF also prints the solution to the problem using the row and column names specified in the MPSX data file (by calling H02BVF).

4 References

[1] (1971) MPSX - Mathematical programming system *Program Number 5734 XM4* IBM Trade Corporation, New York

5 Parameters

1: INFILE — INTEGER *Input*

On entry: the unit number associated with the MPSX data file.

Constraint: $0 \leq$ INFILE ≤ 99.

2: MAXN — INTEGER *Input*

On entry: an upper limit for the number of variables in the problem.

Constraint: MAXN ≥ 1.

3: MAXM — INTEGER *Input*

On entry: an upper limit for the number of constraints (including the objective) in the problem.

Constraint: MAXM ≥ 1.

4: OPTIM — CHARACTER*3 *Input*

On entry: specifies the direction of the optimization. OPTIM must be set to 'MIN' for minimization and to 'MAX' for maximization.

Constraint: OPTIM = 'MIN' or 'MAX'.

5: XBLDEF — ***real*** *Input*

On entry: the default lower bound to be used for the variables in the problem, when none is specified in the BOUNDS section of the MPSX data file. For a standard LP or IP problem XBLDEF would normally be set to zero.

6: XBUDEF — ***real*** *Input*

On entry: the default upper bound to be used for the variables in the problem, when none is specified in the BOUNDS section of the MPSX data file. For a standard LP or IP problem XBUDEF would normally be set to 'infinity' (i.e., XBUDEF $\geq 10^{20}$).

Constraint: XBUDEF $\geq$ XBLDEF.

7: MAXDPT — INTEGER *Input*

On entry: for an IP problem, MAXDPT must specify the maximum depth of the branch and bound tree.

Constraint: MAXDPT ≥ 2.

For an LP problem, MAXDPT is not referenced.

8: MSGLVL — INTEGER *Input*

On entry: the amount of printout produced by E04MFF or H02BBF, as indicated below. For a description of the printed output see Section 8.2 of the document for E04MFF or Section 5.1 of the document for H02BBF (as appropriate). All output is written to the current advisory message unit (as defined by X04ABF).

For an LP problem (E04MFF):

Value	**Definition**
0	No output.
1	The final solution only.
5	One line of output for each iteration (no printout of the final solution).
10	The final solution and one line of output for each iteration.

For an IP problem (H02BBF):

Value	**Definition**
0	No output.
1	The final IP solution only.
5	One line of output for each node investigated and the final IP solution.
10	The original LP solution (first node) with dummy names for the rows and columns, one line of output for each node investigated and the final IP solution with MPSX names for the rows and columns.

9: N — INTEGER *Output*

On exit: n, the actual number of variables in the problem.

10: M — INTEGER *Output*

On exit: m, the actual number of general linear constraints in the problem.

11: X(MAXN) — ***real*** array *Output*

On exit: the solution to the problem, stored in X(1),X(2),...,X(N). X(i) is the value of the variable whose MPSX name is stored in CRNAME(i), for $i = 1, 2, \ldots$,N.

12: CRNAME(MAXN+MAXM) — CHARACTER*8 array *Output*

On exit: the first N elements contain the MPSX names for the variables in the problem.

13: IWORK(LIWORK) — INTEGER array *Output*

On exit: the first (N+M) elements contain ISTATE (the status of the constraints in the working set at the solution). Further details can be found in Section 5 of the document for E04MFF or Section 5 of the document for H02BZF (as appropriate).

14: LIWORK — INTEGER *Input*

On entry: the dimension of the array IWORK as declared in the (sub)program from which H02BFF is called.

Constraints:

For an LP problem, LIWORK $\geq 4 \times$ MAXN + MAXM + 3.

For an IP problem, LIWORK $\geq$ (25+MAXN+MAXM) $\times$ MAXDPT + 7 $\times$ MAXN + 2 $\times$ MAXM + 4.

15: RWORK(LRWORK) — ***real*** array *Output*

On exit: the first (N+M) elements contain BL (the lower bounds), the next (N+M) elements contain BU (the upper bounds) and the next (N+M) elements contain CLAMDA (the Lagrange multipliers). Further details can be found in Section 5 of the document for E04MFF or Section 5 of the document for H02BZF (as appropriate). Note that for an IP problem the contents of BL and BU may not be the same as those originally specified by the user in the MPSX data file and/or via the parameters XBLDEF and XBUDEF.

16: LRWORK — INTEGER *Input*

On entry: the dimension of the array RWORK as declared in the (sub)program from which H02BFF is called.

Constraints:

For an LP problem, LRWORK $\geq 2 \times$ MIN(MAXN,MAXM+1)^2 + MAXM $\times$ MAXN + 12 $\times$ MAXN + 9 $\times$ MAXM.

For an IP problem, LRWORK $\geq$ MAXDPT $\times$ (MAXN+1) + 2 $\times$ MIN(MAXN,MAXM+1)^2 + MAXM $\times$ MAXN + 19 $\times$ MAXN + 15 $\times$ MAXM.

17: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL = $i < 0$

Either MAXM and/or MAXN are too small or the MPSX data file is non-standard and/or corrupt. This corresponds to IFAIL = $-i$ in Section 6 of the document for H02BUF.

IFAIL = 1

X is a weak local minimum. This means that the solution is not unique.

IFAIL = 2

The solution appears to be unbounded. This value of IFAIL implies that a step as large as XBUDEF would have to be taken in order to continue the algorithm. See Section 8.

IFAIL = 3

No feasible point was found, i.e., it was not possible to satisfy all the constraints to within the feasibility tolerance (defined internally as $\sqrt{\text{machine precision}}$). See Section 8.

IFAIL = 4

The maximum number of iterations (defined internally as $\max(50,5(n+m))$) was reached before normal termination occurred. See Section 8.

IFAIL = 5

An input parameter is invalid. Refer to the printed output to determine which parameter must be re-defined.

IFAIL = 6

A serious error has occurred in an internal call to either E04MFF or H02BBF (as appropriate). Check all subroutine calls and array dimensions.

For an IP problem only:

IFAIL = 7

The solution reported is not the optimum solution. See Section 8.

IFAIL = 8

MAXDPT is too small. Try increasing its value (along with that of LIWORK and/or LRWORK if appropriate) and rerun H02BFF.

IFAIL = 9

No feasible integer point was found, i.e., it was not possible to satisfy all the integer variables to within the integer feasibility tolerance (defined internally as 10^{-5}). See Section 8.

7 Accuracy

The routine implements a numerically stable active set strategy and returns solutions that are as accurate as the condition of the problem warrants on the machine.

8 Further Comments

For an LP problem only:

if IFAIL = 2 on exit, users can obtain more information by making separate calls to H02BUF, E04MFF and H02BVF (in that order). Note that this will (by default) cause the final LP solution to be printed twice on the current advisory message unit (see X04ABF), once with dummy names for the rows and columns and once with user supplied names. To suppress the printout of the final LP solution with dummy names for the rows and columns, include the statement

```
CALL E04MHF(' Print Level = 5 ')
```

prior to calling E04MFF.

if IFAIL = 3 on exit, users are recommended to reset the value of the feasibility tolerance and rerun H02BFF. (Further advice is given under the description of IFAIL = 3 in Section 6 of the document for E04MFF). For example, to reset the value of the feasibility tolerance to 0.01, include the statement

```
CALL E04MHF(' Feasibility Tolerance = 0.01 ')
```

prior to calling H02BFF.

if IFAIL = 4 on exit, users are recommended to increase the maximum number of iterations allowed before termination and rerun H02BFF. For example, to increase the maximum number of iterations to 500, include the statement

```
CALL E04MHF(' Iteration Limit = 500 ')
```

prior to calling H02BFF.

Note that H02BUF uses an 'infinite' bound size of 10^{20} in the definition of l and u. In other words, any element of u greater than or equal to 10^{20} will be regarded as $+\infty$ (and similarly any element of l less than or equal to -10^{20} will be regarded as $-\infty$). If this value is deemed to be 'inappropriate', users are recommended to reset the value of the 'infinite' bound size and make any necessary changes to BL and/or BU prior to calling E04MFF. For example, to reset the value of the 'infinite' bound size to 10000, include the statement

```
CALL E04MHF(' Infinite Bound Size = 1.0E+4 ')
```

prior to calling E04MFF.

For an IP problem only:

if IFAIL = 2,3,4,7 or 9 on exit, users can obtain more information by making separate calls to H02BUF, H02BBF, H02BZF and H02BVF (in that order).

Note that H02BUF uses an 'infinite' bound size of 10^{20} in the definition of l and u. In other words, any element of u greater than or equal to 10^{20} will be regarded as $+\infty$ (and similarly any element of l less than or equal to -10^{20} will be regarded as $-\infty$). If this value is deemed to be 'inappropriate', users are recommended to reset the value of the parameter BIGBND (as described in Section 5 of the document for H02BBF) and make any necessary changes to BL and/or BU prior to calling H02BBF.

9 Example

This example solves the same problem as the example for H02BUF, except that it treats it as an IP problem.

One of the applications of integer programming is to the so-called diet problem. Given the nutritional content of a selection of foods, the cost of each food, the amount available of each food and the consumer's minimum daily energy requirements, the problem is to find the cheapest combination. This gives rise to the following problem:

minimize

$$c^T x$$

subject to

$$Ax \geq b,$$
$$0 \leq x \leq u,$$

where

$c = (3\ 24\ 13\ 9\ 20\ 19)^T$, $x = (x_1, x_2, x_3, x_4, x_5, x_6)^T$,

x_1, x_2 and x_6 are real,

x_3, x_4 and x_5 are integer,

$$A = \begin{pmatrix} 110 & 205 & 160 & 160 & 420 & 260 \\ 4 & 32 & 13 & 8 & 4 & 14 \\ 2 & 12 & 54 & 285 & 22 & 80 \end{pmatrix}, \quad b = \begin{pmatrix} 2000 \\ 55 \\ 800 \end{pmatrix} \text{ and}$$

$u = (4\ 3\ 2\ 8\ 2\ 2)^T$.

The rows of A correspond to energy, protein and calcium and the columns of A correspond to oatmeal, chicken, eggs, milk, pie and bacon respectively.

The MPSX data representation of this problem is given in Section 9.2.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02BFF Example Program Text
*     Mark 18 Revised.  NAG Copyright 1997.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MAXN, MAXM
      PARAMETER        (MAXN=50,MAXM=50)
      real             XBLDEF, XBUDEF
      PARAMETER        (XBLDEF=0.0e0,XBUDEF=1.0e+20)
      INTEGER          MAXDPT
      PARAMETER        (MAXDPT=3*MAXN/2)
      INTEGER          MSGLVL
      PARAMETER        (MSGLVL=5)
      INTEGER          LIWORK
      PARAMETER        (LIWORK=(25+MAXN+MAXM)*MAXDPT+2*MAXM+7*MAXN+4)
      INTEGER          LRWORK
      PARAMETER        (LRWORK=MAXDPT*(MAXN+1)
     +                 +2*MAXN**2+MAXM*MAXN+19*MAXN+15*MAXM)
      CHARACTER*3      OPTIM
      PARAMETER        (OPTIM='MIN')
*     .. Local Scalars ..
      INTEGER          IFAIL, INFILE, M, N
*     .. Local Arrays ..
      real             RWORK(LRWORK), X(MAXN)
      INTEGER          IWORK(LIWORK)
      CHARACTER*8      CRNAME(MAXN+MAXM)
*     .. External Subroutines ..
      EXTERNAL         H02BFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02BFF Example Program Results'
```

```
*     Skip heading in data file
      READ (NIN,*)
*
*     Solve the problem
*
      INFILE = NIN
      IFAIL = 0
*
      CALL H02BFF(INFILE,MAXN,MAXM,OPTIM,XBLDEF,XBUDEF,MAXDPT,MSGLVL,N,
     +            M,X,CRNAME,IWORK,LIWORK,RWORK,LRWORK,IFAIL)
*
      STOP
      END
```

9.2 Program Data

```
H02BFF Example Program Data
NAME          DIET
ROWS
 G  ENERGY
 G  PROTEIN
 G  CALCIUM
 N  COST
COLUMNS
    OATMEAL   ENERGY      110.0
    OATMEAL   PROTEIN     4.0
    OATMEAL   CALCIUM     2.0
    OATMEAL   COST        3.0
    CHICKEN   ENERGY      205.0
    CHICKEN   PROTEIN     32.0
    CHICKEN   CALCIUM     12.0
    CHICKEN   COST        24.0
    INTEGER   'MARKER'                'INTORG'
    EGGS      ENERGY      160.0
    EGGS      PROTEIN     13.0
    EGGS      CALCIUM     54.0
    EGGS      COST        13.0
    MILK      ENERGY      160.0
    MILK      PROTEIN     8.0
    MILK      CALCIUM     285.0
    MILK      COST        9.0
    PIE       ENERGY      420.0
    PIE       PROTEIN     4.0
    PIE       CALCIUM     22.0
    PIE       COST        20.0
    INTEGER   'MARKER'                'INTEND'
    BACON     ENERGY      260.0
    BACON     PROTEIN     14.0
    BACON     CALCIUM     80.0
    BACON     COST        19.0
RHS
    DEMANDS   ENERGY      2000.0
    DEMANDS   PROTEIN     55.0
    DEMANDS   CALCIUM     800.0
```

```
BOUNDS
 UI SERVINGS  OATMEAL     4.0
 UI SERVINGS  CHICKEN     3.0
 UP SERVINGS  EGGS        2.0
 UP SERVINGS  MILK        8.0
 UP SERVINGS  PIE         2.0
 UI SERVINGS  BACON       2.0
ENDATA
```

9.3 Program Results

```
H02BFF Example Program Results

*** H02BBF
*** Start of NAG Library implementation details ***

Implementation title: Generalised Base Version
           Precision: FORTRAN double precision
        Product Code: FLBAS18D
                Mark: 18A

*** End of NAG Library implementation details ***

Parameters
----------

Linear constraints......         3        First integer solution..       OFF
Variables...............         6        Max depth of the tree...        75

Feasibility tolerance...  1.05E-08        Print level.............         5
Infinite bound size.....  1.00E+20        EPS (machine precision).  1.11E-16

Integer feasibility tol.  1.00E-05        Iteration limit.........        50
Max number of nodes.....      NONE

** Workspace provided with MAXDPT =    75: LRWORK = 10075  LIWORK =  9679
** Workspace required with MAXDPT =    75: LRWORK =   677  LIWORK =  2587


  *** Optimum LP solution ***    92.50000


  *** Start of tree search ***


 Node  Parent    Obj       Varbl  Value      Lower      Upper      Value     Depth
  No    Node    Value     Chosen Before     Bound      Bound      After
   2     1      93.2         4    4.50       5.00       8.00       5.00        1
   3     1      93.8         4    4.50     0.000E+00    4.00       4.00        1
   4     2      94.8         5    1.81       2.00       2.00       2.00        2
   5     2      96.1         5    1.81     0.000E+00    1.00       1.00        2
   6     3      96.9         6   0.308       1.00       2.00       1.00        2
   7     3      94.5         6   0.308     0.000E+00  0.000E+00  0.000E+00     2
   8     7      96.5         3   0.500       1.00       2.00       1.00        3
   9     7      97.4         3   0.500     0.000E+00  0.000E+00  0.000E+00     3
  10     4      97.0         1    3.27       4.00       4.00       4.00        3
     *** Integer solution ***
```

Node No	Parent Node	Obj Value		Varbl Chosen	Value Before	Lower Bound	Upper Bound	Value After	Depth
11	4	95.7		1	3.27	0.000E+00	3.00	3.00	3
12	11	99.5	CO	4	5.19	6.00	8.00	6.00	4
13	11	96.2		4	5.19	5.00	5.00	5.00	4
14	5	97.3	CO	4	7.13	8.00	8.00	8.00	3
15	5	96.5		4	7.13	5.00	7.00	7.00	3
16	13	107.	CO	6	0.115	1.00	2.00	1.00	5
17	13	96.4		6	0.115	0.000E+00	0.000E+00	0.000E+00	5
18	17	103.	CO	3	0.188	1.00	2.00	1.00	6
19	17	97.5	CO	3	0.188	0.000E+00	0.000E+00	0.000E+00	6
20	15	101.	CO	6	0.769E-01	1.00	2.00	1.00	4
21	15	96.6		6	0.769E-01	0.000E+00	0.000E+00	0.000E+00	4
22	8	97.2	CO	4	3.50	4.00	4.00	4.00	4
23	8	98.5	CO	4	3.50	0.000E+00	3.00	3.00	4
24	21	100.	CO	3	0.125	1.00	2.00	1.00	5
25	21	97.3	CO	3	0.125	0.000E+00	0.000E+00	0.000E+00	5
26	6	97.0	CO	4	2.88	3.00	4.00	3.00	3
27	6	105.	CO	4	2.88	0.000E+00	2.00	2.00	3

*** End of tree search ***

Total of 27 nodes investigated.

Exit H02BBF - Optimum IP solution found.

Final IP objective value = 97.00000

Varbl	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
OATMEAL	EQ	4.00000	4.00000	4.00000	3.000	0.0000E+00
CHICKEN	LL	0.000000E+00	0.000000E+00	3.00000	24.00	0.0000E+00
EGGS	LL	0.000000E+00	0.000000E+00	2.00000	13.00	0.0000E+00
MILK	LL	5.00000	5.00000	8.00000	9.000	0.0000E+00
PIE	EQ	2.00000	2.00000	2.00000	20.00	0.0000E+00
BACON	LL	0.000000E+00	0.000000E+00	2.00000	19.00	0.0000E+00

L Con	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
ENERGY	FR	2080.00	2000.00	None	0.0000E+00	80.00
PROTEIN	FR	64.0000	55.0000	None	0.0000E+00	9.000
CALCIUM	FR	1477.00	800.000	None	0.0000E+00	677.0

H02BUF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

H02BUF reads data for a linear or integer programming problem from an external file which is in standard or compatible MPSX input format.

2 Specification

```
 SUBROUTINE H02BUF(INFILE, MAXN, MAXM, OPTIM, XBLDEF, XBUDEF,
1                  NMOBJ, NMRHS, NMRNG, NMBND, MPSLST, N, M, A, BL,
2                  BU, CVEC, X, INTVAR, CRNAME, NMPROB, IWORK, IFAIL)
 INTEGER           INFILE, MAXN, MAXM, N, M, INTVAR(MAXN),
1                  IWORK(MAXN+MAXM), IFAIL
 real              XBLDEF, XBUDEF, A(MAXM,MAXN), BL(MAXN+MAXM),
1                  BU(MAXN+MAXM), CVEC(MAXN), X(MAXN)
 CHARACTER*3       OPTIM
 CHARACTER*8       NMOBJ, NMRHS, NMRNG, NMBND, CRNAME(MAXN+MAXM),
1                  NMPROB
 LOGICAL           MPSLST
```

3 Description

H02BUF reads linear programming (LP) or integer programming (IP) problem data from an external file which is prepared in standard or compatible MPSX [1] input format and then initializes n (the number of variables), m (the number of general linear constraints), the vectors c, l and u and the m by n matrix A for use with E04MFF or H02BBF, which are designed to solve problems of the form

$$\underset{x \in R^n}{\text{minimize}}\ c^T x \text{ subject to } l \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u.$$

This routine may be followed by calls to either E04MFF (to solve an LP problem) or H02BBF and H02BZF (to solve an IP problem), possibly followed by a call to H02BVF (to print the solution using MPSX names).

Note that H02BUF uses an 'infinite' bound size of 10^{20} in the definition of l and u. In other words, any element of u greater than or equal to 10^{20} will be regarded as $+\infty$ (and similarly any element of l less than or equal to -10^{20} will be regarded as $-\infty$). If this value is deemed to be 'inappropriate', users are recommended to reset the value of either the optional parameter **Infinite BoundSize** (if an LP problem is being solved) or the parameter BIGBND (if an IP problem is being solved) and make any necessary changes to BL and/or BU prior to calling E04MFF or H02BBF (as appropriate).

The documents for H02BVF, E04MFF and/or H02BBF and H02BZF should be consulted for further details.

MPSX input format

The input file of data may only contain two types of lines.

(1) Indicator lines (specifying the type of data which is to follow).
(2) Data lines (specifying the actual data).

The input file must not contain any blank lines. Any characters beyond column 80 are ignored. Indicator lines must not contain leading blank characters (in other words they must begin in column 1). The following displays the order in which the indicator lines must appear in the file:

NAME user-given name
ROWS
    data line(s)
COLUMNS
    data line(s)
RHS
    data line(s)
RANGES (optional)
    data line(s)
BOUNDS (optional)
    data line(s)
ENDATA

The 'user-given name' specifies a name for the problem and must occupy columns 15–22. The name can either be blank or up to a maximum of 8 characters.

A data line follows the same fixed format made up of fields defined below. The contents of the fields may have different significance depending upon the section of data in which they appear.

	Field 1	Field 2	Field 3	Field 4	Field 5	Field 6
Columns	2–3	5–12	15–22	25–36	40–47	50–61
Contents	Code	Name	Name	Value	Name	Value

The names and codes consist of 'alphanumeric' characters (i.e., a–z, A–Z, 0–9, +, −, asterisk (*), blank ( ), colon (:), dollar sign ($) or fullstop (.) only) and the names must not contain leading blank characters. Values are read using Fortran format E12.0. This allows values to be entered in several equivalent forms. For example, 1.2345678, 1.2345678E+0, 123.45678E−2 and 12345678E−07 all represent the same number. It is safest to include an explicit decimal point.

Note that in order to ensure numeric values are interpreted as intended, they should be *right-justified* in the 12-character field, with no trailing blanks. This is because in some situations trailing blanks may be interpreted as zeros and this can dramatically affect the interpretation of the value. This is relevant if the value contains an exponent, or if it contains neither an exponent nor an explicit decimal point. For example, the fields

```
%%%%1.23E-2%
%%%%%%%123%%
```

may be interpreted as 1.23E−20 and 12300 respectively (where % is used to denote a blank). The actual behaviour is system-dependent.

Comment lines are allowed in the data file. These must have an asterisk (*) in column 1 and any characters in columns 2–80. In any data line, a dollar sign ($) as the first character in field 3 or 5 indicates that the information from that point through column 80 consists of comments.

Columns outside the six fields must be blank, except for columns 72–80, whose contents are ignored by the routine. These columns may be used to enter a sequence number. A non-blank character outside the predefined six fields and columns 72–80 is considered to be a major error (IFAIL = 11; see Section 6), unless it is part of a comment.

ROWS Data Lines

These lines specify row (constraint) names and their inequality types (i.e., =, ≥ or ≤).

Field 1:	defines the constraint type. It may be in column 2 or column 3.
N	free row, that is no constraint. It may be used to define the objective row.
G	greater than or equal to (i.e., ≥).
L	less than or equal to (i.e., ≤).
E	exactly equal to (i.e., =).
Field 2:	defines the row name.

Row type N stands for 'Not binding', also known as 'Free'. It can be used to define the objective row. The objective row is a free row that specifies the vector c in the objective function. It is taken to be the first free row, unless some other free row name is specified by the parameter NMOBJ (see Section 5). Note that the objective function must be included in the MPSX data file. Thus the maximum number of constraints (MAXM; see Section 5) in the problem must be $m + 1$.

COLUMNS Data Lines

These lines specify the names to be assigned to the variables (columns) in the constraint matrix A, and define, in terms of column vectors, the actual values of the corresponding matrix elements.

Field 1: blank (ignored)

Field 2: gives the name of the column associated with the elements specified in the following fields.

Field 3: contains the name of a row.

Field 4: used in conjunction with field 3 contains the value of the matrix element.

Field 5: is optional (may be used like field 3).

Field 6: is optional (may be used like field 4).

Note that only non-zero elements of A need to be specified in the COLUMNS section, as any unspecified elements are assumed to be zero.

RHS Data Lines

This section specifies the right-hand side values of the constraint matrix A. The lines specify the name of the RHS (right-hand side) vector given to the problem, the numerical values of the elements of the vector are also defined by the data lines and may appear in any order. The data lines have exactly the same format as the COLUMNS data lines, except that the column name is replaced by the RHS name. Note that any unspecified elements are assumed to be zero.

RANGES Data Lines (optional)

Ranges are used for constraints of the form $l \leq Ax \leq u$, where l and u are finite. The range of the constraint is $r = u - l$. Either l or u must be specified in the RHS section and r must be defined in this section.

The data lines have exactly the same format as the COLUMNS data lines, except that the column name is replaced by the RANGE name.

BOUNDS Data Lines (optional)

These lines specify limits on the values of the variables (l and u in $l \leq x \leq u$). If the variable is not specified in the bound set then it is automatically assumed to lie between default lower and upper bounds (usually 0 and $+\infty$). Like an RHS column which is given a name, the set of variables in one bound set is also given a name.

Field 1:	specifies the type of bound or defines the variable type.
`LO`	lower bound
`UP`	upper bound
`FX`	fixed variable
`FR`	free variable ($-\infty$ to $+\infty$)
`MI`	lower bound is $-\infty$
`PL`	upper bound is $+\infty$. This is the default variable type.
Field 2:	identifies a name for the bound set.
Field 3:	identifies the column name of the variable belonging to this set.
Field 4:	identifies the value of the bound; this has a numerical value only in association with `LO`, `UP`, `FX` in field 1, otherwise it is blank.
Field 5:	is blank and ignored.
Field 6:	is blank and ignored.

Note that if RANGES and BOUNDS sections are both present, the RANGES section must appear first.

Note that if RANGES and BOUNDS sections are both present, the RANGES section must appear first.

Integer problems

In IP problems there are two common integer variable types. (a) 0–1 integer variables which represent 'on' or 'off' situations and (b) General integer variables which are forced to take an integer value, in a specified range, at the optimal integer solution. Integer variables can be defined in the following compatible and standard MPSX forms.

In the compatible MPSX format, the type of integer variables are defined in Field 1 of the BOUNDS section, that is:

Field 1:	specifies the type of the integer variable.
`BV`	0–1 integer variable (bound value is 1.0).
`UI`	general integer variable (bound value is in Field 4).

In the standard MPSX format, the integer variables are treated the same as the 'ordinary' bounded variables, in the BOUNDS section. Integer markers are, however, introduced in the COLUMNS section to specify the integer variables. The indicator lines for these markers are:

	Field 1	Field 2	Field 3	Field 4	Field 5	Field 6
Columns	2–3	5–12	15–22	25–36	40–47	50–61
Contents		INTEGER	'MARKER'		'INTORG'	

to mark the beginning of the integer variables and

	Field 1	Field 2	Field 3	Field 4	Field 5	Field 6
Columns	2–3	5–12	15–22	25–36	40–47	50–61
Contents		INTEGER	'MARKER'		'INTEND'	

to mark the end. That is, any variables between these markers are treated as integer variables. Note that if the (INTEND) indicator line is not specified in the file then all the variables between the (INTORG) indicator line and the end of the COLUMNS section are assumed to be integer variables. The routine accepts both standard and/or compatible MPSX format as a means of specifying integer variables. This is illustrated in Section 9.2 of the document for H02BFF.

4 References

[1] (1971) MPSX - Mathematical programming system *Program Number 5734 XM4* IBM Trade Corporation, New York

5 Parameters

1: INFILE — INTEGER *Input*

On entry: the unit number associated with the MPSX data file.

Constraint: $0 \leq \text{INFILE} \leq 99$.

2: MAXN — INTEGER *Input*

On entry: an upper limit for the number of variables in the problem.

Constraint: $\text{MAXN} \geq 1$.

3: MAXM — INTEGER *Input*

On entry: an upper limit for the number of constraints (including the objective) in the problem.

Constraint: $\text{MAXM} \geq 1$.

4: OPTIM — CHARACTER*3 *Input*

On entry: specifies the direction of the optimization. OPTIM must be set to 'MIN' for minimization and to 'MAX' for maximization.

Constraint: OPTIM = 'MIN' or 'MAX'.

5: XBLDEF — ***real*** *Input*

On entry: the default lower bound to be used for the variables in the problem when none is specified in the BOUNDS section of the MPSX data file. For a standard LP or IP problem XBLDEF would normally be set to zero.

6: XBUDEF — ***real*** *Input*

On entry: the default upper bound to be used for the variables in the problem when none is specified in the BOUNDS section of the MPSX data file. For a standard LP or IP problem XBUDEF would normally be set to 'infinity' (i.e., XBUDEF $\geq 10^{20}$).

Constraint: XBUDEF $\geq$ XBLDEF.

7: NMOBJ — CHARACTER*8 *Input/Output*

On entry: either the name of the objective function to be used for the optimization, or blank (in which case the first objective (free) row in the file is used).

On exit: the name of the objective row as defined in the MPSX data file.

8: NMRHS — CHARACTER*8 *Input/Output*

On entry: either the name of the RHS set to be used for the optimization, or blank (in which case the first RHS set is used).

On exit: the name of the RHS set read in the MPSX data file.

9: NMRNG — CHARACTER*8 *Input/Output*

On entry: either the name of the RANGE set to be used for the optimization, or blank (in which case the first RANGE set (if any) is used).

On exit: the name of the RANGE set read in the MPSX data file. This is blank if the MPSX data file does not have a RANGE set.

10: NMBND — CHARACTER*8 *Input/Output*

On entry: either the name of the BOUNDS set to be used for the optimization, or blank (in which case the first BOUNDS set (if any) is used).

On exit: the name of the BOUNDS set read in the MPSX data file. This is blank if the MPSX data file does not have a BOUNDS set.

11: MPSLST — LOGICAL *Input*

On entry: if MPSLST = .TRUE., then a listing of the input data is sent to the current advisory message unit (as defined by X04ABF). This can be useful for debugging the MPSX data file.

12: N — INTEGER *Output*

On exit: n, the actual number of variables in the problem.

13: M — INTEGER *Output*

On exit: m, the actual number of general linear constraints in the problem.

14: A(MAXM,MAXN) — ***real*** array *Output*

On exit: A, the matrix of general linear constraints.

15: BL(MAXN+MAXM) — ***real*** array *Output*

On exit: l, the lower bounds for all the variables and constraints in the following order. The first N elements of BL contain the bounds on the variables and the next M elements contain the bounds for the general linear constraints (if any). Note that an 'infinite' lower bound is indicated by BL(j) = −1.0E+20 and an equality constraint by BL(j) = BU(j).

16: BU(MAXN+MAXM) — ***real*** array *Output*

On exit: u, the upper bounds for all the variables and constraints in the following order. The first N elements of BU contain the bounds on the variables and the next M elements contain the bounds for the general linear constraints (if any). Note that an 'infinite' upper bound is indicated by BU(j) = 1.0E+20 and an equality constraint by BU(j) = BL(j).

17: CVEC(MAXN) — ***real*** array *Output*

On exit: c, the coefficients of the objective function. The signs of these coefficients are determined by the problem (either LP or IP) and the direction of the optimization (see OPTIM above).

18: X(MAXN) — ***real*** array *Output*

On exit: an initial estimate of the solution to the problem. More precisely, X(j) = 1.0 if j is odd and 0.0 otherwise, for $j = 1, 2, \ldots,$N.

19: INTVAR(MAXN) — INTEGER array *Output*

On exit: indicates which are the integer variables in the problem. More precisely, INTVAR(k) = 1 if x_k is an integer variable, and 0 otherwise, for k = 1,2,...,N.

20: CRNAME(MAXN+MAXM) — CHARACTER*8 array *Output*

On exit: the MPSX names of all the variables and constraints in the problem in the following order. The first N elements contain the MPSX names for the variables and the next M elements contain the MPSX names for the general linear constraints (if any).

21: NMPROB — CHARACTER*8 *Output*

On exit: the name of the problem as defined in the MPSX data file.

22: IWORK(MAXN+MAXM) — INTEGER array *Workspace*

23: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL = 1

There are too many rows present in the data file. Increase MAXM by at least (M − MAXM) and rerun H02BUF.

IFAIL = 2

There are too many columns present in the data file. Increase MAXN by at least (N − MAXN) and rerun H02BUF.

The following error exits (apart from IFAIL = 14) are caused by having either a corrupt or a non-standard MPSX data file. Refer to Section 3 for a detailed description of the MPSX format which can be read by H02BUF. If MPSLST = .TRUE., the last line of printed output refers to the line in the MPSX data file which contains the reported error.

IFAIL = 3

The objective function row was not found. There must be at least one row in the ROWS section with row type N for the objective row.

IFAIL = 4

There are no rows specified in the ROWS section.

IFAIL = 5

An illegal constraint type was detected in the ROWS section. The constraint type must be one of N, L, G or E.

IFAIL = 6

An illegal row name was detected in the ROWS section. Names must be made up of alphanumeric characters with no leading blanks.

IFAIL = 7

An illegal column name was detected in the COLUMNS section. Names must be made up of alphanumeric characters with no leading blanks.

IFAIL = 8

An illegal bound type was detected in the BOUNDS section. The bound type must be one of LO, UP, FX, FR, MI, PL, BV or UI.

IFAIL = 9

An unknown column name was detected in the BOUNDS section. All the column names must be specified in the COLUMNS section.

IFAIL = 10

The last line in the file does not contain the ENDATA line indicator.

IFAIL = 11

An illegal data line was detected in the file. This line is neither a comment line nor a valid data line.

IFAIL = 12

An unknown row name was detected in COLUMNS or RHS or RANGES section. All the row names must be specified in the ROWS section.

IFAIL = 13

There were no columns specified in the COLUMNS section.

IFAIL = 14

An input parameter is invalid.

IFAIL = 15

Incorrect integer marker. In standard MPSX data format, integer variables should be defined between INTORG and INTEND markers.

7 Accuracy

Not applicable.

8 Further Comments

None.

9 Example

This example solves the same problem as the example for H02BFF, except that it treats it as an LP problem.

One of the applications of linear programming is to the so-called diet problem. Given the nutritional content of a selection of foods, the cost of each food, the amount available of each food and the consumer's minimum daily energy requirements, the problem is to find the cheapest combination. This gives rise to the following problem:

minimize

$$c^T x$$

subject to

$$Ax \geq b,$$
$$0 \leq x \leq u,$$

where

$$c = (3\ 24\ 13\ 9\ 20\ 19)^T,\ x = (x_1, x_2, x_3, x_4, x_5, x_6)^T \text{ is real,}$$

$$A = \begin{pmatrix} 110 & 205 & 160 & 160 & 420 & 260 \\ 4 & 32 & 13 & 8 & 4 & 14 \\ 2 & 12 & 54 & 285 & 22 & 80 \end{pmatrix},\quad b = \begin{pmatrix} 2000 \\ 55 \\ 800 \end{pmatrix}$$

and $u = (4\ 3\ 2\ 8\ 2\ 2)^T$.

The rows of A correspond to energy, protein and calcium and the columns of A correspond to oatmeal, chicken, eggs, milk, pie and bacon respectively.

The MPSX representation of the problem is given in Section 9.2.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02BUF Example Program Text
*     Mark 16 Release. NAG Copyright 1993.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MAXN, MAXM
      PARAMETER        (MAXN=50,MAXM=50)
      INTEGER          LDA
      PARAMETER        (LDA=MAXM)
      real             XBUDEF, XBLDEF
      PARAMETER        (XBUDEF=1.0e+20,XBLDEF=0.0e0)
      INTEGER          LIWORK
      PARAMETER        (LIWORK=2*MAXN+3)
      INTEGER          LWORK
      PARAMETER        (LWORK=2*(MAXM+1)**2+7*MAXN+5*MAXM)
      CHARACTER*3      OPTIM
      PARAMETER        (OPTIM='MIN')
*     .. Local Scalars ..
      real             OBJVAL
      INTEGER          IFAIL, INFILE, ITER, M, N
      LOGICAL          MPSLST
      CHARACTER*8      KBLANK, NMBND, NMOBJ, NMPROB, NMRHS, NMRNG
*     .. Local Arrays ..
      real             A(MAXM,MAXN), AX(MAXM), BL(MAXN+MAXM),
     +                 BU(MAXN+MAXM), CLAMDA(MAXN+MAXM), CVEC(MAXN),
     +                 WORK(LWORK), X(MAXN)
```

```
      INTEGER          INTVAR(MAXN), ISTATE(MAXN+MAXM), IWORK(LIWORK)
      CHARACTER*8      CRNAME(MAXN+MAXM)
*     .. External Subroutines ..
      EXTERNAL         E04MFF, E04MHF, H02BUF, H02BVF
*     .. Data statements ..
      DATA             KBLANK/'        '/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02BUF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
*
*     Initialize parameters
*
      INFILE = NIN
      NMPROB = KBLANK
      NMOBJ = KBLANK
      NMRHS = KBLANK
      NMRNG = KBLANK
      NMBND = KBLANK
      MPSLST = .FALSE.
*
      IFAIL = 0
*
*     Convert the MPSX data file for use by E04MFF
*
      CALL H02BUF(INFILE,MAXN,MAXM,OPTIM,XBLDEF,XBUDEF,NMOBJ,NMRHS,
     +            NMRNG,NMBND,MPSLST,N,M,A,BL,BU,CVEC,X,INTVAR,CRNAME,
     +            NMPROB,ISTATE,IFAIL)
*
*     Solve the problem
*
      IFAIL = -1
*
      CALL E04MHF('Print Level = 5')
*
      CALL E04MFF(N,M,A,LDA,BL,BU,CVEC,ISTATE,X,ITER,OBJVAL,AX,CLAMDA,
     +            IWORK,LIWORK,WORK,LWORK,IFAIL)
*
      IF (IFAIL.EQ.0 .OR. IFAIL.EQ.1 .OR. IFAIL.EQ.3) THEN
*
*        Print solution (using MPSX names)
*
         IFAIL = 0
*
         CALL H02BVF(N,M,A,LDA,BL,BU,X,CLAMDA,ISTATE,CRNAME,IFAIL)
*
      ELSE
         WRITE (NOUT,99999) 'E04MFF terminated with IFAIL = ', IFAIL
      END IF
*
      STOP
*
99999 FORMAT (1X,A,I3)
      END
```

9.2 Program Data

```
H02BUF Example Program Data
NAME          DIET
ROWS
 G  ENERGY
 G  PROTEIN
 G  CALCIUM
 N  COST
COLUMNS
    OATMEAL   ENERGY      110.0
    OATMEAL   PROTEIN     4.0
    OATMEAL   CALCIUM     2.0
    OATMEAL   COST        3.0
    CHICKEN   ENERGY      205.0
    CHICKEN   PROTEIN     32.0
    CHICKEN   CALCIUM     12.0
    CHICKEN   COST        24.0
    EGGS      ENERGY      160.0
    EGGS      PROTEIN     13.0
    EGGS      CALCIUM     54.0
    EGGS      COST        13.0
    MILK      ENERGY      160.0
    MILK      PROTEIN     8.0
    MILK      CALCIUM     285.0
    MILK      COST        9.0
    PIE       ENERGY      420.0
    PIE       PROTEIN     4.0
    PIE       CALCIUM     22.0
    PIE       COST        20.0
    BACON     ENERGY      260.0
    BACON     PROTEIN     14.0
    BACON     CALCIUM     80.0
    BACON     COST        19.0
RHS
    DEMANDS   ENERGY      2000.0
    DEMANDS   PROTEIN     55.0
    DEMANDS   CALCIUM     800.0
BOUNDS
 UI SERVINGS  OATMEAL     4.0
 UI SERVINGS  CHICKEN     3.0
 UP SERVINGS  EGGS        2.0
 UP SERVINGS  MILK        8.0
 UP SERVINGS  PIE         2.0
 UI SERVINGS  BACON       2.0
ENDATA
```

9.3 Program Results

```
H02BUF Example Program Results


Calls to E04MHF
---------------

     Print Level = 5

*** E04MFF
*** Start of NAG Library implementation details ***

Implementation title: Generalised Base Version
           Precision: FORTRAN double precision
        Product Code: FLBAS19D
                Mark: 19A

*** End of NAG Library implementation details ***

Parameters
----------

Problem type.....        LP

Linear constraints.....      3       Feasibility tolerance..  1.05E-08
Variables.............       6       Optimality tolerance...  1.72E-13

Infinite bound size....  1.00E+20    COLD start.............
Infinite step size.....  1.00E+20    EPS (machine precision)  1.11E-16

Check frequency........     50       Expand frequency.......        5
Minimum sum of infeas..     NO       Crash tolerance........  1.00E-02

Print level............      5       Iteration limit........       50
Monitoring file........     -1

Workspace provided is     IWORK(     103),  WORK(    5802).
To solve problem we need  IWORK(      15),  WORK(      89).


 Itn     Step Ninf Sinf/Objective  Norm Gz
   0  0.0E+00    3   1.799000E+03  0.0E+00
   1  1.5E-02    1   2.550000E+02  0.0E+00
   2  1.4E-03    0   1.271429E+02  0.0E+00
   3  8.7E-02    0   1.129048E+02  0.0E+00
   4  2.1E-01    0   1.062857E+02  0.0E+00
   5  1.9E+00    0   9.733333E+01  0.0E+00
   6  2.9E+00    0   9.250000E+01  0.0E+00

Exit E04MFF - Optimal LP solution.

Final LP objective value =    92.50000

Exit from LP problem after     6 iterations.


Varbl   State      Value      Lower Bound   Upper Bound    Lagr Mult   Residual
```

OATMEAL	UL	4.00000	0.000000E+00	4.00000	-3.187	0.0000E+00
CHICKEN	LL	0.000000E+00	0.000000E+00	3.00000	12.47	0.0000E+00
EGGS	LL	0.000000E+00	0.000000E+00	2.00000	4.000	0.0000E+00
MILK	FR	4.50000	0.000000E+00	8.00000	0.0000E+00	3.500
PIE	UL	2.00000	0.000000E+00	2.00000	-3.625	0.0000E+00
BACON	LL	0.000000E+00	0.000000E+00	2.00000	4.375	0.0000E+00

L Con	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
ENERGY	LL	2000.00	2000.00	None	5.6250E-02	0.0000E+00
PROTEIN	FR	60.0000	55.0000	None	0.0000E+00	5.000
CALCIUM	FR	1334.50	800.000	None	0.0000E+00	534.5

H02BVF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

H02BVF prints the solution to a linear or integer programming problem computed by E04MFF or H02BBF and H02BZF, with user supplied names for the rows and columns.

2. Specification

```
      SUBROUTINE H02BVF (N, M, A, LDA, BL, BU, X, CLAMDA, ISTATE, CRNAME,
     1                   IFAIL)
      INTEGER           N, M, LDA, ISTATE(N+M), IFAIL
      real              A(LDA,N), BL(N+M), BU(N+M), X(N), CLAMDA(N+M)
      CHARACTER*8       CRNAME(N+M)
```

3. Description

H02BVF prints the solution to a linear or integer programming problem with user supplied names for the rows and columns. All output is written to the current advisory message unit (as defined by X04ABF). The routine must be preceded in the same program by calls to H02BUF and either E04MFF (if an LP problem has been solved) or H02BBF and H02BZF (if an IP problem has been solved). The documents for H02BUF, E04MFF and/or H02BBF and H02BZF should be consulted for further details.

4. References

[1] MPSX – Mathematical Programming System.
Program number 5734 XM4, IBM Trade Corporation, New York, 1971.

5. Parameters

1: N – INTEGER. *Input*

On entry: the number of variables, as returned by H02BUF.

Constraint: N > 0.

2: M – INTEGER. *Input*

On entry: the number of general linear constraints, as returned by H02BUF.

Constraint: M ≥ 0.

3: A(LDA,*) – ***real*** array. *Input*

Note: the second dimension of the array A must be at least at least N when M > 0, and at least 1 when M = 0.

On entry: the matrix of general linear constraints, as returned by H02BUF.

4: LDA – INTEGER. *Input*

On entry: this **must** be the same parameter MAXM as supplied to H02BUF.

Constraint: LDA ≥ max(1,M).

5: BL(N+M) – ***real*** array. *Input*

On entry: the lower bounds for all the constraints, as returned by E04MFF or H02BZF.

6: BU(N+M) – ***real*** array. *Input*

On entry: the upper bounds for all the constraints, as returned by E04MFF or H02BZF.

7: X(N) – ***real*** array. *Input*

On entry: the solution to the problem, as returned by E04MFF or H02BBF.

8: CLAMDA(N+M) – ***real*** array. *Input*

On entry: the Lagrange multipliers (reduced costs) for each constraint with respect to the working set, as returned by E04MFF or H02BZF.

9: ISTATE(N+M) – INTEGER array. *Input*

On entry: the status of every constraint in the working set at the solution, as returned by E04MFF or H02BZF.

10: CRNAME(N+M) – CHARACTER*8 array. *Input*

On entry: the user defined names for all the variables and constraints, as returned by H02BUF.

11: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, $N \leq 0$,
or $M < 0$,
or $LDA < \max(1,M)$.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

See the example for H02BUF.

H02BZF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

Warning: the specification of the parameter LIWORK changed at Mark 16: the minimum dimension of the array IWORK has been increased by N + 3.

1. Purpose

H02BZF extracts more information associated with the solution of an integer programming problem computed by H02BBF.

2. Specification

```
SUBROUTINE H02BZF (N, M, BL, BU, CLAMDA, ISTATE, IWORK, LIWORK, RWORK,
1                  LRWORK, IFAIL)
INTEGER          N, M, ISTATE(N+M), IWORK(LIWORK), LIWORK, LRWORK, IFAIL
real             BL(N+M), BU(N+M), CLAMDA(N+M), RWORK(LRWORK)
```

3. Description

H02BZF extracts the following information associated with the solution of an integer programming problem computed by H02BBF: the upper and lower bounds used for the solution, the Lagrange multipliers (costs), and the status of the variables at the solution.

In the branch and bound method employed by H02BBF, the arrays BL and BU are used to impose restrictions on the values of the integer variables in each sub-problem. That is, if the variable x_j is restricted to take value v_j in a particular sub-problem, then BL(j) = BU(j) = v_j is set in the sub-problem. Thus, on exit from this routine, some of the elements of BL and BU which correspond to integer variables may contain these imposed values, rather than those originally supplied to H02BBF.

4. References

None.

5. Parameters

1: N – INTEGER. *Input*

On entry: this **must** be the same parameter N as supplied to H02BBF.

Constraint: N > 0.

2: M – INTEGER. *Input*

On entry: this **must** be the same parameter M as supplied to H02BBF.

Constraint: M ≥ 0.

3: BL(N+M) – ***real*** array. *Output*

On exit: if H02BBF exits with IFAIL = 0, 7 or 9, the values in the array BL contain the lower bounds imposed on the integer solution for all the constraints. The first N elements contain the lower bounds on the variables, and the next M elements contain the lower bounds for the general linear constraints (if any).

4: BU(N+M) – ***real*** array. *Output*

On exit: if H02BBF exits with IFAIL = 0, 7 or 9, the values in the array BU contain the upper bounds imposed on the integer solution for all the constraints. The first N elements contain the upper bounds on the variables, and the next M elements contain the upper bounds for the general linear constraints (if any).

5: CLAMDA(N+M) – ***real*** array. *Output*

On exit: if H02BBF exits with IFAIL = 0, 7 or 9, the values in the array CLAMDA contain the values of the Lagrange multipliers for each constraint with respect to the current working set. The first N elements contain the multipliers (reduced costs) for the bound constraints on the variables, and the next M elements contain the multipliers (shadow costs) for the general linear constraints (if any).

6: ISTATE(N+M) – INTEGER array. *Output*

On exit: if H02BBF exits with IFAIL = 0, 7 or 9, the values in the array ISTATE indicate the status of the constraints in the working set at an integer solution. Otherwise, ISTATE indicates the composition of the working set at the final iterate. The significance of each possible value of ISTATE(j) is as follows:

ISTATE(j)	**Meaning**
–2	The constraint violates its lower bound by more than TOLFES (the feasibility tolerance, see H02BBF).
–1	The constraint violates its upper bound by more than TOLFES.
0	The constraint is satisfied to within TOLFES, but is not in the working set.
1	This inequality constraint is included in the working set at its lower bound.
2	This inequality constraint is included in the working set at its upper bound.
3	This constraint is included in the working set as an equality. This value of ISTATE can occur only when BL(j) = BU(j).
4	This corresponds to an integer solution being declared with x_j being temporarily fixed at its current value. This value of ISTATE can occur only when IFAIL = 0, 7 or 9 on exit from H02BBF.

7: IWORK(LIWORK) – INTEGER array. *Workspace*

This **must** be the same parameter IWORK as supplied to H02BBF. It is used to pass information from H02BBF to H02BZF and therefore the contents of this array **must not** be changed before calling H02BZF.

8: LIWORK – INTEGER. *Input*

On entry: the dimension of the array IWORK as declared in the (sub)program from which H02BZF is called.

9: RWORK(LRWORK) – ***real*** array. *Workspace*

This **must** be the same parameter RWORK as supplied to H02BBF. It is used to pass information from H02BBF to H02BZF and therefore the contents of this array **must not** be changed before calling H02BZF.

10: LRWORK – INTEGER. *Input*

On entry: the dimension of the array RWORK as declared in the (sub)program from which H02BZF is called.

11: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, N ≤ 0,
or M < 0.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

One of the applications of integer programming is to the so-called diet problem. Given the nutritional content of a selection of foods, the cost of each food, the amount available of each food and the consumer's minimum daily energy requirements, the problem is to find the cheapest combination. This gives rise to the following problem:

minimize

$$c^T x$$

subject to

$$Ax \geq b,$$

$$0 \leq x \leq u,$$

where

$c = (3 \quad 24 \quad 13 \quad 9 \quad 20 \quad 19)^T$, $x = (x_1, x_2, x_3, x_4, x_5, x_6)^T$ is integer,

$$A = \begin{pmatrix} 110 & 205 & 160 & 160 & 420 & 260 \\ 4 & 32 & 13 & 8 & 4 & 14 \\ 2 & 12 & 54 & 285 & 22 & 80 \end{pmatrix}, \quad b = \begin{pmatrix} 2000 \\ 55 \\ 800 \end{pmatrix} \text{ and}$$

$u = (4 \quad 3 \quad 2 \quad 8 \quad 2 \quad 2)^T$.

The rows of A correspond to energy, protein and calcium and the columns of A correspond to oatmeal, chicken, eggs, milk, pie and bacon respectively.

The following program solves the above problem to obtain the optimal integer solution and then examines the effect of increasing the energy required to 2200 units.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02BZF Example Program Text
*     Mark 16 Revised. NAG Copyright 1993.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX
      PARAMETER        (NMAX=10,MMAX=10)
      INTEGER          LDA
      PARAMETER        (LDA=MMAX)
      INTEGER          LIWORK, LRWORK
      PARAMETER        (LIWORK=1000,LRWORK=1000)
*     .. Local Scalars ..
      real             BIGBND, INIVAL, OBJMIP, TOLFES, TOLIV
      INTEGER          I, IFAIL, INTFST, ITMAX, J, M, MAXDPT, MAXNOD,
     +                 MSGLVL, N
*     .. Local Arrays ..
      real             A(LDA,NMAX), BL(NMAX+MMAX), BU(NMAX+MMAX),
     +                 CLAMDA(NMAX+MMAX), CVEC(NMAX), RWORK(LRWORK),
     +                 X(NMAX)
      INTEGER          INTVAR(NMAX), ISTATE(NMAX+MMAX), IWORK(LIWORK)
      CHARACTER*8      NAMES(NMAX+MMAX)
```

```
*     .. External Subroutines ..
      EXTERNAL         H02BBF, H02BZF, OUTSOL
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02BZF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, M
      IF (N.LE.NMAX .AND. M.LE.MMAX) THEN
*
*        Read ITMAX, MSGLVL, MAXNOD, INTFST, MAXDPT, TOLFES, TOLIV,
*        CVEC, A, BIGBND, BL, BU, INTVAR and X from data file
*
         READ (NIN,*) ITMAX, MSGLVL
         READ (NIN,*) MAXNOD
         READ (NIN,*) INTFST, MAXDPT
         READ (NIN,*) TOLFES, TOLIV
         READ (NIN,*) (CVEC(J),J=1,N)
         READ (NIN,*) (NAMES(J),(A(I,J),I=1,M),J=1,N)
         READ (NIN,*) BIGBND
         READ (NIN,*) (BL(I),I=1,N)
         READ (NIN,*) (NAMES(N+I),BL(N+I),I=1,M)
         READ (NIN,*) (BU(I),I=1,N+M)
         READ (NIN,*) (INTVAR(I),I=1,N)
         READ (NIN,*) (X(I),I=1,N)
*
*        Solve the IP problem using H02BBF
*
         IFAIL = -1
*
         CALL H02BBF(ITMAX,MSGLVL,N,M,A,LDA,BL,BU,INTVAR,CVEC,MAXNOD,
     +               INTFST,MAXDPT,TOLIV,TOLFES,BIGBND,X,OBJMIP,IWORK,
     +               LIWORK,RWORK,LRWORK,IFAIL)
*
         IF (IFAIL.EQ.0 .OR. IFAIL.EQ.7 .OR. IFAIL.EQ.9) THEN
            WRITE (NOUT,99999) 'IP objective value = ', OBJMIP
*
*           Get information about the solution
*
            IFAIL = 0
*
            CALL H02BZF(N,M,BL,BU,CLAMDA,ISTATE,IWORK,LIWORK,RWORK,
     +                  LRWORK,IFAIL)
*
*           Print the solution
*
            CALL OUTSOL(N,M,A,LDA,BL,BU,X,ISTATE,CLAMDA,BIGBND,NAMES,
     +                  NOUT)
*
*           Increase the energy requirements and solve the modified IP
*           problem using the current IP solution as the starting point
*
            INIVAL = BL(N+1)
            READ (NIN,*) BL(N+1)
            WRITE (NOUT,99998) 'Increase the energy requirements from',
     +        INIVAL, 'to', BL(N+1)
*
            IFAIL = -1
*
            CALL H02BBF(ITMAX,MSGLVL,N,M,A,LDA,BL,BU,INTVAR,CVEC,MAXNOD,
     +                  INTFST,MAXDPT,TOLIV,TOLFES,BIGBND,X,OBJMIP,
     +                  IWORK,LIWORK,RWORK,LRWORK,IFAIL)
*
            IF (IFAIL.EQ.0 .OR. IFAIL.EQ.7 .OR. IFAIL.EQ.9) THEN
               WRITE (NOUT,99999) 'IP objective value = ', OBJMIP
*
*              Get information about the solution
*
               IFAIL = 0
*
```

```
                CALL H02BZF(N,M,BL,BU,CLAMDA,ISTATE,IWORK,LIWORK,RWORK,
     +                      LRWORK,IFAIL)
*
*               Print the solution
*
                CALL OUTSOL(N,M,A,LDA,BL,BU,X,ISTATE,CLAMDA,BIGBND,NAMES,
     +                      NOUT)
*
              ELSE
                 WRITE (NOUT,99997) ' H02BBF terminated with IFAIL = ',
     +             IFAIL
              END IF
           ELSE
              WRITE (NOUT,99997) ' H02BBF terminated with IFAIL = ', IFAIL
           END IF
         END IF
         STOP
*
99999 FORMAT (//1X,A,1P,G16.4)
99998 FORMAT (//1X,A,2X,1P,G10.4,2X,A,2X,1P,G10.4)
99997 FORMAT (1X,A,I3)
         END
         SUBROUTINE OUTSOL(N,M,A,LDA,BL,BU,X,ISTATE,CLAMDA,BIGBND,NAMES,
     +                     NOUT)
*        .. Scalar Arguments ..
         real              BIGBND
         INTEGER           LDA, M, N, NOUT
*        .. Array Arguments ..
         real              A(LDA,*), BL(N+M), BU(N+M), CLAMDA(N+M), X(N)
         INTEGER           ISTATE(N+M)
         CHARACTER*8       NAMES(N+M)
*        .. Local Scalars ..
         real              B1, B2, RES, RES2, V, WLAM
         INTEGER           IS, J, K
         CHARACTER*80      REC
*        .. Local Arrays ..
         CHARACTER*2       LSTATE(-2:4)
*        .. External Functions ..
         real              sdot
         EXTERNAL          sdot
*        .. Intrinsic Functions ..
         INTRINSIC         ABS
*        .. Data statements ..
         DATA              LSTATE(-2)/'--'/, LSTATE(-1)/'++'/,
        +                  LSTATE(0)/'FR'/, LSTATE(1)/'LL'/,
        +                  LSTATE(2)/'UL'/, LSTATE(3)/'EQ'/,
        +                  LSTATE(4)/'TF'/
*        .. Executable Statements ..
*
         WRITE (NOUT,99999)
         DO 20 J = 1, N + M
            B1 = BL(J)
            B2 = BU(J)
            WLAM = CLAMDA(J)
            IS = ISTATE(J)
            IF (J.LE.N) THEN
*              The variables  x.
               K = J
               V = X(J)
            ELSE
*              The linear constraints  A*x.
               IF (J.EQ.N+1) WRITE (NOUT,99998)
               K = J - N
               V = sdot(N,A(K,1),LDA,X,1)
            END IF
*
*           Print a line for the j-th variable or constraint.
*
            RES = V - B1
            RES2 = B2 - V
```

```
            IF (ABS(RES).GT.ABS(RES2)) RES = RES2
            WRITE (REC,99997) NAMES(J), LSTATE(IS), V, B1, B2, WLAM, RES
            IF (B1.LE.-BIGBND) REC(29:42) = '     None      '
            IF (B2.GE.BIGBND) REC(43:56) = '     None      '
            WRITE (NOUT,'(A)') REC
   20    CONTINUE
         RETURN
*
99999 FORMAT (//1X,'Varbl',3X,'State',5X,'Value',5X,'Lower Bound',3X,
     +       'Upper Bound',4X,'Lagr Mult',3X,'Residual',/)
99998 FORMAT (//1X,'L Con',3X,'State',5X,'Value',5X,'Lower Bound',3X,
     +       'Upper Bound',4X,'Lagr Mult',3X,'Residual',/)
99997 FORMAT (1X,A8,2X,A2,1X,1P,3G14.4,1P,G12.4,1P,G12.4)
      END
```

9.2. Program Data

```
H02BZF Example Program Data
 6  3                                                  :Values of N and M
 0  0                                                  :Values of ITMAX and MSGLVL
 0                                                     :Value of MAXNOD
 0  9                                                  :Values of INTFST and MAXDPT
 0.0  0.0                                              :Values of TOLFES and TOLIV
 3.0  24.0  13.0  9.0  20.0  19.0                      :End of CVEC
 'Oatmeal'    110.0    4.0      2.0
 'Chicken'    205.0   32.0     12.0
 'Eggs'       160.0   13.0     54.0
 'Milk'       160.0    8.0    285.0
 'Pie'        420.0    4.0     22.0
 'Bacon'      260.0   14.0     80.0                          :End of matrix A
 1.0E+20                                                    :Value of BIGBND
 0.0  0.0  0.0  0.0  0.0  0.0
 'Energy'  2000.0  'Protein'  55.0  'Calcium'  800.0        :End of BL
 4.0  3.0  2.0  8.0  2.0  2.0  1.0E+20  1.0E+20  1.0E+20    :End of BU
 1    1    1    1    1    1                               :End of INTVAR
 0.0  0.0  0.0  0.0  0.0  0.0                             :End of X
 2200.0                                          :Change 'Energy' in RHS
```

9.3. Program Results

```
H02BZF Example Program Results


IP objective value =        97.00


Varbl    State     Value      Lower Bound    Upper Bound    Lagr Mult    Residual

Oatmeal    EQ       4.000          4.000          4.000        3.000       0.0000
Chicken    LL     0.0000         0.0000          3.000        24.00       0.0000
Eggs       LL     0.0000         0.0000          2.000        13.00       0.0000
Milk       LL      5.000          5.000          8.000        9.000       0.0000
Pie        EQ      2.000          2.000          2.000        20.00       0.0000
Bacon      LL     0.0000         0.0000          2.000        19.00       0.0000


L Con    State     Value      Lower Bound    Upper Bound    Lagr Mult    Residual

Energy     FR      2080.          2000.           None       0.0000        80.00
Protein    FR      64.00          55.00           None       0.0000       9.000
Calcium    FR      1477.          800.0           None       0.0000       677.0


Increase the energy requirements from   2000.      to   2200.


IP objective value =        106.0
```

Varbl	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
Oatmeal	EQ	4.000	4.000	4.000	3.000	0.0000
Chicken	LL	0.0000	0.0000	3.000	24.00	0.0000
Eggs	LL	0.0000	0.0000	2.000	13.00	0.0000
Milk	LL	6.000	6.000	8.000	9.000	0.0000
Pie	EQ	2.000	2.000	2.000	20.00	0.0000
Bacon	LL	0.0000	0.0000	2.000	19.00	0.0000

L Con	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
Energy	FR	2240.	2200.	None	0.0000	40.00
Protein	FR	72.00	55.00	None	0.0000	17.00
Calcium	FR	1762.	800.0	None	0.0000	962.0

H02CBF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

Note. *This routine uses* optional parameters *to define choices in the problem specification and in the details of the algorithm. If you wish to use* default *settings for all of the optional parameters, you need only read Section 1 to Section 9 of this document. Refer to the additional Section 10, Section 11 and Section 12 for a detailed description of the algorithm, the specification of the optional parameters and a description of the monitoring information produced by the routine.*

1 Purpose

H02CBF solves general quadratic programming problems with integer constraints on the variables. It is not intended for large sparse problems.

2 Specification

```
 SUBROUTINE H02CBF(N, NCLIN, A, LDA, BL, BU, CVEC, H, LDH, QPHESS,
1                  INTVAR, LINTVR, MDEPTH, ISTATE, XS, OBJ, AX,
2                  CLAMDA, STRTGY, IWRK, LIWRK, WRK, LWRK, MONIT,
3                  IFAIL)
 INTEGER           N, NCLIN, LDA, LDH, INTVAR(LINTVR), LINTVR,
1                  MDEPTH, ISTATE(N+NCLIN), STRTGY, IWRK(LIWRK),
2                  LIWRK, LWRK, IFAIL
 real              A(LDA,*), BL(N+NCLIN), BU(N+NCLIN), CVEC(*),
1                  H(LDH,*), XS(N+NCLIN), OBJ, AX(*),
2                  CLAMDA(N+NCLIN), WRK(LWRK)
 EXTERNAL          MONIT, QPHESS
```

3 Description

H02CBF uses a 'Branch and Bound' algorithm in conjunction with E04NFF to try and determine integer solutions to a general quadratic programming problem. Only when the problem is linear and the matrix H is positive definite can the technique be guaranteed to work; but often useful results can be obtained for a wider class of problems.

Branch and bound consists firstly of obtaining a solution without any of the variables $x = (x_1, x_2, \ldots, x_n)^T$ constrained to be integer. Suppose x_1 ought to be integer, but at the optimal value just computed $x_1 = 2.4$. A constraint $x_1 \leq 2$ is added to the system and the second problem solved. A constraint $x_1 \geq 3$ gives rise to a third sub-problem. In a similar manner a whole series of sub-problems may be generated, corresponding to integer constraints on the variables. The sub-problems are all solved using E04NFF.

In practice the routine tries to compute an integer solution as quickly as possible using a depth-first approach, since this helps determine a realistic cut-off value. If we have a cut-off value, say the value of the function at this first integer solution, and any sub-problem, W say, has a solution value greater than this cut-off value, then subsequent sub-problems of W must have solutions greater than the value of the solution at W and therefore need not be computed. Thus a knowledge of a good cut-off value can result in fewer sub-problems being solved and thus speed up the operation of the routine. (See the description of MONIT in Section 5 for details of how users can supply their own cut-off value.)

4 References

[1] Gill P E, Hammarling S, Murray W, Saunders M A and Wright M H (1986) User's guide for LSSOL (Version 1.0) *Report SOL 86-1* Department of Operations Research, Stanford University

[2] Gill P E and Murray W (1978) Numerically stable methods for quadratic programming *Math. Programming* **14** 349–372

[3] Gill P E, Murray W, Saunders M A and Wright M H (1984) Procedures for optimization problems with a mixture of bounds and general linear constraints *ACM Trans. Math. Software* **10** 282–298

[4] Gill P E, Murray W, Saunders M A and Wright M H (1989) A practical anti-cycling procedure for linearly constrained optimization *Math. Programming* **45** 437–474

[5] Gill P E, Murray W, Saunders M A and Wright M H (1991) Inertia-controlling methods for general quadratic programming *SIAM Rev.* **33** 1–36

[6] Pardalos P M and Schnitger G (1988) Checking local optimality in constrained quadratic programming is NP-hard *Operations Research Letters* **7** 33–35

[7] Gill P E, Murray W and Wright M H (1981) *Practical Optimization* Academic Press

5 Parameters

1: N — INTEGER *Input*

On entry: n, the number of variables.

Constraint: N > 0.

2: NCLIN — INTEGER *Input*

On entry: m_L, the number of general linear constraints.

Constraint: NCLIN $\geq$ 0.

3: A(LDA,*) — ***real*** array *Input*

Note: the second dimension of the array A must be at least N when NCLIN > 0, and at least 1 when NCLIN = 0.

On entry: the ith row of A must contain the coefficients of the ith general linear constraint, for $i = 1, 2, \ldots, m_L$.

If NCLIN = 0 then the array A is not referenced.

4: LDA — INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which H02CBF is called.

Constraint: LDA $\geq$ max(1,NCLIN).

5: BL(N+NCLIN) — ***real*** array *Input*

6: BU(N+NCLIN) — ***real*** array *Input*

On entry: BL must contain the lower bounds and BU the upper bounds, for all the constraints in the following order. The first n elements of each array must contain the bounds on the variables, and the next m_L elements the bounds for the general linear constraints (if any). To specify a non-existent lower bound (i.e., $l_j = -\infty$), set BL(j) $\leq -$*bigbnd*, and to specify a non-existent upper bound (i.e., $u_j = +\infty$), set BU(j) $\geq$ *bigbnd*; the default value of *bigbnd* is 10^{20}, but this may be changed by the optional parameter **Infinite Bound Size** (see Section 11.2). To specify the jth constraint as an *equality*, set BL(j) = BU(j) = β, say, where $|\beta| <$ *bigbnd*.

Constraints:

BL(j) $\leq$ BU(j), for $j = 1, 2, \ldots$,N+NCLIN,
$|\beta| <$ *bigbnd* when BL(j) = BU(j) = β.

7: CVEC(*) — ***real*** array *Input*

Note: the dimension of the array CVEC must be at least N when the problem is of type LP, QP2 (the default) or QP4, and at least 1 otherwise.

On entry: the coefficients of the explicit linear term of the objective function when the problem is of type LP, QP2 (the default) and QP4.

If the problem is of type FP, QP1, or QP3, CVEC is not referenced.

8: H(LDH,*) — ***real*** array *Input*

Note: the second dimension of the array H must be at least N if it is to be used to store H explicitly, and at least 1 otherwise.

On entry: H may be used to store the quadratic term H of the QP objective function if desired. In some cases, the user need not use H to store H explicitly (see the specification of subroutine QPHESS below). The elements of H are referenced only by subroutine QPHESS. The number of rows of H is denoted by m, whose default value is n. (The optional parameter **Hessian Rows** may be used to specify a value of $m < n$; see Section 11.2).

If the default version of QPHESS is used and the problem is of type QP1 or QP2 (the default), the first m rows and columns of H must contain the leading m by m rows and columns of the symmetric Hessian matrix H. Only the diagonal and upper triangular elements of the leading m rows and columns of H are referenced. The remaining elements need not be assigned.

If the default version of QPHESS is used and the problem is of type QP3 or QP4, the first m rows of H must contain an m by n upper trapezoidal factor of the symmetric Hessian matrix $H^T H$. The factor need not be of full rank, i.e., some of the diagonal elements may be zero. However, as a general rule, the larger the dimension of the leading non-singular sub-matrix of H, the fewer iterations will be required. Elements outside the upper trapezoidal part of the first m rows of H need not be assigned.

If a non-default version of QPHESS is supplied, then in some cases it may be desirable to use a one-dimensional array to transmit data to QPHESS. (This is illustrated in the example program in Section 9 of the document for H02CCF.) H is then declared as a vector with dimension (LDH), where LDH $\geq$ N $\times$ (N+1)/2.

In other situations, it may be desirable to compute Hx or $H^T Hx$ without accessing H – for example, if H or $H^T H$ is sparse or has special structure. The parameters H and LDH may then refer to any convenient array.

If the problem is of type FP or LP, H is not referenced.

9: LDH — INTEGER *Input*

On entry: the first dimension of the array H as declared in the (sub)program from which H02CBF is called.

Constraints:

if the problem is of type QP1, QP2 (the default), QP3 or QP4, LDH $\geq$ N or at least the value of the optional parameter **Hessian Rows** (default value = n; see Section 11.2).

if the problem is of type FP or LP, LDH $\geq$ 1.

10: QPHESS — SUBROUTINE, supplied by the NAG Fortran Library or the user. *External Procedure*

In general, the user need not provide a version of QPHESS, because a 'default' subroutine with name E04NFU is included in the Library (NFUE04 in some implementations: see the Users' Note for your implementation for details). However, the algorithm of H02CBF requires only the product of H or $H^T H$ and a vector x; and in some cases the user may obtain increased efficiency by providing a version of QPHESS that avoids the need to define the elements of the matrices H or $H^T H$ explicitly.

QPHESS is not referenced if the problem is of type FP or LP, in which case QPHESS may be the routine E04NFU (NFUE04 in some implementations).

Its specification is:

```
SUBROUTINE QPHESS(N, JTHCOL, H, LDH, X, HX)
INTEGER           N, JTHCOL, LDH
real              H(LDH,*), X(N), HX(N)
```

1: N — INTEGER *Input*

On entry: this is the same parameter N as supplied to H02CBF (see above).

2: JTHCOL — INTEGER *Input*

On entry: JTHCOL specifies whether or not the vector x is a column of the identity matrix. If JTHCOL $= j > 0$, then the vector x is the jth column of the identity matrix, and hence Hx or H^THx is the jth column of H or H^TH, respectively, which may in some cases require very little computation and QPHESS may be coded to take advantage of this. However special code is not necessary because x is always stored explicitly in the array X. If JTHCOL $= 0$, x has no special form.

3: H(LDH,*) — ***real*** array *Input*

On entry: this is the same parameter H as supplied to H02CBF (see above).

4: LDH — INTEGER *Input*

On entry: this is the same parameter LDH as supplied to H02CBF (see above).

5: X(N) — ***real*** array *Input*

On entry: the vector x.

6: HX(N) — ***real*** array *Output*

On exit: the product Hx if the problem is of type QP1 or QP2 (the default), or the product H^THx if the problem is of type QP3 or QP4.

QPHESS must be declared as EXTERNAL in the (sub)program from which H02CBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

11: INTVAR(LINTVR) — INTEGER array *Input*

On entry: INTVAR(i) must contain the index of the solution vector x which is required to be integer. For example, if x_1 and x_3 are constrained to take integer values then INTVAR(1) might be set to 1 and INTVAR(2) to 3. The order in which the indices are specified is important, since this determines the order in which the sub-problems are generated. As a rule-of-thumb, the important variables should always be specified first. Thus, in the above example, if x_3 relates to a more important quantity than x_1, then it might be advantageous to set INTVAR(1) = 3 and INTVAR(2) = 1. If k is the smallest integer such that INTVAR(k) is less than or equal to zero then H02CBF assumes that $k-1$ variables are constrained to be integer; components INTVAR($k+1$), ..., INTVAR(LINTVR) are *not* referenced.

12: LINTVR — INTEGER *Input*

On entry: the dimension of the array INTVAR as declared in the calling (sub)program. Often LINTVR is the number of variables that are constrained to be integer.

Constraint: LINTVR > 0.

13: MDEPTH — INTEGER *Input*

On entry: the maximum depth (i.e., number of extra constraints) that H02CBF may insert before admitting failure.

Suggested value: MDEPTH = 3 × N/2.

Constraint: MDEPTH ≥ 1.

14: ISTATE(N+NCLIN) — INTEGER array *Input/Output*

On entry: ISTATE need not be set if the (default) **Cold Start** option is used.

If the **Warm Start** option has been chosen (see Section 11.2), ISTATE specifies the desired status of the constraints at the start of the feasibility phase. More precisely, the first n elements of ISTATE refer to the upper and lower bounds on the variables, and the next m_L elements refer to the general linear constraints (if any). Possible values for ISTATE(j) are as follows:

ISTATE(j)	**Meaning**
0	The corresponding constraint should *not* be in the initial working set.
1	The constraint should be in the initial working set at its lower bound.
2	The constraint should be in the initial working set at its upper bound.
3	The constraint should be in the initial working set as an equality. This value must not be specified unless BL(j) = BU(j).

The values -2, -1 and 4 are also acceptable but will be reset to zero by the routine. If H02CBF has been called previously with the same values of N and NCLIN, ISTATE already contains satisfactory information. (See also the description of the optional parameter **Warm Start** in Section 11.2). The routine also adjusts (if necessary) the values supplied in XS to be consistent with ISTATE.

Constraint: $-2 \leq$ ISTATE(j) ≤ 4, for $j = 1, 2, \ldots,$N+NCLIN.

On exit: the status of the constraints in the working set at the point returned in XS. The significance of each possible value of ISTATE(j) is as follows:

ISTATE(j)	**Meaning**
-2	The constraint violates its lower bound by more than the feasibility tolerance.
-1	The constraint violates its upper bound by more than the feasibility tolerance.
0	The constraint is satisfied to within the feasibility tolerance, but is not in the working set.
1	This inequality constraint is included in the working set at its lower bound.
2	This inequality constraint is included in the working set at its upper bound.
3	This constraint is included in the working set as an equality. This value of ISTATE can occur only when BL(j) = BU(j).
4	This corresponds to optimality being declared with XS(j) being temporarily fixed at its current value. This value of ISTATE can occur only when IFAIL = 1 on exit.

15: XS(N+NCLIN) — ***real*** array *Input/Output*

On entry: an initial estimate of the solution.

On exit: the point at which H02CBF terminated. If IFAIL = 0, 1 or 3, XS contains an estimate of the solution.

16: OBJ — ***real*** *Output*

On exit: the value of the objective function at x if x is feasible, or the sum of infeasibilities at x otherwise. If the problem is of type FP and x is feasible, OBJ is set to zero.

17: AX(*) — ***real*** array *Output*

Note: the dimension of the array AX must be at least max(1,NCLIN).

On exit: the final values of the linear constraints Ax.

If NCLIN = 0 then AX is not referenced.

18: CLAMDA(N+NCLIN) — ***real*** array *Output*

On exit: the values of the Lagrange multipliers for each constraint with respect to the current working set. The first n elements contain the multipliers for the bound constraints on the variables, and the next m_L elements contain the multipliers for the general linear constraints (if any). If ISTATE(j) = 0 (i.e., constraint j is not in the working set), CLAMDA(j) is zero. If x is optimal, CLAMDA(j) should be non-negative if ISTATE(j) = 1, non-positive if ISTATE(j) = 2 and zero if ISTATE(j) = 4.

19: STRTGY — INTEGER *Input*

On entry: STRTGY determines a branching strategy to be used throughout the computation, as follows:

STRTGY	Meaning
0	Always left branch first i.e., impose an upper bound constraint on the variable first.
1	Always right branch first i.e., impose a lower bound constraint on the variable first.
2	Branch towards the nearest integer i.e., if $x_k = 2.4$ then impose an upper bound constraint $x_k \leq 2$, whereas if $x_k = 2.6$ then impose the lower bound constraint $x_k \geq 3.0$.
3	A random choice is made between a left-hand and a right-hand branch.

Constraint: STRTGY = 0, 1, 2 or 3.

20: IWRK(LIWRK) — INTEGER array *Workspace*

21: LIWRK — INTEGER *Input*

On entry: the dimension of the array IWRK as declared in the (sub)program from which H02CBF is called.

Constraint: LIWRK $\geq 2 \times$ N $+ 3 + 2 \times$ MDEPTH.

22: WRK(LWRK) — ***real*** array *Workspace*

23: LWRK — INTEGER *Input*

On entry: the dimension of the array WRK as declared in the (sub)program from which H02CBF is called.

Constraints:

For problems QP2 (the default) and QP4,

LWRK $\geq 2 \times$ N$^2 + 8 \times$ N $+ 5 \times$ NCLIN $+ 4 \times$ MDEPTH if NCLIN > 0,

LWRK $\geq$ N$^2 + 9 \times$ N $+ 4 \times$ MDEPTH if NCLIN $= 0$.

For problems QP1 and QP3,

LWRK $\geq 2 \times$ N$^2 + 8 \times$ N $+ 5 \times$ NCLIN $+ 4 \times$ MDEPTH if NCLIN > 0,

LWRK $\geq$ N$^2 + 8 \times$ N $+ 4 \times$ MDEPTH if NCLIN $= 0$.

If the problem is of type LP,

LWRK $\geq 9 \times$ N $+ 1 + 4 \times$ MDEPTH if NCLIN $= 0$,

LWRK $\geq 2 \times$ N$^2 + 9 \times$ N $+ 5 \times$ NCLIN $+ 4 \times$ MDEPTH if NCLIN $\geq$ N,

LWRK $\geq 2 \times$ (NCLIN+1)$^2 + 9 \times$ N $+ 5 \times$ NCLIN $+ 4 \times$ MDEPTH otherwise.

If the problem is of type FP,

LWRK $\geq 8 \times$ N $+ 1 + 4 \times$ MDEPTH, if NCLIN $= 0$,

LWRK $\geq 2 \times$ N$^2 + 8 \times$ N $+ 5 \times$ NCLIN $+ 4 \times$ MDEPTH if NCLIN $\geq$ N,

LWRK $\geq 2 \times$ (NCLIN+1)$^2 + 8 \times$ N $+ 5 \times$ NCLIN $+ 4 \times$ MDEPTH otherwise.

24: MONIT — SUBROUTINE, supplied by the NAG Fortran Library or the user. *External Procedure*

This routine may be used to print out intermediate output and to affect the course of the computation. Specifically, it allows the user to specify a realistic value for the cut-off value (see Section 3) and to terminate the algorithm. If the user does not require any intermediate output, has no estimate of the cut-off value and requires an exhaustive tree search then MONIT may be the dummy routine H02CBU (CBUH02 in some implementations).

Its specification is:

```
      SUBROUTINE MONIT(INTFND, NODES, DEPTH, OBJ, X(N), BSTVAL,
     1                 BSTSOL(N), BL(N), BU(N), N, HALT, COUNT)
      INTEGER          INTFND, NODES, DEPTH, N, COUNT
      real             OBJ, X(N), BSTVAL, BSTSOL(N), BL(N), BU(N)
      LOGICAL          HALT
```

1: INTFND — INTEGER *Input*

On entry: specifies the number of integer solutions obtained so far.

2: NODES — INTEGER *Input*

On entry: specifies the number of nodes (sub-problems) solved so far.

3: DEPTH — INTEGER *Input*

On entry: specifies the depth in the tree of sub-problems the algorithm has now reached.

4: OBJ — ***real*** *Input*

On entry: specifies the value of the objective function of the end of the latest sub-problem.

5: X(N) — ***real*** array *Input*

On entry: specifies the values of the independent variables at the end of the latest sub-problem.

6: BSTVAL — ***real*** *Input/Output*

On entry: normally specifies the value of the best integer solution found so far.

On exit: may be set a cut-off value by the sophisticated user as follows. Before an integer solution has been found BSTVAL will be set by H02CBF to the largest machine representable number (see X02ALF). If the user knows that the solution being sought is a much smaller number, then BSTVAL may be set to this number as a cut-off value (see Section 3). Beware of setting BSTVAL too small, since then no integer solutions will be discovered. Also make sure that BSTVAL is set using a statement of the form

`IF (INTFND.EQ.0) BSTVAL =` *cut-off value*

on entry to MONIT. This statement will not prevent the normal operation of the algorithm when subsequent integer solutions are found. It would be a grievous mistake to unconditionally set BSTVAL and if you have any doubts whatsoever about the correct use of this parameter then you are strongly recommended to leave it unchanged.

7: BSTSOL(N) — ***real*** array *Input*

On entry: specifies the solution vector which gives rise to the best integer solution value so far discovered.

8: BL(N) — ***real*** array *Input*

On entry: BL(i) specifies the current lower bounds on the variable x_i.

9: BU(N) — ***real*** array *Input*

On entry: BU(i) specifies the current upper bounds on the variable x_i.

10: N — INTEGER *Input*

On entry: specifies the number of variables.

11: HALT — LOGICAL *Input/Output*

On entry: HALT will have the value .FALSE..

On exit: by setting HALT to .TRUE., the user may terminate the algorithm prematurely. This facility may be useful if the user is content with *any* integer solution, or with any integer solution that fits certain criteria. Under these circumstances setting HALT = .TRUE. can save considerable unnecessary computation.

12: COUNT — INTEGER *Input*

On entry: specifies the number of integer solutions found so far.

MONIT must be declared as EXTERNAL in the (sub)program from which H02CBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

25: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error or gives a warning (see Section 6).

For this routine, because the values of output parameters may be useful even if IFAIL $\neq$ 0 on exit, users are recommended to set IFAIL to −1 before entry. **It is then essential to test the value of IFAIL on exit**.

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings specified by the routine:

IFAIL = −1

Algorithm terminated at user request (HALT = .TRUE.).

IFAIL = 1

Input parameter error immediately detected.

IFAIL = 2

No integer solution found. (Check that BSTVAL has not been set too small.)

IFAIL = 3

MDEPTH is too small. Increase the value of MDEPTH and re-enter H02CBF.

IFAIL = 4

The basic problem (without integer constraints) is unbounded.

IFAIL = 5

The basic problem is infeasible.

IFAIL = 6

The basic problem requires too many iterations.

IFAIL = 7

The basic problem has a reduced Hessian which exceeds its assigned dimension.

IFAIL = 8

The basic problem has an invalid parameter setting.

IFAIL = 9

The basic problem, as defined, is not standard.

IFAIL = 10

LIWRK is too small.

IFAIL = 11

LWRK is too small.

IFAIL = 12

An internal error has occurred within the routine. Please contact NAG with details of the call to H02CBF.

7 Accuracy

The routine implements a numerically stable active set strategy and returns solutions that are as accurate as the condition of the problem warrants on the machine.

8 Further Comments

This section contains some comments on scaling and a description of the printed output.

8.1 Scaling

Sensible scaling of the problem is likely to reduce the number of iterations required and make the problem less sensitive to perturbations in the data, thus improving the condition of the problem. In the absence of better information it is usually sensible to make the Euclidean lengths of each constraint of comparable magnitude. See the E04 Chapter Introduction and Gill *et al.*[7] for further information and advice.

8.2 Description of the Printed Output

This section describes the (default) intermediate printout and final printout produced by H02CBF. The intermediate printout is a subset of the monitoring information produced by the routine at every iteration (see Section 12). The level of printed output can be controlled by the user (see the description of the optional parameter **Print Level** in Section 11.2). Note that the intermediate printout and final printout are produced only if **Print Level** ≥ 10 (the default).

The following line of summary output (< 80 characters) is produced at every iteration. In all cases, the values of the quantities printed are those in effect *oncompletion* of the given iteration.

`Itn` is the iteration count.

`Step` is the step taken along the computed search direction. If a constraint is added during the current iteration, `Step` will be the step to the nearest constraint. When the problem is of type LP, the step can be greater than one during the optimality phase.

`Ninf` is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.

`Sinf/Objective` is the value of the current objective function. If x is not feasible, `Sinf` gives a weighted sum of the magnitudes of constraint violations. If x is feasible, `Objective` is the value of the objective function. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which `Ninf` is zero) will give the value of the true objective at the first feasible point. During the optimality phase, the value of the objective function will be non-increasing. During the feasibility phase, the number of constraint infeasibilities will not increase until either a feasible point is found, or the optimality of the multipliers implies that no feasible point exists. Once optimal multipliers are obtained, the number of infeasibilities can increase, but the sum of infeasibilities will either remain constant or be reduced until the minimum sum of infeasibilities is found.

`Norm Gz` is $\|Z_R^T g_{\mathrm{FR}}\|$, the Euclidean norm of the reduced gradient with respect to Z_R (see Section 10.2 and Section 10.4). During the optimality phase, this norm will be approximately zero after a unit step.

The final printout includes a listing of the status of every variable and constraint.

The following describes the printout for each variable. A full stop (.) is printed for any numerical value that is zero.

`Varbl` gives the name (`V`) and index j, for $j = 1, 2, \ldots, n$ of the variable.

`State` gives the state of the variable (`FR` if neither bound is in the working set, `EQ` if a fixed variable, `LL` if on its lower bound, `UL` if on its upper bound, `TF` if temporarily fixed at its current value). If `Value` lies outside the upper or lower bounds by more than the **Feasibility Tolerance** (default value $= \sqrt{\epsilon}$, where ϵ is the ***machine precision***; see Section 11.2), `State` will be `++` or `--` respectively.

A key is sometimes printed before **State** to give some additional information about the state of a variable.

A	*Alternative optimum possible.* The variable is active at one of its bounds, but its Lagrange multiplier is essentially zero. This means that if the variable were allowed to start moving away from its bound, there would be no change to the objective function. The values of the other free variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled **D**), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case the values of the Lagrange multipliers might also change.
D	*Degenerate.* The variable is free, but it is equal to (or very close to) one of its bounds.
I	*Infeasible.* The variable is currently violating one of its bounds by more than the **Feasibility Tolerance**.

Value	is the value of the variable at the final iterate.
Lower Bound	is the lower bound specified for the variable. **None** indicates that $\mathrm{BL}(j) \leq -bigbnd$.
Upper Bound	is the upper bound specified for the variable. **None** indicates that $\mathrm{BU}(j) \geq bigbnd$.
Lagr Mult	is the Lagrange multiplier for the associated bound. This will be zero if **State** is **FR** unless $\mathrm{BL}(j) \leq -bigbnd$ and $\mathrm{BU}(j) \geq bigbnd$, in which case the entry will be blank. If x is optimal, the multiplier should be non-negative if **State** is **LL**, and non-positive if **State** is **UL**.
Slack	is the difference between the variable **Value** and the nearer of its (finite) bounds $\mathrm{BL}(j)$ and $\mathrm{BU}(j)$. A blank entry indicates that the associated variable is not bounded (i.e., $\mathrm{BL}(j) \leq -bigbnd$ and $\mathrm{BU}(j) \geq bigbnd$).

The meaning of the printout for general constraints is the same as that given above for variables, with 'variable' replaced by 'constraint', $\mathrm{BL}(j)$ and $\mathrm{BU}(j)$ are replaced by $\mathrm{BL}(n+j)$ and $\mathrm{BU}(n+j)$ respectively, and with the following change in the heading:

L Con	gives the name (**L**) and index j, for $j = 1, 2, \ldots, m_L$ of the linear constraint.

Note that movement off a constraint (as opposed to a variable moving away from its bound) can be interpreted as allowing the entry in the **Slack** column to become positive.

Numerical values are output with a fixed number of digits; they are not guaranteed to be accurate to this precision.

9 Example

To minimize the quadratic function $f(x) = c^T x + \frac{1}{2} x^T H x$, where

$$c = (-0.02,\ -0.2,\ -0.2,\ -0.2,\ -0.2,\ 0.04,\ 0.04)^T$$

$$H = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & -2 & -2 \end{pmatrix}$$

subject to the bounds

$$\begin{aligned} -0.01 &\leq x_1 \leq 0.01 \\ -0.1 &\leq x_2 \leq 0.15 \\ -0.01 &\leq x_3 \leq 0.03 \\ -0.04 &\leq x_4 \leq 0.02 \\ -0.1 &\leq x_5 \leq 0.05 \\ -0.01 &\leq x_6 \\ -0.01 &\leq x_7 \end{aligned}$$

to the general constraints

$$\begin{array}{rcl}
x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 & = & -0.13 \\
0.15x_1 + 0.04x_2 + 0.02x_3 + 0.04x_4 + 0.02x_5 + 0.01x_6 + 0.03x_7 & \leq & -0.0049 \\
0.03x_1 + 0.05x_2 + 0.08x_3 + 0.02x_4 + 0.06x_5 + 0.01x_6 & \leq & -0.0064 \\
0.02x_1 + 0.04x_2 + 0.01x_3 + 0.02x_4 + 0.02x_5 & \leq & -0.0037 \\
0.02x_1 + 0.03x_2 + 0.01x_5 & \leq & -0.0012 \\
-0.0992 \leq 0.70x_1 + 0.75x_2 + 0.80x_3 + 0.75x_4 + 0.80x_5 + 0.97x_6 & & \\
-0.003 \leq 0.02x_1 + 0.06x_2 + 0.08x_3 + 0.12x_4 + 0.02x_5 + 0.01x_6 + 0.97x_7 & \leq & 0.002
\end{array}$$

and the variable x_4 is constrained to be integer.

The initial point, which is infeasible, is

$$x_0 = (-0.01, -0.03, 0.0, -0.01, -0.1, 0.02, 0.01)^T.$$

The optimal solution (to five figures) is

$$x^* = (-0.01, -0.073328, -0.00025809, 0.0, -0.063354, 0.014109, 0.0028312)^T.$$

The document for H02CCF includes an example program to solve the same problem using some of the optional parameters described in Section 11.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02CBF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT, LINTVR
      PARAMETER        (NIN=5,NOUT=6,LINTVR=1)
      INTEGER          NMAX, NCMAX
      PARAMETER        (NMAX=10,NCMAX=10)
      INTEGER          LDA, LDH
      PARAMETER        (LDA=NCMAX,LDH=NMAX)
      INTEGER          LIWORK, LWORK, MDEPTH
      PARAMETER        (LIWORK=1000,LWORK=10000,MDEPTH=30)
*     .. Local Scalars ..
      real             OBJ
      INTEGER          I, IFAIL, J, N, NCLIN, STRTGY
*     .. Local Arrays ..
      real             A(LDA,NMAX), AX(NCMAX), BL(NMAX+NCMAX),
     +                 BU(NMAX+NCMAX), CLAMDA(NMAX+NCMAX), CVEC(NMAX),
     +                 H(LDH,NMAX), WORK(LWORK), X(NMAX)
      INTEGER          INTVAR(LINTVR), ISTATE(NMAX+NCMAX), IWORK(LIWORK)
*     .. External Subroutines ..
      EXTERNAL         E04NFU, H02CBF, H02CBU, H02CDF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02CBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NCLIN
      IF (N.LE.NMAX .AND. NCLIN.LE.NCMAX) THEN
*
*        Read CVEC, A, BL, BU, X and H from data file
*
         READ (NIN,*) (CVEC(I),I=1,N)
         READ (NIN,*) ((A(I,J),J=1,N),I=1,NCLIN)
         READ (NIN,*) (BL(I),I=1,N+NCLIN)
```

```
         READ (NIN,*) (BU(I),I=1,N+NCLIN)
         READ (NIN,*) (X(I),I=1,N)
         READ (NIN,*) ((H(I,J),J=1,N),I=1,N)
*
         STRTGY = 2
         INTVAR(1) = 4
*
         CALL H02CDF('Nolist')
         CALL H02CDF('Print Level = 0')
*
*        Solve the problem
*
         IFAIL = 0
*
         CALL H02CBF(N,NCLIN,A,LDA,BL,BU,CVEC,H,LDH,E04NFU,INTVAR,
     +               LINTVR,MDEPTH,ISTATE,X,OBJ,AX,CLAMDA,STRTGY,IWORK,
     +               LIWORK,WORK,LWORK,H02CBU,IFAIL)
*
*        Print out the best integer solution found
*
         WRITE (NOUT,99999) OBJ, (I,X(I),I=1,N)
*
      END IF
      STOP
*
99999 FORMAT (' Optimal Integer Value is = ',e20.8,/' Components are ',
     +       /(' x(',I3,') = ',F15.8))
      END
```

9.2 Program Data

```
H02CBF Example Program Data
  7  7                                                  :Values of N and NCLIN
 -0.02  -0.20  -0.20  -0.20  -0.20   0.04   0.04   :End of CVEC
  1.00   1.00   1.00   1.00   1.00   1.00   1.00
  0.15   0.04   0.02   0.04   0.02   0.01   0.03
  0.03   0.05   0.08   0.02   0.06   0.01   0.00
  0.02   0.04   0.01   0.02   0.02   0.00   0.00
  0.02   0.03   0.00   0.00   0.01   0.00   0.00
  0.70   0.75   0.80   0.75   0.80   0.97   0.00
  0.02   0.06   0.08   0.12   0.02   0.01   0.97   :End of matrix A
 -0.01  -0.10     -0.01     -0.04     -0.10     -0.01     -0.01
 -0.13  -1.0E+25  -1.0E+25  -1.0E+25  -1.0E+25  -9.92E-02 -3.0E-03 :End of BL
  0.01   0.15      0.03      0.02      0.05      1.0E+25   1.0E+25
 -0.13  -4.9E-03  -6.4E-03  -3.7E-03  -1.2E-03   1.0E+25   2.0E-03 :End of BU
 -0.01  -0.03   0.00  -0.01  -0.10   0.02   0.01   :End of X
  2.00   0.00   0.00   0.00   0.00   0.00   0.00
  0.00   2.00   0.00   0.00   0.00   0.00   0.00
  0.00   0.00   2.00   2.00   0.00   0.00   0.00
  0.00   0.00   2.00   2.00   0.00   0.00   0.00
  0.00   0.00   0.00   0.00   2.00   0.00   0.00
  0.00   0.00   0.00   0.00   0.00  -2.00  -2.00
  0.00   0.00   0.00   0.00   0.00  -2.00  -2.00   :End of matrix H
```

9.3 Program Results

```
H02CBF Example Program Results
Optimal Integer Value is =       0.37469662E-01
Components are
x(  1) =     -0.01000000
x(  2) =     -0.07332830
x(  3) =     -0.00025809
x(  4) =      0.00000000
x(  5) =     -0.06335433
x(  6) =      0.01410944
x(  7) =      0.00283128
```

The remainder of this document is intended for more advanced users. Section 10 contains a detailed description of the algorithm which may be needed in order to understand Section 11 and Section 12. Section 11 describes the optional parameters which may be set by calls to H02CCF and/or H02CDF. Section 12 describes the quantities which can be requested to monitor the course of the computation.

10 Algorithmic Details

H02CBF implements a basic Branch and bound algorithm (see Section 3) using E04NFF as its basic sub-problem solver. See below for details of its algorithm.

10.1 Overview

H02CBF is based on an inertia-controlling method that maintains a Cholesky factorization of the reduced Hessian (see below). The method is based on that of Gill and Murray [2], and is described in detail by Gill *et al.* [5]. Here we briefly summarize the main features of the method. Where possible, explicit reference is made to the names of variables that are parameters of H02CBF or appear in the printed output. H02CBF has two phases: finding an initial feasible point by minimizing the sum of infeasibilities (the *feasibility phase*), and minimizing the quadratic objective function within the feasible region (the *optimality phase*). The computations in both phases are performed by the same subroutines. The two-phase nature of the algorithm is reflected by changing the function being minimized from the sum of infeasibilities to the quadratic objective function. The feasibility phase does *not* perform the standard simplex method (i.e., it does not necessarily find a vertex), except in the LP case when $m_L \leq n$. Once any iterate is feasible, all subsequent iterates remain feasible.

H02CBF has been designed to be efficient when used to solve a *sequence* of related problems – for example, within a sequential quadratic programming method for nonlinearly constrained optimization (e.g., E04UCF). In particular, the user may specify an initial working set (the indices of the constraints believed to be satisfied exactly at the solution); see the discussion of the optional parameter **Warm Start** in Section 11.2.

In general, an iterative process is required to solve a quadratic program. (For simplicity, we shall always consider a typical iteration and avoid reference to the index of the iteration.) Each new iterate $\bar{x}$ is defined by

$$\bar{x} = x + \alpha p \tag{1}$$

where the *step length* α is a non-negative scalar, and p is called the *search direction*.

At each point x, a working set of constraints is defined to be a linearly independent subset of the constraints that are satisfied 'exactly' (to within the tolerance defined by the optional parameter **Feasibility Tolerance**; see Section 11.2). The working set is the current prediction of the constraints that hold with equality at the solution of a linearly constrained QP problem. The search direction is constructed so that the constraints in the working set remain *unaltered* for any value of the step length. For a bound constraint in the working set, this property is achieved by setting the corresponding element of the search direction to zero. Thus, the associated variable is *fixed*, and specification of the working set induces a partition of x into *fixed* and *free* variables. During a given iteration, the fixed variables are

effectively removed from the problem; since the relevant elements of the search direction are zero, the columns of A corresponding to fixed variables may be ignored.

Let m_W denote the number of general constraints in the working set and let n_{FX} denote the number of variables fixed at one of their bounds (m_W and n_{FX} are the quantities `Lin` and `Bnd` in the monitoring file output from H02CBF; see Section 12). Similarly, let n_{FR} ($n_{FR} = n - n_{FX}$) denote the number of free variables. At every iteration, *the variables are re-ordered so that the last* n_{FX} *variables are fixed*, with all other relevant vectors and matrices ordered accordingly.

10.2 Definition of the Search Direction

Let A_{FR} denote the m_W by n_{FR} sub-matrix of general constraints in the working set corresponding to the free variables, and let p_{FR} denote the search direction with respect to the free variables only. The general constraints in the working set will be unaltered by any move along p if

$$A_{FR}p_{FR} = 0. \tag{2}$$

In order to compute p_{FR}, the *TQ factorization* of A_{FR} is used:

$$A_{FR}Q_{FR} = (0 \;\; T), \tag{3}$$

where T is a non-singular m_W by m_W upper triangular matrix (i.e., $t_{ij} = 0$ if $i > j$), and the non-singular n_{FR} by n_{FR} matrix Q_{FR} is the product of orthogonal transformations (see Gill *et al.* [3]). If the columns of Q_{FR} are partitioned so that

$$Q_{FR} = (Z \;\; Y),$$

where Y is n_{FR} by m_W, then the n_Z ($n_Z = n_{FR} - m_W$) columns of Z form a basis for the null space of A_{FR}. Let n_R be an integer such that $0 \leq n_R \leq n_Z$, and let Z_R denote a matrix whose n_R columns are a subset of the columns of Z. (The integer n_R is the quantity `Zr` in the monitoring output from H02CBF. In many cases, Z_R will include *all* the columns of Z.) The direction p_{FR} will satisfy (2) if

$$p_{FR} = Z_R p_R, \tag{4}$$

where p_R is any n_R-vector.

Let Q denote the n by n matrix

$$Q = \begin{pmatrix} Q_{FR} & \\ & I_{FX} \end{pmatrix},$$

where I_{FX} is the identity matrix of order n_{FX}. Let H_Q and g_Q denote the n by n *transformed Hessian* and *transformed gradient*

$$H_Q = Q^T H Q \;\text{ and }\; g_Q = Q^T(c + Hx)$$

and let the matrix of first n_R rows and columns of H_Q be denoted by H_R and the vector of the first n_R elements of g_Q be denoted by g_R. The quantities H_R and g_R are known as the *reduced Hessian* and *reduced gradient* of $f(x)$, respectively. Roughly speaking, g_R and H_R describe the first and second derivatives of an *unconstrained* problem for the calculation of p_R.

At each iteration, a triangular factorization of H_R is available. If H_R is positive-definite, $H_R = R^T R$, where R is the upper triangular Cholesky factor of H_R. If H_R is not positive-definite, $H_R = R^T D R$, where $D = \text{diag}(1, 1, \ldots, 1, \mu)$, with $\mu \leq 0$.

The computation is arranged so that the reduced-gradient vector is a multiple of e_R, a vector of all zeros except in the last (i.e., n_Rth) position. This allows the vector p_R in (4) to be computed from a single back-substitution

$$Rp_R = \gamma e_R \tag{5}$$

where γ is a scalar that depends on whether or not the reduced Hessian is positive-definite at x. In the positive-definite case, $x + p$ is the minimizer of the objective function subject to the constraints (bounds and general) in the working set treated as equalities. If H_R is not positive-definite, p_R satisfies the conditions

$$p_R^T H_R p_R < 0 \;\text{ and }\; g_R^T p_R \leq 0,$$

which allow the objective function to be reduced by any positive step of the form $x + \alpha p$.

10.3 The Main Iteration

If the reduced gradient is zero, x is a constrained stationary point in the subspace defined by Z. During the feasibility phase, the reduced gradient will usually be zero only at a vertex (although it may be zero at non-vertices in the presence of constraint dependencies). During the optimality phase, a zero reduced gradient implies that x minimizes the quadratic objective when the constraints in the working set are treated as equalities. At a constrained stationary point, Lagrange multipliers λ_C and λ_B for the general and bound constraints are defined from the equations

$$A_{\mathrm{FR}}^T \lambda_C = g_{\mathrm{FR}} \text{ and } \lambda_B = g_{\mathrm{FX}} - A_{\mathrm{FX}}^T \lambda_C. \tag{6}$$

Given a positive constant δ of the order of the ***machine precision***, a Lagrange multiplier λ_j corresponding to an inequality constraint in the working set is said to be *optimal* if $\lambda_j \leq \delta$ when the associated constraint is at its *upper bound*, or if $\lambda_j \geq -\delta$ when the associated constraint is at its *lower bound*. If a multiplier is non-optimal, the objective function (either the true objective or the sum of infeasibilities) can be reduced by deleting the corresponding constraint (with index `Jdel`; see Section 12) from the working set.

If optimal multipliers occur during the feasibility phase and the sum of infeasibilities is non-zero, there is no feasible point, and the user can force H02CBF to continue until the minimum value of the sum of infeasibilities has been found; see the discussion of the optional parameter **Minimum Sum of Infeasibilities** in Section 11.2. At such a point, the Lagrange multiplier λ_j corresponding to an inequality constraint in the working set will be such that $-(1+\delta) \leq \lambda_j \leq \delta$ when the associated constraint is at its *upper bound*, and $-\delta \leq \lambda_j \leq (1+\delta)$ when the associated constraint is at its *lower bound*. Lagrange multipliers for equality constraints will satisfy $|\lambda_j| \leq 1+\delta$.

If the reduced gradient is not zero, Lagrange multipliers need not be computed and the non-zero elements of the search direction p are given by $Z_R p_R$ (see (4) and (5)). The choice of step length is influenced by the need to maintain feasibility with respect to the satisfied constraints. If H_R is positive-definite and $x+p$ is feasible, α will be taken as unity. In this case, the reduced gradient at $\bar{x}$ will be zero, and Lagrange multipliers are computed. Otherwise, α is set to α_{M}, the step to the 'nearest' constraint (with index `Jadd`; see Section 12), which is added to the working set at the next iteration.

Each change in the working set leads to a simple change to A_{FR}: if the status of a general constraint changes, a *row* of A_{FR} is altered; if a bound constraint enters or leaves the working set, a *column* of A_{FR} changes. Explicit representations are recurred of the matrices T, Q_{FR} and R; and of vectors $Q^T g$, and $Q^T c$. The triangular factor R associated with the reduced Hessian is only updated during the optimality phase.

One of the most important features of H02CBF is its control of the conditioning of the working set, whose nearness to linear dependence is estimated by the ratio of the largest to smallest diagonal elements of the TQ factor T (the printed value **`Cond T`**; see Section 12). In constructing the initial working set, constraints are excluded that would result in a large value of **`Cond T`**.

H02CBF includes a rigorous procedure that prevents the possibility of cycling at a point where the active constraints are nearly linearly dependent (see Gill *et al.* [4]). The main feature of the anti-cycling procedure is that the feasibility tolerance is increased slightly at the start of every iteration. This not only allows a positive step to be taken at every iteration, but also provides, whenever possible, a *choice* of constraints to be added to the working set. Let α_{M} denote the maximum step at which $x + \alpha_{\mathrm{M}} p$ does not violate any constraint by more than its feasibility tolerance. All constraints at a distance α ($\alpha \leq \alpha_{\mathrm{M}}$) along p from the current point are then viewed as acceptable candidates for inclusion in the working set. The constraint whose normal makes the largest angle with the search direction is added to the working set.

10.4 Choosing the Initial Working Set

At the start of the optimality phase, a positive-definite H_R can be defined if enough constraints are included in the initial working set. (The matrix with no rows and columns is positive-definite by definition, corresponding to the case when A_{FR} contains n_{FR} constraints.) The idea is to include as many general constraints as necessary to ensure that the reduced Hessian is positive-definite.

Let H_Z denote the matrix of the first n_Z rows and columns of the matrix $H_Q = Q^T H Q$ at the beginning of the optimality phase. A partial Cholesky factorization is used to find an upper triangular matrix

R that is the factor of the largest positive-definite leading sub-matrix of H_Z. The use of interchanges during the factorization of H_Z tends to maximize the dimension of R. (The condition of R may be controlled using the optional parameter **Rank Tolerance**; see Section 11.2.) Let Z_R denote the columns of Z corresponding to R, and let Z be partitioned as $Z = (Z_R \; Z_A)$. A working set for which Z_R defines the null space can be obtained by including *the rows of* Z_A^T as 'artificial constraints'. Minimization of the objective function then proceeds within the subspace defined by Z_R, as described in Section 10.2.

The artificially augmented working set is given by

$$\bar{A}_{\mathrm{FR}} = \begin{pmatrix} Z_A^T \\ A_{\mathrm{FR}} \end{pmatrix}, \tag{7}$$

so that p_{FR} will satisfy $A_{\mathrm{FR}}p_{\mathrm{FR}} = 0$ *and* $Z_A^T p_{\mathrm{FR}} = 0$. By definition of the TQ factorization, $\bar{A}_{\mathrm{FR}}$ *automatically* satisfies the following:

$$\bar{A}_{\mathrm{FR}}Q_{\mathrm{FR}} = \begin{pmatrix} Z_A^T \\ A_{\mathrm{FR}} \end{pmatrix} Q_{\mathrm{FR}} = \begin{pmatrix} Z_A^T \\ A_{\mathrm{FR}} \end{pmatrix} (Z_R \; Z_A \; Y) = (0 \; \bar{T}),$$

where

$$\bar{T} = \begin{pmatrix} I & 0 \\ 0 & T \end{pmatrix},$$

and hence the TQ factorization of (7) is available trivially from T and Q_{FR} without additional expense.

The matrix Z_A is not kept fixed, since its role is purely to define an appropriate null space; the TQ factorization can therefore be updated in the normal fashion as the iterations proceed. No work is required to 'delete' the artificial constraints associated with Z_A when $Z_R^T g_{\mathrm{FR}} = 0$, since this simply involves repartitioning Q_{FR}. The 'artificial' multiplier vector associated with the rows of Z_A^T is equal to $Z_A^T g_{\mathrm{FR}}$, and the multipliers corresponding to the rows of the 'true' working set are the multipliers that would be obtained if the artificial constraints were not present. If an artificial constraint is 'deleted' from the working set, an `A` appears alongside the entry in the `Jdel` column of the monitoring file output (see Section 12).

The number of columns in Z_A and Z_R, the Euclidean norm of $Z_R^T g_{\mathrm{FR}}$, and the condition estimator of R appear in the monitoring file output as `Art`, `Zr`, `Norm Gz` and `Cond Rz` respectively (see Section 12).

Under some circumstances, a different type of artificial constraint is used when solving a linear program. Although the algorithm of H02CBF does not usually perform simplex steps (in the traditional sense), there is one exception: a linear program with fewer general constraints than variables (i.e., $m_L \leq n$). (Use of the simplex method in this situation leads to savings in storage.) At the starting point, the 'natural' working set (the set of constraints exactly or nearly satisfied at the starting point) is augmented with a suitable number of 'temporary' bounds, each of which has the effect of temporarily fixing a variable at its current value. In subsequent iterations, a temporary bound is treated as a standard constraint until it is deleted from the working set, in which case it is never added again. If a temporary bound is 'deleted' from the working set, an `F` (for 'Fixed') appears alongside the entry in the `Jdel` column of the monitoring file output (see Section 12).

11 Optional Parameters

Several optional parameters in H02CBF define choices in the problem specification or the algorithm logic. In order to reduce the number of formal parameters of H02CBF these optional parameters have associated *default values* that are appropriate for most problems. Therefore, the user need only specify those optional parameters whose values are to be different from their default values.

The remainder of this section can be skipped by users who wish to use the default values for *all* optional parameters. A complete list of optional parameters and their default values is given in Section 11.1.

Optional parameters may be specified by calling one, or both, of the routines H02CCF and H02CDF prior to a call to H02CBF.

H02CCF reads options from an external options file, with **Begin** and **End** as the first and last lines respectively and each intermediate line defining a single optional parameter. For example,

```
Begin
  Print Level = 5
End
```

The call

```
CALL H02CCF (IOPTNS, INFORM)
```

can then be used to read the file on unit IOPTNS. INFORM will be zero on successful exit. H02CCF should be consulted for a full description of this method of supplying optional parameters.

H02CDF can be called to supply options directly, one call being necessary for each optional parameter. For example,

```
CALL H02CDF ('Print Level = 5')
```

H02CDF should be consulted for a full description of this method of supplying optional parameters.

All optional parameters not specified by the user are set to their default values. Optional parameters specified by the user are unaltered by H02CBF (unless they define invalid values) and so remain in effect for subsequent calls unless altered by the user.

11.1 Optional Parameter Checklist and Default Values

For easy reference, the following list shows all the valid keywords and their default values. The symbol ϵ represents the ***machine precision*** (see X02AJF).

Optional Parameters	**Default Values**
Check frequency	50
Cold/Warm start	**Cold Start**
Crash tolerance	0.01
Defaults	
Expand frequency	5
Feasibility phase iteration limit	$\max(50, 5(n + m_L))$
Feasibility tolerance	$\sqrt{\epsilon}$
Hessian rows	n
Infinite bound size	10^{20}
Infinite step size	$\max(bigbnd, 10^{20})$
Iteration limit	$\max(50, 5(n + m_L))$
List/Nolist	**List**
Maximum degrees of freedom	n
Minimum sum of infeasibilities	**No**
Monitoring file	-1
Optimality phase iteration limit	$\max(50, 5(n + m_L))$
Optimality tolerance	$\epsilon^{0.8}$
Print level	10
Problem type	QP2
Rank tolerance	100ϵ

11.2 Description of the Optional Parameters

The following list (in alphabetical order) gives the valid options. For each option, we give the keyword, any essential optional qualifiers, the default value, and the definition. The minimum abbreviation of each keyword is underlined. If no characters of an optional qualifier are underlined, the qualifier may be omitted. The letter *a* denotes a phrase (character string) that qualifies an option. The letters *i* and *r* denote INTEGER and ***real*** values required with certain options. The number ϵ is a generic notation for ***machine precision*** (see X02AJF).

Check Frequency i Default = 50

Every ith iteration, a numerical test is made to see if the current solution x satisfies the constraints in the working set. If the largest residual of the constraints in the working set is judged to be too large, the current working set is refactorized and the variables are recomputed to satisfy the constraints more accurately. If $i \leq 0$, the default value is used.

Cold Start Default = **Cold Start**

Warm Start

This option specifies how the initial working set is chosen. With a **Cold Start**, H02CBF chooses the initial working set based on the values of the variables and constraints at the initial point. Broadly speaking, the initial working set will include equality constraints and bounds or inequality constraints that violate or 'nearly' satisfy their bounds (to within **Crash Tolerance**; see below).

With a **Warm Start**, the user must provide a valid definition of every element of the array ISTATE (see Section 5 for the definition of this array). H02CBF will override the user's specification of ISTATE if necessary, so that a poor choice of the working set will not cause a fatal error. For instance, any elements of ISTATE which are set to -2, -1 or 4 will be reset to zero, as will any elements which are set to 3 when the corresponding elements of BL and BU are not equal. A warm start will be advantageous if a good estimate of the initial working set is available – for example, when H02CBF is called repeatedly to solve related problems.

Crash Tolerance r Default = 0.01

This value is used in conjunction with the optional parameter **Cold Start** (the default value) when H02CBF selects an initial working set. If $0 \leq r \leq 1$, the initial working set will include (if possible) bounds or general inequality constraints that lie within r of their bounds. In particular, a constraint of the form $a_j^T x \geq l$ will be included in the initial working set if $|a_j^T x - l| \leq r(1 + |l|)$. If $r < 0$ or $r > 1$, the default value is used.

Defaults

This special keyword may be used to reset all optional parameters to their default values.

Expand Frequency i Default = 5

This option is part of an anti-cycling procedure designed to guarantee progress even on highly degenerate problems.

The strategy is to force a positive step at every iteration, at the expense of violating the constraints by a small amount. Suppose that the value of the optional parameter **Feasibility Tolerance** is δ. Over a period of i iterations, the feasibility tolerance actually used by H02CBF (i.e., the *working* feasibility tolerance) increases from 0.5δ to δ (in steps of $0.5\delta/i$).

At certain stages the following 'resetting procedure' is used to remove constraint infeasibilities. First, all variables whose upper or lower bounds are in the working set are moved exactly onto their bounds. A count is kept of the number of non-trivial adjustments made. If the count is positive, iterative refinement is used to give variables that satisfy the working set to (essentially) ***machine precision***. Finally, the working feasibility tolerance is reinitialized to 0.5δ.

If a problem requires more than i iterations, the resetting procedure is invoked and a new cycle of i iterations is started with i incremented by 10. (The decision to resume the feasibility phase or optimality phase is based on comparing any constraint infeasibilities with δ.)

The resetting procedure is also invoked when H02CBF reaches an apparently optimal, infeasible or unbounded solution, unless this situation has already occurred twice. If any non-trivial adjustments are made, iterations are continued.

If $i \leq 0$, the default value is used. If $i \geq 9999999$, no anti-cycling procedure is invoked.

Feasibility Phase Iteration Limit i_1 Default = $\max(50, 5(n + m_L))$

Optimality Phase Iteration Limit i_2 Default = $\max(50, 5(n + m_L))$

The scalars i_1 and i_2 specify the maximum number of iterations allowed in the feasibility and optimality phases. **Optimality Phase Iteration Limit** is equivalent to **Iteration Limit**. Setting $i_1 = 0$ and

Print Level > 0 means that the workspace needed will be computed and printed, but no iterations will be performed. If $i_1 < 0$ or $i_2 < 0$, the default value is used.

Feasibility Tolerance r Default $= \sqrt{\epsilon}$

If $r \geq \epsilon$, r defines the maximum acceptable *absolute* violation in each constraint at a 'feasible' point. For example, if the variables and the coefficients in the general constraints are of order unity, and the latter are correct to about 6 decimal digits, it would be appropriate to specify r as 10^{-6}. If $0 \leq r < \epsilon$, the default value is used.

H02CBF attempts to find a feasible solution before optimizing the objective function. If the sum of infeasibilities cannot be reduced to zero, the optional parameter **Minimum Sum of Infeasibilities** (see below) can be used to find the minimum value of the sum. Let `Sinf` be the corresponding sum of infeasibilities. If `Sinf` is quite small, it may be appropriate to raise r by a factor of 10 or 100. Otherwise, some error in the data should be suspected.

Note that a 'feasible solution' is a solution that satisfies the current constraints to within the tolerance r.

Hessian Rows i Default $= n$

Note that this option does not apply to problems of type FP or LP.

This specifies m, the number of rows of the Hessian matrix H. The default value of m is n, the number of variables of the problem.

If the problem is of type QP, m will usually be n, the number of variables. However, a value of m less than n is appropriate for QP3 or QP4 if H is an upper trapezoidal matrix with m rows. Similarly, m may be used to define the dimension of a leading block of non-zeros in the Hessian matrices of QP1 or QP2, in which case the last $n - m$ rows and columns of H are assumed to be zero. In the QP case, m should not be greater than n; if it is, the last $m - n$ rows of H are ignored.

If $i < 0$ or $i > n$, the default value is used.

Infinite Bound Size r Default $= 10^{20}$

If $r > 0$, r defines the 'infinite' bound *bigbnd* in the definition of the problem constraints. Any upper bound greater than or equal to *bigbnd* will be regarded as plus infinity (and similarly any lower bound less than or equal to $-$*bigbnd* will be regarded as minus infinity). If $r \leq 0$, the default value is used.

Infinite Step Size r Default $= \max(bigbnd, 10^{20})$

If $r > 0$, r specifies the magnitude of the change in variables that will be considered a step to an unbounded solution. (Note that an unbounded solution can occur only when the Hessian is not positive-definite.) If the change in x during an iteration would exceed the value of r, the objective function is considered to be unbounded below in the feasible region. If $r \leq 0$, the default value is used.

Iteration Limit i Default $= \max(50, 5(n + m_L))$

Iters

Itns

See **Feasibility Phase Iteration Limit** above.

List Default = **List**

Nolist

Normally each optional parameter specification is printed as it is supplied. **Nolist** may be used to suppress the printing and **List** may be used to restore printing.

Maximum Degrees of Freedom i Default $= n$

Note that this option does not apply to problems of type FP or LP.

This places a limit on the storage allocated for the triangular factor R of the reduced Hessian H_R. Ideally, i should be set slightly larger than the value of n_R expected at the solution. It need not be larger than $m_N + 1$, where m_N is the number of variables that appear nonlinearly in the quadratic objective function. For many problems it can be much smaller than m_N.

For quadratic problems, a minimizer may lie on any number of constraints, so that n_R may vary between 1 and n. The default value of i is therefore the number of variables n. If **Hessian Rows** m is specified, the default value of i is the same number, m.

Minimum Sum of Infeasibilities **No** Default = No

Minimum Sum of Infeasibilities **Yes**

If no feasible point exists for the constraints, this option is used to control whether or not H02CBF will calculate a point that minimizes the constraint violations. If **Minimum Sum of Infeasibilities** = No, H02CBF will terminate as soon as it is evident that no feasible point exists for the constraints. The final point will generally not be the point at which the sum of infeasibilities is minimized. If **Minimum Sum of Infeasibilities** = Yes, H02CBF will continue until the sum of infeasibilities is minimized.

Monitoring File i Default = -1

If $i \geq 0$ and **Print Level** ≥ 5 (see below), monitoring information produced by H02CBF at every iteration is sent to a file with logical unit number i. If $i < 0$ and/or **Print Level** < 5, no monitoring information is produced.

Optimality Phase Iteration Limit i Default = $\max(50, 5(n + m_L))$

See **Feasibility Phase Iteration Limit** above.

Optimality Tolerance r Default = $\epsilon^{0.8}$

If $r \geq \epsilon$, r defines the tolerance used to determine if the bounds and general constraints have the right 'sign' for the solution to be judged to be optimal.

If $0 \leq r < \epsilon$, the default value is used.

Print Level i Default = 10

The value of i controls the amount of printout produced by H02CBF, as indicated below. A detailed description of the printed output is given in Section 8.2 (summary output at each iteration and the final solution) and Section 12 (monitoring information at each iteration). If $i < 0$, the default value is used.

The following printout is sent to the current advisory message unit (as defined by X04ABF):

i	**Output**
0	No output.
1	The final solution only.
5	One line of summary output (< 80 characters; see Section 8.2) for each iteration (no printout of the final solution).
≥ 10	The final solution and one line of summary output for each iteration.

The following printout is sent to the logical unit number defined by the optional parameter **Monitoring File** (see above):

i	**Output**
< 5	No output.
≥ 5	One long line of output (> 80 characters; see Section 12) for each iteration (no printout of the final solution).
≥ 20	At each iteration, the Lagrange multipliers, the variables x, the constraint values Ax and the constraint status.
≥ 30	At each iteration, the diagonal elements of the upper triangular matrix T associated with the TQ factorization (3) (see Section 10.2) of the working set, and the diagonal elements of the upper triangular matrix R.

If **Print Level** ≥ 5 and the unit number defined by **Monitoring File** is the same as that defined by X04ABF, then the summary output is suppressed.

Problem Type a Default = QP2

This option specifies the type of objective function to be minimized during the optimality phase. The following are the five optional keywords and the dimensions of the arrays that must be specified in order to define the objective function:

LP	H not referenced, CVEC(N) required;
QP1	H(LDH,*) symmetric, CVEC not referenced;

QP2 H(LDH,*) symmetric, CVEC(N) required;
QP3 H(LDH,*) upper trapezoidal, CVEC not referenced;
QP4 H(LDH,*) upper trapezoidal, CVEC(N) required.

For problems of type FP, the objective function is omitted and neither H nor CVEC are referenced.

The following keywords are also acceptable. The minimum abbreviation of each keyword is underlined.

a	**Option**
Quadratic	QP2
Linear	LP
Feasible	FP

In addition, the keyword QP is equivalent to the default option QP2.

If $H = 0$, i.e., the objective function is purely linear, the efficiency of H02CBF may be increased by specifying *a* as LP.

Rank Tolerance r Default = 100ϵ

Note that this option does not apply to problems of type FP or LP.

This parameter enables the user to control the condition number of the triangular factor R (see Section 10). If ρ_i denotes the function $\rho_i = \max\{|R_{11}|, |R_{22}|, \ldots, |R_{ii}|\}$, the dimension of R is defined to be smallest index i such that $|R_{i+1,i+1}| \leq \sqrt{r}|\rho_{i+1}|$. If $r \leq 0$, the default value is used.

Warm Start

See **Cold Start** above.

12 Description of Monitoring Information

This section describes the long line of output (> 80 characters) which forms part of the monitoring information produced by H02CBF. (See also the description of the optional parameters **Monitoring File** and **Print Level** in Section 11.2). The level of printed output can be controlled by the user.

To aid interpretation of the printed results, the following convention is used for numbering the constraints: indices 1 through n refer to the bounds on the variables, and indices $n + 1$ through $n + m_L$ refer to the general constraints. When the status of a constraint changes, the index of the constraint is printed, along with the designation `L` (lower bound), `U` (upper bound), `E` (equality), `F` (temporarily fixed variable) or `A` (artificial constraint).

When **Print Level** ≥ 5 and **Monitoring File** ≥ 0, the following line of output is produced at every iteration on the unit number specified by **Monitoring File**. In all cases, the values of the quantities printed are those in effect *on completion* of the given iteration.

`Itn` is the iteration count.

`Jdel` is the index of the constraint deleted from the working set. If `Jdel` is zero, no constraint was deleted.

`Jadd` is the index of the constraint added to the working set. If `Jadd` is zero, no constraint was added.

`Step` is the step taken along the computed search direction. If a constraint is added during the current iteration (i.e., `Jadd` is positive), `Step` will be the step to the nearest constraint. When the problem is of type LP, the step can be greater than one during the optimality phase.

`Ninf` is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.

`Sinf/Objective` is the value of the current objective function. If x is not feasible, `Sinf` gives a weighted sum of the magnitudes of constraint violations. If x is feasible, `Objective` is the value of the objective function. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which `Ninf` is zero) will give the value of the true objective at the first feasible point. During the optimality phase, the value of the objective function will be non-increasing. During the feasibility phase, the number of constraint infeasibilities will not increase until either a feasible point is found, or the optimality of the multipliers implies that no feasible point exists. Once optimal multipliers are obtained, the number of infeasibilities can increase, but the sum of infeasibilities will either remain constant or be reduced until the minimum sum of infeasibilities is found.

`Bnd` is the number of simple bound constraints in the current working set.

`Lin` is the number of general linear constraints in the current working set.

`Art` is the number of artificial constraints in the working set, i.e., the number of columns of Z_A (see Section 10.4).

`Zr` is the number of columns of Z_R (see Section 10.2). `Zr` is the dimension of the subspace in which the objective function is currently being minimized. The value of `Zr` is the number of variables minus the number of constraints in the working set; i.e., `Zr` $= n -$ (`Bnd` $+$ `Lin` $+$ `Art`). The value of n_Z, the number of columns of Z (see Section 10.2) can be calculated as $n_Z = n -$ (`Bnd` $+$ `Lin`). A zero value of n_Z implies that x lies at a vertex of the feasible region.

`Norm Gz` is $\|Z_R^T g_{\mathrm{FR}}\|$, the Euclidean norm of the reduced gradient with respect to Z_R. During the optimality phase, this norm will be approximately zero after a unit step.

`NOpt` is the number of non-optimal Lagrange multipliers at the current point. `NOpt` is not printed if the current x is infeasible or no multipliers have been calculated. At a minimizer, `NOpt` will be zero.

`Min Lm` is the value of the Lagrange multiplier associated with the deleted constraint. If `Min Lm` is negative, a lower bound constraint has been deleted, if `Min Lm` is positive, an upper bound constraint has been deleted. If no multipliers are calculated during a given iteration, `Min Lm` will be zero.

`Cond T` is a lower bound on the condition number of the working set.

`Cond Rz` is a lower bound on the condition number of the triangular factor R (the Cholesky factor of the current reduced Hessian; see Section 10.2). If the problem is specified to be of type LP, `Cond Rz` is not printed.

`Rzz` is the last diagonal element μ of the matrix D associated with the $R^T DR$ factorization of the reduced Hessian H_R (see Section 10.2). `Rzz` is only printed if H_R is not positive-definite (in which case $\mu \neq 1$). If the printed value of `Rzz` is small in absolute value, then H_R is approximately singular. A negative value of `Rzz` implies that the objective function has negative curvature on the current working set.

H02CCF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

To supply optional parameters to H02CBF from an external file.

2 Specification

```
SUBROUTINE H02CCF(IOPTNS, INFORM)
INTEGER           IOPTNS, INFORM
```

3 Description

H02CCF may be used to supply values for optional parameters to H02CBF. H02CCF reads an external file and each line of the file defines a single optional parameter. It is only necessary to supply values for those parameters whose values are to be different from their default values.

Each optional parameter is defined by a single character string of up to 72 characters, consisting of one or more items. The items associated with a given option must be separated by spaces, or equal signs [=]. Alphabetic characters may be upper or lower case. The string

```
Print level = 1
```

is an example of a string used to set an optional parameter. For each option the string contains one or more of the following items:

(a) a mandatory keyword;
(b) a phrase that qualifies the keyword;
(c) a number that specifies an INTEGER or ***real*** value. Such numbers may be up to 16 contiguous characters in Fortran 77's I, F, E or D formats, terminated by a space if this is not the last item on the line.

Blank strings and comments are ignored. A comment begins with an asterisk (*) and all subsequent characters in the string are regarded as part of the comment.

The file containing the options must start with **begin** and must finish with **end**. An example of a valid options file is:

```
Begin * Example options file
 Print level = 10
End
```

Normally each line of the file is printed as it is read, on the current advisory message unit (see X04ABF), but printing may be suppressed using the keyword **nolist**. To suppress printing of **begin**, **nolist** must be the first option supplied as in the file:

```
Begin
 Nolist
 Print level = 10
End
```

Printing will automatically be turned on again after a call to H02CBF and may be turned on again at any time by the user by using the keyword **list**.

Optional parameter settings are preserved following a call to H02CBF, and so the keyword **defaults** is provided to allow the user to reset all the optional parameters to their default values prior to a subsequent call to H02CBF.

A complete list of optional parameters, their abbreviations, synonyms and default values is given in Section 11 of the document for H02CBF.

4 References

None.

5 Parameters

1: IOPTNS — INTEGER *Input*

On entry: the unit number of the options file to be read.

Constraint: $0 \leq \text{IOPTNS} \leq 99$.

2: INFORM — INTEGER *Output*

On exit: contains zero if the options file has been successfully read and a value > 0 otherwise, as indicated below.

INFORM = 1

IOPTNS is not in the range $[0, 99]$.

INFORM = 2

begin was found, but end-of-file was found before **end** was found.

INFORM = 3

end-of-file was found before **begin** was found.

6 Error Indicators and Warnings

If a line is not recognized as a valid option, then a warning message is output on the current advisory message unit (see X04ABF).

7 Accuracy

Not applicable.

8 Further Comments

H02CDF may also be used to supply optional parameters to H02CBF. Note that if E04NFF is used in the same program as H02CBF, then in general H02CCF will also affect the options used by E04NFF.

9 Example

This example solves the same problem as the example for H02CBF, but in addition illustrates the use of H02CCF and H02CDF to set optional parameters for H02CBF.

In this example the options file read by H02CCF is appended to the data file for the program (see Section 9.2). It would usually be more convenient in practice to keep the data file and the options file separate.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02CCF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT, LINTVR
```

```
      PARAMETER        (NIN=5,NOUT=6,LINTVR=1)
      INTEGER          NMAX, NCMAX
      PARAMETER        (NMAX=10,NCMAX=10)
      INTEGER          LDA, LDH
      PARAMETER        (LDA=NCMAX,LDH=NMAX)
      INTEGER          LIWORK, LWORK, MDEPTH
      PARAMETER        (LIWORK=1000,LWORK=10000,MDEPTH=30)
*     .. Local Scalars ..
      real             OBJ
      INTEGER          I, IFAIL, INFORM, J, N, NCLIN, STRTGY
*     .. Local Arrays ..
      real             A(LDA,NMAX), AX(NCMAX), BL(NMAX+NCMAX),
     +                 BU(NMAX+NCMAX), CLAMDA(NMAX+NCMAX), CVEC(NMAX),
     +                 H(LDH,NMAX), WORK(LWORK), X(NMAX)
      INTEGER          INTVAR(LINTVR), ISTATE(NMAX+NCMAX), IWORK(LIWORK)
*     .. External Subroutines ..
      EXTERNAL         E04NFU, H02CBF, H02CBU, H02CCF, H02CDF, X04ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02CCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NCLIN
      IF (N.LE.NMAX .AND. NCLIN.LE.NCMAX) THEN
*
*        Read CVEC, A, BL, BU, X and H from data file
*
         READ (NIN,*) (CVEC(I),I=1,N)
         READ (NIN,*) ((A(I,J),J=1,N),I=1,NCLIN)
         READ (NIN,*) (BL(I),I=1,N+NCLIN)
         READ (NIN,*) (BU(I),I=1,N+NCLIN)
         READ (NIN,*) (X(I),I=1,N)
         READ (NIN,*) ((H(I,J),J=1,N),I=1,N)
*
*        Set four options using H02CDF
*
         CALL H02CDF(' Print Level = 1 ')
*
         CALL H02CDF(' Check Frequency = 10 ')
*
         CALL H02CDF(' Crash Tolerance = 0.05 ')
*
         CALL H02CDF(' Infinite Bound Size = 1.0D+25 ')
*
*        Set the unit number for advisory messages to NOUT
*
         CALL X04ABF(1,NOUT)
*
*        Read the options file for the remaining options
*
         CALL H02CCF(NIN,INFORM)
*
         IF (INFORM.NE.0) THEN
            WRITE (NOUT,99998) 'H02CCF terminated with INFORM = ',
     +        INFORM
            STOP
         END IF
*
         STRTGY = 2
```

```
         INTVAR(1) = 4
*
         CALL H02CDF('Nolist')
         CALL H02CDF('Print Level = 0')
*
*        Solve the problem
*
         IFAIL = 1
*
         CALL H02CBF(N,NCLIN,A,LDA,BL,BU,CVEC,H,LDH,E04NFU,INTVAR,
     +               LINTVR,MDEPTH,ISTATE,X,OBJ,AX,CLAMDA,STRTGY,IWORK,
     +               LIWORK,WORK,LWORK,H02CBU,IFAIL)
*
*        Print out the best integer solution found
*
         WRITE (NOUT,99999) OBJ, (I,X(I),I=1,N)
*
      END IF
*
      STOP
*
99999 FORMAT (//' Optimal Integer Value is = ',e20.8,/' Components ar',
     +       'e ',/(' x(',I3,') = ',F15.8))
99998 FORMAT (A,I3)
      END
```

9.2 Program Data

```
H02CCF Example Program Data
  7  7                                                  :Values of N and NCLIN
 -0.02  -0.20  -0.20  -0.20  -0.20   0.04   0.04   :End of CVEC
  1.00   1.00   1.00   1.00   1.00   1.00   1.00
  0.15   0.04   0.02   0.04   0.02   0.01   0.03
  0.03   0.05   0.08   0.02   0.06   0.01   0.00
  0.02   0.04   0.01   0.02   0.02   0.00   0.00
  0.02   0.03   0.00   0.00   0.01   0.00   0.00
  0.70   0.75   0.80   0.75   0.80   0.97   0.00
  0.02   0.06   0.08   0.12   0.02   0.01   0.97   :End of matrix A
 -0.01  -0.10     -0.01     -0.04     -0.10     -0.01     -0.01
 -0.13  -1.0E+25  -1.0E+25  -1.0E+25  -1.0E+25  -9.92E-02 -3.0E-03 :End of BL
  0.01   0.15      0.03      0.02      0.05      1.0E+25   1.0E+25
 -0.13  -4.9E-03  -6.4E-03  -3.7E-03  -1.2E-03   1.0E+25   2.0E-03 :End of BU
 -0.01  -0.03   0.00  -0.01  -0.10   0.02   0.01   :End of X
  2.00   0.00   0.00   0.00   0.00   0.00   0.00
  0.00   2.00   0.00   0.00   0.00   0.00   0.00
  0.00   0.00   2.00   2.00   0.00   0.00   0.00
  0.00   0.00   2.00   2.00   0.00   0.00   0.00
  0.00   0.00   0.00   0.00   2.00   0.00   0.00
  0.00   0.00   0.00   0.00   0.00  -2.00  -2.00
  0.00   0.00   0.00   0.00   0.00  -2.00  -2.00   :End of matrix H
Begin   Example options file for H02CCF
   Feasibility Phase Iteration Limit = 5  *  (Default = 70)
   Optimality Phase Iteration Limit = 10  *  (Default = 70)
End
```

9.3 Program Results

```
H02CCF Example Program Results


Calls to H02CDF
---------------

      Print Level = 1
      Check Frequency = 10
      Crash Tolerance = 0.05
      Infinite Bound Size = 1.0E+25


OPTIONS file
------------

     Begin   Example options file for H02CCF
        Feasibility Phase Iteration Limit = 5  *  (Default = 70)
        Optimality Phase Iteration Limit = 10  *  (Default = 70)
     End


Optimal Integer Value is =       0.37469662E-01
Components are
x(  1) =     -0.01000000
x(  2) =     -0.07332830
x(  3) =     -0.00025809
x(  4) =      0.00000000
x(  5) =     -0.06335433
x(  6) =      0.01410944
x(  7) =      0.00283128
```

H02CDF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

To supply individual optional parameters to H02CBF.

2 Specification

```
SUBROUTINE H02CDF(STRING)
CHARACTER*(*)      STRING
```

3 Description

H02CDF may be used to supply values for optional parameters to H02CBF. It is only necessary to call H02CDF for those parameters whose values are to be different from their default values. One call to H02CDF sets one parameter value.

Each optional parameter is defined by a single character string of up to 72 characters, consisting of one or more items. The items associated with a given option must be separated by spaces, or equal signs [=]. Alphabetic characters may be upper or lower case. The string

```
Print level = 1
```

is an example of a string used to set an optional parameter. For each option the string contains one or more of the following items:

(a) a mandatory keyword;
(b) a phrase that qualifies the keyword;
(c) a number that specifies an INTEGER or ***real*** value. Such numbers may be up to 16 contiguous characters in Fortran 77's I, F, E or D formats, terminated by a space if this is not the last item on the line.

Blank strings and comments are ignored. A comment begins with an asterisk (*) and all subsequent characters in the string are regarded as part of the comment.

Normally, each user-specified option is printed as it is defined, on the current advisory message unit (see X04ABF), but this printing may be suppressed using the keyword **nolist**. Thus the statement

```
CALL H02CDF ('Nolist')
```

suppresses printing of this and subsequent options. Printing will automatically be turned on again after a call to H02CBF, and may be turned on again at any time by the user, by using the keyword **list**.

Optional parameter settings are preserved following a call to H02CBF, and so the keyword **defaults** is provided to allow the user to reset all the optional parameters to their default values by the statement,

```
CALL H02CDF ('Defaults')
```

prior to a subsequent call to H02CBF.

A complete list of optional parameters, their abbreviations, synonyms and default values is given in Section 11 of the document for H02CBF.

4 References

None.

5 Parameters

1: STRING — CHARACTER*(*) *Input*

On entry: a single valid option string (as described in Section 3 above and in Section 11 of the document for H02CBF).

6 Error Indicators and Warnings

If a line is not recognized as a valid option, then a warning message is output on the current advisory message unit (see X04ABF).

7 Accuracy

Not applicable.

8 Further Comments

H02CCF may also be used to supply optional parameters to H02CBF. Note that if E04NFF is used in the same program as H02CBF, then in general H02CCF will also affect the options used by E04NFF.

9 Example

See the example for H02CCF.

H02CEF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

Note. *This routine uses* optional parameters *to define choices in the problem specification and in the details of the algorithm. If you wish to use* default *settings for all of the optional parameters, you need only read Section 1 to Section 9 of this document. Refer to the additional Section 10, Section 11 and Section 12 for a description of the algorithm, the specification of the optional parameters and a description of the monitoring information produced by the routine.*

1 Purpose

H02CEF obtains integer solutions to sparse linear programming and quadratic programming problems.

2 Specification

```
      SUBROUTINE H02CEF(N, M, NNZ, IOBJ, NCOLH, QPHX, A, HA, KA, BL, BU,
     1                  START, NAMES, NNAME, CRNAME, NS, XS, INTVAR,
     2                  LINTVR, MDEPTH, ISTATE, MINIZ, MINZ, OBJ,
     3                  CLAMDA, STRTGY, IZ, LENIZ, Z, LENZ, MONIT, IFAIL)
      INTEGER           N, M, NNZ, IOBJ, NCOLH, HA(NNZ), KA(N+1), NNAME,
     1                  NS, INTVAR(LINTVR), LINTVR, MDEPTH, ISTATE(N+M),
     2                  MINIZ, MINZ, STRTGY, IZ(LENIZ), LENIZ, LENZ,
     3                  IFAIL
      real              A(NNZ), BL(N+M), BU(N+M), XS(N+M), OBJ,
     1                  CLAMDA(N+M), Z(LENZ)
      CHARACTER*8       NAMES(5), CRNAME(NNAME)
      CHARACTER*1       START
      EXTERNAL          QPHX, MONIT
```

3 Description

H02CEF is designed to obtain integer solutions to a class of quadratic programming problems addressed by E04NKF. Specifically it solves the following problem:

$$\underset{x \in R^n}{\text{minimize}}\ f(x) \text{ subject to } l \leq \begin{Bmatrix} x \\ Ax \end{Bmatrix} \leq u, \tag{1}$$

where $x = (x_1, x_2, \ldots, x_n)^T$ is a set of variables (some of which may be required to be integer), A is an m by n matrix and the objective function $f(x)$ may be specified in a variety of ways depending upon the particular problem to be solved. The optional parameter **Maximize** (see Section 11.2) may be used to specify an alternative problem in which $f(x)$ is maximized. The possible forms for $f(x)$ are listed in Table 1 below, in which the prefixes LP and QP stand for 'linear programming' and 'quadratic programming' respectively, c is an n element vector and H is the n by n second-derivative matrix $\nabla^2 f(x)$ (the *Hessian matrix*).

Problem type	**Objective function** $f(x)$	**Hessian matrix** H
LP	$c^T x$	Not applicable
QP	$c^T x + \frac{1}{2} x^T H x$	Symmetric positive semi-definite

Table 1

For LP and QP problems, the unique global minimum value of $f(x)$ is found. For QP problems, you must also provide a subroutine that computes Hx for any given vector x. (H need not be stored explicitly.)

(It is not expected that the feasibility problem of E04NKF would be relevant here.)

The routine employs a 'Branch and Bound' method to enforce the integer constraints. In this technique the problem is first solved without the integer constraints. If a variable is found to be non-integral when it is required to have an integer value then two additional problems are constructed. One bounds the

variable above by the nearest integer value below the optimal value previously obtained. The second problem is formed by bounding the variable below by the nearest integer value above the optimal value. This process is continued until an integer solution is found. At this point the user may elect to stop, or may continue to search for better integer solutions by examining any other sub-problems that remain to be explained.

In practice the routine tries to compute an integer solution as quickly as possible using a depth-first approach, since this helps determine a realistic cut-off value. If we have a cut-off value, say the value of the function at this first integer solution, and any sub-problem, W say, has a solution value greater than this cut-off value, then subsequent sub-problems of W must have solutions greater than the value of the solution at W and therefore need not be computed. Thus a knowledge of a good cut-off value can result in fewer sub-problems being solved and thus speed up the operation of the routine. (See the description of MONIT in Section 5 for details of how users can supply their own cut-off value.)

Each sub-problem is solved using E04NKF. The user is referred to the routine document for E04NKF for details of the algorithm used.

4 References

[1] Gill P E, Murray W and Saunders M A (1996) SNOPT: An SQP Algorithm for Large-scale Constrained Optimization *Numerical Analysis Report 96-2.* Department of Mathematics, University of California, San Diego

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[4] Gill P E, Murray W, Saunders M A and Wright M H (1989) A practical anti-cycling procedure for linearly constrained optimization *Math. Programming* **45** 437–474

[5] Gill P E, Murray W, Saunders M A and Wright M H (1991) Inertia-controlling methods for general quadratic programming *SIAM Rev.* **33** 1–36

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[7] Hall J A J and McKinnon K I M (1996) The Simplest Examples where the Simplex Method Cycles and Conditions where EXPAND Fails to Prevent Cycling *Report MS 96-010.* Department of Mathematics and Statistics, University of Edinburgh

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5 Parameters

1: N — INTEGER *Input*

On entry: n, the number of variables (excluding slacks). This is the number of columns in the linear constraint matrix A.

Constraint: $\mathrm{N} \geq 1$.

2: M — INTEGER *Input*

On entry: m, the number of general linear constraints (or slacks). This is the number of rows in A, including the free row (if any; see IOBJ below).

Constraint: $\mathrm{M} \geq 1$.

3: NNZ — INTEGER *Input*

On entry: the number of non-zero elements in A.

Constraint: $1 \leq \mathrm{NNZ} \leq \mathrm{N} \times \mathrm{M}$.

4: IOBJ — INTEGER *Input*

On entry: if IOBJ > 0, row IOBJ of A is a free row containing the non-zero elements of the vector c appearing in the linear objective term $c^T x$. If IOBJ $= 0$, there is no free row – i.e., the problem is either an FP problem (in which case IOBJ must be set to zero), or a QP problem with $c = 0$.

Constraint: $0 \leq$ IOBJ $\leq$ M.

5: NCOLH — INTEGER *Input*

On entry: n_H, the number of leading non-zero columns of the Hessian matrix H. For FP and LP problems, NCOLH must be set to zero.

Constraint: $0 \leq$ NCOLH $\leq$ N.

6: QPHX — SUBROUTINE, supplied by the NAG Fortran Library or the user. *External Procedure*

For QP problems, you must supply a version of QPHX to compute the matrix product Hx. If H has rows and columns consisting entirely of zeros, it is most efficient to order the variables $x = (y \;\; z)^T$ so that

$$Hx = \begin{pmatrix} H_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} H_1 y \\ 0 \end{pmatrix},$$

where the nonlinear variables y appear first as shown. For LP problems, QPHX will never be called by H02CEF and hence QPHX may be the dummy routine E04NKU (NKUE04 in some implementations).

Its specification is:

```
SUBROUTINE QPHX(NSTATE, NCOLH, X, HX)
INTEGER          NSTATE, NCOLH
real             X(NCOLH), HX(NCOLH)
```

1: NSTATE — INTEGER *Input*

On entry: if NSTATE $= 1$, then H02CEF is calling QPHX for the first time on a sub-problem. This parameter setting allows you to save computation time if certain data must be read or calculated only once. If NSTATE ≥ 2, then H02CEF is calling QPHX for the last time. This parameter setting allows you to perform some additional computation on the final sub-problem solution. In general, the last call to QPHX is made with NSTATE $= 2 +$ IFAIL (see Section 6). Otherwise, NSTATE $= 0$.

2: NCOLH — INTEGER *Input*

On entry: this is the same parameter NCOLH as supplied to H02CEF (see above).

3: X(NCOLH) — ***real*** array *Input*

On entry: the first NCOLH elements of the vector x.

4: HX(NCOLH) — ***real*** array *Output*

On exit: the product Hx.

QPHX must be declared as EXTERNAL in the (sub)program from which H02CEF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

7: A(NNZ) — ***real*** array *Input*

On entry: the non-zero elements of A, ordered by increasing column index. Note that multiple elements with the same row and column indices are not allowed.

8: HA(NNZ) — INTEGER array *Input*

On entry: HA(i) must contain the row index of the non-zero element stored in A(i), for $i = 1, 2, \ldots,$NNZ. Note that the row indices for a column may be supplied in any order.

Constraint: $1 \leq$ HA(i) $\leq$ M, for $i = 1, 2, \ldots,$NNZ.

9: KA(N+1) — INTEGER array *Input*

On entry: KA(j) must contain the index in A of the start of the jth column, for $j = 1, 2, \ldots$,N. To specify the jth column as empty, set KA(j) = KA($j + 1$). Note that the first and last elements of KA must be such that KA(1) = 1 and KA(N+1) = NNZ + 1.

Constraints:

KA(1) = 1,
KA(j) $\geq$ 1 for $j = 2, 3, \ldots$,N,
KA(N+1) = NNZ + 1,
$0 \leq$ KA($j + 1$) − KA(j) $\leq$ M for $j = 1, 2, \ldots$,N.

10: BL(N+M) — ***real*** array *Input*

On entry: l, the lower bounds for all the variables and general constraints, in the following order. The first N elements of BL must contain the bounds on the variables x, and the next M elements the bounds for the general linear constraints Ax (or slacks s) and the free row (if any). To specify a non-existent lower bound (i.e., $l_j = -\infty$), set BL(j) $\leq -bigbnd$, where *bigbnd* is the value of the optional parameter **Infinite Bound Size** (default value = 10^{20}; see Section 11.2). To specify the jth constraint as an *equality*, set BL(j) = BU(j) = β, say, where $|\beta| <$ *bigbnd*. Note that the lower bound corresponding to the free row must be set to $-\infty$ and stored in BL(N+IOBJ).

Constraints:

BL(N+IOBJ) $\leq -bigbnd$ when IOBJ > 0.
(See also the description for BU below.)

11: BU(N+M) — ***real*** array *Input*

On entry: u, the upper bounds for all the variables and general constraints, in the following order. The first N elements of BL must contain the bounds on the variables x, and the next M elements the bounds for the general linear constraints Ax (or slacks s) and the free row (if any). To specify a non-existent upper bound (i.e., $u_j = +\infty$), set BU(j) $\geq$ *bigbnd*. Note that the upper bound corresponding to the free row must be set to $+\infty$ and stored in BU(N+IOBJ).

Constraints:

BU(N+IOBJ) $\geq$ *bigbnd* when IOBJ > 0,
BL(j) $\leq$ BU(j), for $j = 1, 2, \ldots$,N+M,
$|\beta| <$ *bigbnd* when BL(j) = BU(j) = β.

12: START — CHARACTER*1 *Input*

On entry: indicates how a starting basis is to be obtained as follows.

If START = 'C', then an internal crash procedure will be used to choose an initial basis matrix B.
If START = 'W', then a basis is already defined in ISTATE (probably from a previous call).

Constraint: START = 'C' or 'W'.

13: NAMES(5) — CHARACTER*8 *Input*

On entry: a set of names associated with the so-called MPSX form of the problem as follows:

NAMES(1) must contain the name for the problem (or be blank);
NAMES(2) must contain the name for the free row (or be blank);
NAMES(3) must contain the name for the constraint right-hand side (or be blank);
NAMES(4) must contain the name for the ranges (or be blank);
NAMES(5) must contain the name for the bounds (or be blank).

(These names are used in the monitoring file output; see Section 12.)

14: NNAME — INTEGER *Input*

On entry: the number of column (i.e., variable) and row names supplied in CRNAME as follows.

If NNAME = 1, there are no names. Default names will be used in the printed output.
If NNAME = N+M, all names must be supplied.

Constraint: NNAME = 1 or N+M.

15: CRNAME(NNAME) — CHARACTER*8 array *Input*

On entry: the optional column and row names, respectively as follows.

If NNAME = 1, CRNAME is not referenced and the printed output will use default names for the columns and rows.
If NNAME = N+M, the first N elements must contain the names for the columns and the next M elements must contain the names for the rows. Note that the name for the free row (if any) must be stored in CRNAME(N+IOBJ).

16: NS — INTEGER *Input/Output*

On entry: n_S, the number of superbasics. For QP problems, NS need not be specified if START = 'C', but must retain its value from a previous call when START = 'W'. For FP and LP problems, NS need not be initialized.

On exit: the final number of superbasics. This will be zero for FP and LP problems.

17: XS(N+M) — ***real*** array *Input/Output*

On entry: the initial values of the variables and slacks (x, s). (See the description for ISTATE below.)

On exit: XS(i) contains the final value of x_i, for $i = 1, 2, \ldots, n$.

18: INTVAR(LINTVR) — INTEGER array *Input*

On entry: INTVAR specifies which components of the solution vector x are constrained to be integer. Specifically, if k elements of x are required to take integer values then INTVAR(i) = l_i for $i = 1, 2, \ldots, k$, where l_i is the integer index such that x_{l_i} is integer. If $k <$ LINTVR then INTVAR($k + 1$) must be set to -1 to signal the end of the integer variable indices.

The order in which the indices of those components of x required to be integer is presented determines the order in which the sub-problems are treated and solved. As such it can be a powerful tool to assist the routine in achieving a solution efficiently. The general advice is to enter the important integer variables in the model early in INTVAR; secondary or less important variables should be entered near the end of the list. However some experimentation might be required to find the optimal order.

19: LINTVR — INTEGER *Input*

On entry: k, the number of components of x required to be integer. If $k = 0$, then LINTVR must be set to 1 and INTVAR(1) set to -1.

20: MDEPTH — INTEGER *Input*

On entry: MDEPTH specifies the maximum depth the tree of sub-problems may be developed.

Suggested value: MDEPTH = 2 × N + 20.

Constraint: MDEPTH > 0.

21: ISTATE(N+M) — INTEGER array *Input/Output*

On entry: if START = 'C', the first N elements of ISTATE and XS must specify the initial states and values, respectively, of the variables x. (The slacks s need not be initialized.) An internal crash procedure is then used to select an initial basis matrix B. The initial basis matrix will be triangular (neglecting certain small elements in each column). It is chosen from various rows and columns of columns of $(A - I)$. Possible values for ISTATE(j) are as follows:

ISTATE(j)	**State of XS(j) during crash procedure**
0 or 1	Eligible for the basis
2	Ignored
3	Eligible for the basis (given preference over 0 or 1)
4 or 5	Ignored

If nothing special is known about the problem, or there is no wish to provide special information, you may set ISTATE(j) = 0 and XS(j) = 0.0 for $j = 1, 2, \ldots$,N. All variables will then be eligible for the initial basis. Less trivially, to say that the jth variable will probably be equal to one of its bounds, set ISTATE(j) = 4 and XS(j) = BL(j) or ISTATE(j) = 5 and XS(j) = BU(j) as appropriate.

Following the crash procedure, variables for which ISTATE(j) = 2 are made superbasic. Other variables not selected for the basis are then made nonbasic at the value XS(j) if BL(j) $\leq$ XS(j) $\leq$ BU(j), or at the value BL(j) or BU(j) closest to XS(j).

If START = 'W', ISTATE and XS must specify the initial states and values, respectively, of the variables and slacks (x, s). If H02CEF has been called previously with the same values of N and M, ISTATE already contains satisfactory information.

Constraints:

If START = 'C', $0 \leq$ ISTATE(j) ≤ 5 for $j = 1, 2, \ldots$,N.
If START = 'W', $0 \leq$ ISTATE(j) ≤ 3 for $j = 1, 2, \ldots$,N+M.

On exit: the final states of the variables and slacks (x, s) from the solution of the last sub-problem tackled. The significance of each possible value of ISTATE(j) is as follows:

ISTATE(j)	**State of variable j**	**Normal value of XS(j)**
0	Nonbasic	BL(j)
1	Nonbasic	BU(j)
2	Superbasic	Between BL(j) and BU(j)
3	Basic	Between BL(j) and BU(j)

If NINF = 0, basic and superbasic variables may be outside their bounds by as much as the value of the optional parameter **Feasibility Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$, where ϵ is the ***machine precision***; see Section 11.2). Note that unless the optional parameter **Scale Option** = 0 (default value = 2; see Section 11.2) is specified, the **Feasibility Tolerance** applies to the variables of the scaled problem. In this case, the variables of the original problem may be as much as 0.1 outside their bounds, but this is unlikely unless the problem is very badly scaled.

Very occasionally some nonbasic variables may be outside their bounds by as much as the **Feasibility Tolerance**, and there may be some nonbasic variables for which XS(j) lies strictly between its bounds.

If NINF > 0, some basic and superbasic variables may be outside their bounds by an arbitrary amount (bounded by SINF if **Scale Option** = 0).

22: MINIZ — INTEGER *Output*

On exit: the minimum value of LENIZ required to start solving the problem. If IFAIL = 14, H02CEF may be called again with LENIZ suitably larger than MINIZ. (The bigger the better, since it is not certain how much workspace the basis factors need.)

23: MINZ — INTEGER *Output*

On exit: the minimum value of LENZ required to start solving the problem. If IFAIL = 15, H02CEF may be called again with LENZ suitably larger than MINZ. (The bigger the better, since it is not certain how much workspace the basis factors need.)

24: OBJ — ***real*** *Output*

On exit: the value of the objective function. If NINF = 0, OBJ includes the quadratic objective term $\frac{1}{2}x^THx$ (if any). If NINF > 0, OBJ is just the linear objective term c^Tx (if any). For FP problems, OBJ is set to zero.

25: CLAMDA(N+M) — ***real*** array *Output*

On exit: a set of Lagrange multipliers for the bounds on the variables and the general constraints. More precisely, the first N elements contain the multipliers (*reduced costs*) for the bounds on the variables, and the next M elements contain the multipliers (*shadow prices*) for the general linear constraints.

26: STRTGY — INTEGER *Input*

On entry: STRTGY defines the branching strategy adopted by the routine.

If STRTGY = 0, each sub-problem first explored imposes a tighter upper bound on the component of x;
if STRTGY = 1, each sub-problem first explored imposes a tighter lower bound on the component of x;
if STRTGY = 2, each branch explored imposes a tighter upper bound on the component of x if its fractional part is less than 0.5, otherwise it imposes a tighter lower bound;
if STRTGY = 3, a random choice is made between first exploring a tighter lower bound or a tighter upper bound sub-problem.

Constraint: STRTGY = 0, 1, 2 or 3.

27: IZ(LENIZ) — INTEGER array *Workspace*

28: LENIZ — INTEGER *Input*

On entry: the dimension of the array IZ as declared in the (sub)program from which H02CEF is called.

Constraint: LENIZ $\geq$ 1.

29: Z(LENZ) — ***real*** array *Workspace*

30: LENZ — INTEGER *Input*

On entry: the dimension of the array Z as declared in the (sub)program from which H02CEF is called.

Constraint: LENZ $\geq$ 1.

The amounts of workspace provided (i.e., LENIZ and LENZ) and required (i.e., MINIZ and MINZ) are (by default) output on the current advisory message unit (as defined by X04ABF). Since the minimum values of LENIZ and LENZ required to start solving the problem are returned in MINIZ and MINZ, respectively, you may prefer to obtain appropriate values from the output of a preliminary run with LENIZ and LENZ set to 1. (H02CEF will then terminate with IFAIL = 14.)

31: MONIT — SUBROUTINE, supplied by the NAG Fortran Library or the user. *External Procedure*

To provide feed-back to the user on the progress of the Branch and Bound process. Additionally MONIT provides, via its parameter HALT, the ability to terminate the process. (The user might choose to do this when an integer solution is found, rather than search for a better solution.) If the user does not require any intermediate output then MONIT may be the dummy routine H02CEY (CEYH02 in some implementations).

Its specification is:

```
      SUBROUTINE MONIT(INTFND, NODES, DEPTH, OBJ, X, BSTVAL, BSTSOL, BL,
     1                 BU, N, HALT, COUNT)
      INTEGER          INTFND, NODES, DEPTH, N, COUNT
      real             OBJ, X(N), BSTVAL, BSTSOL(N), BL(N), BU(N)
      LOGICAL          HALT
```

1: INTFND — INTEGER *Input*

On entry: INTFND contains the number of integer solutions obtained so far.

2: NODES — INTEGER *Input*

On entry: NODES contains the number of nodes (sub-problems) solved so far.

3: DEPTH — INTEGER *Input*

On entry: DEPTH contains the depth reached in the tree of problems.

4: OBJ — ***real*** *Input*

On entry: OBJ contains the solution value to the sub-problem at this node.

5: X(N) — ***real*** array *Input*

On entry: X contains the solution vector to the sub-problem at this node.

6: BSTVAL — ***real*** *Input/Output*

On entry: BSTVAL contains the value of the objective function corresponding to the best integer solution obtained so far. If no integer solution has been found BSTVAL contains the largest machine representable number (see X02ALF).

On exit: may be set to a cut-off value by the sophisticated user as follows. Before an integer solution has been found BSTVAL will be set by H02CEF to the largest machine representable number (see X02ALF). If the user knows that the solution being sought is a much smaller number, then BSTVAL may be set to this number as a cut-off value (see Section 3). Beware of setting BSTVAL too small, since then no integer solutions will be discovered. Also make sure that BSTVAL is set using a statement of the form

`IF (INTFND.EQ.0) BSTVAL =` *cut-off value*

on entry to MONIT. This statement will not prevent the normal operation of the algorithm when subsequent integer solutions are found. It would be a grievous mistake to unconditionally set BSTVAL and if you have any doubts whatsoever about the correct use of this parameter then you are strongly recommended to leave it unchanged.

7: BSTSOL(N) — ***real*** array *Input*

On entry: BSTSOL contains the value of the best integer solution obtained so far.

8: BL(N) — ***real*** array *Input*

On entry: BL contains the current lower bounds on the variables at this point.

9: BU(N) — ***real*** array *Input*

On entry: BU contains the current upper bounds on the variables at this point.

10: N — INTEGER *Input*

On entry: N contains the number of variables in the minimization problem.

11: HALT — LOGICAL *Output*

On exit: If HALT is set to .TRUE. E04NFF will be brought to a halt with IFAIL exit −1.

12: COUNT — INTEGER *Input/Output*

COUNT may be used by the user to save the last value of INTFND. If a subsequent call of MONIT has a value of INTFND which is greater than COUNT, then the user knows that a new integer solution has been found at this node.

MONIT must be declared as EXTERNAL in the (sub)program from which H02CEF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

32: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings specified by the routine:

IFAIL = −1

Halted at user request.

IFAIL = 0

Successful exit.

IFAIL = 1

Input parameter error immediately detected.

IFAIL = 2

No integer solution found.

IFAIL = 3

MDEPTH is too small.

IFAIL = 4

The problem is unbounded (or badly scaled). The objective function is not bounded below in the feasible region.

IFAIL = 5

The problem is infeasible. The general constraints cannot all be satisfied simultaneously to within the value of the optional parameter **Feasibility Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$, where ϵ is the ***machine precision***; see Section 11.2).

IFAIL = 6

Too many iterations. The value of the optional parameter **Iteration Limit** (default value = $\max(50, 5(n+m))$; see Section 11.2) is too small.

IFAIL = 7

The reduced Hessian matrix $Z^T H Z$ (see Section 10.2) exceeds its assigned dimension. The value of the optional parameter **Superbasics Limit** (default value = $\min(n_H + 1, n)$; see Section 11.2) is too small.

IFAIL = 8

The Hessian matrix H appears to be indefinite. Check that subroutine QPHX has been coded correctly and that all relevant elements of Hx have been assigned their correct values.

IFAIL = 9

An input parameter is invalid.

IFAIL = 10

Numerical error in trying to satisfy the general constraints. The basis is very ill-conditioned.

IFAIL = 11

Not enough integer workspace for the basis factors. Increase LENIZ and rerun H02CEF.

IFAIL = 12

Not enough real workspace for the basis factors. Increase LENZ and rerun H02CEF.

IFAIL = 13

The basis is singular after 15 attempts to factorize it (adding slacks where necessary). Either the problem is badly scaled or the value of the optional parameter **LU Factor Tolerance** (default value = 100.0) is too large.

IFAIL = 14

Not enough integer workspace to start solving the problem. Increase LENIZ to at least MINIZ and rerun H02CEF.

IFAIL = 15

Not enough real workspace to start solving the problem. Increase LENZ to at least MINZ and rerun H02CEF.

IFAIL = 16

An internal error has occurred. Contact NAG with details of your program.

7 Accuracy

The routine implements a numerically stable active-set strategy and returns solutions that are as accurate as the condition of the problem warrants on the machine.

8 Further Comments

This section contains a description of the printed output.

8.1 Description of the Printed Output

This section describes the (default) intermediate printout and final printout produced by H02CEF. The intermediate printout is a subset of the monitoring information produced by the routine at every iteration (see Section 12). The level of printed output can be controlled by the user (see the description of the optional parameter **Print Level** in Section 11.2). Note that the intermediate printout and final printout are produced only if **Print Level** ≥ 10 (the default).

The following line of summary output (< 80 characters) is produced at every iteration. In all cases, the values of the quantities printed are those in effect *oncompletion* of the given iteration.

`Itn`	is the iteration count.
`Step`	is the step taken along the computed search direction.
`Ninf`	is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.
`Sinf/Objective`	is the value of the current objective function. If x is not feasible, `Sinf` gives the sum of the magnitudes of constraint violations. If x is feasible, `Objective` is the value of the objective function. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which `Ninf` is zero) will give the value of the true objective at the first feasible point. During the optimality phase, the value of the objective function will be non-increasing. During the feasibility phase, the number of constraint infeasibilities will not increase until either a feasible point is found, or the optimality of the multipliers implies that no feasible point exists.
`Norm rg`	is $\|d_S\|$, the Euclidean norm of the reduced gradient (see Section 10.3). During the optimality phase, this norm will be approximately zero after a unit step. For FP and LP problems, `Norm rg` is not printed.

The final printout includes a listing of the status of every variable and constraint.

The following describes the printout for each variable. A full stop (.) is printed for any numerical value that is zero.

Variable gives the name of the variable. If NNAME = 1, a default name is assigned to the jth variable for $j = 1, 2, \ldots, n$. If NNAME = N + M, the name supplied in CRNAME(j) is assigned to the jth variable.

State gives the state of the variable (**LL** if nonbasic on its lower bound, **UL** if nonbasic on its upper bound, **EQ** if nonbasic and fixed, **FR** if nonbasic and strictly between its bounds, **BS** if basic and **SBS** if superbasic).

A key is sometimes printed before **State** to give some additional information about the state of a variable. Note that unless the optional parameter **Scale Option** = 0 (default value = 2; see Section 11.2) is specified, the tests for assigning a key are applied to the variables of the scaled problem.

- **A** *Alternative optimum possible.* The variable is nonbasic, but its reduced gradient is essentially zero. This means that if the variable were allowed to start moving away from its bound, there would be no change in the value of the objective function. The values of the other free variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled **D**), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the Lagrange multipliers *might* also change.
- **D** *Degenerate.* The variable is basic or superbasic, but it is equal to (or very close to) one of its bounds.
- **I** *Infeasible.* The variable is basic or superbasic and is currently violating one of its bounds by more than the value of the optional parameter **Feasibility Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$, where ϵ is the ***machine precision***; see Section 11.2).
- **N** *Not precisely optimal.* The variable is nonbasic or superbasic. If the value of the reduced gradient for the variable exceeds the value of the optional parameter **Optimality Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$; see Section 11.2), the solution would not be declared optimal because the reduced gradient for the variable would not be considered negligible.

Value is the value of the variable at the final iterate.

Lower Bound is the lower bound specified for the variable. **None** indicates that BL(j) $\leq -bigbnd$.

Upper Bound is the upper bound specified for the variable. **None** indicates that BU(j) $\geq bigbnd$.

Lagr Mult is the Lagrange multiplier for the associated bound. This will be zero if **State** is **FR**. If x is optimal, the multiplier should be non-negative if **State** is **LL**, non-positive if **State** is **UL**, and zero if **State** is **BS** or **SBS**.

Residual is the difference between the variable **Value** and the nearer of its (finite) bounds BL(j) and BU(j). A blank entry indicates that the associated variable is not bounded (i.e., BL(j) $\leq -bigbnd$ and BU(j) $\geq bigbnd$).

The meaning of the printout for linear constraints is the same as that given above for variables, with 'variable' replaced by 'constraint', n replaced by m, CRNAME(j) replaced by CRNAME($n + j$), BL(j) and BU(j) are replaced by BL($n + j$) and BU($n + j$) respectively, and with the following change in the heading:

Constrnt gives the name of the linear constraint.

Note that movement off a constraint (as opposed to a variable moving away from its bound) can be interpreted as allowing the entry in the **Residual** column to become positive.

Numerical values are output with a fixed number of digits; they are not guaranteed to be accurate to this precision.

9 Example

To minimize the quadratic function $f(x) = c^T x + \frac{1}{2} x^T H x$, where

$$c = (-200.0,\ -2000.0,\ -2000.0,\ -2000.0,\ -2000.0,\ 400.0,\ 400.0)^T$$

$$H = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 2 & 2 \end{pmatrix}$$

subject to the bounds

$$\begin{aligned} 0 &\leq x_1 \leq 200 \\ 0 &\leq x_2 \leq 2500 \\ 400 &\leq x_3 \leq 800 \\ 100 &\leq x_4 \leq 700 \\ 0 &\leq x_5 \leq 1500 \\ 0 &\leq x_6 \\ 0 &\leq x_7 \end{aligned}$$

to the linear constraints

$$\begin{aligned} x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 &= 2000 \\ 0.15x_1 + 0.04x_2 + 0.02x_3 + 0.04x_4 + 0.02x_5 + 0.01x_6 + 0.03x_7 &\leq 60 \\ 0.03x_1 + 0.05x_2 + 0.08x_3 + 0.02x_4 + 0.06x_5 + 0.01x_6 &\leq 100 \\ 0.02x_1 + 0.04x_2 + 0.01x_3 + 0.02x_4 + 0.02x_5 &\leq 40 \\ 0.02x_1 + 0.03x_2 + 0.01x_5 &\leq 30 \\ 1500 \leq 0.70x_1 + 0.75x_2 + 0.80x_3 + 0.75x_4 + 0.80x_5 + 0.97x_6 & \\ 250 \leq 0.02x_1 + 0.06x_2 + 0.08x_3 + 0.12x_4 + 0.02x_5 + 0.01x_6 + 0.97x_7 &\leq 300 \end{aligned}$$

and the variables x_2, x_3, x_4, x_5, x_6, x_7, are constrained to be integer.

The initial point, which is infeasible, is

$$x_0 = (0.0,\ 0.0,\ 0.0,\ 0.0,\ 0.0,\ 0.0,\ 0.0)^T.$$

The optimal solution (to five figures) is

$$x^* = (0.0,\ 355.0,\ 645.0,\ 164.0,\ 410.0,\ 275.0,\ 151.0)^T.$$

One bound constraint and one linear constraint are active at the solution. Note that the Hessian matrix H is positive semi-definite.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02CEF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX, NNZMAX, LENIZ, LENZ, LINTVR, MM
      PARAMETER        (NMAX=100,MMAX=100,NNZMAX=100,LENIZ=100000,
     +                 LENZ=100000,LINTVR=10,MM=2000)
*     .. Local Scalars ..
      real             OBJ
      INTEGER          I, ICOL, IFAIL, IOBJ, J, JCOL, M, MINIZ, MINZ, N,
```

```
     +                NCOLH, NNAME, NNZ, NS, STRTGY
      CHARACTER       START
*     .. Local Arrays ..
      real            A(NNZMAX), BL(NMAX+MMAX), BU(NMAX+MMAX),
     +                CLAMDA(NMAX+MMAX), XS(NMAX+MMAX), Z(LENZ)
      INTEGER         HA(NNZMAX), INTVAR(LINTVR), ISTATE(NMAX+MMAX),
     +                IZ(LENIZ), KA(NMAX+1)
      CHARACTER*8     CRNAME(NMAX+MMAX), NAMES(5)
*     .. External Subroutines ..
      EXTERNAL        H02CEF, H02CGF, MONIT, QPHX
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02CEF Example Program Results'
*     Skip heading in data file.
      READ (NIN,*)
      READ (NIN,*) N, M
      IF (N.LE.NMAX .AND. M.LE.MMAX) THEN
*
*        Read NNZ, IOBJ, NCOLH, START and NNAME from data file.
*
         READ (NIN,*) NNZ, IOBJ, NCOLH, START, NNAME
*
*        Read NAMES and CRNAME from data file.
*
         READ (NIN,*) (NAMES(I),I=1,5)
         READ (NIN,*) (CRNAME(I),I=1,NNAME)
*
*        Read the matrix A from data file. Set up KA.
*
         JCOL = 1
         KA(JCOL) = 1
         DO 40 I = 1, NNZ
*
*           Element ( HA( I ), ICOL ) is stored in A( I ).
*
            READ (NIN,*) A(I), HA(I), ICOL
*
            IF (ICOL.EQ.JCOL+1) THEN
*
*              Index in A of the start of the ICOL-th column equals I.
*
               KA(ICOL) = I
               JCOL = ICOL
            ELSE IF (ICOL.GT.JCOL+1) THEN
*
*              Index in A of the start of the ICOL-th column equals I,
*              but columns JCOL+1,JCOL+2,...,ICOL-1 are empty. Set the
*              corresponding elements of KA to I.
*
               DO 20 J = JCOL + 1, ICOL - 1
                  KA(J) = I
   20          CONTINUE
               KA(ICOL) = I
               JCOL = ICOL
            END IF
   40    CONTINUE
         KA(N+1) = NNZ + 1
*
*        Read BL, BU, ISTATE and XS from data file.
```

```
*
         READ (NIN,*) (BL(I),I=1,N+M)
         READ (NIN,*) (BU(I),I=1,N+M)
         READ (NIN,*) (ISTATE(I),I=1,N)
         READ (NIN,*) (XS(I),I=1,N)
*
         STRTGY = 3
         INTVAR(1) = 2
         INTVAR(2) = 3
         INTVAR(3) = 4
         INTVAR(4) = 5
         INTVAR(5) = 6
         INTVAR(6) = 7
         INTVAR(7) = -1
*
         CALL H02CGF('NoList')
         CALL H02CGF('Print Level = 0')
*
*        Solve the QP problem.
*
         IFAIL = 0
*
         CALL H02CEF(N,M,NNZ,IOBJ,NCOLH,QPHX,A,HA,KA,BL,BU,START,NAMES,
     +               NNAME,CRNAME,NS,XS,INTVAR,LINTVR,MM,ISTATE,MINIZ,
     +               MINZ,OBJ,CLAMDA,STRTGY,IZ,LENIZ,Z,LENZ,MONIT,IFAIL)
*
*        Print out the best integer solution found
*
         WRITE (NOUT,99999) OBJ, (I,XS(I),I=1,N)
      END IF
      STOP
*
99999 FORMAT (' Optimal Integer Value is = ',e20.8,/' Components are ',
     +       /(' x(',I3,') = ',F10.2))
99998 FORMAT (1X,A,I3)
      END
*
      SUBROUTINE QPHX(NSTATE,NCOLH,X,HX)
*
*     Routine to compute H*x. (In this version of QPHX, the Hessian
*     matrix H is not referenced explicitly.)
*
*     .. Parameters ..
      real             TWO
      PARAMETER        (TWO=2.0e+0)
*     .. Scalar Arguments ..
      INTEGER          NCOLH, NSTATE
*     .. Array Arguments ..
      real             HX(NCOLH), X(NCOLH)
*     .. Executable Statements ..
      HX(1) = TWO*X(1)
      HX(2) = TWO*X(2)
      HX(3) = TWO*(X(3)+X(4))
      HX(4) = HX(3)
      HX(5) = TWO*X(5)
      HX(6) = TWO*(X(6)+X(7))
      HX(7) = HX(6)
*
```

```
      END
*
      SUBROUTINE MONIT(INTFND,NODES,DEPTH,OBJ,X,BSTVAL,BSTSOL,BL,BU,N,
     +                 HALT,COUNT)
*     .. Parameters ..
      real             CUTOFF
      PARAMETER        (CUTOFF=-1847510.0e+0)
*     .. Scalar Arguments ..
      real             BSTVAL, OBJ
      INTEGER          COUNT, DEPTH, INTFND, N, NODES
      LOGICAL          HALT
*     .. Array Arguments ..
      real             BL(N), BSTSOL(N), BU(N), X(N)
*     .. Executable Statements ..
      IF (INTFND.EQ.0) BSTVAL = CUTOFF
*
      END
```

9.2 Program Data

```
H02CEF Example Program Data
 7  8            :Values of N and M
48  8  7  'C'  15 :Values of NNZ, IOBJ, NCOLH, START and NNAME
'        '  '        '  '        '  '        '  '        ' :End of NAMES
'...X1...'  '...X2...'  '...X3...'  '...X4...'  '...X5...'
'...X6...'  '...X7...'  '..ROW1..'  '..ROW2..'  '..ROW3..'
'..ROW4..'  '..ROW5..'  '..ROW6..'  '..ROW7..'  '..COST..' :End of CRNAME
    0.02   7   1
    0.02   5   1
    0.03   3   1
    1.00   1   1
    0.70   6   1
    0.02   4   1
    0.15   2   1
 -200.00   8   1
    0.06   7   2
    0.75   6   2
    0.03   5   2
    0.04   4   2
    0.05   3   2
    0.04   2   2
    1.00   1   2
-2000.00   8   2
    0.02   2   3
    1.00   1   3
    0.01   4   3
    0.08   3   3
    0.08   7   3
    0.80   6   3
-2000.00   8   3
    1.00   1   4
    0.12   7   4
    0.02   3   4
    0.02   4   4
    0.75   6   4
    0.04   2   4
-2000.00   8   4
```

```
    0.01   5   5
    0.80   6   5
    0.02   7   5
    1.00   1   5
    0.02   2   5
    0.06   3   5
    0.02   4   5
-2000.00   8   5
    1.00   1   6
    0.01   2   6
    0.01   3   6
    0.97   6   6
    0.01   7   6
  400.00   8   6
    0.97   7   7
    0.03   2   7
    1.00   1   7
  400.00   8   7                                                :End of matrix A
 0.0       0.0       4.0E+02   1.0E+02  0.0      0.0      0.0       2.0E+03
-1.0E+25  -1.0E+25  -1.0E+25  -1.0E+25  1.5E+03  2.5E+02 -1.0E+25 :End of BL
 2.0E+02   2.5E+03   8.0E+02   7.0E+02  1.5E+03  1.0E+25  1.0E+25   2.0E+03
 6.0E+01   1.0E+02   4.0E+01   3.0E+01  1.0E+25  3.0E+02  1.0E+25 :End of BU
 0    0    0    0    0    0    0    0   :End of ISTATE
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0 :End of XS
```

9.3 Program Results

```
H02CEF Example Program Results
Optimal Integer Value is =      -0.18475180E+07
Components are
x(  1) =       0.00
x(  2) =     355.00
x(  3) =     645.00
x(  4) =     164.00
x(  5) =     410.00
x(  6) =     275.00
x(  7) =     151.00
```

The remainder of this document is intended for more advanced users. Section 10 contains a detailed algorithm description that may be needed in order to understand Section 11 and Section 12. Section 11 describes the optional parameters that may be set by calls to H02CFF and/or H02CGF. Section 12 describes the quantities that can be requested to monitor the course of the computation.

10 Algorithmic Details

This section contains a description of the method used by H02CEF.

10.1 Overview

H02CEF employs a Branch and Bound technique (see Section 3) based on an inertia-controlling method to solve the sub-problems that maintains a Cholesky factorization of the reduced Hessian (see below). The method is similar to that of Gill and Murray [3], and is described in detail by Gill *et al.* [5]. Here we briefly summarize the main features of the method. Where possible, explicit reference is made to the names of variables that are parameters of the routine or appear in the printed output.

The method used has two distinct phases: finding an initial feasible point by minimizing the sum of infeasibilities (the *feasibility phase*), and minimizing the quadratic objective function within the feasible region (the *optimality phase*). The computations in both phases are performed by the same subroutines. The two-phase nature of the algorithm is reflected by changing the function being minimized from the sum of infeasibilities (the printed quantity `Sinf`; see Section 12) to the quadratic objective function (the printed quantity `Objective`; see Section 12).

In general, an iterative process is required to solve a quadratic program. Given an iterate (x, s) in both the original variables x and the slack variables s, a new iterate $(\bar{x}, \bar{s})$ is defined by

$$\begin{pmatrix} \bar{x} \\ \bar{s} \end{pmatrix} = \begin{pmatrix} x \\ s \end{pmatrix} + \alpha p, \tag{2}$$

where the *step length* α is a non-negative scalar (the printed quantity `Step`; see Section 12), and p is called the *search direction*. (For simplicity, we shall consider a typical iteration and avoid reference to the index of the iteration.) Once an iterate is feasible (i.e., satisfies the constraints), all subsequent iterates remain feasible.

10.2 Definition of the Working Set and Search Direction

At each iterate (x, s), a *working set* of constraints is defined to be a linearly independent subset of the constraints that are satisfied 'exactly' (to within the value of the optional parameter **Feasibility Tolerance**; see Section 11.2). The working set is the current prediction of the constraints that hold with equality at a solution of the LP or QP problem. Let m_W denote the number of constraints in the working set (including bounds), and let W denote the associated m_W by $(n + m)$ *working set matrix* consisting of the m_W gradients of the working set constraints.

The search direction is defined so that constraints in the working set remain *unaltered* for any value of the step length. It follows that p must satisfy the identity

$$Wp = 0. \tag{3}$$

This characterization allows p to be computed using any n by n_Z full-rank matrix Z that spans the null space of W. (Thus, $n_Z = n - m_W$ and $WZ = 0$.) The null space matrix Z is defined from a sparse LU factorization of part of W (see (6) and (7) below). The direction p will satisfy (3) if

$$p = Zp_Z, \tag{4}$$

where p_Z is any n_Z-vector.

The working set contains the constraints $Ax - s = 0$ and a subset of the upper and lower bounds on the variables (x, s). Since the gradient of a bound constraint $x_j \geq l_j$ or $x_j \leq u_j$ is a vector of all zeros except for ± 1 in position j, it follows that the working set matrix contains the rows of $(A - I)$ and the unit rows associated with the upper and lower bounds in the working set.

The working set matrix W can be represented in terms of a certain column partition of the matrix $(A - I)$. As in Section 3 we partition the constraints $Ax - s = 0$ so that

$$Bx_B + Sx_S + Nx_N = 0, \tag{5}$$

where B is a square non-singular basis and x_B, x_S and x_N are the basic, superbasic and nonbasic variables respectively. The nonbasic variables are equal to their upper or lower bounds at (x, s), and the superbasic variables are independent variables that are chosen to improve the value of the current objective function. The number of superbasic variables is n_S (the printed quantity `Ns`; see Section 12). Given values of x_N and x_S, the basic variables x_B are adjusted so that (x, s) satisfies (5).

If P is a permutation matrix such that $(A - I)P = (B \;\; S \;\; N)$, then the working set matrix W satisfies

$$WP = \begin{pmatrix} B & S & N \\ 0 & 0 & I_N \end{pmatrix}, \tag{6}$$

where I_N is the identity matrix with the same number of columns as N.

The null space matrix Z is defined from a sparse LU factorization of part of W. In particular, Z is maintained in 'reduced gradient' form, using the LUSOL package (see Gill *et al.*[6]) to maintain sparse

LU factors of the basis matrix B that alters as the working set W changes. Given the permutation P, the null space basis is given by

$$Z = P \begin{pmatrix} -B^{-1}S \\ I \\ 0 \end{pmatrix}. \tag{7}$$

This matrix is used only as an operator, i.e., it is never computed explicitly. Products of the form Zv and $Z^T g$ are obtained by solving with B or B^T. This choice of Z implies that n_Z, the number of 'degrees of freedom' at (x, s), is the same as n_S, the number of superbasic variables.

Let g_Z and H_Z denote the *reduced gradient* and *reduced Hessian* of the objective function:

$$g_Z = Z^T g \text{ and } H_Z = Z^T H Z, \tag{8}$$

where g is the objective gradient at (x, s). Roughly speaking, g_Z and H_Z describe the first and second derivatives of an n_S-dimensional *unconstrained* problem for the calculation of p_Z. (The condition estimator of H_Z is the quantity **Cond Hz** in the monitoring file output; see Section 12.)

At each iteration, an upper triangular factor R is available such that $H_Z = R^T R$. Normally, R is computed from $R^T R = Z^T H Z$ at the start of the optimality phase and then updated as the QP working set changes. For efficiency, the dimension of R should not be excessive (say, $n_S \leq 1000$). This is guaranteed if the number of nonlinear variables is 'moderate'.

If the QP problem contains linear variables, H is positive semi-definite and R may be singular with at least one zero diagonal element. However, an inertia-controlling strategy is used to ensure that only the last diagonal element of R can be zero. (See Gill *et al.* [5] for a discussion of a similar strategy for indefinite quadratic programming.)

If the initial R is singular, enough variables are fixed at their current value to give a non-singular R. This is equivalent to including temporary bound constraints in the working set. Thereafter, R can become singular only when a constraint is deleted from the working set (in which case no further constraints are deleted until R becomes non-singular).

10.3 The Main Iteration

If the reduced gradient is zero, (x, s) is a constrained stationary point on the working set. During the feasibility phase, the reduced gradient will usually be zero only at a vertex (although it may be zero elsewhere in the presence of constraint dependencies). During the optimality phase, a zero reduced gradient implies that x minimizes the quadratic objective function when the constraints in the working set are treated as equalities. At a constrained stationary point, Lagrange multipliers λ are defined from the equations

$$W^T \lambda = g(x). \tag{9}$$

A Lagrange multiplier λ_j corresponding to an inequality constraint in the working set is said to be *optimal* if $\lambda_j \leq \sigma$ when the associated constraint is at its *upper bound*, or if $\lambda_j \geq -\sigma$ when the associated constraint is at its *lower bound*, where σ depends on the value of the optional parameter **Optimality Tolerance** (see Section 11.2). If a multiplier is non-optimal, the objective function (either the true objective or the sum of infeasibilities) can be reduced by continuing the minimization with the corresponding constraint excluded from the working set. (This step is sometimes referred to as 'deleting' a constraint from the working set.) If optimal multipliers occur during the feasibility phase but the sum of infeasibilities is non-zero, there is no feasible point and the routine terminates immediately with IFAIL = 3 (see Section 6).

The special form (6) of the working set allows the multiplier vector λ, the solution of (9), to be written in terms of the vector

$$d = \begin{pmatrix} g \\ 0 \end{pmatrix} - (A - I)^T \pi = \begin{pmatrix} g - A^T \pi \\ \pi \end{pmatrix}, \tag{10}$$

where π satisfies the equations $B^T \pi = g_B$, and g_B denotes the basic elements of g. The elements of π are the Lagrange multipliers λ_j associated with the equality constraints $Ax - s = 0$. The vector d_N of nonbasic elements of d consists of the Lagrange multipliers λ_j associated with the upper and lower bound constraints in the working set. The vector d_S of superbasic elements of d is the reduced gradient g_Z in (8). The vector d_B of basic elements of d is zero, by construction. (The Euclidean norm of d_S and

the final values of d_S, g and π are the quantities **Norm rg**, **Reduced Gradnt**, **Obj Gradient** and **Dual Activity** in the monitoring file output; see Section 12.)

If the reduced gradient is not zero, Lagrange multipliers need not be computed and the search direction is given by $p = Zp_Z$ (see (7) and (11)). The step length is chosen to maintain feasibility with respect to the satisfied constraints.

There are two possible choices for p_Z, depending on whether or not H_Z is singular. If H_Z is non-singular, R is non-singular and p_Z in (4) is computed from the equations

$$R^T R p_Z = -g_Z, \tag{11}$$

where g_Z is the reduced gradient at x. In this case, $(x, s) + p$ is the minimizer of the objective function subject to the working set constraints being treated as equalities. If $(x, s)+p$ is feasible, α is defined to be unity. In this case, the reduced gradient at $(\bar{x}, \bar{s})$ will be zero, and Lagrange multipliers are computed at the next iteration. Otherwise, α is set to α_M, the step to the 'nearest' constraint along p. This constraint is added to the working set at the next iteration.

If H_Z is singular, then R must also be singular, and an inertia-controlling strategy is used to ensure that only the last diagonal element of R is zero. (See Gill *et al.* [5] for a discussion of a similar strategy for indefinite quadratic programming.) In this case, p_Z satisfies

$$p_Z^T H_Z p_Z = 0 \text{ and } g_Z^T p_Z \leq 0, \tag{12}$$

which allows the objective function to be reduced by any step of the form $(x, s) + \alpha p$, where $\alpha > 0$. The vector $p = Zp_Z$ is a direction of unbounded descent for the QP problem in the sense that the QP objective is linear and decreases without bound along p. If no finite step of the form $(x, s) + \alpha p$ (where $\alpha > 0$) reaches a constraint not in the working set, the QP problem is unbounded and the routine terminates immediately with IFAIL = 2 (see Section 6). Otherwise, α is defined as the maximum feasible step along p and a constraint active at $(x, s) + \alpha p$ is added to the working set for the next iteration.

10.4 Miscellaneous

If the basis matrix is not chosen carefully, the condition of the null space matrix Z in (7) could be arbitrarily high. To guard against this, the routine implements a 'basis repair' feature in which the LUSOL package (see Gill *et al.*[6]) is used to compute the rectangular factorization

$$(B \;\; S)^T = LU, \tag{13}$$

returning just the permutation P that makes PLP^T unit lower triangular. The pivot tolerance is set to require $|PLP^T|_{ij} \leq 2$, and the permutation is used to define P in (6). It can be shown that $||Z||$ is likely to be little more than unity. Hence, Z should be well-conditioned *regardless of the condition of* W. This feature is applied at the beginning of the optimality phase if a potential $B - S$ ordering is known.

The EXPAND procedure (see Gill *et al.* [4]) is used to reduce the possibility of cycling at a point where the active constraints are nearly linearly dependent. Although there is no absolute guarantee that cycling will not occur, the probability of cycling is extremely small (see Hall and McKinnon [7]). The main feature of EXPAND is that the feasibility tolerance is increased at the start of every iteration. This allows a positive step to be taken at every iteration, perhaps at the expense of violating the bounds on (x, s) by a small amount.

Suppose that the value of the optional parameter **Feasibility Tolerance** (see Section 11.2) is δ. Over a period of K iterations (where K is the value of the optional parameter **Expand Frequency**; see Section 11.2), the feasibility tolerance actually used by H02CEF (i.e., the *working* feasibility tolerance) increases from 0.5δ to δ (in steps of $0.5\delta/K$).

At certain stages the following 'resetting procedure' is used to remove small constraint infeasibilities. First, all nonbasic variables are moved exactly onto their bounds. A count is kept of the number of non-trivial adjustments made. If the count is non-zero, the basic variables are recomputed. Finally, the working feasibility tolerance is reinitialized to 0.5δ.

If a problem requires more than K iterations, the resetting procedure is invoked and a new cycle of iterations is started. (The decision to resume the feasibility phase or optimality phase is based on comparing any constraint infeasibilities with δ.)

The resetting procedure is also invoked when H02CEF reaches an apparently optimal, infeasible or unbounded solution, unless this situation has already occurred twice. If any non-trivial adjustments are made, iterations are continued.

The EXPAND procedure not only allows a positive step to be taken at every iteration, but also provides a potential *choice* of constraints to be added to the working set. All constraints at a distance α (where $\alpha \leq \alpha_M$) along p from the current point are then viewed as acceptable candidates for inclusion in the working set. The constraint whose normal makes the largest angle with the search direction is added to the working set. This strategy helps keep the basis matrix B well-conditioned.

11 Optional Parameters

Several optional parameters in H02CEF define choices in the problem specification or the algorithm logic. In order to reduce the number of formal parameters of H02CEF these optional parameters have associated *default values* that are appropriate for most problems. Therefore, the user need only specify those optional parameters whose values are to be different from their default values.

The remainder of this section can be skipped by users who wish to use the default values for *all* optional parameters. A complete list of optional parameters and their default values is given in Section 11.1.

Optional parameters may be specified by calling one, or both, of the routines H02CFF and H02CGF prior to a call to H02CEF.

H02CFF reads options from an external options file, with **Begin** and **End** as the first and last lines respectively and each intermediate line defining a single optional parameter. For example,

```
Begin
  Print Level = 5
End
```

The call

```
CALL H02CFF (IOPTNS, INFORM)
```

can then be used to read the file on unit IOPTNS. INFORM will be zero on successful exit. H02CFF should be consulted for a full description of this method of supplying optional parameters.

H02CGF can be called to supply options directly, one call being necessary for each optional parameter. For example,

```
CALL H02CGF ('Print Level = 5')
```

H02CGF should be consulted for a full description of this method of supplying optional parameters.

All optional parameters not specified by the user are set to their default values. Optional parameters specified by the user are unaltered by H02CEF (unless they define invalid values) and so remain in effect for subsequent calls unless altered by the user.

11.1 Optional Parameter Checklist and Default Values

For easy reference, the following list shows all the valid keywords and their default values. The symbol ϵ represents the ***machine precision*** (see X02AJF).

Optional Parameters	**Default Values**
Check frequency	60
Crash option	2
Crash tolerance	0.1
Defaults	
Expand frequency	10000
Factorization frequency	100

Feasibility tolerance	$\max(10^{-6}, \sqrt{\epsilon})$
Infinite bound size	10^{20}
Infinite step size	$\max(bigbnd, 10^{20})$
Iteration limit	$\max(50, 5(n+m))$
List/Nolist	**List**
LU factor tolerance	100.0
LU singularity tolerance	$\epsilon^{0.67}$
LU update tolerance	10.0
Maximize/Minimize	**Minimize**
Monitoring file	-1
Optimality tolerance	$\max(10^{-6}, \sqrt{\epsilon})$
Partial price	10
Pivot tolerance	$\epsilon^{0.67}$
Print level	10
Scale option	2
Scale tolerance	0.9
Superbasics limit	$\min(n_H + 1, n)$
Rank tolerance	100ϵ

11.2 Description of the Optional Parameters

The following list (in alphabetical order) gives the valid options. For each option, we give the keyword, any essential optional qualifiers, the default value, and the definition. The minimum abbreviation of each keyword is underlined. If no characters of an optional qualifier are underlined, the qualifier may be omitted. The letters i and r denote INTEGER and ***real*** values required with certain options. The default value of an option is used whenever the condition $|i| \geq 100000000$ is satisfied. The number ϵ is a generic notation for ***machine precision*** (see X02AJF).

Check Frequency i Default = 60

Every ith iteration after the most recent basis factorization, a numerical test is made to see if the current solution (x, s) satisfies the linear constraints $Ax - s = 0$. If the largest element of the residual vector $r = Ax - s$ is judged to be too large, the current basis is refactorized and the basic variables recomputed to satisfy the constraints more accurately. If $i < 0$, the default value is used. If $i = 0$, the value $i = 99999999$ is used and effectively no checks are made.

Crash Option i Default = 2

Note that this option does not apply when START = 'W' (see Section 5).

If START = 'C', an internal crash procedure is used to select an initial basis from various rows and columns of the constraint matrix $(A - I)$. The value of i determines which rows and columns are initially eligible for the basis, and how many times the crash procedure is called. If $i = 0$, the all-slack basis $B = -I$ is chosen. If $i = 1$, the crash procedure is called once (looking for a triangular basis in all rows and columns of the linear constraint matrix A). If $i = 2$, the crash procedure is called twice (looking at any *equality* constraints first followed by any *inequality* constraints). If $i < 0$ or $i > 2$, the default value is used.

If $i = 1$ or 2, certain slacks on inequality rows are selected for the basis first. (If $i = 2$, numerical values are used to exclude slacks that are close to a bound.) The crash procedure then makes several passes through the columns of A, searching for a basis matrix that is essentially triangular. A column is assigned to 'pivot' on a particular row if the column contains a suitably large element in a row that has not yet been assigned. (The pivot elements ultimately form the diagonals of the triangular basis.) For remaining unassigned rows, slack variables are inserted to complete the basis.

Crash Tolerance r Default = 0.1

This value allows the crash procedure to ignore certain 'small' non-zero elements in the constraint matrix A while searching for a triangular basis. For each column of A, if a_{max} is the largest element in the column, other non-zeros in that column are ignored if they are less than (or equal to) $a_{max} \times r$.

When $r > 0$, the basis obtained by the crash procedure may not be strictly triangular, but it is likely to be non-singular and almost triangular. The intention is to obtain a starting basis with more column

variables and fewer (arbitrary) slacks. A feasible solution may be reached earlier for some problems. If $r < 0$ or $r \geq 1$, the default value is used.

Defaults

This special keyword may be used to reset all optional parameters to their default values.

Expand Frequency i Default = 10000

This option is part of an anti-cycling procedure (see Section 10.4) designed to allow progress even on highly degenerate problems.

For LP problems, the strategy is to force a positive step at every iteration, at the expense of violating the constraints by a small amount. Suppose that the value of the optional parameter **Feasibility Tolerance** is δ. Over a period of i iterations, the feasibility tolerance actually used by H02CEF (i.e., the *working* feasibility tolerance) increases from 0.5δ to δ (in steps of $0.5\delta/i$).

For QP problems, the same procedure is used for iterations in which there is only one superbasic variable. (Cycling can only occur when the current solution is at a vertex of the feasible region.) Thus, zero steps are allowed if there is more than one superbasic variable, but otherwise positive steps are enforced.

Increasing the value of i helps reduce the number of slightly infeasible nonbasic basic variables (most of which are eliminated during the resetting procedure). However, it also diminishes the freedom to choose a large pivot element (see **Pivot Tolerance** below).

If $i < 0$, the default value is used. If $i = 0$, the value $i = 99999999$ is used and effectively no anti-cycling procedure is invoked.

Factorization Frequency i Default = 100

If $i > 0$, at most i basis changes will occur between factorizations of the basis matrix. For LP problems, the basis factors are usually updated at every iteration. For QP problems, fewer basis updates will occur as the solution is approached. The number of iterations between basis factorizations will therefore increase. During these iterations a test is made regularly according to the value of **Check Frequency** (see above) to ensure that the linear constraints $Ax - s = 0$ are satisfied. If necessary, the basis will be refactorized before the limit of i updates is reached. If $i \leq 0$, the default value is used.

Feasibility Tolerance r Default = $\max(10^{-6}, \sqrt{\epsilon})$

If $r \geq \epsilon$, r defines the maximum acceptable *absolute* violation in each constraint at a 'feasible' point (including slack variables). For example, if the variables and the coefficients in the linear constraints are of order unity, and the latter are correct to about 5 decimal digits, it would be appropriate to specify r as 10^{-5}. If $r < \epsilon$, the default value is used.

H02CEF attempts to find a feasible solution before optimizing the objective function. If the sum of infeasibilities cannot be reduced to zero, the problem is assumed to be *infeasible*. Let **Sinf** be the corresponding sum of infeasibilities. If **Sinf** is quite small, it may be appropriate to raise r by a factor of 10 or 100. Otherwise, some error in the data should be suspected. Note that the routine does *not* attempt to find the minimum value of **Sinf**.

If the constraints and variables have been scaled (see **Scale Option** below), then feasibility is defined in terms of the scaled problem (since it is more likely to be meaningful).

Infinite Bound Size r Default = 10^{20}

If $r > 0$, r defines the 'infinite' bound *bigbnd* in the definition of the problem constraints. Any upper bound greater than or equal to *bigbnd* will be regarded as plus infinity (and similarly any lower bound less than or equal to $-$*bigbnd* will be regarded as minus infinity). If $r \leq 0$, the default value is used.

Infinite Step Size r Default = $\max(bigbnd, 10^{20})$

If $r > 0$, r specifies the magnitude of the change in variables that will be considered a step to an unbounded solution. (Note that an unbounded solution can occur only when the Hessian is not positive-definite.) If the change in x during an iteration would exceed the value of r, the objective function is considered to be unbounded below in the feasible region. If $r \leq 0$, the default value is used.

Iteration Limit i Default = $\max(50, 5(n+m))$

Iters

Itns

The value of i specifies the maximum number of iterations allowed before termination. Setting $i = 0$ and **Print Level** > 0 means that the workspace needed to start solving the problem will be computed and printed, but no iterations will be performed. If $i < 0$, the default value is used.

List Default = **List**

Nolist

Normally each optional parameter specification is printed as it is supplied. **Nolist** may be used to suppress the printing and **List** may be used to restore printing.

LU Factor Tolerance r_1 Default = 100.0

LU Update Tolerance r_2 Default = 10.0

The values of r_1 and r_2 affect the stability and sparsity of the basis factorization $B = LU$, during refactorization and updates respectively. The lower triangular matrix L is a product of matrices of the form

$$\begin{pmatrix} 1 & \\ \mu & 1 \end{pmatrix}$$

where the multipliers μ will satisfy $|\mu| \leq r_i$. The default values of r_1 and r_2 usually strike a good compromise between stability and sparsity. For large and relatively dense problems, setting r_1 and r_2 to 25 (say) may give a marked improvement in sparsity without impairing stability to a serious degree. Note that for band matrices it may be necessary to set r_1 in the range $1 \leq r_1 < 2$ in order to achieve stability. If $r_1 < 1$ or $r_2 < 1$, the default value is used.

LU Singularity Tolerance r Default = $\epsilon^{0.67}$

If $r > 0$, r defines the singularity tolerance used to guard against ill-conditioned basis matrices. Whenever the basis is refactorized, the diagonal elements of U are tested as follows. If $|u_{jj}| \leq r$ or $|u_{jj}| < r \times \max_i |u_{ij}|$, the jth column of the basis is replaced by the corresponding slack variable. If $r \leq 0$, the default value is used.

Maximize Default = **Minimize**

Minimize

This option specifies the required direction of the optimization. It applies to both linear and nonlinear terms (if any) in the objective function. Note that if two problems are the same except that one minimizes $f(x)$ and the other maximizes $-f(x)$, their solutions will be the same but the signs of the dual variables π_i and the reduced gradients d_j (see Section 10.3) will be reversed.

Monitoring File i Default = -1

If $i \geq 0$ and **Print Level** > 0 (see below), monitoring information produced by H02CEF is sent to a file with logical unit number i. If $i < 0$ and/or **Print Level** $= 0$, the default value is used and hence no monitoring information is produced.

Optimality Tolerance r Default = $\max(10^{-6}, \sqrt{\epsilon})$

If $r \geq \epsilon$, r is used to judge the size of the reduced gradients $d_j = g_j - \pi^T a_j$. By definition, the reduced gradients for basic variables are always zero. Optimality is declared if the reduced gradients for any nonbasic variables at their lower or upper bounds satisfy $-r \times \max(1, \| \pi \|) \leq d_j \leq r \times \max(1, \| \pi \|)$, and if $|d_j| \leq r \times \max(1, \| \pi \|)$ for any superbasic variables. If $r < \epsilon$, the default value is used.

Partial Price i Default = 10

Note that this option does not apply to QP problems.

This option is recommended for large FP or LP problems that have significantly more variables than constraints (i.e., $n \gg m$). It reduces the work required for each pricing operation (i.e., when a nonbasic variable is selected to enter the basis). If $i = 1$, all columns of the constraint matrix $(A - I)$ are searched. If $i > 1$, A and $-I$ are partitioned to give i roughly equal segments A_j, K_j, for $j = 1, 2, \ldots, p$ (modulo p). If the previous pricing search was successful on A_{j-1}, K_{j-1}, the next search begins on the segments

A_j, K_j. If a reduced gradient is found that is larger than some dynamic tolerance, the variable with the largest such reduced gradient (of appropriate sign) is selected to enter the basis. If nothing is found, the search continues on the next segments A_{j+1}, K_{j+1}, and so on. If $i \leq 0$, the default value is used.

Pivot Tolerance r Default = $\epsilon^{0.67}$

If $r > 0$, r is used to prevent columns entering the basis if they would cause the basis to become almost singular. If $r \leq 0$, the default value is used.

Print Level i Default = 10

The value of i controls the amount of printout produced by H02CEF, as indicated below. A detailed description of the printed output is given in Section 8.1 (summary output at each iteration and the final solution) and Section 12 (monitoring information at each iteration). Note that the summary output will not exceed 80 characters per line and that the monitoring information will not exceed 120 characters per line. If $i < 0$, the default value is used. The following printout is sent to the current advisory message unit (as defined by X04ABF):

i	**Output**
0	No output.
1	The final solution only.
5	One line of summary output for each iteration (no printout of the final solution).
≥ 10	The final solution and one line of summary output for each iteration.

The following printout is sent to the logical unit number defined by the optional parameter **Monitoring File** (see above):

i	**Output**
0	No output.
1	The final solution only.
5	One long line of output for each iteration (no printout of the final solution).
≥ 10	The final solution and one long line of output for each iteration.
≥ 20	The final solution, one long line of output for each iteration, matrix statistics (initial status of rows and columns, number of elements, density, biggest and smallest elements, etc.), details of the scale factors resulting from the scaling procedure (if **Scale Option** = 1 or 2; see below), basis factorization statistics and details of the initial basis resulting from the crash procedure (if START = 'C'; see Section 5).

If **Print Level** > 0 and the unit number defined by **Monitoring File** is the same as that defined by X04ABF, then the summary output is suppressed.

Scale Option i Default = 2

This option enables you to scale the variables and constraints using an iterative procedure due to Fourer (see [8]), which attempts to compute row scales r_i and column scales c_j such that the scaled matrix coefficients $\bar{a}_{ij} = a_{ij} \times (c_j/r_i)$ are as close as possible to unity. This may improve the overall efficiency of the routine on some problems. (The lower and upper bounds on the variables and slacks for the scaled problem are redefined as $\bar{l}_j = l_j/c_j$ and $\bar{u}_j = u_j/c_j$ respectively, where $c_j \equiv r_{j-n}$ if $j > n$.)

If $i = 0$, no scaling is performed. If $i = 1$, all rows and columns of the constraint matrix A are scaled. If $i = 2$, an additional scaling is performed that may be helpful when the solution x is large; it takes into account columns of $(A - I)$ that are fixed or have positive lower bounds or negative upper bounds. If $i < 0$ or $i > 2$, the default value is used.

Scale Tolerance r Default = 0.9

Note that this option does not apply when **Scale Option** = 0 (see above).

If $0 < r < 1$, r is used to control the number of scaling passes to be made through the constraint matrix A. At least 3 (and at most 10) passes will be made. More precisely, let a_p denote the largest column ratio (i.e., 'biggest' element/'smallest' element in some sense) after the pth scaling pass through A. The scaling procedure is terminated if $a_p \geq a_{p-1} \times r$ for some $p \geq 3$. Thus, increasing the value of r from 0.9 to 0.99 (say) will probably increase the number of passes through A. If $r \leq 0$ or $r \geq 1$, the default value is used.

Superbasics Limit i Default = $\min(n_H + 1, n)$

Note that this option does not apply to FP or LP problems.

The value of i specifies 'how nonlinear' you expect the QP problem to be. If $i \leq 0$, the default value is used.

12 Description of Monitoring Information

This section describes the intermediate printout and final printout which constitutes the monitoring information produced by H02CEF. (See also the description of the optional parameters **Monitoring File** and **Print Level** in Section 11.2). The level of printed output can be controlled by the user.

When **Print Level** = 5 or ≥ 10 and **Monitoring File**≥ 0, the following line of intermediate printout (< 120 characters) is produced at every iteration on the unit number specified by **Monitoring File**. Unless stated otherwise, the values of the quantities printed are those in effect *on completion* of the given iteration.

`Itn` is the iteration count.

`pp` is the partial price indicator. The variable selected by the last pricing operation came from the pp-th partition of A and $-I$. Note that pp is reset to zero whenever the basis is refactorized.

`dj` is the value of the reduced gradient (or reduced cost) for the variable selected by the pricing operation at the start of the current iteration.

`+S` is the variable selected by the pricing operation to be added to the superbasic set.

`-S` is the variable chosen to leave the superbasic set.

`-B` is the variable removed from the basis (if any) to become nonbasic.

`-B` is the variable chosen to leave the set of basics (if any) in a special basic $\leftrightarrow$ superbasic swap. The entry under `-S` has become basic if this entry is non-zero, and nonbasic otherwise. The swap is done to ensure that there are no superbasic slacks.

`Step` is the value of the step length α taken along the computed search direction p. The variables x have been changed to $x + \alpha p$. If a variable is made superbasic during the current iteration (i.e., `+S` is positive), `Step` will be the step to the nearest bound. During the optimality phase, the step can be greater than unity only if the reduced Hessian is not positive-definite.

`Pivot` is the rth element of a vector y satisfying $By = a_q$ whenever a_q (the qth column of the constraint matrix $(A - I)$) replaces the rth column of the basis matrix B. Wherever possible, `Step` is chosen so as to avoid extremely small values of `Pivot` (since they may cause the basis to be nearly singular). In extreme cases, it may be necessary to increase the value of the optional parameter **Pivot Tolerance** (default value = $\epsilon^{0.67}$, where ϵ is the ***machine precision***; see Section 11.2) to exclude very small elements of y from consideration during the computation of `Step`.

`Ninf` is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.

`Sinf/Objective` is the value of the current objective function. If x is not feasible, `Sinf` gives the sum of the magnitudes of constraint violations. If x is feasible, `Objective` is the value of the objective function. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which `Ninf` is zero) will give the value of the true objective at the first feasible point. During the optimality phase, the value of the objective function will be non-increasing. During the feasibility phase, the number of constraint infeasibilities will not increase until either a feasible point is found, or the optimality of the multipliers implies that no feasible point exists.

`L` is the number of non-zeros in the basis factor L. Immediately after a basis factorization $B = LU$, this is `lenL`, the number of subdiagonal elements in the columns of a lower triangular matrix. Further non-zeros are added to `L` when various columns of B are later replaced. (Thus, `L` increases monotonically.)

`U` is the number of non-zeros in the basis factor U. Immediately after a basis factorization, this is `lenU`, the number of diagonal and superdiagonal elements in the rows of an upper triangular matrix. As columns of B are replaced, the matrix U is maintained explicitly (in sparse form). The value of `U` may fluctuate up or down; in general, it will tend to increase.

`Ncp` is the number of compressions required to recover workspace in the data structure for U. This includes the number of compressions needed during the previous basis factorization. Normally, `Ncp` should increase very slowly. If it does not, increase LENZ by at least `L + U` and rerun H02CEF (possibly using START = 'W'; see Section 5).

`Norm rg` is $\|d_S\|$, the Euclidean norm of the reduced gradient (see Section 10.3) at the start of the current iteration. During the optimality phase, this norm will be approximately zero after a unit step. For FP and LP problems, **Norm rg** is not printed.

`Ns` is the current number of superbasic variables. For FP and LP problems, **Ns** is not printed.

`Cond Hz` is a lower bound on the condition number of the reduced Hessian (see Section 10.2). The larger this number, the more difficult the problem. For FP and LP problems, **Cond Hz** is not printed.

When **Print Level** ≥ 20 and **Monitoring File** ≥ 0, the following lines of intermediate printout (< 120 characters) are produced on the unit number specified by **Monitoring File** whenever the matrix B or $B_S = (B \;\; S)^T$ is factorized. Gaussian elimination is used to compute an LU factorization of B or B_S, where PLP^T is a lower triangular matrix and PUQ is an upper triangular matrix for some permutation matrices P and Q. The factorization is stabilized in the manner described under the optional parameter **LU Factor Tolerance** (default value = 100.0; see Section 11.2).

`Factorize` is the factorization count.

`Demand` is a code giving the reason for the present factorization as follows:

Code	Meaning
0	First LU factorization.
1	Number of updates reached the value of the optional parameter **Factorization Frequency** (default value = 100; see Section 11.2).
2	Excessive non-zeros in updated factors.
7	Not enough storage to update factors.
10	Row residuals too large (see the description for the optional parameter **Check Frequency** in Section 11.2).
11	Ill-conditioning has caused inconsistent results.

`Iteration` is the iteration count.

`Nonlinear` is the number of nonlinear variables in B (not printed if B_S is factorized).

`Linear` is the number of linear variables in B (not printed if B_S is factorized).

`Slacks` is the number of slack variables in B (not printed if B_S is factorized).

`Elems` is the number of non-zeros in B (not printed if B_S is factorized).

`Density` is the percentage non-zero density of B (not printed if B_S is factorized). More precisely, **Density** $= 100\times$ **Elems**/(**Nonlinear** + **Linear** + **Slacks**)^2.

`Compressns` is the number of times the data structure holding the partially factorized matrix needed to be compressed, in order to recover unused workspace. Ideally, it should be zero. If it is more than 3 or 4, increase LENIZ and LENZ and rerun H02CEF (possibly using START = 'W'; see Section 5).

`Merit` is the average Markowitz merit count for the elements chosen to be the diagonals of PUQ. Each merit count is defined to be $(c-1)(r-1)$, where c and r are the number of non-zeros in the column and row containing the element at the time it is selected to be the next diagonal. **Merit** is the average of **m** such quantities. It gives an indication of how much work was required to preserve sparsity during the factorization.

`lenL` is the number of non-zeros in L.

`lenU` is the number of non-zeros in U.

`Increase` is the percentage increase in the number of non-zeros in L and U relative to the number of non-zeros in B. More precisely, `Increase` = $100 \times$ (`lenL` + `lenU` − `Elems`)/`Elems`.

`m` is the number of rows in the problem. Note that `m` = `Ut` + `Lt` + `bp`.

`Ut` is the number of triangular rows of B at the top of U.

`d1` is the number of columns remaining when the density of the basis matrix being factorized reached 0.3.

`Lmax` is the maximum subdiagonal element in the columns of L (not printed if B_S is factorized). This will not exceed the value of the **LU Factor Tolerance**.

`Bmax` is the maximum non-zero element in B (not printed if B_S is factorized).

`BSmax` is the maximum non-zero element in B_S (not printed if B is factorized).

`Umax` is the maximum non-zero element in U, excluding elements of B that remain in U unchanged. (For example, if a slack variable is in the basis, the corresponding row of B will become a row of U without modification. Elements in such rows will not contribute to `Umax`. If the basis is strictly triangular, *none* of the elements of B will contribute, and `Umax` will be zero.)
Ideally, `Umax` should not be significantly larger than `Bmax`. If it is several orders of magnitude larger, it may be advisable to reset the **LU Factor Tolerance** to a value near 1.0.
`Umax` is not printed if B_S is factorized.

`Umin` is the magnitude of the smallest diagonal element of PUQ (not printed if B_S is factorized).

`Growth` is the value of the ratio `Umax`/`Bmax`, which should not be too large.
Providing `Lmax` is not large (say < 10.0), the ratio max(`Bmax`, `Umax`)/`Umin` is an estimate of the condition number of B. If this number is extremely large, the basis is nearly singular and some numerical difficulties could occur in subsequent computations. (However, an effort is made to avoid near singularity by using slacks to replace columns of B that would have made `Umin` extremely small, and the modified basis is refactorized.)
`Growth` is not printed if B_S is factorized.

`Lt` is the number of triangular columns of B at the beginning of L.

`bp` is the size of the 'bump' or block to be factorized nontrivially after the triangular rows and columns have been removed.

`d2` is the number of columns remaining when the density of the basis matrix being factorized reached 0.6.

When **Print Level** ≥ 20 and **Monitoring File** ≥ 0, the following lines of intermediate printout (< 80 characters) are produced on the unit number specified by **Monitoring File** whenever START = 'C' (see Section 5). They refer to the number of columns selected by the crash procedure during each of several passes through A, whilst searching for a triangular basis matrix.

`Slacks` is the number of slacks selected initially.

`Free cols` is the number of free columns in the basis.

`Preferred` is the number of 'preferred' columns in the basis (i.e., ISTATE(j) = 3 for some $j \leq n$).

`Unit` is the number of unit columns in the basis.

`Double` is the number of double columns in the basis.

`Triangle` is the number of triangular columns in the basis.

`Pad` is the number of slacks used to pad the basis.

When **Print Level** ≥ 20 and **Monitoring File** ≥ 0, the following lines of intermediate printout (< 80 characters) are produced on the unit number specified by **Monitoring File**. They refer to the elements of the NAMES array (see Section 5).

`Name` gives the name for the problem (blank if none).

`Status` gives the exit status for the problem (i.e., `Optimal soln`, `Weak soln`, `Unbounded`, `Infeasible`, `Excess itns`, `Error condn` or `Feasble soln`) followed by details of the direction of the optimization (i.e., `(Min)` or `(Max)`).

`Objective`	gives the name of the free row for the problem (blank if none).
`RHS`	gives the name of the constraint right-hand side for the problem (blank if none).
`Ranges`	gives the name of the ranges for the problem (blank if none).
`Bounds`	gives the name of the bounds for the problem (blank if none).

When **Print Level** = 1 or $\geq$ 10 and **Monitoring File** $\geq$ 0, the following lines of final printout (< 120 characters) are produced on the unit number specified by **Monitoring File**.

Let a_j denote the jth column of A, for $j = 1, 2, \ldots, n$. The following describes the printout for each column (or variable). A full stop (.) is printed for any numerical value that is zero.

`Number`	is the column number j. (This is used internally to refer to x_j in the intermediate output.)
`Column`	gives the name of x_j.
`State`	gives the state of x_j (`LL` if nonbasic on its lower bound, `UL` if nonbasic on its upper bound, `EQ` if nonbasic and fixed, `FR` if nonbasic and strictly between its bounds, `BS` if basic and `SBS` if superbasic).

A key is sometimes printed before `State` to give some additional information about the state of x_j. Note that unless the optional paramter **Scale Option** = 0 (default value = 2; see Section 11.2) is specified, the tests for assigning a key are applied to the variables of the scaled problem.

`A`	*Alternative optimum possible.* x_j is nonbasic, but its reduced gradient is essentially zero. This means that if x_j were allowed to start moving away from its bound, there would be no change in the value of the objective function. The values of the basic and superbasic variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled `D`), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the Lagrange multipliers *might* also change.
`D`	*Degenerate.* x_j is basic or superbasic, but it is equal to (or very close to) one of its bounds.
`I`	*Infeasible.* x_j is basic or superbasic and is currently violating one of its bounds by more than the value of the optional parameter **Feasibility Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$, where ϵ is the ***machine precision***; see Section 11.2).
`N`	*Not precisely optimal.* x_j is nonbasic or superbasic. If the value of the reduced gradient for x_j exceeds the value of the optional parameter **Optimality Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$), the solution would not be declared optimal because the reduced gradient for x_j would not be considered negligible.

`Activity`	is the value of x_j at the final iterate.
`Obj Gradient`	is the value of g_j at the final iterate. For FP problems, g_j is set to zero.
`Lower Bound`	is the lower bound specified for x_j. **None** indicates that $\mathrm{BL}(j) \leq -bigbnd$.
`Upper Bound`	is the upper bound specified for x_j. **None** indicates that $\mathrm{BU}(j) \geq bigbnd$.
`Reduced Gradnt`	is the value of d_j at the final iterate (see Section 10.3). For FP problems, d_j is set to zero.
`m + j`	is the value of $m + j$.

Let v_i denote the ith row of A, for $i = 1, 2, \ldots, m$. The following describes the printout for each row (or constraint). A full stop (.) is printed for any numerical value that is zero.

`Number`	is the value of $n + i$. (This is used internally to refer to s_i in the intermediate output.)
`Row`	gives the name of v_i.
`State`	gives the state of v_i (`LL` if active on its lower bound, `UL` if active on its upper bound, `EQ` if active and fixed, `BS` if inactive when s_i is basic and `SBS` if inactive when s_i is superbasic).

A key is sometimes printed before **State** to give some additional information about the state of s_i. Note that unless the optional parameter **Scale Option** = 0 (default value = 2; see Section 11.2) is specified, the tests for assigning a key are applied to the variables of the scaled problem.

- **A** *Alternative optimum possible.* s_i is nonbasic, but its reduced gradient is essentially zero. This means that if s_i were allowed to start moving away from its bound, there would be no change in the value of the objective function. The values of the basic and superbasic variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled **D**), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the dual variables (or Lagrange multipliers) *might* also change.
- **D** *Degenerate.* s_i is basic or superbasic, but it is equal to (or very close to) one of its bounds.
- **I** *Infeasible.* s_i is basic or superbasic and is currently violating one of its bounds by more than the value of the optional parameter **Feasibility Tolerance** (default value = 10^{-6}; see Section 11.2).
- **N** *Not precisely optimal.* s_i is nonbasic or superbasic. If the value of the reduced gradient for s_i exceeds the value of the optional parameter **Optimality Tolerance** (default value = $\max(10^{-6}, \sqrt{\epsilon})$), the solution would not be declared optimal because the reduced gradient for s_i would not be considered negligible.

Activity is the value of v_i at the final iterate.

Slack Activity is the value by which v_i differs from its nearest bound. (For the free row (if any), it is set to **Activity**.)

Lower Bound is the lower bound specified for v_i. **None** indicates that $\mathrm{BL}(n+j) \leq -bigbnd$.

Upper Bound is the upper bound specified for v_i. **None** indicates that $\mathrm{BU}(n+j) \geq bigbnd$.

Dual Activity is the value of the dual variable π_i (the Lagrange multiplier for v_i; see Section 10.3). For FP problems, π_i is set to zero.

i gives the index i of v_i.

Numerical values are output with a fixed number of digits; they are not guaranteed to be accurate to this precision.

H02CFF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

To supply optional parameters to H02CEF from an external file.

2 Specification

```
SUBROUTINE H02CFF(IOPTNS, INFORM)
INTEGER           IOPTNS, INFORM
```

3 Description

H02CFF may be used to supply values for optional parameters to H02CEF. H02CFF reads an external file and each line of the file defines a single optional parameter. It is only necessary to supply values for those parameters whose values are to be different from their default values.

Each optional parameter is defined by a single character string of up to 72 characters, consisting of one or more items. The items associated with a given option must be separated by spaces, or equal signs [=]. Alphabetic characters may be upper or lower case. The string

```
Print level = 1
```

is an example of a string used to set an optional parameter. For each option the string contains one or more of the following items:

(a) a mandatory keyword;
(b) a phrase that qualifies the keyword;
(c) a number that specifies an INTEGER or ***real*** value. Such numbers may be up to 16 contiguous characters in Fortran 77's I, F, E or D formats, terminated by a space if this is not the last item on the line.

Blank strings and comments are ignored. A comment begins with an asterisk (*) and all subsequent characters in the string are regarded as part of the comment.

The file containing the options must start with **begin** and must finish with **end**. An example of a valid options file is:

```
Begin * Example options file
 Print Level = 1
End
```

Normally each line of the file is printed as it is read, on the current advisory message unit (see X04ABF), but printing may be suppressed using the keyword **nolist**. To suppress printing of **begin**, **nolist** must be the first option supplied as in the file:

```
Begin
 Nolist
 Print Level = 1
End
```

Printing will automatically be turned on again after a call to H02CEF and may be turned on again at any time using the keyword **list**.

Optional parameter settings are preserved following a call to H02CEF, and so the keyword **defaults** is provided to allow the user to reset all the optional parameters to their default values prior to a subsequent call to H02CEF.

A complete list of optional parameters, their abbreviations, synonyms and default values is given in Section 11 of the document for H02CEF.

4 References

None.

5 Parameters

1: IOPTNS — INTEGER *Input*

On entry: the unit number of the options file to be read.

Constraint: $0 \leq \text{IOPTNS} \leq 99$.

2: INFORM — INTEGER *Output*

On exit: contains zero if the options file has been successfully read and a value > 0 otherwise, as indicated below.

INFORM = 1

IOPTNS is not in the range $[0, 99]$.

INFORM = 2

begin was found, but end-of-file was found before **end** was found.

INFORM = 3

end-of-file was found before **begin** was found.

6 Error Indicators and Warnings

If a line is not recognized as a valid option, then a warning message is output on the current advisory message unit (see X04ABF).

7 Accuracy

Not applicable.

8 Further Comments

H02CGF may also be used to supply optional parameters to H02CEF. Note that if E04NKF is used in the same program as H02CEF, then in general H02CFF will also affect the options used by E04NKF.

9 Example

This example solves the same problem as the example for H02CEF, but in addition illustrates the use of H02CFF and H02CGF to set optional parameters for H02CEF.

In this example the options file read by H02CFF is appended to the data file for the program (see Section 9.2). It would usually be more convenient in practice to keep the data file and the options file separate.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H02CFF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT
```

```
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX, NNZMAX, LENIZ, LENZ, LINTVR, MM
      PARAMETER        (NMAX=100,MMAX=100,NNZMAX=100,LENIZ=100000,
     +                 LENZ=100000,LINTVR=10,MM=2000)
*     .. Local Scalars ..
      real             OBJ
      INTEGER          I, ICOL, IFAIL, INFORM, IOBJ, J, JCOL, M, MINIZ,
     +                 MINZ, N, NCOLH, NNAME, NNZ, NS, STRTGY
      CHARACTER        START
*     .. Local Arrays ..
      real             A(NNZMAX), BL(NMAX+MMAX), BU(NMAX+MMAX),
     +                 CLAMDA(NMAX+MMAX), XS(NMAX+MMAX), Z(LENZ)
      INTEGER          HA(NNZMAX), INTVAR(LINTVR), ISTATE(NMAX+MMAX),
     +                 IZ(LENIZ), KA(NMAX+1)
      CHARACTER*8      CRNAME(NMAX+MMAX), NAMES(5)
*     .. External Subroutines ..
      EXTERNAL         H02CEF, H02CFF, H02CGF, MONIT, QPHX, X04ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H02CFF Example Program Results'
*     Skip heading in data file.
      READ (NIN,*)
      READ (NIN,*) N, M
      IF (N.LE.NMAX .AND. M.LE.MMAX) THEN
*
*        Read NNZ, IOBJ, NCOLH, START and NNAME from data file.
*
         READ (NIN,*) NNZ, IOBJ, NCOLH, START, NNAME
*
*        Read NAMES and CRNAME from data file.
*
         READ (NIN,*) (NAMES(I),I=1,5)
         READ (NIN,*) (CRNAME(I),I=1,NNAME)
*
*        Read the matrix A from data file. Set up KA.
*
         JCOL = 1
         KA(JCOL) = 1
         DO 40 I = 1, NNZ
*
*           Element ( HA( I ), ICOL ) is stored in A( I ).
*
            READ (NIN,*) A(I), HA(I), ICOL
*
            IF (ICOL.EQ.JCOL+1) THEN
*
*              Index in A of the start of the ICOL-th column equals I.
*
               KA(ICOL) = I
               JCOL = ICOL
            ELSE IF (ICOL.GT.JCOL+1) THEN
*
*              Index in A of the start of the ICOL-th column equals I,
*              but columns JCOL+1,JCOL+2,...,ICOL-1 are empty. Set the
*              corresponding elements of KA to I.
*
               DO 20 J = JCOL + 1, ICOL - 1
                  KA(J) = I
   20          CONTINUE
```

```
                KA(ICOL) = I
                JCOL = ICOL
              END IF
   40       CONTINUE
            KA(N+1) = NNZ + 1
*
*           Read BL, BU, ISTATE and XS from data file.
*
            READ (NIN,*) (BL(I),I=1,N+M)
            READ (NIN,*) (BU(I),I=1,N+M)
            READ (NIN,*) (ISTATE(I),I=1,N)
            READ (NIN,*) (XS(I),I=1,N)
*
*           Set three options using H02CGF.
*
            CALL H02CGF(' Check Frequency = 10 ')
*
            CALL H02CGF(' Feasibility Tolerance = 0.00001 ')
*
            CALL H02CGF(' Infinite Bound Size = 1.0D+25 ')
*
*           Set the unit number for advisory messages to NOUT.
*
            CALL X04ABF(1,NOUT)
*
*           Read the options file for the remaining options.
*
            CALL H02CFF(NIN,INFORM)
*
            IF (INFORM.NE.0) THEN
               WRITE (NOUT,99999) 'H02CFF terminated with INFORM = ',
     +           INFORM
               STOP
            END IF
*
            STRTGY = 3
            INTVAR(1) = 2
            INTVAR(2) = 3
            INTVAR(3) = 4
            INTVAR(4) = 5
            INTVAR(5) = 6
            INTVAR(6) = 7
            INTVAR(7) = -1
*
            CALL H02CGF('NoList')
            CALL H02CGF('Print Level = 0')
*
*           Solve the QP problem.
*
            IFAIL = 0
*
            CALL H02CEF(N,M,NNZ,IOBJ,NCOLH,QPHX,A,HA,KA,BL,BU,START,NAMES,
     +                  NNAME,CRNAME,NS,XS,INTVAR,LINTVR,MM,ISTATE,MINIZ,
     +                  MINZ,OBJ,CLAMDA,STRTGY,IZ,LENIZ,Z,LENZ,MONIT,IFAIL)
*
*           Print out the best integer solution found
*
            WRITE (NOUT,99999) OBJ, (I,XS(I),I=1,N)
```

```
      END IF
      STOP
*
99999 FORMAT (' Optimal Integer Value is = ',e20.8,/' Components are ',
     +       /(' x(',I3,') = ',F10.2))
99998 FORMAT (1X,A,I3)
      END
*
      SUBROUTINE QPHX(NSTATE,NCOLH,X,HX)
*
*     Routine to compute H*x. (In this version of QPHX, the Hessian
*     matrix H is not referenced explicitly.)
*
*     .. Parameters ..
      real            TWO
      PARAMETER       (TWO=2.0e+0)
*     .. Scalar Arguments ..
      INTEGER         NCOLH, NSTATE
*     .. Array Arguments ..
      real            HX(NCOLH), X(NCOLH)
*     .. Executable Statements ..
      HX(1) = TWO*X(1)
      HX(2) = TWO*X(2)
      HX(3) = TWO*(X(3)+X(4))
      HX(4) = HX(3)
      HX(5) = TWO*X(5)
      HX(6) = TWO*(X(6)+X(7))
      HX(7) = HX(6)
*
      END
*
      SUBROUTINE MONIT(INTFND,NODES,DEPTH,OBJ,X,BSTVAL,BSTSOL,BL,BU,N,
     +                 HALT,COUNT)
*     .. Parameters ..
      real            CUTOFF
      PARAMETER       (CUTOFF=-1840000.0e+0)
*     .. Scalar Arguments ..
      real            BSTVAL, OBJ
      INTEGER         COUNT, DEPTH, INTFND, N, NODES
      LOGICAL         HALT
*     .. Array Arguments ..
      real            BL(N), BSTSOL(N), BU(N), X(N)
*     .. Executable Statements ..
      IF (INTFND.EQ.0) BSTVAL = CUTOFF
*
      END
```

9.2 Program Data

```
H02CFF Example Program Data
 7  8             :Values of N and M
48  8  7  'C'  15 :Values of NNZ, IOBJ, NCOLH, START and NNAME
'        '  '        '  '        '  '        '  '        ' :End of NAMES
'...X1...'  '...X2...'  '...X3...'  '...X4...'  '...X5...'
'...X6...'  '...X7...'  '..ROW1..'  '..ROW2..'  '..ROW3..'
'..ROW4..'  '..ROW5..'  '..ROW6..'  '..ROW7..'  '..COST..' :End of CRNAME
   0.02   7   1
```

```
    0.02   5   1
    0.03   3   1
    1.00   1   1
    0.70   6   1
    0.02   4   1
    0.15   2   1
 -200.00   8   1
    0.06   7   2
    0.75   6   2
    0.03   5   2
    0.04   4   2
    0.05   3   2
    0.04   2   2
    1.00   1   2
-2000.00   8   2
    0.02   2   3
    1.00   1   3
    0.01   4   3
    0.08   3   3
    0.08   7   3
    0.80   6   3
-2000.00   8   3
    1.00   1   4
    0.12   7   4
    0.02   3   4
    0.02   4   4
    0.75   6   4
    0.04   2   4
-2000.00   8   4
    0.01   5   5
    0.80   6   5
    0.02   7   5
    1.00   1   5
    0.02   2   5
    0.06   3   5
    0.02   4   5
-2000.00   8   5
    1.00   1   6
    0.01   2   6
    0.01   3   6
    0.97   6   6
    0.01   7   6
  400.00   8   6
    0.97   7   7
    0.03   2   7
    1.00   1   7
  400.00   8   7                                          :End of matrix A
 0.0       0.0       4.0E+02   1.0E+02  0.0      0.0      0.0       2.0E+03
-1.0E+25  -1.0E+25  -1.0E+25  -1.0E+25  1.5E+03  2.5E+02 -1.0E+25 :End of BL
 2.0E+02   2.5E+03   8.0E+02   7.0E+02  1.5E+03  1.0E+25  1.0E+25   2.0E+03
 6.0E+01   1.0E+02   4.0E+01   3.0E+01  1.0E+25  3.0E+02  1.0E+25 :End of BU
 0    0    0    0    0    0    0    0   :End of ISTATE
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0 :End of XS
Begin
  Iteration Limit = 125 * (Default = 75)
  Print Level = 1       * (Default = 10)
End
```

9.3 Program Results

```
H02CFF Example Program Results


Calls to H02CGF
---------------

      Check Frequency = 10
      Feasibility Tolerance = 0.00001
      Infinite Bound Size = 1.0E+25


OPTIONS file
------------

     Begin
       Iteration Limit = 125 * (Default = 75)
       Print Level = 1       * (Default = 10)
     End
Optimal Integer Value is =      -0.18475180E+07
Components are
x(  1) =       0.00
x(  2) =     355.00
x(  3) =     645.00
x(  4) =     164.00
x(  5) =     410.00
x(  6) =     275.00
x(  7) =     151.00
```

H02CGF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

To supply individual optional parameters to H02CEF.

2 Specification

```
SUBROUTINE H02CGF(STRING)
CHARACTER*(*)     STRING
```

3 Description

H02CGF may be used to supply values for optional parameters to H02CEF. It is only necessary to call H02CGF for those parameters whose values are to be different from their default values. One call to H02CGF sets one parameter value.

Each optional parameter is defined by a single character string of up to 72 characters, consisting of one or more items. The items associated with a given option must be separated by spaces, or equal signs [=]. Alphabetic characters may be upper or lower case. The string

```
Print level = 1
```

is an example of a string used to set an optional parameter. For each option the string contains one or more of the following items:

(a) a mandatory keyword;
(b) a phrase that qualifies the keyword;
(c) a number that specifies an INTEGER or ***real*** value. Such numbers may be up to 16 contiguous characters in Fortran 77's I, F, E or D formats, terminated by a space if this is not the last item on the line.

Blank strings and comments are ignored. A comment begins with an asterisk (*) and all subsequent characters in the string are regarded as part of the comment.

Normally, each user-specified option is printed as it is defined, on the current advisory message unit (see X04ABF), but this printing may be suppressed using the keyword **nolist**. Thus the statement

```
CALL H02CGF ('Nolist')
```

suppresses printing of this and subsequent options. Printing will automatically be turned on again after a call to H02CEF, and may be turned on again at any time using the keyword **list**.

Optional parameter settings are preserved following a call to H02CEF, and so the keyword **defaults** is provided to allow the user to reset all the optional parameters to their default values by the statement,

```
CALL H02CGF ('Defaults')
```

prior to a subsequent call to H02CEF.

A complete list of optional parameters, their abbreviations, synonyms and default values is given in Section 11 of the document for H02CEF.

4 References

None.

5 Parameters

1: STRING — CHARACTER*(*) *Input*

On entry: a single valid option string (as described in Section 3 above and in Section 11 of the document for H02CEF).

6 Error Indicators and Warnings

If a line is not recognized as a valid option, then a warning message is output on the current advisory message unit (see X04ABF).

7 Accuracy

Not applicable.

8 Further Comments

H02CFF may also be used to supply optional parameters to H02CEF. Note that if E04NKF is used in the same program as H02CEF, then in general H02CFF will also affect the options used by E04NKF.

9 Example

See the example for H02CEF.

H03ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

H03ABF solves the classical Transportation ('Hitchcock') problem.

2. Specification

```
      SUBROUTINE H03ABF (KOST, MMM, MA, MB, M, K15, MAXIT, K7, K9, NUMIT,
     1                   K6, K8, K11, K12, Z, IFAIL)
      INTEGER          KOST(MMM,MB), MMM, MA, MB, M, K15(M), MAXIT,
     1                 K7(M), K9(M), NUMIT, K6(M), K8(M), K11(M), K12(M),
     2                 IFAIL
      real             Z
```

3. Description

H03ABF solves the Transportation problem by minimizing

$$z = \sum_i \sum_j c_{ij} x_{ij}.$$

subject to the constraints

$$\sum_j x_{ij} = A_i \qquad \text{(Availabilities)}$$

$$\sum_i x_{ij} = B_j \qquad \text{(Requirements)}$$

where the x_{ij} can be interpreted as quantities of goods sent from source i to destination j, for $i = 1,2,...,m_a$; $j = 1,2,...,m_b$, at a cost of c_{ij} per unit, and it is assumed that $\sum_i A_i = \sum_j B_j$ and $x_{ij} \geq 0$.

H03ABF uses the 'stepping stone' method, modified to accept degenerate cases.

4. References

[1] HADLEY, G.
Linear Programming.
Addison-Wesley, New York, 1962.

5. Parameters

1: KOST(MMM,MB) – INTEGER array. *Input*

On entry: the coefficients c_{ij}, for $i = 1,2,...,m_a$; $j = 1,2,...,m_b$.

2: MMM – INTEGER. *Input*

On entry: the first dimension of the array KOST as declared in the (sub)program from which H03ABF is called.

Constraint: MMM ≥ MA.

3: MA – INTEGER. *Input*

On entry: the number of sources, m_a.

Constraint: MA ≥ 1.

4: MB – INTEGER. *Input*

On entry: the number of destinations, m_b.

Constraint: MB ≥ 1.

5: M – INTEGER. *Input*

On entry: the value of $m_a + m_b$.

6: K15(M) – INTEGER array. *Input/Output*

On entry: K15(i) must be set to the availabilities A_i, for $i = 1,2,...,m_a$; and K15(m_a+j) must be set to the requirements B_j, for $j = 1,2,...,m_b$.

On exit: the contents of K15 are undefined.

7: MAXIT – INTEGER. *Input*

On entry: the maximum number of iterations allowed.

Constraint: MAXIT ≥ 1.

8: K7(M) – INTEGER array. *Workspace*

9: K9(M) – INTEGER array. *Workspace*

10: NUMIT – INTEGER. *Output*

On exit: the number of iterations performed.

11: K6(M) – INTEGER array. *Output*

On exit: K6(k), for $k = 1,2,...,m_a+m_b-1$, contains the source indices of the optimal solution (see K11 below).

12: K8(M) – INTEGER array. *Output*

On exit: K8(k), for $k = 1,2,...,m_a+m_b-1$, contains the destination indices of the optimal solution (see K11 below).

13: K11(M) – INTEGER array. *Output*

On exit: K11(k), for $k = 1,2,...,m_a+m_b-1$, contains the optimal quantities x_{ij} which, sent from source i = K6(k) to destination j = K8(k), minimize z.

14: K12(M) – INTEGER array. *Output*

On exit: K12(k), for $k = 1,2,...,m_a+m_b-1$, contains the unit cost c_{ij} associated with the route from source i = K6(k) to destination j = K8(k).

15: Z – ***real***. *Output*

On exit: the value of the minimized total cost.

16: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry the sum of the availabilities does not equal the sum of the requirements.

IFAIL = 2

During computation MAXIT has been exceeded.

IFAIL = 3

On entry, MAXIT < 1.

IFAIL = 4

On entry, MA < 1,
or MB < 1,
or M ≠ MA + MB,
or MA > MMM.

7. Accuracy

All operations are performed in integer arithmetic so that there are no rounding errors.

8. Further Comments

An accurate estimate of the run time for a particular problem is difficult to achieve.

9. Example

A company has three warehouses and three stores. The warehouses have a surplus of 12 units of a given commodity divided among them as follows:

Warehouse	Surplus
1	1
2	5
3	6

The stores altogether need 12 units of commodity, with the following requirements:

Store	Requirement
1	4
2	4
3	4

Costs of shipping one unit of the commodity from warehouse *i* to store *j* are displayed in the following matrix:

		Store		
		1	2	3
Warehouse	1	8	8	11
	2	5	8	14
	3	4	3	10

It is required to find the units of commodity to be moved from the warehouses to the stores, such that the transportation costs are minimized. The maximum number of iterations allowed is 200.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     H03ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MAMAX, MBMAX, M, MMM
      PARAMETER        (MAMAX=5,MBMAX=5,M=MAMAX+MBMAX,MMM=MAMAX)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             Z
      INTEGER          I, IFAIL, J, L, MA, MB
```

```
*     .. Local Arrays ..
      INTEGER          K11(M), K12(M), K15(M), K6(M), K7(M), K8(M),
     +                 K9(M), KOST(MMM,MBMAX)
*     .. External Subroutines ..
      EXTERNAL         H03ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H03ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) MA, MB
      IF (MA.GT.0 .AND. MA.LE.MAMAX .AND. MB.GT.0 .AND. MB.LE.MBMAX)
     +    THEN
         READ (NIN,*) (K15(I),I=1,MA+MB)
         DO 20 I = 1, MA
            READ (NIN,*) (KOST(I,J),J=1,MB)
   20    CONTINUE
         IFAIL = 0
*
         CALL H03ABF(KOST,MMM,MA,MB,MA+MB,K15,200,K7,K9,L,K6,K8,K11,K12,
     +               Z,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,99999) 'Total cost = ', Z
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Goods from  to'
         WRITE (NOUT,*)
         WRITE (NOUT,99998) (K11(I),K6(I),K8(I),I=1,MA+MB-1)
      END IF
      STOP
*
99999 FORMAT (1X,A,F5.1)
99998 FORMAT (1X,I3,I6,I5)
      END
```

9.2. Program Data

```
H03ABF Example Program Data
    3    3
    1    5    6    4    4    4
    8    8   11
    5    8   14
    4    3   10
```

9.3. Program Results

```
 H03ABF Example Program Results

 Total cost =  77.0

 Goods from  to

   4     3    2
   2     3    3
   1     2    3
   1     1    3
   4     2    1
```

H03ADF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

H03ADF finds the shortest path through a directed or undirected acyclic network using Dijkstra's algorithm.

2 Specification

```
 SUBROUTINE H03ADF(N, NS, NE, DIRECT, NNZ, D, IROW, ICOL, SPLEN,
1                  PATH, IWORK, WORK, IFAIL)
 INTEGER           N, NS, NE, NNZ, IROW(NNZ), ICOL(NNZ),
1                  PATH(N), IWORK(3*N+1), IFAIL
 real              D(NNZ), SPLEN, WORK(2*N)
 LOGICAL           DIRECT
```

3 Description

This routine attempts to find the shortest path through a **directed** or **undirected acyclic** network, which consists of a set of points called **vertices** and a set of curves called **arcs** that connect certain pairs of distinct vertices. An acyclic network is one in which there are no paths connecting a vertex to itself. An arc whose origin vertex is i and whose destination vertex is j can be written as $i \rightarrow j$. In an undirected network the arcs $i \rightarrow j$ and $j \rightarrow i$ are equivalent (i.e., $i \leftrightarrow j$), whereas in a directed network they are different. Note that the shortest path may not be unique and in some cases may not even exist (e.g. if the network is disconnected).

The network is assumed to consist of n vertices which are labelled by the integers $1, 2, \ldots, n$. The lengths of the arcs between the vertices are defined by the n by n **distance matrix** D, in which the element d_{ij} gives the length of the arc $i \rightarrow j$; $d_{ij} = 0$ if there is no arc connecting vertices i and j (as is the case for an acyclic network when $i = j$). Thus the matrix D is usually **sparse**. For example, if $n = 4$ and the network is directed, then

$$D = \begin{pmatrix} 0 & d_{12} & d_{13} & d_{14} \\ d_{21} & 0 & d_{23} & d_{24} \\ d_{31} & d_{32} & 0 & d_{34} \\ d_{41} & d_{42} & d_{43} & 0 \end{pmatrix}.$$

If the network is undirected, D is **symmetric** since $d_{ij} = d_{ji}$ (i.e., the length of the arc $i \rightarrow j \equiv$ the length of the arc $j \rightarrow i$).

The method used by H03ADF is described in detail in Section 8.

4 References

[1] Dijkstra E W (1959) A note on two problems in connection with graphs *Numer. Math.* **1** 269–271

5 Parameters

1: N — INTEGER *Input*

On entry: n, the number of vertices.

Constraint: N $\geq$ 2.

2: NS — INTEGER *Input*

3: NE — INTEGER *Input*

On entry: n_s and n_e, the labels of the first and last vertices, respectively, between which the shortest path is sought.

Constraints:

$1 \leq \text{NS} \leq \text{N}$,
$1 \leq \text{NE} \leq \text{N}$,
$\text{NS} \neq \text{NE}$.

4: DIRECT — LOGICAL *Input*

On entry: indicates whether the network is directed or undirected as follows:

if DIRECT = .TRUE., the network is directed;
if DIRECT = .FALSE., the network is undirected.

5: NNZ — INTEGER *Input*

On entry: the number of non-zero elements in the distance matrix D.

Constraints:

if DIRECT = .TRUE., $1 \leq \text{NNZ} \leq \text{N} \times (\text{N}-1)$;
if DIRECT = .FALSE., $1 \leq \text{NNZ} \leq \text{N} \times (\text{N}-1)/2$.

6: D(NNZ) — ***real*** array *Input*

On entry: the non-zero elements of the distance matrix D, ordered by increasing row index and increasing column index within each row. More precisely, D(k) must contain the value of the non-zero element with indices (IROW(k),ICOL(k)); this is the length of the arc from the vertex with label IROW(k) to the vertex with label ICOL(k). Elements with the same row and column indices are not allowed. If DIRECT = .FALSE., then only those non-zero elements in the strict upper triangle of D need be supplied since $d_{ij} = d_{ji}$. (F11ZAF may be used to sort the elements of an arbitrarily ordered matrix into the required form. This is illustrated in Section 9.)

Constraint: D(k) > 0.0, for $k = 1, 2, \ldots,$NNZ.

7: IROW(NNZ) — INTEGER array *Input*

8: ICOL(NNZ) — INTEGER array *Input*

On entry: IROW(k) and ICOL(k) must contain the row and column indices, respectively, for the non-zero element stored in D(k).

Constraints:

IROW and ICOL must satisfy the following constraints (which may be imposed by a call to F11ZAF):
IROW($k-1$) < IROW(k), or
IROW($k-1$) = IROW(k) and ICOL($k-1$) < ICOL(k), for $k = 2, 3, \ldots,$NNZ.
In addition, if DIRECT = .TRUE., $1 \leq$ IROW(k) $\leq$ N, $1 \leq$ ICOL(k) $\leq$ N and IROW(k) $\neq$ ICOL(k);
if DIRECT = .FALSE., $1 \leq$ IROW(k) < ICOL(k) $\leq$ N.

9: SPLEN — ***real*** *Output*

On exit: the length of the shortest path between the specified vertices n_s and n_e.

10: PATH(N) — INTEGER array *Output*

On exit: contains details of the shortest path between the specified vertices n_s and n_e. More precisely, NS = PATH(1) $\rightarrow$ PATH(2) $\rightarrow \ldots \rightarrow$ PATH(p) = NE for some $p \leq n$. The remaining $(n-p)$ elements are set to zero.

11: IWORK(3*N+1) — INTEGER array *Workspace*

12: WORK(2*N) — ***real*** array *Workspace*

13: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL = 1

On entry, N < 2,
or NS < 1,
or NS > N,
or NE < 1,
or NE > N,
or NS = NE.

IFAIL = 2

On entry, NNZ > N × (N−1) when DIRECT = .TRUE.,
or NNZ > N × (N−1)/2 when DIRECT = .FALSE.,
or NNZ < 1.

IFAIL = 3

On entry, IROW(k) < 1 or IROW(k) > N or ICOL(k) < 1 or ICOL(k) > N or IROW(k) = ICOL(k) for some k when DIRECT = .TRUE..

IFAIL = 4

On entry, IROW(k) < 1 or IROW(k) ≥ ICOL(k) or ICOL(k) > N for some k when DIRECT = .FALSE..

IFAIL = 5

On entry, D(k) ≤ 0.0 for some k.

IFAIL = 6

On entry, IROW($k-1$) > IROW(k) or IROW($k-1$) = IROW(k) and ICOL($k-1$) > ICOL(k) for some k.

IFAIL = 7

On entry, IROW($k-1$) = IROW(k) and ICOL($k-1$) = ICOL(k) for some k.

IFAIL = 8

No connected network exists between vertices NS and NE.

7 Accuracy

The results are exact, except for the obvious rounding errors in summing the distances in the length of the shortest path.

8 Further Comments

This routine is based upon Dijkstra's algorithm (see [1]), which attempts to find a path $n_s \rightarrow n_e$ between two specified vertices n_s and n_e of shortest length $d(n_s, n_e)$.

The algorithm proceeds by assigning labels to each vertex, which may be **temporary** or **permanent**. A temporary label can be changed, whereas a permanent one cannot. For example, if vertex p has a permanent label (q, r), then r is the distance $d(n_s, r)$ and q is the previous vertex on a shortest length $n_s \rightarrow p$ path. If the label is temporary, then it has the same meaning but it refers only to the shortest $n_s \rightarrow p$ path found so far. A shorter one may be found later, in which case the label may become permanent.

The algorithm consists of the following steps.

(1) Assign the permanent label $(-, 0)$ to vertex n_s and temporary labels $(-, \infty)$ to every other vertex. Set $k = n_s$ and go to (2).

(2) Consider each vertex y adjacent to vertex k with a temporary label in turn. Let the label at k be (p, q) and at $y(r, s)$. If $q + d_{ky} < s$, then a new temporary label $(k, q + d_{ky})$ is assigned to vertex y; otherwise no change is made in the label of y. When all vertices y with temporary labels adjacent to k have been considered, go to (3).

(3) From the set of temporary labels, select the one with the smallest second component and declare that label to be permanent. The vertex it is attached to becomes the new vertex k. If $k = n_e$ go to (4). Otherwise go to (2) unless no new vertex can be found (e.g. when the set of temporary labels is 'empty' but $k \neq n_e$, in which case no connected network exists between vertices n_s and n_e).

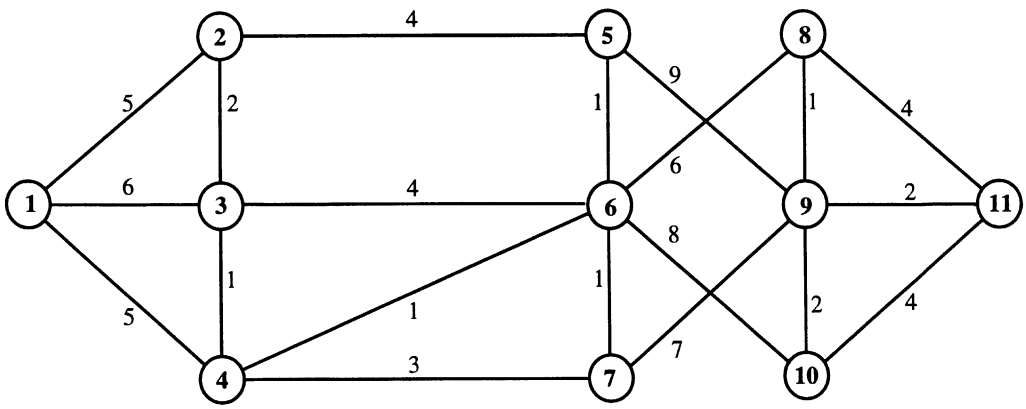
(4) To find the shortest path, let (y, z) denote the label of vertex n_e. The column label (z) gives $d(n_s, n_e)$ while the row label (y) then links back to the previous vertex on a shortest length $n_s \rightarrow n_e$ path. Go to vertex y. Suppose that the (permanent) label of vertex y is (w, x), then the next previous vertex is w on a shortest length $n_s \rightarrow y$ path. This process continues until vertex n_s is reached. Hence the shortest path is

$$n_s \rightarrow \ldots \rightarrow w \rightarrow y \rightarrow n_e,$$

which has length $d(n_s, n_e)$.

9 Example

To find the shortest path between vertices 1 and 11 for the undirected network



9.1 Program Text

```
*     H03ADF Example Program Text
*     Mark 18 Release. NAG Copyright 1997.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
```

```
      INTEGER          NMAX, NNZMAX
      PARAMETER        (NMAX=100,NNZMAX=1000)
      CHARACTER        DUP, ZERO
      PARAMETER        (DUP='Fail',ZERO='Remove')
*     .. Local Scalars ..
      real             SPLEN
      INTEGER          IFAIL, J, LENC, N, NE, NNZ, NS
      LOGICAL          DIRECT
*     .. Local Arrays ..
      real             D(NNZMAX), WORK(2*NMAX)
      INTEGER          ICOL(NNZMAX), IROW(NNZMAX), IWORK(3*NMAX+1),
     +                 PATH(NMAX)
*     .. External Subroutines ..
      EXTERNAL         F11ZAF, H03ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'H03ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NS, NE, NNZ, DIRECT
      IF (N.LE.NMAX .AND. NNZ.LE.NNZMAX) THEN
*
*        Read D, IROW and ICOL from data file.
*
         READ (NIN,*) (D(J),IROW(J),ICOL(J),J=1,NNZ)
*
*        Reorder the elements of D into the form required by H03ADF.
*
         IFAIL = 0
         CALL F11ZAF(N,NNZ,D,IROW,ICOL,DUP,ZERO,IWORK,IWORK(N+2),IFAIL)
*
*        Find the shortest path between vertices NS and NE.
*
         IFAIL = 0
         CALL H03ADF(N,NS,NE,DIRECT,NNZ,D,IROW,ICOL,SPLEN,PATH,IWORK,
     +               WORK,IFAIL)
*
         IF (IFAIL.EQ.0) THEN
*
*           Print details of shortest path.
*
            DO 20 J = 0, N - 1
               IF (PATH(J+1).EQ.0) THEN
                  LENC = J
                  GO TO 40
               END IF
   20       CONTINUE
            LENC = N
   40       CONTINUE
            WRITE (NOUT,99999) 'Shortest path = ', (PATH(J),J=1,LENC)
            WRITE (NOUT,99998) 'Length of shortest path = ', SPLEN
         END IF
      END IF
      STOP
*
99999 FORMAT (/1X,A,10(I2,:'  to '))
99998 FORMAT (/1X,A,G16.6)
      END
```

9.2 Program Data

```
H03ADF Example Program Data
11  1  11  20  F   :Values of N, NS, NE, NNZ and DIRECT
6.0   6   8
1.0   8   9
2.0   9  11
4.0   2   5
1.0   3   4
6.0   1   3
4.0   3   6
1.0   4   6
2.0   2   3
3.0   4   7
5.0   1   2
7.0   6  10
1.0   5   6
4.0   8  11
9.0   5   9
1.0   6   7
8.0   7   9
4.0  10  11
2.0   9  10
5.0   1   4        :End of D, IROW, ICOL
```

9.3 Program Results

```
H03ADF Example Program Results

Shortest path =  1  to  4  to  6  to  8  to  9  to 11

Length of shortest path =      15.0000
```

Chapter M01 – Sorting

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
M01CAF	12	Sort a vector, real numbers
M01CBF	12	Sort a vector, integer numbers
M01CCF	12	Sort a vector, character data
M01DAF	12	Rank a vector, real numbers
M01DBF	12	Rank a vector, integer numbers
M01DCF	12	Rank a vector, character data
M01DEF	12	Rank rows of a matrix, real numbers
M01DFF	12	Rank rows of a matrix, integer numbers
M01DJF	12	Rank columns of a matrix, real numbers
M01DKF	12	Rank columns of a matrix, integer numbers
M01DZF	12	Rank arbitrary data
M01EAF	12	Rearrange a vector according to given ranks, real numbers
M01EBF	12	Rearrange a vector according to given ranks, integer numbers
M01ECF	12	Rearrange a vector according to given ranks, character data
M01EDF	19	Rearrange a vector according to given ranks, complex numbers
M01ZAF	12	Invert a permutation
M01ZBF	12	Check validity of a permutation
M01ZCF	12	Decompose a permutation into cycles

Chapter M01

Sorting

Contents

1 Scope of the Chapter

This chapter is concerned with sorting numeric or character data. It handles only the simplest types of data structure and it is concerned only with **internal** sorting – that is, sorting a set of data which can all be stored within the program.

Users with large files of data or complicated data structures to be sorted should use a comprehensive sorting program or package.

2 Background to the Problems

The usefulness of sorting is obvious (perhaps a little too obvious, since sorting can be expensive and is sometimes done when not strictly necessary). Sorting may traditionally be associated with data processing and non-numerical programming, but it has many uses within the realm of numerical analysis. For example, within the NAG Fortran Library, sorting is used to arrange eigenvalues in ascending order of absolute value; in the manipulation of sparse matrices and in the ranking of observations for nonparametric statistics.

The general problem may be defined as follows. We are given N items of data

$$R_1, R_2, \ldots, R_N.$$

Each item R_i contains a key K_i which can be ordered relative to any other key according to some specified criterion (for example, ascending numeric value). The problem is to determine a permutation

$$p(1), p(2), \ldots, p(N)$$

which puts the keys in order:

$$K_{p(1)} \leq K_{p(2)} \leq \ldots \leq K_{p(N)}$$

Sometimes we may wish actually to **rearrange** the items so that their keys are in order; for other purposes we may simply require a table of **indices** so that the items can be referred to in sorted order; or yet again we may require a table of **ranks**, that is, the positions of each item in the sorted order.

For example, given the single-character items, to be sorted into alphabetic order:

E B A D C

the indices of the items in sorted order are

3 2 5 4 1

and the ranks of the items are

5 2 1 4 3.

Indices may be converted to ranks, and vice versa, by simply computing the inverse permutation.

The items may consist solely of the key (each item may simply be a number). On the other hand, the items may contain additional information (for example, each item may be an eigenvalue of a matrix and its associated eigenvector, the eigenvalue being the key). In the latter case there may be many distinct items with equal keys, and it may be important to preserve the original order among them (if this is achieved, the sorting is called '**stable**').

There are a number of ingenious algorithms for sorting. For a fascinating discussion of them, and of the whole subject, see Knuth [1].

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

Four categories of routines are provided:

– routines which rearrange the data into sorted order (M01C-);

- routines which determine the ranks of the data, leaving the data unchanged (M01D-);
- routines which rearrange the data according to pre-determined ranks (M01E-);
- service routines (M01Z-).

In the first two categories, routines are provided for ***real*** and integer numeric data, and for character data. In the third category there are routines for rearranging ***real***, ***complex***, integer and character data. Utilities for the manipulation of sparse matrices can be found in Chapter F11.

If the task is simply to rearrange a one-dimensional array of data into sorted order, then an M01C- routine should be used, since this requires no extra workspace and is faster than any other method. There are no M01C- routines for more complicated data structures, because the cost of rearranging the data is likely to outstrip the cost of comparisons. Instead, a combination of M01D- and M01E- routines, or some other approach, must be used as described below.

For many applications it is in fact preferable to separate the task of determining the sorted order (ranking) from the task of rearranging data into a pre-determined order; the latter task may not need to be performed at all. Frequently it may be sufficient to refer to the data in sorted order via an index vector, without rearranging it. Frequently also one set of data (e.g. a column of a matrix) is used for determining a set of ranks, which are then applied to other data (e.g. the remaining columns of the matrix).

To determine the ranks of a set of data, use an M01D- routine. Routines are provided for ranking one-dimensional arrays, and for ranking rows or columns of two-dimensional arrays. For ranking an arbitrary data structure, use M01DZF, which is, however, much less efficient than the other M01D- routines.

To create an index vector so that data can be referred to in sorted order, first call an M01D- routine to determine the ranks, and then call M01ZAF to convert the vector of ranks into an index vector.

To rearrange data according to pre-determined ranks: use an M01E- routine if the data is stored in a one-dimensional array; or if the data is stored in a more complicated structure

either use an index vector to generate a new copy of the data in the desired order

or rearrange the data without using extra storage by first calling M01ZCF and then using the simple code-framework given in the document for M01ZCF (assuming that the elements of data all occupy equal storage).

Examples of these operations can be found in the routine documents of the relevant routines.

4 Index

5 Routines Withdrawn or Scheduled for Withdrawal

Since Mark 13 the following routines have been withdrawn. Advice on replacing calls to these routines is given in the document 'Advice on Replacement Calls for Withdrawn/Superseded Routines'.

M01AAF	M01ABF	M01ACF	M01ADF	M01AEF	M01AFF
M01AGF	M01AHF	M01AJF	M01AKF	M01ALF	M01AMF
M01ANF	M01APF	M01AQF	M01ARF	M01BAF	M01BBF
M01BCF	M01BDF				

6 References

[1] Knuth D E (1973) *The Art of Computer Programming (Volume 3)* Addison–Wesley (2nd Edition)

M01CAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01CAF rearranges a vector of ***real*** numbers into ascending or descending order.

2. Specification

```
SUBROUTINE M01CAF (RV, M1, M2, ORDER, IFAIL)
INTEGER          M1, M2, IFAIL
real             RV(M2)
CHARACTER*1      ORDER
```

3. Description

M01CAF is based on Singleton's implementation of the 'median-of-three' Quicksort algorithm [2], but with two additional modifications. First, small subfiles are sorted by an insertion sort on a separate final pass (Sedgewick [1]). Second, if a subfile is partitioned into two very unbalanced subfiles, the larger of them is flagged for special treatment: before it is partitioned, its end-points are swapped with two random points within it; this makes the worst case behaviour extremely unlikely.

4. References

[1] SEDGEWICK, R.
Implementing Quicksort programs.
Comm. ACM 21, pp. 847-857, 1978.

[2] SINGLETON, R.C.
An efficient algorithm for sorting with minimal storage: Algorithm 347.
Comm. ACM 12, pp. 185-187, 1969.

5. Parameters

1: RV(M2) – ***real*** array. *Input/Output*

On entry: elements M1 to M2 of RV must contain ***real*** values to be sorted.

On exit: these values are rearranged into sorted order.

2: M1 – INTEGER. *Input*

On entry: the index of the first element of RV to be sorted.

Constraint: M1 > 0.

3: M2 – INTEGER. *Input*

On entry: the index of the last element of RV to be sorted.

Constraint: M2 ≥ M1.

4: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the values will be sorted into ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 − M1 + 1. The worst case time is proportional to n^2 but this is extremely unlikely to occur.

9. Example

The example program reads a list of ***real*** numbers and sorts them into ascending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01CAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX
      PARAMETER        (NMAX=100)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, N
*     .. Local Arrays ..
      real             RV(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01CAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.GE.1 .AND. N.LE.NMAX) THEN
         READ (NIN,*) (RV(I),I=1,N)
         IFAIL = 0
*
```

```
         CALL M01CAF(RV,1,N,'Ascending',IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Sorted numbers'
         WRITE (NOUT,*)
         WRITE (NOUT,99999) (RV(I),I=1,N)
      END IF
      STOP
*
99999 FORMAT (1X,10F7.1)
      END
```

9.2. Program Data

```
M01CAF Example Program Data
16
1.3 5.9 4.1 2.3 0.5 5.8 1.3 6.5
2.3 0.5 6.5 9.9 2.1 1.1 1.2 8.6
```

9.3. Program Results

```
 M01CAF Example Program Results

 Sorted numbers

     0.5    0.5    1.1    1.2    1.3    1.3    2.1    2.3    2.3    4.1
     5.8    5.9    6.5    6.5    8.6    9.9
```

M01CBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01CBF rearranges a vector of integer numbers into ascending or descending order.

2. Specification

```
SUBROUTINE M01CBF (IV, M1, M2, ORDER, IFAIL)
INTEGER          IV(M2), M1, M2, IFAIL
CHARACTER*1      ORDER
```

3. Description

M01CBF is based on Singleton's implementation of the 'median-of-three' Quicksort algorithm [2], but with two additional modifications. First, small subfiles are sorted by an insertion sort on a separate final pass (Sedgewick [1]). Second, if a subfile is partitioned into two very unbalanced subfiles, the larger of them is flagged for special treatment: before it is partitioned, its end-points are swapped with two random points within it; this makes the worst case behaviour extremely unlikely.

4. References

[1] SEDGEWICK, R.
Implementing Quicksort programs.
Comm. ACM 21, pp. 847-857, 1978.

[2] SINGLETON, R.C.
An efficient algorithm for sorting with minimal storage: Algorithm 347.
Comm. ACM 12, pp. 185-187, 1969.

5. Parameters

1: IV(M2) – INTEGER array. *Input/Output*

On entry: elements M1 to M2 of IV must contain integer values to be sorted.

On exit: these values are rearranged into sorted order.

2: M1 – INTEGER. *Input*

On entry: the index of the first element of IV to be sorted.

Constraint: M1 > 0.

3: M2 – INTEGER. *Input*

On entry: the index of the last element of IV to be sorted.

Constraint: M2 ≥ M1.

4: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the values will be sorted into ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 − M1 + 1. The worst case time is proportional to n^2 but this is extremely unlikely to occur.

9. Example

The example program reads a list of integers and sorts them into descending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01CBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX
      PARAMETER        (NMAX=100)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, N
*     .. Local Arrays ..
      INTEGER          IV(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01CBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01CBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.GE.1 .AND. N.LE.NMAX) THEN
         READ (NIN,*) (IV(I),I=1,N)
         IFAIL = 0
*
         CALL M01CBF(IV,1,N,'Descending',IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Sorted numbers'
         WRITE (NOUT,*)
         WRITE (NOUT,99999) (IV(I),I=1,N)
      END IF
      STOP
*
99999 FORMAT (1X,10I7)
      END
```

9.2. Program Data

```
M01CBF Example Program Data
16
23 45 45 67 69 90 999 1
78 112 24 69 96 99 45 78
```

9.3. Program Results

```
 M01CBF Example Program Results

 Sorted numbers

     999     112      99      96      90      78      78      69      69      67
      45      45      45      24      23       1
```

M01CCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01CCF rearranges a vector of character data so that a specified substring is in ASCII or reverse ASCII order.

2. Specification

```
SUBROUTINE M01CCF (CH, M1, M2, L1, L2, ORDER, IFAIL)
INTEGER        M1, M2, L1, L2, IFAIL
CHARACTER*1    ORDER
CHARACTER*(*) CH(M2)
```

3. Description

M01CCF is based on Singleton's implementation of the 'median-of-three' Quicksort algorithm [2], but with two additional modifications. First, small subfiles are sorted by an insertion sort on a separate final pass (Sedgewick [1]). Second, if a subfile is partitioned into two very unbalanced subfiles, the larger of them is flagged for special treatment: before it is partitioned, its end-points are swapped with two random points within it; this makes the worst case behaviour extremely unlikely.

Only the substring (L1:L2) of each element of the array CH is used to determine the sorted order, but the entire elements are rearranged into sorted order.

4. References

[1] SEDGEWICK, R.
Implementing Quicksort programs.
Comm. ACM 21, pp. 847-857, 1978.

[2] SINGLETON, R.C.
An efficient algorithm for sorting with minimal storage: Algorithm 347.
Comm. ACM 12, pp. 185-187, 1969.

5. Parameters

1: CH(M2) – CHARACTER*(*) array. *Input/Output*

On entry: elements M1 to M2 of CH must contain character data to be sorted.

Constraint: the length of each element of CH must not exceed 255.

On exit: these values are rearranged into sorted order.

2: M1 – INTEGER. *Input*

On entry: the index of the first element of CH to be sorted.

Constraint: M1 > 0.

3: M2 – INTEGER. *Input*

On entry: the index of the last element of CH to be sorted.

Constraint: M2 ≥ M1.

4: L1 – INTEGER. *Input*

5: L2 – INTEGER. *Input*

On entry: only the substring (L1:L2) of each element of CH is to be used in determining the sorted order.

Constraint: $0 < L1 \leq L2 \leq LEN(CH(1))$.

6: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the values will be sorted into ASCII order; if ORDER is 'R' or 'r', into reverse ASCII order.

Constraint: ORDER = 'A', 'a', 'R' or 'r'.

7: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2,
or L2 < 1,
or L1 < 1,
or L1 > L2,
or L2 > LEN(CH(1)).

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'R' or 'r'.

IFAIL = 3

On entry, the length of each element of CH exceeds 255.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 – M1 + 1. The worst case time is proportional to n^2, but this is extremely unlikely to occur.

The routine relies on the Fortran 77 intrinsic functions LLT and LGT to order characters according to the ASCII collating sequence.

9. Example

The example program reads a file of 12-character records, and sorts them into reverse ASCII order on characters 7 to 12.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01CCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX
      PARAMETER        (MMAX=100)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, L1, L2, M
*     .. Local Arrays ..
      CHARACTER*12     CH(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01CCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01CCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      DO 20 M = 1, MMAX
         READ (NIN,'(A)',END=40) CH(M)
   20 CONTINUE
   40 M = M - 1
      L1 = 7
      L2 = 12
      IFAIL = 0
*
      CALL M01CCF(CH,1,M,L1,L2,'Reverse ASCII',IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Records sorted on columns ', L1, '  to ', L2
      WRITE (NOUT,*)
      WRITE (NOUT,99998) (CH(I),I=1,M)
      STOP
*
99999 FORMAT (1X,A,I2,A,I2)
99998 FORMAT (1X,A)
      END
```

9.2. Program Data

```
M01CCF Example Program Data
A02AAF   289
A02ABF   523
A02ACF   531
C02ADF   169
C02AEF   599
C05ADF  1351
C05AGF   240
C05AJF   136
C05AVF   211
C05AXF   183
C05AZF  2181
```

9.3. Program Results

```
M01CCF Example Program Results

Records sorted on columns  7  to 12

C05AZF  2181
C05ADF  1351
C02AEF   599
A02ACF   531
A02ABF   523
A02AAF   289
C05AGF   240
C05AVF   211
C05AXF   183
C02ADF   169
C05AJF   136
```

M01DAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DAF ranks a vector of ***real*** numbers in ascending or descending order.

2. Specification

```
SUBROUTINE M01DAF (RV, M1, M2, ORDER, IRANK, IFAIL)
INTEGER          M1, M2, IRANK(M2), IFAIL
real             RV(M2)
CHARACTER*1      ORDER
```

3. Description

M01DAF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal elements preserve their ordering in the input data.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: RV(M2) – ***real*** array. *Input*

On entry: elements M1 to M2 of RV must contain ***real*** values to be ranked.

2: M1 – INTEGER. *Input*

On entry: the index of the first element of RV to be ranked.

Constraint: M1 > 0.

3: M2 – INTEGER. *Input*

On entry: the index of the last element of RV to be ranked.

Constraint: M2 ≥ M1.

4: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the values will be ranked in ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

5: IRANK(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of IRANK contain the ranks of the corresponding elements of RV. Note that the ranks are in the range M1 to M2: thus, if RV(i) is the first element in the rank order, IRANK(i) is set to M1.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 – M1 + 1.

9. Example

The example program reads a list of ***real*** numbers and ranks them in ascending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX
      PARAMETER        (NMAX=100)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, N
*     .. Local Arrays ..
      real             RV(NMAX)
      INTEGER          IRANK(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.GE.1 .AND. N.LE.NMAX) THEN
         READ (NIN,*) (RV(I),I=1,N)
         IFAIL = 0
*
```

```
         CALL M01DAF(RV,1,N,'Ascending',IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) '   Data   Ranks'
         WRITE (NOUT,*)
         DO 20 I = 1, N
            WRITE (NOUT,99999) RV(I), IRANK(I)
   20    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,F7.1,I7)
      END
```

9.2. Program Data

```
M01DAF Example Program Data
12
5.3 4.6 7.8 1.7 5.3 9.9 3.2 4.3 7.8 4.5 1.2 7.6
```

9.3. Program Results

```
 M01DAF Example Program Results

    Data   Ranks

     5.3       7
     4.6       6
     7.8      10
     1.7       2
     5.3       8
     9.9      12
     3.2       3
     4.3       4
     7.8      11
     4.5       5
     1.2       1
     7.6       9
```

M01DBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DBF ranks a vector of integer numbers in ascending or descending order.

2. Specification

```
SUBROUTINE M01DBF (IV, M1, M2, ORDER, IRANK, IFAIL)
INTEGER        IV(M2), M1, M2, IRANK(M2), IFAIL
CHARACTER*1    ORDER
```

3. Description

M01DBF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal elements preserve their ordering in the input data.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: IV(M2) – INTEGER array. *Input*

On entry: elements M1 to M2 of IV must contain integer values to be ranked.

2: M1 – INTEGER. *Input*

On entry: the index of the first element of IV to be ranked.

Constraint: M1 > 0.

3: M2 – INTEGER. *Input*

On entry: M2 must specify the index of the last element of IV to be ranked.

Constraint: M2 ≥ M1.

4: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the values will be ranked in ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

5: IRANK(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of IRANK contain the ranks of the corresponding elements of IV. Note that the ranks are in the range M1 to M2: thus, if IV(i) is the first element in the rank order, IRANK(i) is set to M1.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 − M1 + 1.

9. Example

The example program reads a list of integers and ranks them in descending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX
      PARAMETER        (NMAX=100)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, N
*     .. Local Arrays ..
      INTEGER          IRANK(NMAX), IV(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.GE.1 .AND. N.LE.NMAX) THEN
         READ (NIN,*) (IV(I),I=1,N)
         IFAIL = 0
*
```

```
         CALL M01DBF(IV,1,N,'Descending',IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) '   Data   Ranks'
         WRITE (NOUT,*)
         DO 20 I = 1, N
            WRITE (NOUT,99999) IV(I), IRANK(I)
   20    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,2I7)
      END
```

9.2. Program Data

```
M01DBF Example Program Data
12
34 44 89 64 69 69 23 1 999 65 22 76
```

9.3. Program Results

```
 M01DBF Example Program Results

    Data   Ranks

      34       9
      44       8
      89       2
      64       7
      69       4
      69       5
      23      10
       1      12
     999       1
      65       6
      22      11
      76       3
```

M01DCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DCF ranks a vector of character data in ASCII or reverse ASCII order of a specified substring.

2. Specification

```
SUBROUTINE M01DCF (CH, M1, M2, L1, L2, ORDER, IRANK, IFAIL)
INTEGER        M1, M2, L1, L2, IRANK(M2), IFAIL
CHARACTER*1    ORDER
CHARACTER*(*) CH(M2)
```

3. Description

M01DCF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal elements preserve their ordering in the input data.

Only the substring (L1:L2) of each element of the array CH is used to determine the rank order.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: CH(M2) – CHARACTER*(*) array. *Input*

On entry: elements M1 to M2 of CH must contain character data to be ranked.

Constraint: the length of each element of CH must not exceed 255.

2: M1 – INTEGER. *Input*

On entry: the index of the first element of CH to be ranked.

Constraint: M1 > 0.

3: M2 – INTEGER. *Input*

On entry: the index of the last element of CH to be ranked.

Constraint: M2 ≥ M1.

4: L1 – INTEGER. *Input*

5: L2 – INTEGER. *Input*

On entry: only the substring (L1:L2) of each element of CH is to be used in determining the rank order.

Constraint: 0 < L1 ≤ L2 ≤ LEN(CH(1))

6: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the values will be ranked in ASCII order; if ORDER is 'R' or 'r', in reverse ASCII order.

Constraint: ORDER = 'A', 'a', 'R' or 'r'.

7: IRANK(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of IRANK contain the ranks of the corresponding elements of CH. Note that the ranks are in the range M1 to M2: thus, if CH(i) is the first element in the rank order, IRANK(i) is set to M1.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2,
or L2 < 1,
or L1 < 1,
or L1 > L2,
or L2 > LEN(CH(1)).

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'R' or 'r'.

IFAIL = 3

On entry, the length of each element of CH exceeds 255.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 – M1 + 1.

The routine relies on the Fortran 77 intrinsic functions LLT and LGT to order characters according to the ASCII collating sequence.

9. Example

The example program reads a file of 12-character records, and ranks them in reverse ASCII order on characters 7 to 12.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX
      PARAMETER        (MMAX=100)
```

```
*     .. Local Scalars ..
      INTEGER          I, IFAIL, L1, L2, M
*     .. Local Arrays ..
      INTEGER          IRANK(MMAX)
      CHARACTER*12     CH(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      DO 20 M = 1, MMAX
         READ (NIN,'(A)',END=40) CH(M)
   20 CONTINUE
   40 M = M - 1
      L1 = 7
      L2 = 12
      IFAIL = 0
*
      CALL M01DCF(CH,1,M,L1,L2,'Reverse ASCII',IRANK,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Records ranked on columns ', L1, '  to ', L2
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Data            Ranks'
      WRITE (NOUT,*)
      WRITE (NOUT,99998) (CH(I),IRANK(I),I=1,M)
      STOP
*
99999 FORMAT (1X,A,I2,A,I2)
99998 FORMAT (1X,A,I7)
      END
```

9.2. Program Data

```
M01DCF Example Program Data
A02AAF   289
A02ABF   523
A02ACF   531
C02ADF   169
C02AEF   599
C05ADF  1351
C05AGF   240
C05AJF   136
C05AVF   211
C05AXF   183
C05AZF  2181
```

9.3. Program Results

```
 M01DCF Example Program Results

 Records ranked on columns  7  to 12

 Data            Ranks

 A02AAF   289      6
 A02ABF   523      5
 A02ACF   531      4
 C02ADF   169     10
 C02AEF   599      3
 C05ADF  1351      2
 C05AGF   240      7
 C05AJF   136     11
 C05AVF   211      8
 C05AXF   183      9
 C05AZF  2181      1
```

M01DEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DEF ranks the rows of a matrix of ***real*** numbers in ascending or descending order.

2. Specification

```
SUBROUTINE M01DEF (RM, LDM, M1, M2, N1, N2, ORDER, IRANK, IFAIL)
INTEGER          LDM, M1, M2, N1, N2, IRANK(M2), IFAIL
real             RM(LDM,N2)
CHARACTER*1      ORDER
```

3. Description

M01DEF ranks rows M1 to M2 of a matrix, using the data in columns N1 to N2 of those rows. The ordering is determined by first ranking the data in column N1, then ranking any tied rows according to the data in column N1 + 1, and so on up to column N2.

M01DEF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal rows preserve their ordering in the input data.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: RM(LDM,N2) – ***real*** array. *Input*

On entry: columns N1 to N2 of rows M1 to M2 of RM must contain ***real*** data to be ranked.

2: LDM – INTEGER. *Input*

On entry: the first dimension of the array RM as declared in the (sub)program from which M01DEF is called.

Constraint: LDM ≥ M2.

3: M1 – INTEGER. *Input*

On entry: the index of the first row of RM to be ranked.

Constraint: M1 > 0.

4: M2 – INTEGER. *Input*

On entry: the index of the last row of RM to be ranked.

Constraint: M2 ≥ M1.

5: N1 – INTEGER. *Input*

On entry: the index of the first column of RM to be used.

Constraint: N1 > 0.

6: N2 – INTEGER. *Input*

On entry: the index of the last column of RM to be used.

Constraint: N2 ≥ N1.

7: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the rows will be ranked in ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

8: IRANK(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of IRANK contain the ranks of the corresponding rows of RM. Note that the ranks are in the range M1 to M2: thus, if the ith row of RM is the first in the rank order, IRANK(i) is set to M1.

9: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or N2 < 1,
or M1 < 1,
or M1 > M2,
or N1 < 1,
or N1 > N2,
or LDM < M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 – M1 + 1.

9. Example

The example program reads a matrix of ***real*** numbers and ranks the rows in ascending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      real             RM(MMAX,NMAX)
      INTEGER          IRANK(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX) THEN
         DO 20 I = 1, M
            READ (NIN,*) (RM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
         CALL M01DEF(RM,MMAX,1,M,1,N,'Ascending',IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Data                          Ranks'
         WRITE (NOUT,*)
         DO 40 I = 1, M
            WRITE (NOUT,99999) (RM(I,J),J=1,N), IRANK(I)
   40    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,3F7.1,I11)
      END
```

9.2. Program Data

```
M01DEF Example Program Data
12 3
6.0 5.0 4.0
5.0 2.0 1.0
2.0 4.0 9.0
4.0 9.0 6.0
4.0 9.0 5.0
4.0 1.0 2.0
3.0 4.0 1.0
2.0 4.0 6.0
1.0 6.0 4.0
9.0 3.0 2.0
6.0 2.0 5.0
4.0 9.0 6.0
```

9.3. Program Results

```
M01DEF Example Program Results

Data                          Ranks

     6.0     5.0     4.0         11
     5.0     2.0     1.0          9
     2.0     4.0     9.0          3
     4.0     9.0     6.0          7
     4.0     9.0     5.0          6
     4.0     1.0     2.0          5
     3.0     4.0     1.0          4
     2.0     4.0     6.0          2
     1.0     6.0     4.0          1
     9.0     3.0     2.0         12
     6.0     2.0     5.0         10
     4.0     9.0     6.0          8
```

M01DFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DFF ranks the rows of a matrix of integer numbers in ascending or descending order.

2. Specification

```
SUBROUTINE M01DFF (IM, LDM, M1, M2, N1, N2, ORDER, IRANK, IFAIL)
INTEGER          IM(LDM,N2), LDM, M1, M2, N1, N2, IRANK(M2), IFAIL
CHARACTER*1      ORDER
```

3. Description

M01DFF ranks rows M1 to M2 of a matrix, using the data in columns N1 to N2 of those rows. The ordering is determined by first ranking the data in column N1, then ranking any tied rows according to the data in column N1 + 1, and so on up to column N2.

M01DFF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal rows preserve their ordering in the input data.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: IM(LDM,N2) – INTEGER array. *Input*

On entry: columns N1 to N2 of rows M1 to M2 of IM must contain INTEGER data to be ranked.

2: LDM – INTEGER. *Input*

On entry: the first dimension of the array IM as declared in the (sub)program from which M01DFF is called.

Constraint: LDM ≥ M2.

3: M1 – INTEGER. *Input*

On entry: the index of the first row of IM to be ranked.

Constraint: M1 > 0.

4: M2 – INTEGER. *Input*

On entry: the index of the last row of IM to be ranked.

Constraint: M2 ≥ M1.

5: N1 – INTEGER. *Input*

On entry: the index of the first column of IM to be used.

Constraint: N1 > 0.

6: N2 – INTEGER. *Input*

On entry: the index of the last column of IM to be used.

Constraint: N2 ≥ N1.

7: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the rows will be ranked in ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

8: IRANK(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of IRANK contain the ranks of the corresponding rows of IM. Note that the ranks are in the range M1 to M2: thus, if the *i*th row of IM is the first in the rank order, IRANK(*i*) is set to M1.

9: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or N2 < 1,
or M1 < 1,
or M1 > M2,
or N1 < 1,
or N1 > N2,
or LDM < M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 – M1 + 1.

9. Example

The example program reads a matrix of integers and ranks the rows in descending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DFF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      INTEGER          IM(MMAX,NMAX), IRANK(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DFF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX) THEN
         DO 20 I = 1, M
            READ (NIN,*) (IM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
         CALL M01DFF(IM,MMAX,1,M,1,N,'Descending',IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Data                          Ranks'
         WRITE (NOUT,*)
         DO 40 I = 1, M
            WRITE (NOUT,99999) (IM(I,J),J=1,N), IRANK(I)
   40    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,3I7,I11)
      END
```

9.2. Program Data

```
M01DFF Example Program Data
12 3
6 5 4
5 2 1
2 4 9
4 9 6
4 9 5
4 1 2
3 4 1
2 4 6
1 6 4
9 3 2
6 2 5
4 9 6
```

9.3. Program Results

```
M01DFF Example Program Results

Data                        Ranks

     6     5     4            2
     5     2     1            4
     2     4     9           10
     4     9     6            5
     4     9     5            7
     4     1     2            8
     3     4     1            9
     2     4     6           11
     1     6     4           12
     9     3     2            1
     6     2     5            3
     4     9     6            6
```

M01DJF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DJF ranks the columns of a matrix of ***real*** numbers in ascending or descending order.

2. Specification

```
SUBROUTINE M01DJF (RM, LDM, M1, M2, N1, N2, ORDER, IRANK, IFAIL)
INTEGER          LDM, M1, M2, N1, N2, IRANK(N2), IFAIL
real             RM(LDM,N2)
CHARACTER*1      ORDER
```

3. Description

M01DJF ranks columns N1 to N2 of a matrix, using the data in rows M1 to M2 of those columns. The ordering is determined by first ranking the data in row M1, then ranking any tied columns according to the data in row M1 + 1, and so on up to row M2.

M01DJF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal columns preserve their ordering in the input data.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: RM(LDM,N2) – ***real*** array. *Input*

On entry: rows M1 to M2 of columns N1 to N2 of RM must contain ***real*** data to be ranked.

2: LDM – INTEGER. *Input*

On entry: the first dimension of the array RM as declared in the (sub)program from which M01DJF is called.

Constraint: LDM ≥ M2.

3: M1 – INTEGER. *Input*

On entry: the index of the first row of RM to be used.

Constraint: M1 > 0.

4: M2 – INTEGER. *Input*

On entry: the index of the last row of RM to be used.

Constraint: M2 ≥ M1.

5: N1 – INTEGER. *Input*

On entry: the index of the first column of RM to be ranked.

Constraint: N1 > 0.

6: N2 – INTEGER. *Input*

On entry: the index of the last column of RM to be ranked.

Constraint: N2 ≥ N1.

7: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the columns will be ranked in ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

8: IRANK(N2) – INTEGER array. *Output*

On exit: elements N1 to N2 of IRANK contain the ranks of the corresponding columns of RM. Note that the ranks are in the range N1 to N2: thus, if the ith column of RM is the first in the rank order, IRANK(i) is set to N1.

9: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or N2 < 1,
or M1 < 1,
or M1 > M2,
or N1 < 1,
or N1 > N2,
or LDM < M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = N2 – N1 + 1.

9. Example

The example program reads a matrix of ***real*** numbers and ranks the columns in ascending order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DJF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      real             RM(MMAX,NMAX)
      INTEGER          IRANK(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DJF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DJF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX) THEN
         DO 20 I = 1, M
            READ (NIN,*) (RM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
         CALL M01DJF(RM,MMAX,1,M,1,N,'Ascending',IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Data'
         WRITE (NOUT,*)
         DO 40 I = 1, M
            WRITE (NOUT,99999) (RM(I,J),J=1,N)
   40    CONTINUE
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Ranks'
         WRITE (NOUT,*)
         WRITE (NOUT,99998) (IRANK(I),I=1,N)
      END IF
      STOP
*
99999 FORMAT (1X,12F6.1)
99998 FORMAT (1X,12I6)
      END
```

9.2. Program Data

```
M01DJF Example Program Data
3 12
5.0 4.0 3.0 2.0 2.0 1.0 9.0 4.0 4.0 2.0 2.0 1.0
3.0 8.0 2.0 5.0 5.0 6.0 9.0 8.0 9.0 5.0 4.0 1.0
9.0 1.0 6.0 1.0 2.0 4.0 8.0 1.0 2.0 2.0 6.0 2.0
```

9.3. Program Results

```
M01DJF Example Program Results

Data

   5.0    4.0    3.0    2.0    2.0    1.0    9.0    4.0    4.0    2.0    2.0    1.0
   3.0    8.0    2.0    5.0    5.0    6.0    9.0    8.0    9.0    5.0    4.0    1.0
   9.0    1.0    6.0    1.0    2.0    4.0    8.0    1.0    2.0    2.0    6.0    2.0

Ranks

    11      8      7      4      5      2     12      9     10      6      3      1
```

M01DKF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DKF ranks the columns of a matrix of integer numbers in ascending or descending order.

2. Specification

```
SUBROUTINE M01DKF (IM, LDM, M1, M2, N1, N2, ORDER, IRANK, IFAIL)
INTEGER        IM(LDM,N2), LDM, M1, M2, N1, N2, IRANK(N2), IFAIL
CHARACTER*1    ORDER
```

3. Description

M01DKF ranks columns N1 to N2 of a matrix, using the data in rows M1 to M2 of those columns. The ordering is determined by first ranking the data in row M1, then ranking any tied columns according to the data in row M1 + 1, and so on up to row M2.

M01DKF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10. The ranking is stable: equal columns preserve their ordering in the input data.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973

5. Parameters

1: IM(LDM,N2) – INTEGER array. *Input*

On entry: rows M1 to M2 of columns N1 to N2 of IM must contain integer data to be ranked.

2: LDM – INTEGER. *Input*

On entry: the first dimension of the array IM as declared in the (sub)program from which M01DKF is called.

Constraint: LDM ≥ M2.

3: M1 – INTEGER. *Input*

On entry: the index of the first row of IM to be used.

Constraint: M1 > 0.

4: M2 – INTEGER. *Input*

On entry: the index of the last row of IM to be used.

Constraint: M2 ≥ M1.

5: N1 – INTEGER. *Input*

On entry: the index of the first column of IM to be ranked.

Constraint: N1 > 0.

6: N2 – INTEGER. *Input*

On entry: the index of the last column of IM to be ranked.

Constraint: N2 ≥ N1.

7: ORDER – CHARACTER*1. *Input*

On entry: if ORDER is 'A' or 'a', the columns will be ranked in ascending (i.e. non-decreasing) order; if ORDER is 'D' or 'd', into descending order.

Constraint: ORDER = 'A', 'a', 'D' or 'd'.

8: IRANK(N2) – INTEGER array. *Output*

On exit: elements N1 to N2 of IRANK contain the ranks of the corresponding columns of IM. Note that the ranks are in the range N1 to N2: thus, if the ith column of IM is the first in the rank order, IRANK(i) is set to N1.

9: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or N2 < 1,
or M1 < 1,
or M1 > M2,
or N1 < 1,
or N1 > N2,
or LDM < M2.

IFAIL = 2

On entry, ORDER is not 'A', 'a', 'D' or 'd'.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = N2 – N1 + 1.

9. Example

The example program reads a matrix of integers and ranks the columns in descending order.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DKF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      INTEGER          IM(MMAX,NMAX), IRANK(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DKF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DKF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX) THEN
         DO 20 I = 1, M
            READ (NIN,*) (IM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
         CALL M01DKF(IM,MMAX,1,M,1,N,'Descending',IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Data'
         WRITE (NOUT,*)
         DO 40 I = 1, M
            WRITE (NOUT,99999) (IM(I,J),J=1,N)
   40    CONTINUE
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Ranks'
         WRITE (NOUT,*)
         WRITE (NOUT,99999) (IRANK(I),I=1,N)
      END IF
      STOP
*
99999 FORMAT (1X,12I6)
      END
```

9.2. Program Data

```
M01DKF Example Program Data
3 12
5 4 3 2 2 1 9 4 4 2 2 1
3 8 2 5 5 6 9 8 9 5 4 1
9 1 6 1 2 4 8 1 2 2 6 2
```

9.3. Program Results

```
 M01DKF Example Program Results

 Data

      5     4     3     2     2     1     9     4     4     2     2     1
      3     8     2     5     5     6     9     8     9     5     4     1
      9     1     6     1     2     4     8     1     2     2     6     2

 Ranks

      2     4     6     9     7    11     1     5     3     8    10    12
```

M01DZF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01DZF ranks arbitrary data according to a user-supplied comparison routine.

2. Specification

```
SUBROUTINE M01DZF (COMPAR, M1, M2, IRANK, IFAIL)
INTEGER          M1, M2, IRANK(M2), IFAIL
LOGICAL          COMPAR
EXTERNAL         COMPAR
```

3. Description

M01DZF is a general-purpose routine for ranking arbitrary data. M01DZF does not access the data directly; instead it calls a user-supplied routine COMPAR to determine the relative ordering of any two data items. The data items are identified simply by an integer in the range M1 to M2.

M01DZF uses a variant of list-merging, as described by Knuth [1] pp. 165-166. The routine takes advantage of natural ordering in the data, and uses a simple list insertion in a preparatory pass to generate ordered lists of length at least 10.

4. References

[1] KNUTH, D.E.
The Art of Computer Programming, (Vol. 3, Sorting and Searching).
Addison Wesley, 1973.

5. Parameters

1: COMPAR – LOGICAL FUNCTION, supplied by the user. *External Procedure*

COMPAR must specify the relative ordering of any two data items; it must return .TRUE. if item I must come strictly **after** item J in the rank ordering.

Its specification is:

```
LOGICAL FUNCTION  COMPAR(I, J)
INTEGER           I, J
```

1: I – INTEGER. *Input*

2: J – INTEGER. *Input*

On entry: I and J identify the data items to be compared.

Constraint: M1 ≤ I, J ≤ M2.

COMPAR must be declared as EXTERNAL in the (sub)program from which M01DZF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: M1 and M2 must specify the range of data items to be ranked, and the range of ranks to be assigned. Specifically, M01DZF ranks the data items identified by integers in the range M1 to M2, and assigns ranks in the range M1 to M2 which are stored in elements M1 to M2 of IRANK.

Constraint: 0 < M1 ≤ M2.

4: IRANK(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of IRANK contain the ranks of the data items M1 to M2. Note that the ranks are in the range M1 to M2: thus, if item i is first in the rank ordering, IRANK(i) contains M1.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to $n \times \log n$, where n = M2 – M1 + 1; it will usually be dominated by the time taken in COMPAR.

9. Example

The example program reads records, each of which contains an integer key and a ***real*** number. The program ranks the records first of all in ascending order of the integer key; records with equal keys are ranked in descending order of the ***real*** number if the key is negative, in ascending order of the ***real*** number if the key is positive, and in their original order if the key is zero. After calling M01DZF, the program calls M01ZAF to convert the ranks to indices, and prints the records in rank order. Note the use of COMMON to communicate the data between the main program and the function COMPAR.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01DZF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX
      PARAMETER        (NMAX=100)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Arrays in Common ..
      real             RV(NMAX)
      INTEGER          IV(NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, N
*     .. Local Arrays ..
      INTEGER          IRANK(NMAX)
*     .. External Functions ..
      LOGICAL          COMPAR
      EXTERNAL         COMPAR
```

```
*     .. External Subroutines ..
      EXTERNAL          M01DZF, M01ZAF
*     .. Common blocks ..
      COMMON            RV, IV
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01DZF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.GE.1 .AND. N.LE.NMAX) THEN
         READ (NIN,*) (IV(I),RV(I),I=1,N)
         IFAIL = 0
*
         CALL M01DZF(COMPAR,1,N,IRANK,IFAIL)
         CALL M01ZAF(IRANK,1,N,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) '   Data in sorted order'
         WRITE (NOUT,*)
         DO 20 I = 1, N
            WRITE (NOUT,99999) IV(IRANK(I)), RV(IRANK(I))
   20    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,I7,F7.1)
      END
*
      LOGICAL FUNCTION COMPAR(I,J)
*     .. Parameters ..
      INTEGER                 NMAX
      PARAMETER               (NMAX=100)
*     .. Scalar Arguments ..
      INTEGER                 I, J
*     .. Arrays in Common ..
      real                    RV(NMAX)
      INTEGER                 IV(NMAX)
*     .. Common blocks ..
      COMMON                  RV, IV
*     .. Executable Statements ..
      IF (IV(I).NE.IV(J)) THEN
         COMPAR = IV(I) .GT. IV(J)
      ELSE
         IF (IV(I).LT.0) THEN
            COMPAR = RV(I) .LT. RV(J)
         ELSE IF (IV(I).GT.0) THEN
            COMPAR = RV(I) .GT. RV(J)
         ELSE
            COMPAR = I .LT. J
         END IF
      END IF
      RETURN
      END
```

9.2. Program Data

```
M01DZF Example Program Data
12
 2   3.0
 1   4.0
-1   6.0
 0   5.0
 2   2.0
-2   7.0
 0   4.0
 1   3.0
 1   5.0
-1   2.0
 1   0.0
 2   1.0
```

9.3. Program Results

```
M01DZF Example Program Results

   Data in sorted order

     -2     7.0
     -1     6.0
     -1     2.0
      0     4.0
      0     5.0
      1     0.0
      1     3.0
      1     4.0
      1     5.0
      2     1.0
      2     2.0
      2     3.0
```

M01EAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01EAF rearranges a vector of ***real*** numbers into the order specified by a vector of ranks.

2. Specification

```
SUBROUTINE M01EAF (RV, M1, M2, IRANK, IFAIL)
INTEGER          M1, M2, IRANK(M2), IFAIL
real             RV(M2)
```

3. Description

M01EAF is designed to be used typically in conjunction with the M01D- ranking routines. After one of the M01D- routines has been called to determine a vector of ranks, M01EAF can be called to rearrange a vector of ***real*** numbers into the rank order. If the vector of ranks has been generated in some other way, then M01ZBF should be called to check its validity before M01EAF is called.

4. References

None.

5. Parameters

1: RV(M2) – ***real*** array. *Input/Output*

On entry: elements M1 to M2 of RV must contain ***real*** values to be rearranged.

On exit: these values are rearranged into rank order. For example, if IRANK(i) = M1, then the initial value of RV(i) is moved to RV(M1).

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: M1 and M2 must specify the range of the ranks supplied in IRANK and the elements of RV to be rearranged.

Constraint: $0 < \text{M1} \leq \text{M2}$.

4: IRANK(M2) – INTEGER array. *Input*

On entry: elements M1 to M2 of IRANK must contain a permutation of the integers M1 to M2, which are interpreted as a vector of ranks.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

Elements M1 to M2 of IRANK contain a value outside the range M1 to M2.

IFAIL = 3

Elements M1 to M2 of IRANK contain a repeated value.

If IFAIL = 2 or 3, elements M1 to M2 of IRANK do not contain a permutation of the integers M1 to M2. On exit, the contents of RV may be corrupted. To check the validity of IRANK without the risk of corrupting RV, use M01ZBF.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to n, where $n = M2 - M1 + 1$.

9. Example

The example program reads a matrix of ***real*** numbers and rearranges its rows so that the elements of the kth column are in ascending order. To do this, the program first calls M01DAF to rank the elements of the kth column, and then calls M01EAF to rearrange each column into the order specified by the ranks. The value of k is read from the data-file.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01EAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, K, M, N
*     .. Local Arrays ..
      real             RM(MMAX,NMAX)
      INTEGER          IRANK(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DAF, M01EAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01EAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N, K
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX .AND.
     +    K.GE.1 .AND. K.LE.N) THEN
         DO 20 I = 1, M
            READ (NIN,*) (RM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
```

```
         CALL M01DAF(RM(1,K),1,M,'Ascending',IRANK,IFAIL)
*
         DO 40 J = 1, N
*
            CALL M01EAF(RM(1,J),1,M,IRANK,IFAIL)
*
   40    CONTINUE
         WRITE (NOUT,*)
         WRITE (NOUT,99999) 'Matrix sorted on column', K
         WRITE (NOUT,*)
         DO 60 I = 1, M
            WRITE (NOUT,99998) (RM(I,J),J=1,N)
   60    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,A,I3)
99998 FORMAT (1X,3F7.1)
      END
```

9.2. Program Data

```
M01EAF Example Program Data
12 3 1
6.0 5.0 4.0
5.0 2.0 1.0
2.0 4.0 9.0
4.0 9.0 6.0
4.0 9.0 5.0
4.0 1.0 2.0
3.0 4.0 1.0
2.0 4.0 6.0
1.0 6.0 4.0
9.0 3.0 2.0
6.0 2.0 5.0
4.0 9.0 6.0
```

9.3. Program Results

```
 M01EAF Example Program Results

 Matrix sorted on column  1

     1.0    6.0    4.0
     2.0    4.0    9.0
     2.0    4.0    6.0
     3.0    4.0    1.0
     4.0    9.0    6.0
     4.0    9.0    5.0
     4.0    1.0    2.0
     4.0    9.0    6.0
     5.0    2.0    1.0
     6.0    5.0    4.0
     6.0    2.0    5.0
     9.0    3.0    2.0
```

M01EBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01EBF rearranges a vector of integer numbers into the order specified by a vector of ranks.

2. Specification

```
SUBROUTINE M01EBF (IV, M1, M2, IRANK, IFAIL)
INTEGER        IV(M2), M1, M2, IRANK(M2), IFAIL
```

3. Description

M01EBF is designed to be used typically in conjunction with the M01D- ranking routines. After one of the M01D- routines has been called to determine a vector of ranks, M01EBF can be called to rearrange a vector of integer numbers into the rank order. If the vector of ranks has been generated in some other way, then M01ZBF should be called to check its validity before M01EBF is called.

4. References

None.

5. Parameters

1: IV(M2) – INTEGER array. *Input/Output*

On entry: elements M1 to M2 of IV must contain integer values to be rearranged.

On exit: these values are rearranged into rank order. For example, if IRANK(i) = M1, then the initial value of IV(i) is moved to IV(M1).

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: M1 and M2 specify the range of the ranks supplied in IRANK and the elements of IV to be rearranged.

Constraint: $0 < M1 \leq M2$.

4: IRANK(M2) – INTEGER array. *Input*

On entry: elements M1 to M2 of IRANK must contain a permutation of the integers M1 to M2, which are interpreted as a vector of ranks.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

Elements M1 to M2 of IRANK contain a value outside the range M1 to M2.

IFAIL = 3

Elements M1 to M2 of IRANK contain a repeated value.

If IFAIL = 2 or 3, elements M1 to M2 of IRANK do not contain a permutation of the integers M1 to M2. On exit, the contents of IV may be corrupted. To check the validity of IRANK without the risk of corrupting IV, use M01ZBF.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to n, where $n = M2 - M1 + 1$.

9. Example

The example program reads a matrix of integers and rearranges its rows so that the elements of the kth column are in ascending order. To do this, the program first calls M01DBF to rank the elements of the kth column, and then calls M01EBF to rearrange each column into the order specified by the ranks. The value of k is read from the data-file.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01EBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, K, M, N
*     .. Local Arrays ..
      INTEGER          IM(MMAX,NMAX), IRANK(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DBF, M01EBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01EBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N, K
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX .AND.
     +    K.GE.1 .AND. K.LE.N) THEN
         DO 20 I = 1, M
            READ (NIN,*) (IM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
         CALL M01DBF(IM(1,K),1,M,'Ascending',IRANK,IFAIL)
*
         DO 40 J = 1, N
*
```

```
            CALL M01EBF(IM(1,J),1,M,IRANK,IFAIL)
*
   40     CONTINUE
          WRITE (NOUT,*)
          WRITE (NOUT,99999) 'Matrix sorted on column', K
          WRITE (NOUT,*)
          DO 60 I = 1, M
             WRITE (NOUT,99998) (IM(I,J),J=1,N)
   60     CONTINUE
       END IF
       STOP
*
99999 FORMAT (1X,A,I3)
99998 FORMAT (1X,3I7)
      END
```

9.2. Program Data

```
M01EBF Example Program Data
12 3 1
6 5 4
5 2 1
2 4 9
4 9 6
4 9 5
4 1 2
3 4 1
2 4 6
1 6 4
9 3 2
6 2 5
4 9 6
```

9.3. Program Results

```
 M01EBF Example Program Results

 Matrix sorted on column  1

        1       6       4
        2       4       9
        2       4       6
        3       4       1
        4       9       6
        4       9       5
        4       1       2
        4       9       6
        5       2       1
        6       5       4
        6       2       5
        9       3       2
```

M01ECF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01ECF rearranges a vector of character data into the order specified by a vector of ranks.

2. Specification

```
SUBROUTINE M01ECF (CH, M1, M2, IRANK, IFAIL)
INTEGER          M1, M2, IRANK(M2), IFAIL
CHARACTER*(*) CH(M2)
```

3. Description

M01ECF is designed to be used typically in conjunction with the M01D- ranking routines. After one of the M01D- routines has been called to determine a vector of ranks, M01ECF can be called to rearrange a vector of character data into the rank order. If the vector of ranks has been generated in some other way, then M01ZBF should be called to check its validity before M01ECF is called.

4. References

None.

5. Parameters

1: CH(M2) – CHARACTER*(*) array. *Input/Output*

On entry: elements M1 to M2 of CH must contain character data to be rearranged.

Constraint: the length of each element of CH must not exceed 255.

On exit: these values are rearranged into rank order. For example, if IRANK(i) = M1, then the initial value of CH(i) is moved to CH(M1).

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: the range of the ranks supplied in IRANK and the elements of CH to be rearranged.

Constraint: $0 < M1 \leq M2$.

4: IRANK(M2) – INTEGER array. *Input*

On entry: elements M1 to M2 of IRANK must contain a permutation of the integers M1 to M2, which are interpreted as a vector of ranks.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

On entry, the length of each element of CH exceeds 255.

IFAIL = 3

Elements M1 to M2 of IRANK contain a value outside the range M1 to M2.

IFAIL = 4

Elements M1 to M2 of IRANK contain a repeated value.

If IFAIL = 3 or 4, elements M1 to M2 of IRANK do not contain a permutation of the integers M1 to M2. On exit, the contents of CH may be corrupted. To check the validity of IRANK without the risk of corrupting CH, use M01ZBF.

7. Accuracy

Not applicable.

8. Further Comments

The average time taken by the routine is approximately proportional to n, where $n = M2 - M1 + 1$.

9. Example

The example program reads a file of 12-character records, each of which contains in characters 1 to 6 a name of a NAG routine, and in characters 7 to 12 an integer frequency. The program first calls M01DBF to rank the integers in descending order, and then calls M01ECF to rearrange the names into the order specified by the ranks.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01ECF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX
      PARAMETER        (MMAX=100)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, M
*     .. Local Arrays ..
      INTEGER          IFREQ(MMAX), IRANK(MMAX)
      CHARACTER*6      CH(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DBF, M01ECF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01ECF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      DO 20 M = 1, MMAX
         READ (NIN,99999,END=40) CH(M), IFREQ(M)
   20 CONTINUE
   40 M = M - 1
      IFAIL = 0
*
```

```
      CALL M01DBF(IFREQ,1,M,'Descending',IRANK,IFAIL)
      CALL M01ECF(CH,1,M,IRANK,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Names in order of frequency'
      WRITE (NOUT,*)
      WRITE (NOUT,99998) (CH(I),I=1,M)
      STOP
*
99999 FORMAT (A6,I6)
99998 FORMAT (1X,A)
      END
```

9.2. Program Data

```
M01ECF Example Program Data
A02AAF   289
A02ABF   523
A02ACF   531
C02ADF   169
C02AEF   599
C05ADF  1351
C05AGF   240
C05AJF   136
C05AVF   211
C05AXF   183
C05AZF  2181
```

9.3. Program Results

```
 M01ECF Example Program Results

 Names in order of frequency

 C05AZF
 C05ADF
 C02AEF
 A02ACF
 A02ABF
 A02AAF
 C05AGF
 C05AVF
 C05AXF
 C02ADF
 C05AJF
```

M01EDF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

M01EDF rearranges a vector of ***complex*** numbers into the order specified by a vector of ranks.

2 Specification

```
SUBROUTINE M01EDF(CV, M1, M2, IRANK, IFAIL)
INTEGER           M1, M2, IRANK(M2), IFAIL
complex           CV(M2)
```

3 Description

M01EDF is designed to be used typically in conjunction with the M01D- ranking routines. After one of the M01D- routines has been called to determine a vector of ranks, M01EDF can be called to rearrange a vector of complex numbers into the rank order. If the vector of ranks has been generated in some other way, then M01ZBF should be called to check its validity before M01EDF is called.

4 References

None.

5 Parameters

1: CV(M2) — ***complex*** array *Input/Output*

On entry: elements M1 to M2 of CV must contain ***complex*** values to be rearranged.

On exit: these values are rearranged into rank order. For example, if IRANK(i) = M1, then the initial value of CV(i) is moved to CV(M1).

2: M1 — INTEGER *Input*

3: M2 — INTEGER *Input*

On entry: M1 and M2 must specify the range of the ranks supplied in IRANK and the elements of CV to be rearranged.

Constraint: $0 < \text{M1} \leq \text{M2}$.

4: IRANK(M2) — INTEGER array *Input*

On entry: elements M1 to M2 of IRANK must contain a permutation of the integers M1 to M2, which are interpreted as a vector of ranks.

5: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

Elements M1 to M2 of IRANK contain a value outside the range M1 to M2.

IFAIL = 3

Elements M1 to M2 of IRANK contain a repeated value.

If IFAIL = 2 or 3, elements M1 to M2 of IRANK do not contain a permutation of the integers M1 to M2. On exit, the contents of CV may be corrupted. To check the validity of IRANK without the risk of corrupting CV, use M01ZBF.

7 Accuracy

Not applicable.

8 Further Comments

The average time taken by the routine is approximately proportional to n, where $n = \mathrm{M2} - \mathrm{M1} + 1$.

9 Example

The example program reads a matrix of ***complex*** numbers and rearranges its rows so that the elements in the kth column are in ascending order of modulus. To do this, the program first calls M01DDF to rank the moduli of the elements in the kth column, and then calls M01EDF to rearrange each column into the order specified by the ranks. The value of k is read from the data-file.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01EDF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, K, M, N
      CHARACTER*30     STRING
*     .. Local Arrays ..
      complex          CM(MMAX,NMAX)
      real             CMOD(MMAX)
      INTEGER          IRANK(MMAX)
*     .. External Subroutines ..
```

```
      EXTERNAL         M01DAF, M01EDF, X04DAF
*     .. Intrinsic Functions ..
      INTRINSIC        ABS
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01EDF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N, K
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX .AND.
     +    K.GE.1 .AND. K.LE.N) THEN
*
*        Read matrix from data file.
*
         DO 20 I = 1, M
            READ (NIN,*) (CM(I,J),J=1,N)
   20    CONTINUE
*
*        Calculate the moduli of the elements in the K-th column.
*
         DO 40 I = 1, M
            CMOD(I) = ABS(CM(I,K))
   40    CONTINUE
*
*        Rearrange the rows so that the elements in the K-th column
*        are in ascending order of modulus.
*
         IFAIL = 0
*
         CALL M01DAF(CMOD,1,M,'Ascending',IRANK,IFAIL)
*
*        Rearrange each column into the order specified by IRANK.
*
         DO 60 J = 1, N
            IFAIL = 0
*
            CALL M01EDF(CM(1,J),1,M,IRANK,IFAIL)
*
   60    CONTINUE
*
*        Print the results.
*
         WRITE (NOUT,*)
         WRITE (STRING,99999) 'Matrix sorted on column', K
         IFAIL = 0
*
         CALL X04DAF('General',' ',M,N,CM,MMAX,STRING,IFAIL)
*
      END IF
      STOP
*
99999 FORMAT (1X,A,I3)
      END
```

9.2 Program Data

```
M01EDF Example Program Data
12 3 2
(6.0, 1.0) (5.0,-2.0) (4.0, 4.0)
(5.0,-3.0) (2.0,-2.0) (1.0, 1.0)
(2.0, 2.0) (4.0, 1.0) (9.0,-3.0)
(4.0, 2.0) (9.0, 6.0) (6.0, 4.0)
(4.0, 0.0) (9.0, 3.0) (5.0, 1.0)
(4.0,-8.0) (1.0, 5.0) (2.0, 1.0)
(3.0,-3.0) (4.0,-5.0) (1.0, 0.0)
(2.0, 4.0) (4.0,-2.0) (6.0,-1.0)
(1.0, 1.0) (6.0, 1.0) (4.0, 0.0)
(9.0, 1.0) (3.0, 3.0) (2.0,-4.0)
(6.0,-1.0) (2.0, 3.0) (5.0,-3.0)
(4.0,-5.0) (9.0, 9.0) (6.0, 7.0)
```

9.3 Program Results

```
M01EDF Example Program Results

 Matrix sorted on column  2
                1          2          3
 1       5.0000     2.0000     1.0000
        -3.0000    -2.0000     1.0000

 2       6.0000     2.0000     5.0000
        -1.0000     3.0000    -3.0000

 3       2.0000     4.0000     9.0000
         2.0000     1.0000    -3.0000

 4       9.0000     3.0000     2.0000
         1.0000     3.0000    -4.0000

 5       2.0000     4.0000     6.0000
         4.0000    -2.0000    -1.0000

 6       4.0000     1.0000     2.0000
        -8.0000     5.0000     1.0000

 7       6.0000     5.0000     4.0000
         1.0000    -2.0000     4.0000

 8       1.0000     6.0000     4.0000
         1.0000     1.0000     0.0000

 9       3.0000     4.0000     1.0000
        -3.0000    -5.0000     0.0000

10       4.0000     9.0000     5.0000
         0.0000     3.0000     1.0000

11       4.0000     9.0000     6.0000
         2.0000     6.0000     4.0000

12       4.0000     9.0000     6.0000
        -5.0000     9.0000     7.0000
```

M01ZAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01ZAF inverts a permutation, and hence converts a rank vector to an index vector, or vice versa.

2. Specification

```
SUBROUTINE M01ZAF (IPERM, M1, M2, IFAIL)
INTEGER        IPERM(M2), M1, M2, IFAIL
```

3. Description

There are two common ways of describing a permutation using an integer vector IPERM. The first uses ranks: IPERM(i) holds the position to which the ith data element should be moved in order to sort the data; in other words its rank in the sorted order. The second uses indices: IPERM(i) holds the current position of the data element which would occur in ith position in sorted order. For example, given the values

3.5 5.9 2.9 0.5

to be sorted in ascending order, the ranks would be

3 4 2 1

and the indices would be

4 3 1 2

The M01D- routines generate ranks, and the M01E- routines require ranks to be supplied to specify the re-ordering. However if it is desired simply to refer to the data in sorted order without actually re-ordering them, indices are more convenient than ranks (see the example in Section 9).

M01ZAF can be used to convert ranks to indices, or indices to ranks, as the two permutations are inverses of one another.

4. References

None.

5. Parameters

1: IPERM(M2) – INTEGER array. *Input/Output*

On entry: elements M1 to M2 of IPERM must contain a permutation of the integers M1 to M2.

On exit: these elements contain the inverse permutation of the integers M1 to M2.

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: M1 and M2 must specify the range of elements used in the array IPERM and the range of values in the permutation, as specified under IPERM.

Constraint: $0 < M1 \leq M2$.

4: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

Elements M1 to M2 of IPERM contain a value outside the range M1 to M2.

IFAIL = 3

Elements M1 to M2 of IPERM contain a repeated value.

If IFAIL = 2 or 3, elements M1 to M2 of IPERM do not contain a permutation of the integers M1 to M2; on exit these elements are usually corrupted. To check the validity of a permutation without the risk of corrupting it, use M01ZBF.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

The example program reads a matrix of ***real*** numbers and prints its rows in ascending order as ranked by M01DEF. The program first calls M01DEF to rank the rows, and then calls M01ZAF to convert the rank vector to an index vector, which is used to refer to the rows in sorted order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01ZAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      real             RM(MMAX,NMAX)
      INTEGER          IPERM(MMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DEF, M01ZAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01ZAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX) THEN
         DO 20 I = 1, M
            READ (NIN,*) (RM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
```

```
         CALL M01DEF(RM,MMAX,1,M,1,N,'Ascending',IPERM,IFAIL)
         CALL M01ZAF(IPERM,1,M,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Matrix sorted by rows'
         WRITE (NOUT,*)
         DO 40 I = 1, M
            WRITE (NOUT,99999) (RM(IPERM(I),J),J=1,N)
   40    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,3F7.1)
      END
```

9.2. Program Data

```
M01ZAF Example Program Data
12 3
6.0 5.0 4.0
5.0 2.0 1.0
2.0 4.0 9.0
4.0 9.0 6.0
4.0 9.0 5.0
4.0 1.0 2.0
3.0 4.0 1.0
2.0 4.0 6.0
1.0 6.0 4.0
9.0 3.0 2.0
6.0 2.0 5.0
4.0 9.0 6.0
```

9.3. Program Results

```
 M01ZAF Example Program Results

 Matrix sorted by rows

     1.0     6.0     4.0
     2.0     4.0     6.0
     2.0     4.0     9.0
     3.0     4.0     1.0
     4.0     1.0     2.0
     4.0     9.0     5.0
     4.0     9.0     6.0
     4.0     9.0     6.0
     5.0     2.0     1.0
     6.0     2.0     5.0
     6.0     5.0     4.0
     9.0     3.0     2.0
```

M01ZBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01ZBF checks the validity of a permutation.

2. Specification

```
SUBROUTINE M01ZBF (IPERM, M1, M2, IFAIL)
INTEGER        IPERM(M2), M1, M2, IFAIL
```

3. Description

M01ZBF can be used to check the validity of user-supplied ranks or indices, without the ranks or indices being corrupted.

4. References

None.

5. Parameters

1: IPERM(M2) – INTEGER array. *Input*

On entry: elements M1 to M2 of IPERM must be set to values which are supposed to be a permutation of the integers M1 to M2. If they are a valid permutation, the routine exits with IFAIL = 0.

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: the range of elements used in the array IPERM and the range of values in the permutation, as specified under IPERM.

Constraint: $0 < M1 \leq M2$.

4: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

Elements M1 to M2 of IPERM contain a value outside the range M1 to M2.

IFAIL = 3

Elements M1 to M2 of IPERM contain a repeated value.

If IFAIL = 2 or 3, elements M1 to M2 of IPERM do not contain a permutation of the integers M1 to M2.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

The example program reads in a vector of ***real*** numbers, and a vector of ranks; it calls M01ZBF to check the validity of the ranks before calling M01EAF to rearrange the ***real*** numbers into the specified order.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01ZBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NMAX
      PARAMETER        (NMAX=100)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, N
*     .. Local Arrays ..
      real             RV(NMAX)
      INTEGER          IRANK(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01EAF, M01ZBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01ZBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.GE.1 .AND. N.LE.NMAX) THEN
         READ (NIN,*) (RV(I),I=1,N)
         READ (NIN,*) (IRANK(I),I=1,N)
         IFAIL = 0
*
         CALL M01ZBF(IRANK,1,N,IFAIL)
         CALL M01EAF(RV,1,N,IRANK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Numbers in rank order'
         WRITE (NOUT,*)
         WRITE (NOUT,99999) (RV(I),I=1,N)
      END IF
      STOP
*
99999 FORMAT (1X,10F7.1)
      END
```

9.2. Program Data

```
M01ZBF Example Program Data
12
5.3 4.6 7.8 1.7 5.3 9.9 3.2 4.3 7.8 4.5 1.2 7.6
  7   6  10   2   8  12   3   4  11   5   1   9
```

9.3. Program Results

```
M01ZBF Example Program Results

Numbers in rank order

    1.2    1.7    3.2    4.3    4.5    4.6    5.3    5.3    7.6    7.8
    7.8    9.9
```

M01ZCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

M01ZCF decomposes a permutation into cycles, as an aid to re-ordering ranked data.

2. Specification

```
SUBROUTINE M01ZCF (IPERM, M1, M2, ICYCL, IFAIL)
INTEGER        IPERM(M2), M1, M2, ICYCL(M2), IFAIL
```

3. Description

M01ZCF is provided as an aid to re-ordering arbitrary data structures without using additional storage. However users should consider carefully whether it is necessary to rearrange their data, or whether it would be simpler and more efficient to refer to the data in sorted order using an index vector, or to create a copy of the data in sorted order.

To rearrange data into a different order without using additional storage, the simplest method is to decompose the permutation which specifies the new order, into cycles; and then to do a cyclic permutation of the data items in each cycle. (This is the method used by the M01E- re-ordering routines.) Given a vector IRANK which specifies the ranks of the data (as generated by the M01D- routines), M01ZCF generates a new vector ICYCL, in which the permutation is represented in its component cycles, with the first element of each cycle negated. For example, the permutation

5 7 4 2 1 6 3

is composed of the cycles

(1 5) (2 7 3 4) (6)

and the vector ICYCL generated by M01ZCF contains

–1 5 –2 7 3 4 –6

In order to rearrange the data according to the specified ranks:

item 6 must be left in place;

items 1 and 5 must be interchanged;

items 4, 2, 7 and 3 must be moved one place round the cycle.

The complete rearrangement can be achieved by the following code:

```
      DO 10 K = M1, M2
         I = ICYCL(K)
         IF (I.LT.0) THEN
            J = -I
         ELSE
            [swap items I and J]
         ENDIF
   10 CONTINUE
```

4. References

None.

5. Parameters

1: IPERM(M2) – INTEGER array. *Input*

On entry: elements M1 to M2 of IPERM must contain a permutation of the integers M1 to M2.

2: M1 – INTEGER. *Input*

3: M2 – INTEGER. *Input*

On entry: M1 and M2 must specify the range of elements used in the array IPERM and the range of values in the permutation, as specified under IPERM.

Constraint: $0 < M1 \leq M2$.

4: ICYCL(M2) – INTEGER array. *Output*

On exit: elements M1 to M2 of ICYCL contain a representation of the permutation as a list of cycles, with the first integer in each cycle negated. (See Section 3.)

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M2 < 1,
or M1 < 1,
or M1 > M2.

IFAIL = 2

Elements M1 to M2 of IPERM contain a value outside the range M1 to M2.

IFAIL = 3

Elements M1 to M2 of IPERM contain a repeated value.

If IFAIL = 2 or 3, elements M1 to M2 of IPERM do not contain a permutation of the integers M1 to M2.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

The example program reads a matrix of ***real*** numbers and rearranges its columns so that the elements of the lth row are in ascending order. To do this, the program first calls M01DJF to rank the elements of the lth row, and then calls M01ZCF to decompose the rank vector into cycles. It then rearranges the columns using the framework of code suggested in Section 3. The value of l is read from the data-file.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     M01ZCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=20,NMAX=20)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             T
      INTEGER          I, IFAIL, II, J, K, L, M, N
*     .. Local Arrays ..
      real             RM(MMAX,NMAX)
      INTEGER          ICYCL(NMAX), IRANK(NMAX)
*     .. External Subroutines ..
      EXTERNAL         M01DJF, M01ZCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'M01ZCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N, L
      IF (M.GE.1 .AND. M.LE.MMAX .AND. N.GE.1 .AND. N.LE.NMAX .AND.
     +    L.GE.1 .AND. L.LE.M) THEN
         DO 20 I = 1, M
            READ (NIN,*) (RM(I,J),J=1,N)
   20    CONTINUE
         IFAIL = 0
*
         CALL M01DJF(RM,MMAX,L,L,1,N,'Ascending',IRANK,IFAIL)
         CALL M01ZCF(IRANK,1,N,ICYCL,IFAIL)
*
         DO 60 K = 1, N
            I = ICYCL(K)
            IF (I.LT.0) THEN
               J = -I
            ELSE
*              Swap columns I and J
               DO 40 II = 1, M
                  T = RM(II,J)
                  RM(II,J) = RM(II,I)
                  RM(II,I) = T
   40          CONTINUE
            END IF
   60    CONTINUE
         WRITE (NOUT,*)
         WRITE (NOUT,99999) 'Matrix sorted on row', L
         WRITE (NOUT,*)
         DO 80 I = 1, M
            WRITE (NOUT,99998) (RM(I,J),J=1,N)
   80    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,A,I3)
99998 FORMAT (1X,12F6.1)
      END
```

9.2. Program Data

```
M01ZCF Example Program Data
3 12 3
5.0 4.0 3.0 2.0 2.0 1.0 9.0 4.0 4.0 2.0 2.0 1.0
3.0 8.0 2.0 5.0 5.0 6.0 9.0 8.0 9.0 5.0 4.0 1.0
9.0 1.0 6.0 1.0 2.0 4.0 8.0 1.0 2.0 2.0 6.0 2.0
```

9.3. Program Results

```
M01ZCF Example Program Results

Matrix sorted on row  3

   4.0   2.0   4.0   2.0   4.0   2.0   1.0   1.0   3.0   2.0   9.0   5.0
   8.0   5.0   8.0   5.0   9.0   5.0   1.0   6.0   2.0   4.0   9.0   3.0
   1.0   1.0   1.0   2.0   2.0   2.0   2.0   4.0   6.0   6.0   8.0   9.0
```

Chapter P01 – Error Trapping

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
P01ABF	12	Return value of error indicator/terminate with error message

Chapter P01

Error Trapping

Contents

1 Scope of the Chapter

This chapter is concerned with the trapping of error, failure or warning conditions by NAG Library routines. This introduction document describes the commonly occurring parameter IFAIL.

2 Background to the Problems

2.1 Errors, Failure and Warning Conditions

The error, failure or warning conditions considered here are those that can be detected by explicit coding in a Library routine. Such conditions must be anticipated by the author of the routine. They should not be confused with run-time errors detected by the compiling system, e.g. detection of overflow or failure to assign an initial value to a variable.

In the rest of this document we use the word 'error' to cover all types of error, failure or warning conditions detected by the routine. They fall roughly into three classes.

(i) On entry to the routine the value of a parameter is out of range. This means that it is not useful, or perhaps even meaningful, to begin computation.
(ii) During computation the routine decides that it cannot yield the desired results, and indicates a failure condition. For example, a matrix inversion routine will indicate a failure condition if it considers that the matrix is singular and so cannot be inverted.
(iii) Although the routine completes the computation and returns results, it cannot guarantee that the results are completely reliable; it therefore returns a warning. For example, an optimization routine may return a warning if it cannot guarantee that it has found a local minimum.

All three classes of errors are handled in the same way by the Library.

Each error which can be detected by a Library routine is associated with a number. These numbers, with explanations of the errors, are listed in Section 6 (Error Indicators and Warnings) in the routine document. Unless the document specifically states to the contrary, the user should not assume that the routine necessarily tests for the occurrence of the errors in their order of error number, i.e., the detection of an error does not imply that other errors have or have not been detected.

2.2 The IFAIL Parameter

Most of the NAG Library routines which can be called directly by the user have a parameter called IFAIL. This parameter is concerned with the NAG Library error trapping mechanism (and, for some routines, with controlling the output of error messages and advisory messages).

IFAIL has **two** purposes:

(i) to allow the user to specify what action the Library routine should take if an error is detected;
(ii) to inform the user of the outcome of the call of the routine.

For purpose (i), the user **must** assign a value to IFAIL before the call to the Library routine. Since IFAIL is reset by the routine for purpose (ii), the parameter must be the name of a variable, **not** a literal or constant.

The value assigned to IFAIL before entry should be either 0 (**hard fail** option), or 1 or – 1 (**soft fail** option). If after completing its computation the routine has not detected an error, IFAIL is reset to 0 to indicate a **successful call.** Control returns to the calling program in the normal way. If the routine does detect an error, its action depends on whether the hard or soft fail option was chosen.

2.3 Hard Fail Option

If the user sets IFAIL to 0 before calling the Library routine, execution of the program will terminate if the routine detects an error. Before the program is stopped, this error message is output:

```
** ABNORMAL EXIT from NAG Library routine XXXXXX: IFAIL = n

** NAG hard failure - execution terminated
```

where **XXXXXX** is the routine name, and **n** is the number associated with the detected error. An explanation of error number **n** is given in Section 6 of the routine document **XXXXXX**.

In addition, most routines output explanatory error messages immediately before the standard termination message shown above.

In some implementations of the NAG Library, when the hard fail option is invoked, the error message may be accompanied by dump or tracing information. The output channel used for the output of the error message is determined by X04AAF.

The hard fail option should be selected if the user is in any doubt about continuing the execution of the program after an unsuccessful call to a NAG Library routine.

2.4 Soft Fail Option

To select this option, the user must set IFAIL to 1 or −1 before calling the Library routine.

If the routine detects an error, IFAIL is reset to the associated error number; further computation within the routine is suspended and control returns to the calling program.

If the user sets IFAIL to 1, then no error message is output (**silent exit**).

If the user sets IFAIL to −1 (**noisy exit**), then before control is returned to the calling program, the following error message is output:

```
** ABNORMAL EXIT from NAG Library routine XXXXXX: IFAIL = n

** NAG soft failure - control returned
```

In addition, most routines output explanatory error messages immediately before the above standard message.

It is most important to test the value of IFAIL on exit if the soft fail option is selected. A non-zero exit value of IFAIL implies that the call was not successful so it is imperative that the user's program be coded to take appropriate action. That action may simply be to print IFAIL with an explanatory caption and then terminate the program. Many of the example programs in Section 9 of the routine documents have IFAIL-exit tests of this form. In the more ambitious case, where the user wishes his or her program to continue, it is essential that the program can branch to a point at which it is **sensible** to resume computation.

The soft fail option puts the onus on the user to handle any errors detected by the Library routine. With the proviso that the user is able to implement it **properly**, it is clearly more flexible than the hard fail option since it allows computation to continue in the case of errors. In particular there are at least two cases where its flexibility is useful:

(i) where additional information about the error or the progress of computation is returned via some of the other parameters;
(ii) exceptionally, certain routine documents may advise further calls with IFAIL left with its value on exit after the first call of the routine. In such cases the user should not reset the IFAIL-exit value between calls;
(iii) in some routines, 'partial' success can be achieved, e.g. a probable solution found but not all conditions fully satisfied, so the routine returns a warning. On the basis of the advice in Section 6 and elsewhere in the routine document, the user may decide that this partially successful call is adequate for certain purposes.

2.5 Historical Note

The error handling mechanism described above was introduced into the NAG Library at Mark 12. It supersedes the earlier mechanism which for most routines allowed IFAIL to be set by the user to 0 or 1 only. The new mechanism is compatible with the old except that the details of the messages output on hard failure have changed. The new mechanism also allows the user to set IFAIL to −1 (soft failure, noisy exit).

A few routines (introduced mainly at Marks 7 and 8) use IFAIL in a different way to control the output of error messages, and also of advisory messages (see Chapter X04). In those routines IFAIL is regarded as a decimal integer whose least significant digits are denoted *ba* with the following significance:

$a = 0$: hard failure $a = 1$: soft failure
$b = 0$: silent exit $b = 1$: noisy exit

Details are given in the documents of the relevant routines; for those routines this alternative use of IFAIL remains valid.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

To implement the error mechanism described in Section 2, NAG Library routines call P01ABF.

This routine is therefore primarily of interest only to writers of NAG Fortran Library software. It is included in the general user manual for completeness. Users need not know how to call P01ABF directly though they may be aware of its existence.

P01ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

P01ABF either returns the value of IERROR (soft failure), or terminates execution of the program (hard failure). Diagnostic messages may be output.

2. Specification

```
INTEGER FUNCTION P01ABF (IFAIL, IERROR, SRNAME, NREC, REC)
INTEGER           IFAIL, IERROR, NREC
CHARACTER*(*) SRNAME, REC(*)
```

3. Description

P01ABF is intended for use by other NAG Fortran Library routines. If a routine does not terminate normally, P01ABF is called to provide uniform handling of error or warning conditions. Associated with abnormal termination are error or warning indicators, which are listed in Section 6 of the routine documents. P01ABF is called with the indicator value stored in IERROR and the name of the calling library routine in SRNAME. Messages relating to the reason for termination may optionally be supplied in the array REC. The action of P01ABF then depends on the entry values of IFAIL and IERROR.

If IERROR = 0 (successful termination), the value 0 is simply returned through the routine name. No message is output.

Non-zero values of IERROR indicate abnormal termination and the action taken depends on the value of IFAIL.

If IFAIL = –1 or 1, the value of IERROR is returned through the routine name (soft failure); if IFAIL = 0, then execution of the user's program is terminated without returning to the calling routine (hard failure).

If IFAIL = 1, then no output occurs from P01ABF (silent exit). If IFAIL = 0 or –1, then P01ABF writes messages to the unit number specified by a call to X04AAF (noisy exit). Any messages supplied by the calling routine in the array REC are output first, followed by a record of the form

```
** ABNORMAL EXIT from NAG Fortran Library routine XXXXXX: IFAIL =      n
```

where XXXXXX is the value of SRNAME and n is the value of IERROR. For soft failure this is followed by the record

```
** NAG soft failure: control returned
```

and for hard failure by

```
** NAG hard failure: execution terminated
```

See also Section 8 concerning compatibility with error-handling mechanisms in the NAG Fortran Library before Mark 12.

4. References

None.

5. Parameters

1: IFAIL – INTEGER. *Input*

On entry: the value of IFAIL determines the action of the routine as described in Section 3.

2: IERROR – INTEGER. *Input*

On entry: the value of the error or warning indicator. Unless IFAIL = 0, the value of IERROR is returned through the routine name.

3: SRNAME – CHARACTER*(*). *Input*

On entry: the name of the routine which has called P01ABF. If this is a NAG Fortran Library routine, the length of SRNAME is always 6.

4: NREC – INTEGER. *Input*

On entry: the number of elements (records) in the array REC.

Constraint: NREC ≥ 0.

5: REC(*) – CHARACTER*(*) array. *Input*

Note: the dimension of REC must be greater than or equal to max(1,NREC).

On entry: an internal file. Unless IFAIL = 1, or NREC = 0, the first NREC elements of REC are written to the unit determined by X04AAF. If NREC = 0, then REC is not referenced.

6. Error Indicators and Warnings

None.

7. Accuracy

Not applicable.

8. Further Comments

P01ABF was introduced at Mark 12 of the NAG Fortran Library, to supersede the earlier error-handling P01AAF. P01ABF is compatible with P01AAF except that the details of the messages printed on hard failure have changed.

Compatibility includes even those routines (introduced mainly at Marks 7 and 8) which used IFAIL in a different way to control the output of messages. In those routines IFAIL is regarded as a decimal integer whose least significant two digits are denoted ba with the following meanings:

a = 0: hard failure a = 1: soft failure
b = 0: silent exit b = 1: noisy exit

However this aspect of P01ABF will not, and should not, be used in future.

9. Example

In the simple program below, the subroutine MYSQRT uses P01ABF in the way in which it is usually employed by a NAG Fortran Library routine. Within MYSQRT, error number 1 is associated with an attempt to find a real square root of a negative number. The first call illustrates soft failure with a silent exit, the second call soft failure with a noisy exit and the third call hard failure. Output from the main program is all in upper case characters; output from P01ABF uses lower case characters.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     P01ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Scalars ..
      real             Y
      INTEGER          IFAIL
*     .. External Subroutines ..
      EXTERNAL         MYSQRT
```

```
*     .. Executable Statements ..
      WRITE (NOUT,*) 'P01ABF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'Soft failure, silent exit - message output from the main program'
      IFAIL = 1
      CALL MYSQRT(-1.0e0,Y,IFAIL)
      IF (IFAIL.EQ.0) THEN
         WRITE (NOUT,99999) Y
      ELSE
         WRITE (NOUT,*)
     +     'Attempt to take the square root of a negative number'
      END IF
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Soft failure, noisy exit'
      IFAIL = -1
      CALL MYSQRT(-2.0e0,Y,IFAIL)
      IF (IFAIL.EQ.0) THEN
         WRITE (NOUT,99999) Y
      END IF
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Hard failure, noisy exit'
      IFAIL = 0
      CALL MYSQRT(-3.0e0,Y,IFAIL)
      WRITE (NOUT,99999) Y
      STOP
*
99999 FORMAT (1X,F10.4)
      END
*
      SUBROUTINE MYSQRT(X,Y,IFAIL)
*     Simple routine to compute square root
*     .. Parameters ..
      CHARACTER*6       SRNAME
      PARAMETER         (SRNAME='MYSQRT')
*     .. Scalar Arguments ..
      real              X, Y
      INTEGER           IFAIL
*     .. Local Arrays ..
      CHARACTER*51      REC(1)
*     .. External Functions ..
      INTEGER           P01ABF
      EXTERNAL          P01ABF
*     .. Intrinsic Functions ..
      INTRINSIC         SQRT
*     .. Executable Statements ..
      IF (X.GE.0.0e0) THEN
         Y = SQRT(X)
         IFAIL = 0
      ELSE
         WRITE (REC,99999) '** Attempt to take the square root of ', X
         IFAIL = P01ABF(IFAIL,1,SRNAME,1,REC)
      END IF
      RETURN
*
99999 FORMAT (1X,A,1P,e12.5)
      END
```

9.2. Program Data

None.

9.3. Program Results

```
P01ABF Example Program Results

Soft failure, silent exit - message output from the main program
Attempt to take the square root of a negative number

Soft failure, noisy exit
** Attempt to take the square root of -2.00000E+00
** ABNORMAL EXIT from NAG Library routine MYSQRT: IFAIL =      1
** NAG soft failure - control returned

Hard failure, noisy exit
** Attempt to take the square root of -3.00000E+00
** ABNORMAL EXIT from NAG Library routine MYSQRT: IFAIL =      1
** NAG hard failure - execution terminated
```

Chapter S – Approximations of Special Functions

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
S01BAF	14	$\ln(1+x)$
S01EAF	14	Complex exponential, e^z
S07AAF	1	$\tan x$
S09AAF	1	$\arcsin x$
S09ABF	3	$\arccos x$
S10AAF	3	$\tanh x$
S10ABF	4	$\sinh x$
S10ACF	4	$\cosh x$
S11AAF	4	$\text{arctanh} x$
S11ABF	4	$\text{arcsinh} x$
S11ACF	4	$\text{arccosh} x$
S13AAF	1	Exponential integral $E_1(x)$
S13ACF	2	Cosine integral $\text{Ci}(x)$
S13ADF	5	Sine integral $\text{Si}(x)$
S14AAF	1	Gamma function
S14ABF	8	Log Gamma function
S14ACF	14	$\psi(x) - \ln x$
S14ADF	14	Scaled derivatives of $\psi(x)$
S14BAF	14	Incomplete gamma functions $P(a,x)$ and $Q(a,x)$
S15ABF	3	Cumulative normal distribution function $P(x)$
S15ACF	4	Complement of cumulative normal distribution function $Q(x)$
S15ADF	4	Complement of error function $\text{erfc}(x)$
S15AEF	4	Error function $\text{erf}(x)$
S15AFF	7	Dawson's integral
S15DDF	14	Scaled complex complement of error function, $\exp(-z^2)\text{erfc}(-iz)$
S17ACF	1	Bessel function $Y_0(x)$
S17ADF	1	Bessel function $Y_1(x)$
S17AEF	5	Bessel function $J_0(x)$
S17AFF	5	Bessel function $J_1(x)$
S17AGF	8	Airy function $\text{Ai}(x)$
S17AHF	8	Airy function $\text{Bi}(x)$
S17AJF	8	Airy function $\text{Ai}'(x)$
S17AKF	8	Airy function $\text{Bi}'(x)$
S17DCF	13	Bessel functions $Y_{\nu+a}(z)$, real $a \geq 0$, complex z, $\nu = 0, 1, 2, \ldots$
S17DEF	13	Bessel functions $J_{\nu+a}(z)$, real $a \geq 0$, complex z, $\nu = 0, 1, 2, \ldots$
S17DGF	13	Airy functions $\text{Ai}(z)$ and $\text{Ai}'(z)$, complex z
S17DHF	13	Airy functions $\text{Bi}(z)$ and $\text{Bi}'(z)$, complex z
S17DLF	13	Hankel functions $H^{(j)}_{\nu+a}(z)$, $j = 1, 2$, real $a \geq 0$, complex z, $\nu = 0, 1, 2, \ldots$
S18ACF	1	Modified Bessel function $K_0(x)$
S18ADF	1	Modified Bessel function $K_1(x)$
S18AEF	5	Modified Bessel function $I_0(x)$
S18AFF	5	Modified Bessel function $I_1(x)$
S18CCF	10	Modified Bessel function $e^x K_0(x)$
S18CDF	10	Modified Bessel function $e^x K_1(x)$
S18CEF	10	Modified Bessel function $e^{-\lvert x\rvert} I_0(x)$
S18CFF	10	Modified Bessel function $e^{-\lvert x\rvert} I_1(x)$
S18DCF	13	Modified Bessel functions $K_{\nu+a}(z)$, real $a \geq 0$, complex z, $\nu = 0, 1, 2, \ldots$
S18DEF	13	Modified Bessel functions $I_{\nu+a}(z)$, real $a \geq 0$, complex z, $\nu = 0, 1, 2, \ldots$
S19AAF	11	Kelvin function ber x

S19ABF	11	Kelvin function bei x
S19ACF	11	Kelvin function ker x
S19ADF	11	Kelvin function kei x
S20ACF	5	Fresnel integral $S(x)$
S20ADF	5	Fresnel integral $C(x)$
S21BAF	8	Degenerate symmetrised elliptic integral of 1st kind $R_C(x, y)$
S21BBF	8	Symmetrised elliptic integral of 1st kind $R_F(x, y, z)$
S21BCF	8	Symmetrised elliptic integral of 2nd kind $R_D(x, y, z)$
S21BDF	8	Symmetrised elliptic integral of 3rd kind $R_J(x, y, z, r)$
S21CAF	15	Jacobian elliptic functions sn, cn and dn

Chapter S

Approximations of Special Functions

Contents

1 Scope of the Chapter

This chapter is concerned with the provision of some commonly occurring physical and mathematical functions.

2 Background to the Problems

The majority of the routines in this chapter approximate real-valued functions of a single real argument, and the techniques involved are described in Section 2.1. In addition the chapter contains routines for elliptic integrals (see Section 2.2), Bessel and Airy functions of a complex argument (see Section 2.3), exponential of a complex argument, and complementary error function of a complex argument.

2.1 Functions of a Single Real Argument

Most of the routines for functions of a single real argument have been based on truncated Chebyshev expansions. This method of approximation was adopted as a compromise between the conflicting requirements of efficiency and ease of implementation on many different machine ranges. For details of the reasons behind this choice and the production and testing procedures followed in constructing this chapter see Schonfelder [7].

Basically, if the function to be approximated is $f(x)$, then for $x \in [a, b]$ an approximation of the form

$$f(x) = g(x) {\sum_{r=0}}' C_r T_r(t)$$

is used ($\sum'$ denotes, according to the usual convention, a summation in which the first term is halved), where $g(x)$ is some suitable auxiliary function which extracts any singularities, asymptotes and, if possible, zeros of the function in the range in question and $t = t(x)$ is a mapping of the general range $[a, b]$ to the specific range $[-1, +1]$ required by the Chebyshev polynomials, $T_r(t)$. For a detailed description of the properties of the Chebyshev polynomials see Clenshaw [5] and Fox and Parker [6].

The essential property of these polynomials for the purposes of function approximation is that $T_n(t)$ oscillates between ± 1 and it takes its extreme values $n + 1$ times in the interval $[-1, +1]$. Therefore, provided the coefficients C_r decrease in magnitude sufficiently rapidly the error made by truncating the Chebyshev expansion after n terms is approximately given by

$$E(t) \simeq C_n T_n(t).$$

That is, the error oscillates between $\pm C_n$ and takes its extreme value $n+1$ times in the interval in question. Now this is just the condition that the approximation be a mini-max representation, one which minimizes the maximum error. By suitable choice of the interval, $[a, b]$, the auxiliary function, $g(x)$, and the mapping of the independent variable, $t(x)$, it is almost always possible to obtain a Chebyshev expansion with rapid convergence and hence truncations that provide near mini-max polynomial approximations to the required function. The difference between the true mini-max polynomial and the truncated Chebyshev expansion is seldom sufficiently great enough to be of significance.

The evaluation of the Chebyshev expansions follows one of two methods. The first and most efficient, and hence the most commonly used, works with the equivalent simple polynomial. The second method, which is used on the few occasions when the first method proves to be unstable, is based directly on the truncated Chebyshev series, and uses backward recursion to evaluate the sum. For the first method, a suitably truncated Chebyshev expansion (truncation is chosen so that the error is less than the ***machine precision***) is converted to the equivalent simple polynomial. That is, we evaluate the set of coefficients b_r such that

$$y(t) = \sum_{r=0}^{n-1} b_r t^r = {\sum_{r=0}^{n-1}}' C_r T_r(t).$$

The polynomial can then be evaluated by the efficient Horner's method of nested multiplications,

$$y(t) = (b_0 + t(b_1 + t(b_2 + \ldots t(b_{n-2} + t b_{n-1}))) \ldots).$$

This method of evaluation results in efficient routines but for some expansions there is considerable loss of accuracy due to cancellation effects. In these cases the second method is used. It is well known that if

$$\begin{aligned} b_{n-1} &= C_{n-1} \\ b_{n-2} &= 2tb_{n-1} + C_{n-2} \\ b_j &= 2tb_{j+1} - b_{j+2} + C_j, \quad j = n-3, n-4, \ldots, 0 \end{aligned}$$

then

$$\sum_{r=0}^{\prime} C_r T_r(t) = \tfrac{1}{2}(b_0 - b_2)$$

and this is always stable. This method is most efficiently implemented by using three variables cyclically and explicitly constructing the recursion.

That is,

$$\begin{aligned} \alpha &= C_{n-1} \\ \beta &= 2t\alpha + C_{n-2} \\ \gamma &= 2t\beta - \alpha + C_{n-3} \\ \alpha &= 2t\gamma - \beta + C_{n-4} \\ \beta &= 2t\alpha - \gamma + C_{n-5} \\ &\ldots \\ &\ldots \\ \text{say } \alpha &= 2t\gamma - \beta + C_2 \\ \beta &= 2t\alpha - \gamma + C_1 \\ y(t) &= t\beta - \alpha + \tfrac{1}{2}C_0 \end{aligned}$$

The auxiliary functions used are normally functions compounded of simple polynomial (usually linear) factors extracting zeros, and the primary compiler-provided functions, sin, cos, ln, exp, sqrt, which extract singularities and/or asymptotes or in some cases basic oscillatory behaviour, leaving a smooth well-behaved function to be approximated by the Chebyshev expansion which can therefore be rapidly convergent.

The mappings of $[a, b]$ to $[-1, +1]$ used range from simple linear mappings to the case when b is infinite, and considerable improvement in convergence can be obtained by use of a bilinear form of mapping. Another common form of mapping is used when the function is even; that is, it involves only even powers in its expansion. In this case an approximation over the whole interval $[-a, a]$ can be provided using a mapping $t = 2(x/a)^2 - 1$. This embodies the evenness property but the expansion in t involves all powers and hence removes the necessity of working with an expansion with half its coefficients zero.

For many of the routines an analysis of the error in principle is given, namely, if E and ∇ are the absolute errors in function and argument and ϵ and δ are the corresponding relative errors, then

$$\begin{aligned} E &\simeq |f'(x)|\nabla \\ E &\simeq |xf'(x)|\delta \\ \epsilon &\simeq \left|\frac{xf'(x)}{f(x)}\right|\delta. \end{aligned}$$

If we ignore errors that arise in the argument of the function by propagation of data errors etc., and consider only those errors that result from the fact that a real number is being represented in the

computer in floating-point form with finite precision, then δ is bounded and this bound is independent of the magnitude of x. For example, on an 11-digit machine

$$|\delta| \leq 10^{-11}.$$

(This of course implies that the absolute error $\nabla = x\delta$ is also bounded but the bound is now dependent on x.) However, because of this the last two relations above are probably of more interest. If possible the relative error propagation is discussed; that is, the behaviour of the error amplification factor $|xf'(x)/f(x)|$ is described, but in some cases, such as near zeros of the function which cannot be extracted explicitly, absolute error in the result is the quantity of significance and here the factor $|xf'(x)|$ is described. In general, testing of the functions has shown that their error behaviour follows fairly well these theoretical error behaviours. In regions where the error amplification factors are less than or of the order of one, the errors are slightly larger than the above predictions. The errors are here limited largely by the finite precision of arithmetic in the machine, but ϵ is normally no more than a few times greater than the bound on δ. In regions where the amplification factors are large, of order ten or greater, the theoretical analysis gives a good measure of the accuracy obtainable.

It should be noted that the definitions and notations used for the functions in this chapter are all taken from Abramowitz and Stegun [1]. Users are strongly recommended to consult this book for details before using the routines in this chapter.

2.2 Approximations to Elliptic Integrals

The functions provided here are symmetrised variants of the classic elliptic integrals. These alternative definitions have been suggested by Carlson (see [2], [3] and [4]) and he also developed the basic algorithms used in this chapter.

The standard integral of the first kind is represented by

$$R_F(x,y,z) = \frac{1}{2}\int_0^\infty \frac{dt}{\sqrt{(t+x)(t+y)(t+z)}},$$

where $x, y, z \geq 0$ and at most one may be equal to zero.

The normalisation factor, $\frac{1}{2}$, is chosen so as to make

$$R_F(x,x,x) = 1/\sqrt{x}.$$

If any two of the variables are equal, R_F degenerates into the second function

$$R_C(x,y) = R_F(x,y,y) = \frac{1}{2}\int_0^\infty \frac{dt}{\sqrt{t+x}(t+y)},$$

where the argument restrictions are now $x \geq 0$ and $y \neq 0$.

This function is related to the logarithm or inverse hyperbolic functions if $0 < y < x$, and to the inverse circular functions if $0 \leq x \leq y$.

The integrals of the second kind are defined by

$$R_D(x,y,z) = \frac{3}{2}\int_0^\infty \frac{dt}{\sqrt{(t+x)(t+y)(t+z)^3}}$$

with $z > 0$, $x \geq 0$ and $y \geq 0$, but only one of x or y may be zero.

The function is a degenerate special case of the integral of the third kind

$$R_J(x,y,z,\rho) = \frac{3}{2}\int_0^\infty \frac{dt}{\sqrt{(t+x)(t+y)(t+z)}(t+\rho)}$$

with $\rho \neq 0$ and $x, y, z \geq 0$ with at most one equality holding. Thus $R_D(x,y,z) = R_J(x,y,z,z)$. The normalisation of both these functions is chosen so that

$$R_D(x,x,x) = R_J(x,x,x,x) = 1/(x\sqrt{x}).$$

The algorithms used for all these functions are based on duplication theorems. These allow a recursion system to be established which constructs a new set of arguments from the old using a combination of arithmetic and geometric means. The value of the function at the original arguments can then be simply related to the value at the new arguments. These recursive reductions are used until the arguments differ from the mean by an amount small enough for a Taylor series about the mean to give sufficient accuracy when retaining terms of order less than six. Each step of the recurrences reduces the difference from the mean by a factor of four, and as the truncation error is of order six, the truncation error goes like $(4096)^{-n}$, where n is the number of iterations.

The above forms can be related to the more traditional canonical forms (see Abramowitz and Stegun [1], 17.2).

If we write $q = \cos^2\phi$, $r = 1 - m.\sin^2\phi$, $s = 1 + n.\sin^2\phi$, where $0 < \phi \leq \frac{1}{2}\pi$, we have:

the elliptic integral of the first kind:

$$F(\phi|m) = \int_0^{\sin\phi} (1-t^2)^{-1/2}(1-mt^2)^{-1/2}dt = \sin\phi.R_F(q,r,1);$$

the elliptic integral of the second kind:

$$\begin{aligned} E(\phi|m) &= \int_0^{\sin\phi} (1-t^2)^{-1/2}(1-mt^2)^{1/2}dt \\ &= \sin\phi.R_F(q,r,1) - \tfrac{1}{3}m.\sin^3\phi.R_D(q,r,1) \end{aligned}$$

the elliptic integral of the third kind:

$$\begin{aligned} \Pi(n;\phi|m) &= \int_0^{\sin\phi} (1-t^2)^{-1/2}(1-mt^2)^{-1/2}(1+nt^2)^{-1}dt \\ &= \sin\phi.R_F(q,r,1) - \tfrac{1}{3}n.\sin^3\phi.R_J(q,r,1,s). \end{aligned}$$

Also the complete elliptic integral of the first kind:

$$K(m) = \int_0^{\pi/2} (1-m.\sin^2\theta)^{-1/2}d\theta = R_F(0,1-m,1);$$

the complete elliptic integral of the second kind:

$$E(m) = \int_0^{\pi/2} (1-m.\sin^2\theta)^{1/2}d\theta = R_F(0,1-m,1) - \tfrac{1}{3}m.R_D(0,1-m,1).$$

2.3 Bessel and Airy Functions of a Complex Argument

The routines for Bessel and Airy functions of a real argument are based on Chebyshev expansions, as described in Section 2.1. The routines for functions of a complex argument, however, use different methods. These routines relate all functions to the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ computed in the right-half complex plane, including their analytic continuations. I_ν and K_ν are computed by different methods according to the values of z and ν. The methods include power series, asymptotic expansions and Wronskian evaluations. The relations between functions are based on well known formulae (see Abramowitz and Stegun [1]).

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

3.1 Elliptic Integrals

IMPORTANT ADVICE: users who encounter elliptic integrals in the course of their work are strongly recommended to look at transforming their analysis directly to one of the Carlson forms, rather than to

the traditional canonical Legendre forms. In general, the extra symmetry of the Carlson forms is likely to simplify the analysis, and these symmetric forms are much more stable to calculate.

The routine S21BAF for R_C is largely included as an auxiliary to the other routines for elliptic integrals. This integral essentially calculates elementary functions, e.g.

$$\begin{aligned}
\ln x &= (x-1).R_C\left(\left(\frac{1+x}{2}\right)^2, x\right), \quad x > 0; \\
\arcsin x &= x.R_C(1-x^2, 1), \ |x| \leq 1; \\
\operatorname{arcsinh} x &= x.R_C(1+x^2, 1), \text{ etc.}
\end{aligned}$$

In general this method of calculating these elementary functions is not recommended as there are usually much more efficient specific routines available in the Library. However, S21BAF may be used, for example, to compute $\ln x/(x-1)$ when x is close to 1, without the loss of significant figures that occurs when $\ln x$ and $x-1$ are computed separately.

3.2 Bessel and Airy Functions

For computing the Bessel functions $J_\nu(x)$, $Y_\nu(x)$, $I_\nu(x)$ and $K_\nu(x)$ where x is real and $\nu = 0$ or 1, special routines are provided, which are much faster than the more general routines that allow a complex argument and arbitrary real $\nu \geq 0$. Similarly, special routines are provided for computing the Airy functions and their derivatives $\mathrm{Ai}(x)$, $\mathrm{Bi}(x)$, $\mathrm{Ai}'(x)$, $\mathrm{Bi}'(x)$ for a real argument which are much faster than the routines for complex arguments.

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Tangent, hyperbolic	S10AAF
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5 References

[1] Abramowitz M and Stegun I A (1972) *Handbook of Mathematical Functions* Dover Publications (3rd Edition)

[2] Carlson B C (1965) On computing elliptic integrals and functions *J. Math. Phys.* **44** 36–51

[3] Carlson B C (1977) *Special Functions of Applied Mathematics* Academic Press

[4] Carlson B C (1977) Elliptic integrals of the first kind *SIAM J. Math. Anal.* **8** 231–242

[5] Clenshaw C W (1962) Mathematical tables *Chebyshev Series for Mathematical Functions* HMSO

[6] Fox L and Parker I B (1968) *Chebyshev Polynomials in Numerical Analysis* Oxford University Press

[7] Schonfelder J L (1976) The production of special function routines for a multi-machine library *Softw. Pract. Exper.* **6 (1)**

S01BAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S01BAF returns a value of the shifted logarithmic function, $\ln(1+x)$, via the routine name.

2. Specification

```
real FUNCTION S01BAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine computes values of $\ln(1+x)$, retaining full relative precision even when $|x|$ is small. The routine is based on the Chebyshev expansion

$$\ln\frac{1+p^2+2p\bar{x}}{1+p^2-2p\bar{x}} = 4\sum_{k=0}^{\infty}\frac{p^{2k+1}}{2k+1}T_{2k+1}(\bar{x}).$$

Setting $\bar{x} = \dfrac{x(1+p^2)}{2p(x+2)}$, and choosing $p = \dfrac{q-1}{q+1}$, $q = \sqrt[4]{2}$ the expansion is valid in the domain $x \in \left[\dfrac{1}{\sqrt{2}}-1, \sqrt{2}-1\right]$. Outside this domain, $\ln(1+x)$ is computed by the Fortran intrinsic logarithmic function.

4. References

[1] LYUSTERNIK, L.A., CHERVONENKIS, O.A. and YANPOLSKII, A.R.
Handbook for Computing Elementary Functions, p. 57.
Pergamon Press, 1965.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > −1.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, X ≤ −1.0.

The result is returned as zero.

7. Accuracy

The returned result should be accurate almost to ***machine precision***, with a limit of about 20 significant figures due to the precision of internal constants. Note however that if x lies very close to -1.0 and is not exact (for example if x is the result of some previous computation and has been rounded), then precision will be lost in the computation of $1 + x$, and hence $\ln(1+x)$, in S01BAF.

8. Further Comments

Empirical tests show that the time taken for a call of S01BAF usually lies between about 1.25 and 2.5 times the time for a call to the standard Fortran function LOG.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S01BAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. External Functions ..
      real             S01BAF
      EXTERNAL         S01BAF
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S01BAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '       X           Y'
   20 READ (NIN,*,END=40) X
      IFAIL = 0
*
      Y = S01BAF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.4)
      END
```

9.2. Program Data

```
S01BAF Example Program Data
  2.50E+0
  1.25E-1
 -9.06E-1
  1.29E-3
 -7.83E-6
  1.00E-9
```

9.3. Program Results

```
S01BAF Example Program Results

      X           Y
 2.5000E+00  1.2528E+00
 1.2500E-01  1.1778E-01
-9.0600E-01 -2.3645E+00
 1.2900E-03  1.2892E-03
-7.8300E-06 -7.8300E-06
 1.0000E-09  1.0000E-09
```

S01EAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S01EAF evaluates the exponential function e^z, for ***complex*** z.

2. Specification

complex FUNCTION S01EAF (Z, IFAIL)
INTEGER IFAIL
complex Z

3. Description

This routine evaluates the exponential function e^z, taking care to avoid machine overflow, and giving a warning if the result cannot be computed to more than half precision. The function is evaluated as $e^z = e^x(\cos y + i \sin y)$, where x and y are the real and imaginary parts respectively of z.

Since $\cos y$ and $\sin y$ are less than or equal to 1 in magnitude, it is possible that e^x may overflow although $e^x \cos y$ or $e^x \sin y$ does not. In this case the alternative formula $\text{sign}(\cos y)e^{x+\ln|\cos y|}$ is used for the real part of the result, and $\text{sign}(\sin y)e^{x+\ln|\sin y|}$ for the imaginary part. If either part of the result still overflows, a warning is returned through parameter IFAIL.

If Im z is too large, precision may be lost in the evaluation of $\sin y$ and $\cos y$. Again, a warning is returned through IFAIL.

4. References

None.

5. Parameters

1: Z – ***complex***. *Input*

On entry: the argument z of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

The real part of the result overflows, and is set to the largest safe number with the correct sign. The imaginary part of the result is meaningful.

IFAIL = 2

The imaginary part of the result overflows, and is set to the largest safe number with the correct sign. The real part of the result is meaningful.

IFAIL = 3

Both real and imaginary parts of the result overflow, and are set to the largest safe number with the correct signs.

IFAIL = 4

The computed result is accurate to less than half precision, due to the size of Im z.

IFAIL = 5

The computed result has no precision, due to the size of Im z, and is set to zero.

7. Accuracy

Accuracy is limited in general only by the accuracy of the Fortran intrinsic functions in the computation of $\sin y$, $\cos y$ and e^x, where x = Re z, y = Im z. As y gets larger, precision will probably be lost due to argument reduction in the evaluation of the sine and cosine functions, until the warning error IFAIL = 4 occurs when y gets larger than $\sqrt{1/\varepsilon}$, where ε is the ***machine precision***. Note that on some machines, the intrinsic functions SIN and COS will not operate on arguments larger than about $\sqrt{1/\varepsilon}$, and so IFAIL can never return as 4.

In the comparatively rare event that the result is computed by the formulae $\text{sign}(\cos y)e^{x+\ln|\cos y|}$ and $\text{sign}(\sin y)e^{x+\ln|\sin y|}$, a further small loss of accuracy may be expected due to rounding errors in the logarithmic function.

8. Further Comments

None.

9. Example

The following program reads values of the argument z from a file, evaluates the function at each value of z and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S01EAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          W, Z
      INTEGER          IFAIL
*     .. External Functions ..
      complex          S01EAF
      EXTERNAL         S01EAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S01EAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     + '                Z                                   exp(Z)'
   20 READ (NIN,*,END=40) Z
      IFAIL = 0
*
      W = S01EAF(Z,IFAIL)
*
      WRITE (NOUT,99999) Z, W
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,'(',F12.4,',',F12.4,')      (',F12.4,',',F12.4,')')
      END
```

9.2. Program Data

```
S01EAF Example Program Data
( 1.0, 0.0)
(-0.5, 2.0)
( 0.0,-2.0)
(-2.5,-1.5)
```

9.3. Program Results

```
S01EAF Example Program Results

                Z                                  exp(Z)
(      1.0000,      0.0000)      (      2.7183,      0.0000)
(     -0.5000,      2.0000)      (     -0.2524,      0.5515)
(      0.0000,     -2.0000)      (     -0.4161,     -0.9093)
(     -2.5000,     -1.5000)      (      0.0058,     -0.0819)
```

S07AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S07AAF returns the value of the circular tangent, $\tan x$, via the routine name.

2. Specification

```
real FUNCTION S07AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the circular tangent of its argument, $\tan x$. It is based on the Chebyshev expansion

$$\tan\theta = \theta\, y(t) = \theta {\sum_{r=0}}' c_r T_r(t)$$

where $-\frac{\pi}{4} < \theta < \frac{\pi}{4}$ and $-1 < t < +1$, $\quad t = 2\left(\frac{4\theta}{\pi}\right)^2 - 1.$

The reduction to the standard range is accomplished by taking

$$x = N\pi/2 + \theta$$

where N is an integer and $-\frac{\pi}{4} < \theta < \frac{\pi}{4}$,

i.e. $\theta = x - \left(\frac{2x}{\pi}\right)\frac{\pi}{2}$ where $N = \left[\frac{2x}{\pi}\right]$ = the nearest integer to $\frac{2x}{\pi}$.

From the properties of $\tan x$ it follows that

$$\tan x = \left\{\begin{matrix} \tan\theta, & N \text{ even} \\ -1/\tan\theta, & N \text{ odd} \end{matrix}\right\}$$

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.3, p. 71, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument that is too large; the default result returned is zero.

IFAIL = 2

The routine has been called with an argument that is too close to an odd multiple of $\pi/2$, at which the function is infinite; the routine returns a value with the correct sign but a more or less arbitrary but large magnitude (see Section 7).

7. Accuracy

If δ and ε are the relative errors in the argument and result respectively, then in principle

$$\varepsilon \geq \frac{2x}{\sin 2x}\ \delta.$$

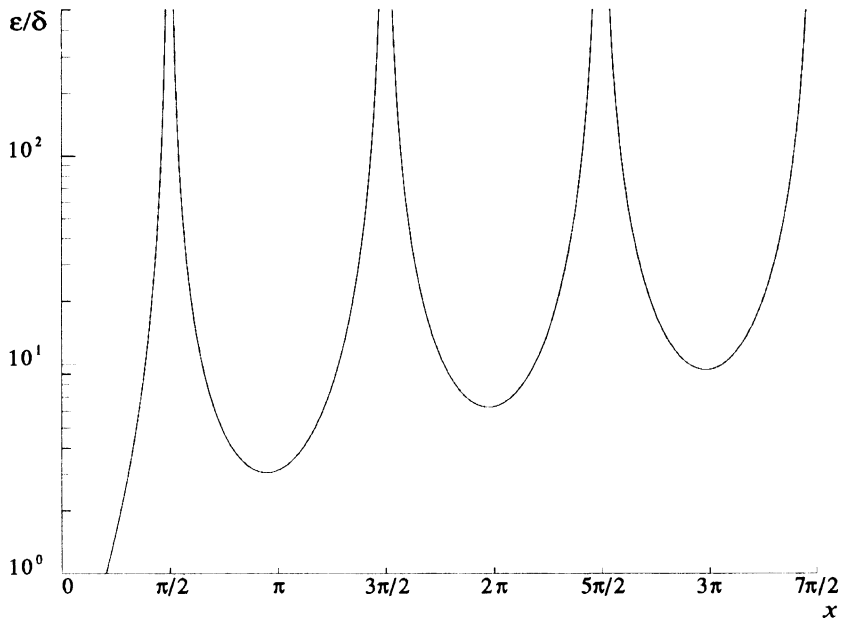
That is a relative error in the argument, x, is amplified by at least a factor $2x/\sin 2x$ in the result.

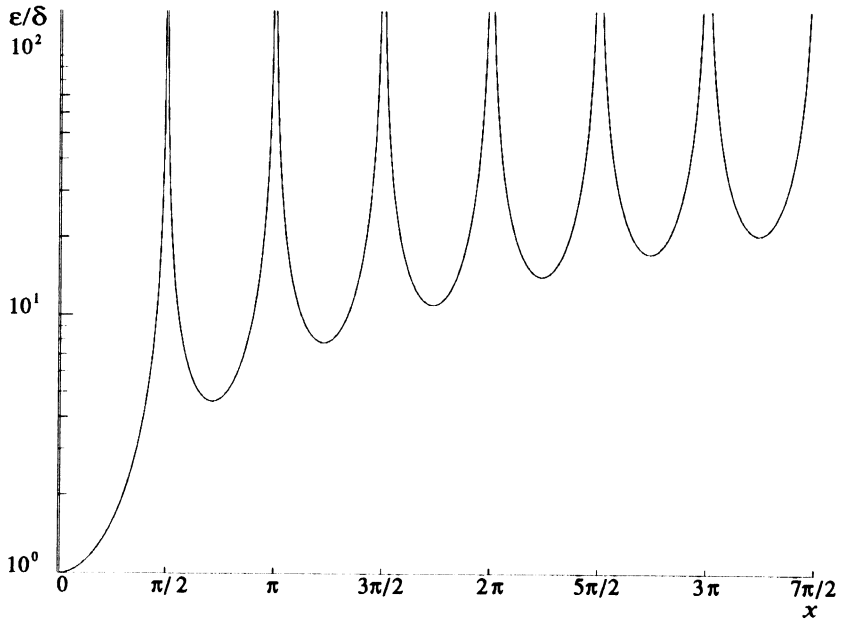
Similarly if E is the absolute error in the result this is given by

$$E \geq \frac{x}{\cos^2 x}\ \delta.$$

The equalities should hold if δ is greater than the ***machine precision*** (δ is a result of data errors etc.) but if δ is simply the round off error in the machine it is possible that internal calculation rounding will lose an extra figure.

The graphs below show the behaviour of these amplification factors.





In the principal range it is possible to preserve relative accuracy even near the zero of $\tan x$ at $x = 0$ but at the other zeros only absolute accuracy is possible. Near the infinities of $\tan x$ both the relative and absolute errors become infinite and the routine must fail (error 2).

If N is odd and $|\theta| \leq xF_2$ the routine could not return better than two figures and in all probability would produce a result that was in error in its most significant figure. Therefore the routine fails and it returns the value

$$-\text{sign}\theta\left(\frac{1}{|xF_2|}\right) \simeq -\text{sign}\theta \tan\left(\frac{\pi}{2}-|xF_2|\right)$$

which is the value of the tangent at the nearest argument for which a valid call could be made.

Accuracy is also unavoidably lost if the routine is called with a large argument. If $|x| > F_1$ the routine fails (error 1) and returns zero. (See the Users' Note for your implementation for specific values of F_1 and F_2).

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S07AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
```

```
*     .. External Functions ..
      real               S07AAF
      EXTERNAL           S07AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S07AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y          IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S07AAF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S07AAF Example Program Data
            -2.0
            -0.5
             1.0
             3.0
             1.5708
```

9.3. Program Results

```
 S07AAF Example Program Results

      X           Y          IFAIL

  -2.000E+00   2.185E+00       0
  -5.000E-01  -5.463E-01       0
   1.000E+00   1.557E+00       0
   3.000E+00  -1.425E-01       0
   1.571E+00  -2.722E+05       0
```

S09AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S09AAF returns the value of the inverse circular sine, $\arcsin x$, via the routine name. The value is in the principal range $(-\pi/2, \pi/2)$

2. Specification

```
real FUNCTION S09AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the inverse circular sine, $\arcsin x$. It is based on the Chebyshev expansion

$$\arcsin x = x \times y(x) = x \sum_{r=0}' a_r T_r(t)$$

where $-\frac{1}{\sqrt{2}} \leq x \leq \frac{1}{\sqrt{2}}$ and $t = 4x^2 - 1$.

For $x^2 \leq \frac{1}{2}$, $\arcsin x = x \times y(x)$.

For $\frac{1}{2} < x^2 \leq 1$, $\arcsin x = \text{sign}\, x \left\{ \frac{\pi}{2} - \arcsin\sqrt{1-x^2} \right\}$.

For $x^2 > 1$, $\arcsin x$ is undefined and the routine fails.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.4, p. 79, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: $|X| \leq 1.0$.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument greater than 1.0 in absolute value; $\arcsin x$ is undefined and the routine returns zero.

7. Accuracy

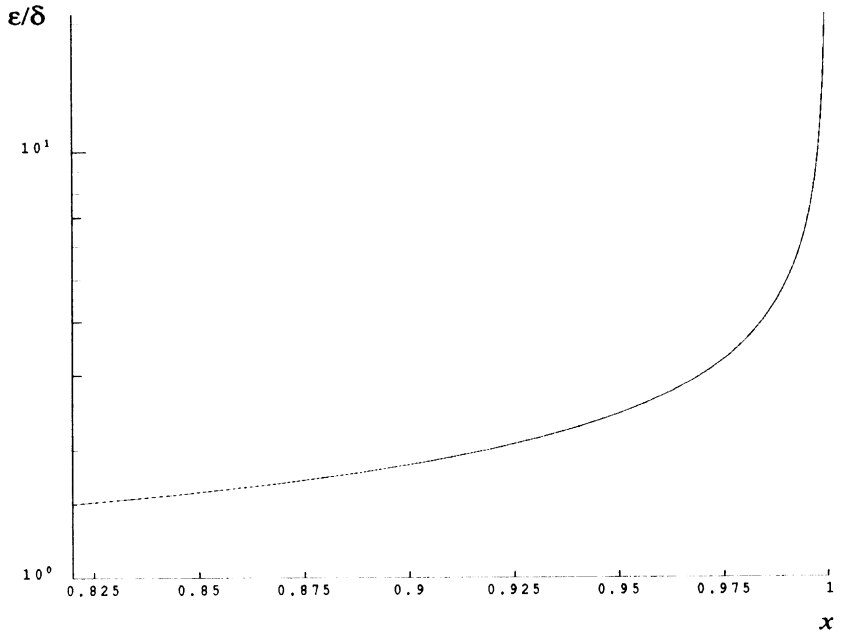
If δ and ε are the relative errors in the argument and result, respectively, then in principle

$$|\varepsilon| \simeq \left| \frac{x}{\arcsin x \sqrt{1-x^2}} \times \delta \right|.$$

That is, a relative error in the argument x, is amplified by at least a factor $\dfrac{x}{\arcsin x \sqrt{1-x^2}}$ in the result.

The equality should hold if δ is greater than the ***machine precision*** (δ is a result of data errors etc.) but if δ is produced simply by round off error in the machine it is possible that rounding in internal calculations may lose an extra figure in the result.

This factor stays close to one except near $|x| = 1$ where its behaviour is shown in the following graph.



For $|x|$ close to unity, $1 - |x| \sim \delta$, the above analysis is no longer applicable owing to the fact that both argument and result are subject to finite bounds, ($|x| \leq 1$ and $|\arcsin x| \leq \frac{1}{2}\pi$). In this region $\varepsilon \sim \sqrt{\delta}$, that is the result will have approximately half as many correct significant figures as the argument.

For $|x| = 1$ the result will be correct to full ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S09AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S09AAF
      EXTERNAL         S09AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S09AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S09AAF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S09AAF Example Program Data
            -0.5
             0.1
             0.9
             2.0
            -1.5
```

9.3. Program Results

```
 S09AAF Example Program Results

      X           Y        IFAIL

  -5.000E-01  -5.236E-01       0
   1.000E-01   1.002E-01       0
   9.000E-01   1.120E+00       0
   2.000E+00   0.000E+00       1
  -1.500E+00   0.000E+00       1
```

S09ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S09ABF returns the value of the inverse circular cosine, arccos x, via the routine name; the result is in the principal range $(0,\pi)$.

2. Specification

```
real FUNCTION S09ABF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the inverse circular cosine, arccos x. It is based on the Chebyshev expansion

$$\arcsin x = x \times y(t) = x \sum_{r=0}{}' a_r T_r(t)$$

where $\frac{-1}{\sqrt{2}} \leq x \leq \frac{1}{\sqrt{2}}$, and $t = 4x^2 - 1$.

For $x^2 \leq \frac{1}{2}$, $\arccos x = \frac{\pi}{2} - \arcsin x$.

For $-1 \leq x < \frac{-1}{\sqrt{2}}$, $\arccos x = \pi - \arcsin\sqrt{1-x^2}$.

For $\frac{1}{\sqrt{2}} < x \leq 1$, $\arccos x = \arcsin\sqrt{1-x^2}$.

For $|x| > 1$, arccos x is undefined and the routine fails.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.4., p. 79, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: |X| ≤ 1.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

S09ABF has been called with |X| > 1.0, for which arccos is undefined. A zero result is returned.

7. Accuracy

If δ and ε are the relative errors in the argument and the result, respectively, then in principle

$$|\varepsilon| \simeq \left| \frac{x}{\arccos x \sqrt{1-x^2}} \times \delta \right|.$$

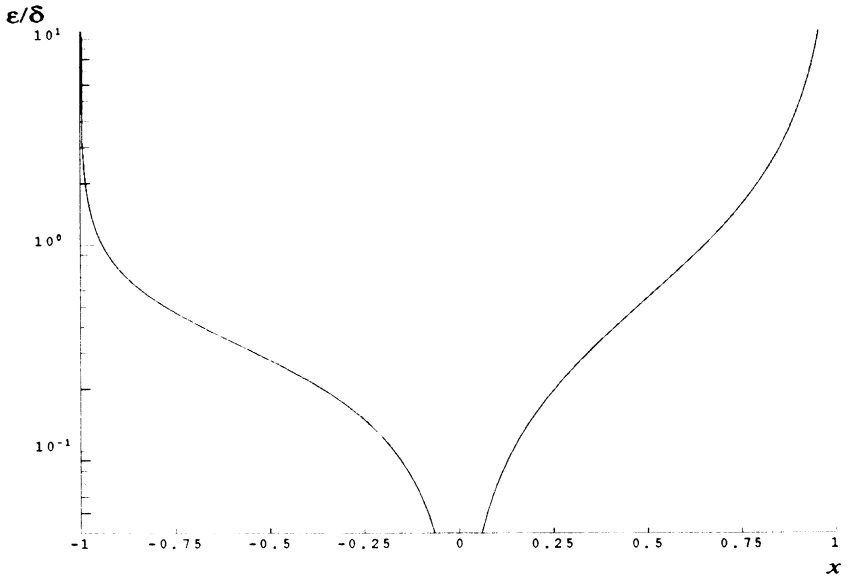
The equality should hold if δ is greater than the ***machine precision*** (δ is due to data errors etc.), but if δ is due simply to round-off in the machine it is possible that rounding etc. in internal calculations may lose one extra figure.

The behaviour of the amplification factor $\dfrac{x}{\arccos x \sqrt{1-x^2}}$ is shown in the graph below.

In the region of $x = 0$ this factor tends to zero and the accuracy will be limited by the ***machine precision***. For $|x|$ close to one, $1 - |x| \sim \delta$, the above analysis is not applicable owing to the fact that both the argument and the result are bounded $|x| \leq 1$, $0 \leq \arccos x \leq \pi$.

In the region of $x \sim -1$ we have $\varepsilon \sim \sqrt{\delta}$, that is the result will have approximately half as many correct significant figures as the argument.

In the region $x \sim +1$, we have that the absolute error in the result, E, is given by $E \sim \sqrt{\delta}$, that is the result will have approximately half as many decimal places correct as there are correct figures in the argument.



8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S09ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S09ABF
      EXTERNAL         S09ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S09ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S09ABF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S09ABF Example Program Data
            -0.5
             0.1
             0.9
             2.0
            -1.5
```

9.3. Program Results

```
 S09ABF Example Program Results

      X           Y        IFAIL

  -5.000E-01   2.094E+00       0
   1.000E-01   1.471E+00       0
   9.000E-01   4.510E-01       0
   2.000E+00   0.000E+00       1
  -1.500E+00   0.000E+00       1
```

S10AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S10AAF returns a value for the hyperbolic tangent, $\tanh x$, via the routine name.

2. Specification

```
real FUNCTION S10AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the hyperbolic tangent of its argument, $\tanh x$.

For $|x| \leq 1$ it is based on the Chebyshev expansion

$$\tanh x = x \times y(t) = x \sum_{r=0}' a_r T_r(t)$$

where $-1 \leq x \leq 1$, $-1 \leq t \leq 1$, and $t = 2x^2 - 1$.

For $1 < |x| < E_1$ (See the Users' Note for your implementation for value of E_1)

$$\tanh x = \frac{e^{2x} - 1}{e^{2x} + 1}$$

For $|x| \geq E_1$, $\tanh x = \text{sign}\, x$ to within the representation accuracy of the machine and so this approximation is used.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.5, p. 83, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with the other routines in this chapter.

7. Accuracy

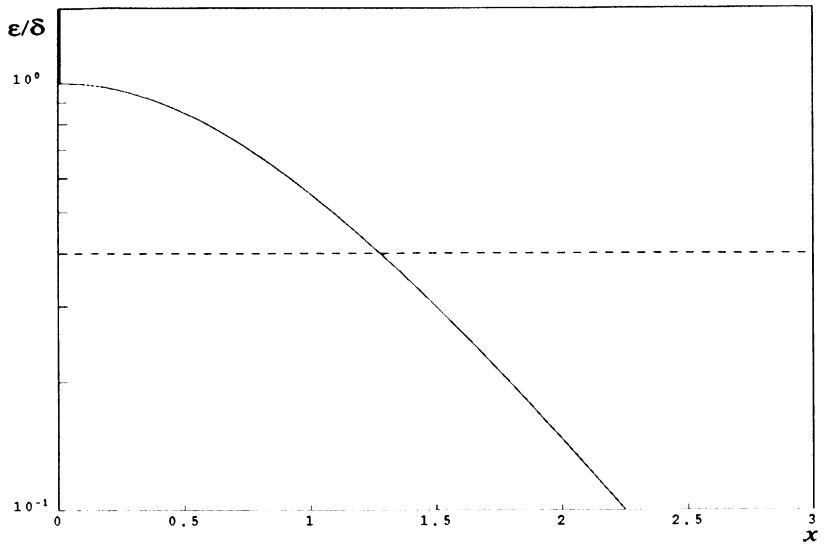
If δ and ε are the relative errors in the argument and the result respectively, then in principle,

$$|\varepsilon| \simeq \left| \frac{2x}{\sinh 2x} \delta \right|.$$

That is, a relative error in the argument, x, is amplified by a factor approximately $\frac{2x}{\sinh 2x}$, in the result.

The equality should hold if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is due simply to the round-off in the machine representation it is possible that an extra figure may be lost in internal calculation round-off.

The behaviour of the amplification factor is shown in the following graph:



It should be noted that this factor is always less than or equal to 1.0 and away from $x = 0$ the accuracy will eventually be limited entirely by the precision of machine representation.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S10AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S10AAF
      EXTERNAL         S10AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S10AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S10AAF(X,IFAIL)
*
```

```
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S10AAF Example Program Data
           -20.0
            -5.0
             0.5
             5.0
```

9.3. Program Results

```
 S10AAF Example Program Results

      X            Y         IFAIL

  -2.000E+01  -1.000E+00       0
  -5.000E+00  -9.999E-01       0
   5.000E-01   4.621E-01       0
   5.000E+00   9.999E-01       0
```

S10ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S10ABF returns the value of the hyperbolic sine, $\sinh x$, via the routine name.

2. Specification

```
real FUNCTION S10ABF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the hyperbolic sine of its argument, $\sinh x$.

For $|x| \leq 1$ it uses the Chebyshev expansion

$$\sinh x = x \times y(t) = x \sum_{r=0}' a_r T_r(t)$$

where $t = 2x^2 - 1$.

For $1 < |x| \leq E_1$, $\quad \sinh x = \frac{1}{2}(e^x - e^{-x})$

where E_1 is a machine-dependent constant, details of which are given in the Users' Note for your implementation.

For $|x| > E_1$, the routine fails owing to the danger of setting overflow in calculating e^x. The result returned for such calls is $\sinh(\text{sign}\, x E_1)$, i.e. it returns the result for the nearest valid argument.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.5, p. 83, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument too large in absolute magnitude. There is a danger of setting overflow. The result is the value of sinh at the closest argument for which a valid call could be made. (See Section 3 and the Users' Note for your implementation).

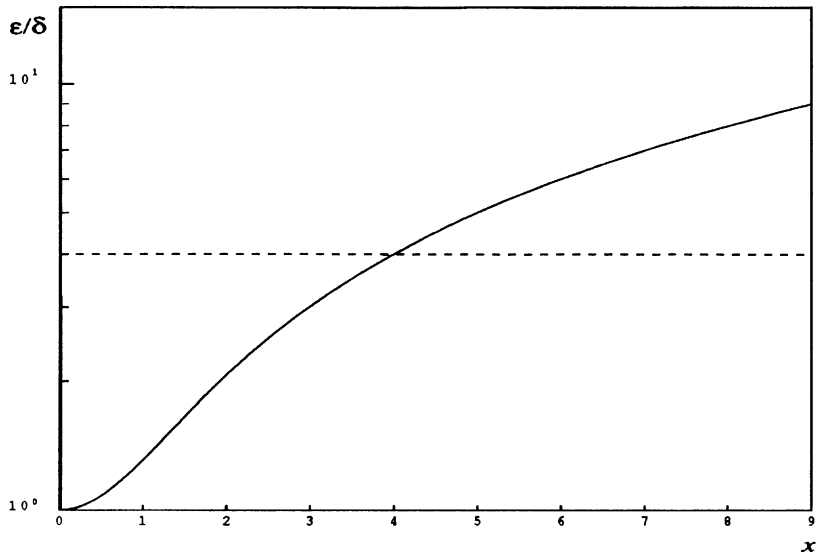
7. Accuracy

If δ and ε are the relative errors in the argument and result, respectively, then in principle

$$|\varepsilon| \simeq |x \coth x \times \delta|.$$

That is the relative error in the argument, x, is amplified by a factor, approximately $x \coth x$. The equality should hold if δ is greater than the ***machine precision*** (δ is a result of data errors etc.) but, if δ is simply a result of round-off in the machine representation of x, then it is possible that an extra figure may be lost in internal calculation round-off.

The behaviour of the error amplification factor can be seen in the following graph:



It should be noted that for $|x| \geq 2$

$$\varepsilon \sim x\delta = \Delta$$

where Δ is the absolute error in the argument.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S10ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S10ABF
      EXTERNAL         S10ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S10ABF Example Program Results'
```

```
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S10ABF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S10ABF Example Program Data
          -10.0
           -0.5
            0.0
            0.5
           25.0
```

9.3. Program Results

```
 S10ABF Example Program Results

      X           Y         IFAIL

  -1.000E+01  -1.101E+04       0
  -5.000E-01  -5.211E-01       0
   0.000E+00   0.000E+00       0
   5.000E-01   5.211E-01       0
   2.500E+01   3.600E+10       0
```

S10ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S10ACF returns the value of the hyperbolic cosine, $\cosh x$, via the routine name.

2. Specification

```
real FUNCTION S10ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the hyperbolic cosine, $\cosh x$.

For $|x| \leq E_1$, $\quad \cosh x = \frac{1}{2}(e^x + e^{-x})$.

For $|x| > E_1$, the routine fails owing to danger of setting overflow in calculating e^x. The result returned for such calls is $\cosh E_1$, i.e. it returns the result for the nearest valid argument. The value of machine-dependent constant E_1 may be given in the Users' Note for your implementation.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.5, p. 83, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument too large in absolute magnitude. There is a danger of overflow. The result returned is the value of $\cosh x$ at the nearest valid argument.

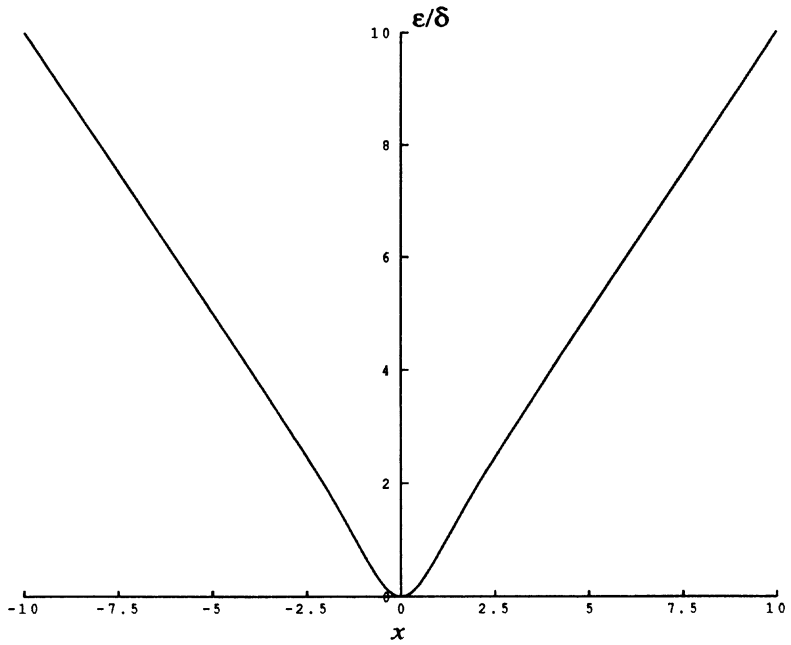
7. Accuracy

If δ and ε are the relative errors in the argument and result, respectively, then in principle

$$\varepsilon \simeq x \tanh x \times \delta.$$

That is, the relative error in the argument, x, is amplified by a factor, at least $x \tanh x$. The equality should hold if δ is greater than the ***machine precision*** (δ is due to data errors etc.) but if δ is simply a result of round-off in the machine representation of x then it is possible that an extra figure may be lost in internal calculation round-off.

The behaviour of the error amplification factor is shown by the following graph:



It should be noted that near $x = 0$ where this amplification factor tends to zero the accuracy will be limited eventually by the machine precision. Also for $|x| \geq 2$

$$\varepsilon \sim x\delta = \Delta$$

where Δ is the absolute error in the argument x.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S10ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S10ACF
      EXTERNAL         S10ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S10ACF Example Program Results'
```

```
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S10ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S10ACF Example Program Data
          -10.0
           -0.5
            0.0
            0.5
           25.0
```

9.3. Program Results

```
 S10ACF Example Program Results

      X           Y         IFAIL

  -1.000E+01   1.101E+04       0
  -5.000E-01   1.128E+00       0
   0.000E+00   1.000E+00       0
   5.000E-01   1.128E+00       0
   2.500E+01   3.600E+10       0
```

S11AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S11AAF returns the value of the inverse hyperbolic tangent, arctanh x, via the routine name.

2. Specification

```
real FUNCTION S11AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the inverse hyperbolic tangent of its argument, arctanh x.

For $x^2 \leq \frac{1}{2}$ it is based on the Chebyshev expansion

$$\text{arctanh}\, x = x \times y(t) = x \sum_{r=0}' a_r T_r(t)$$

where $-\frac{1}{\sqrt{2}} \leq x \leq \frac{1}{\sqrt{2}}$, $\quad -1 \leq t \leq 1$, $\quad$ and $t = 4x^2 - 1$.

For $\frac{1}{2} < x^2 < 1$, it uses

$$\text{arctanh}\, x = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right).$$

For $|x| \geq 1$, the routine fails as arctanh x is undefined.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.6, p. 86, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: |X| < 1.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument greater than or equal to 1.0 in magnitude, for which arctanh is not defined. The result is returned as zero.

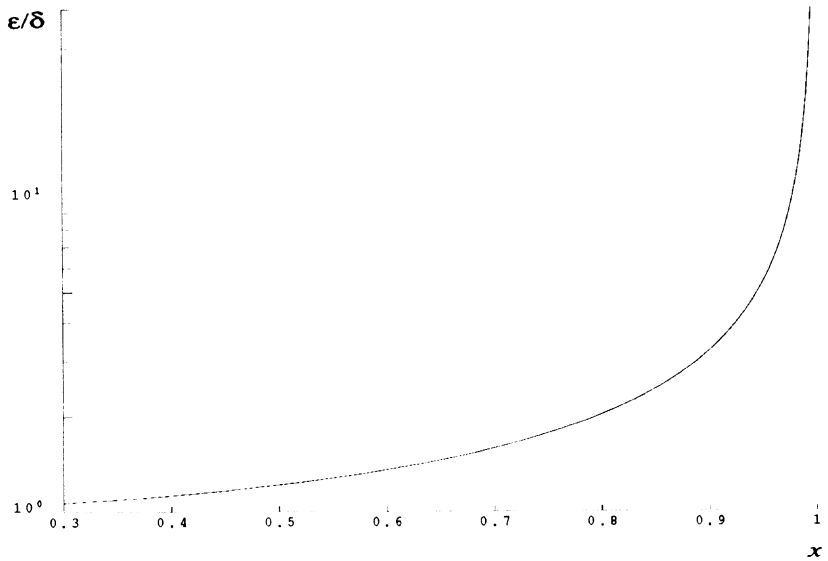
7. Accuracy

If δ and ε are the relative errors in the argument and result, respectively, then in principle

$$|\varepsilon| \simeq \left| \frac{x}{(1-x^2)\operatorname{arctanh} x} \times \delta \right|.$$

That is, the relative error in the argument, x, is amplified by at least a factor $\dfrac{x}{(1-x^2)\operatorname{arctanh} x}$ in the result. The equality should hold if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is simply due to round-off in the machine representation then it is possible that an extra figure may be lost in internal calculation round-off.

The behaviour of the amplification factor is shown in the following graph:



The factor is not significantly greater than one except for arguments close to $|x| = 1$. However in the region where $|x|$ is close to one, $1 - |x| \sim \delta$, the above analysis is inapplicable since x is bounded by definition, $|x| < 1$. In this region where arctanh is tending to infinity we have

$$\varepsilon \sim 1/\ln \delta$$

which implies an obvious, unavoidable serious loss of accuracy near $|x| \sim 1$, e.g. if x and 1 agree to 6 significant figures, the result for $\operatorname{arctanh} x$ would be correct to at most about one figure.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S11AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S11AAF
      EXTERNAL         S11AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S11AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S11AAF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S11AAF Example Program Data
            -0.5
             0.0
             0.5
            -0.9999
             3.0
```

9.3. Program Results

```
 S11AAF Example Program Results

      X           Y         IFAIL

  -5.000E-01  -5.493E-01       0
   0.000E+00   0.000E+00       0
   5.000E-01   5.493E-01       0
  -9.999E-01  -4.952E+00       0
   3.000E+00   0.000E+00       1
```

S11ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S11ABF returns the value of the inverse hyperbolic sine, $\operatorname{arcsinh} x$, via the routine name.

2. Specification

```
real FUNCTION S11ABF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the inverse hyperbolic sine of its argument, $\operatorname{arcsinh} x$.

For $|x| \leq 1$ it is based on the Chebyshev expansion

$$\operatorname{arcsinh} x = x \times y(t) = x \sum_{r=0}{}' c_r T_r(t), \qquad \text{where } t = 2x^2 - 1.$$

For $|x| > 1$ it uses the fact that

$$\operatorname{arcsinh} x = \operatorname{sign} x \times \ln\left(|x| + \sqrt{x^2+1}\right).$$

This form is used directly for $1 < |x| < 10^k$, where $k = n/2 + 1$, and the machine uses approximately n decimal place arithmetic.

For $|x| \geq 10^k$, $\sqrt{x^2+1}$ is equal to $|x|$ to within the accuracy of the machine and hence we can guard against premature overflow and, without loss of accuracy, calculate

$$\operatorname{arcsinh} x = \operatorname{sign} x \times (\ln 2 + \ln |x|).$$

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.6, p. 86, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with the other routines in this chapter.

7. Accuracy

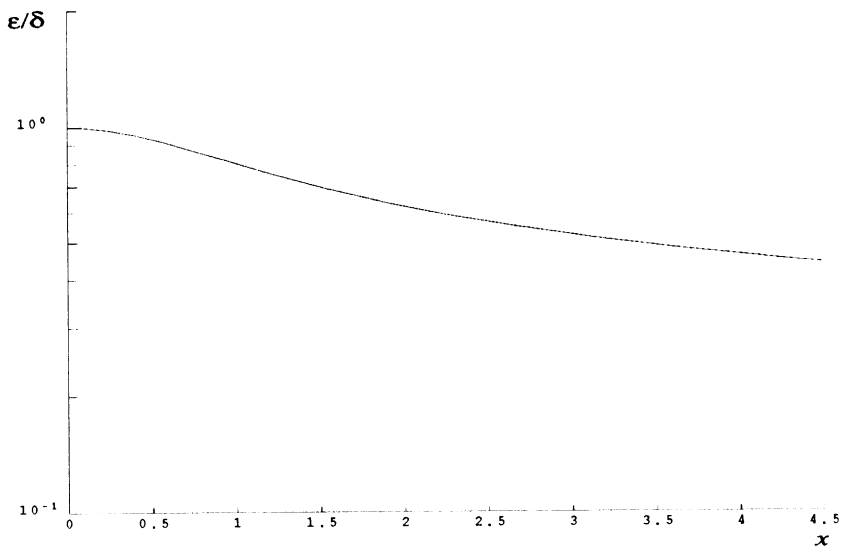
If δ and ε are the relative errors in the argument and the result, respectively, then in principle

$$|\varepsilon| \simeq \left| \frac{x}{\sqrt{1+x^2}\ \operatorname{arcsinh} x} \delta \right|.$$

That is, the relative error in the argument, x, is amplified by a factor at least $\frac{x}{\sqrt{1+x^2}\ \operatorname{arcsinh} x}$, in the result.

The equality should hold if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is simply due to round-off in the machine representation it is possible that an extra figure may be lost in internal calculation round-off.

The behaviour of the amplification factor is shown in the following graph:



It should be noted that this factor is always less than or equal to one. For large x we have the absolute error in the result, E, in principle, given by

$$E \sim \delta.$$

This means that eventually accuracy is limited by ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S11ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
```

```
*     .. External Functions ..
      real                 S11ABF
      EXTERNAL             S11ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S11ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S11ABF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S11ABF Example Program Data
            -2.0
            -0.5
             1.0
             6.0
```

9.3. Program Results

```
 S11ABF Example Program Results

      X           Y         IFAIL

  -2.000E+00  -1.444E+00       0
  -5.000E-01  -4.812E-01       0
   1.000E+00   8.814E-01       0
   6.000E+00   2.492E+00       0
```

S11ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S11ACF returns the value of the inverse hyperbolic cosine, $\text{arccosh}\, x$, via the routine name. The result is in the principal positive branch.

2. Specification

```
real FUNCTION S11ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the inverse hyperbolic cosine, $\text{arccosh}\, x$. It is based on the relation

$$\text{arccosh}\, x = \ln(x+\sqrt{x^2-1}).$$

This form is used directly for $1 < x < 10^k$, where $k = n/2 + 1$, and the machine uses approximately n decimal place arithmetic.

For $x \geq 10^k$, $\sqrt{x^2-1}$ is equal to $\sqrt{x}$ to within the accuracy of the machine and hence we can guard against premature overflow and, without loss of accuracy, calculate

$$\text{arccosh}\, x = \ln 2 + \ln x.$$

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 4.6, p. 86, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

Constraint: X $\geq$ 1.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

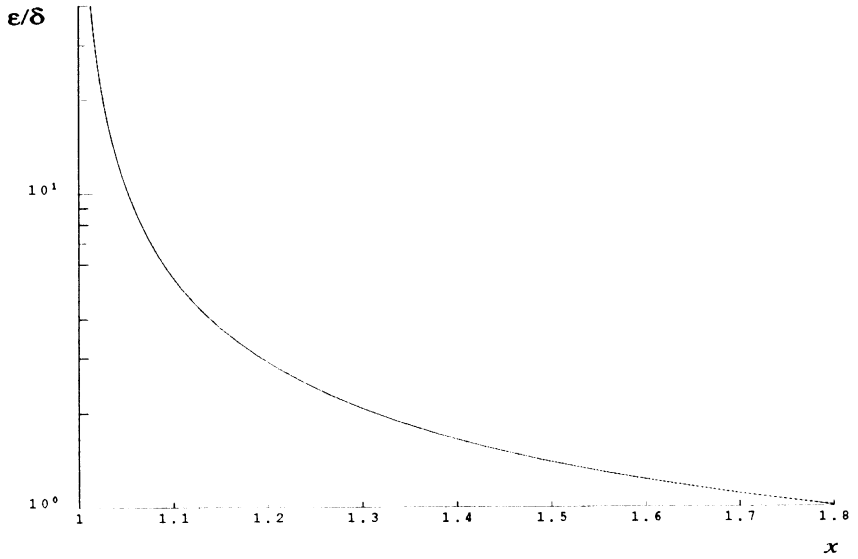
The routine has been called with an argument less than 1.0, for which $\text{arccosh}\, x$ is not defined. The result returned is zero.

7. Accuracy

If δ and ε are the relative errors in the argument and result respectively, then in principle

$$|\varepsilon| \simeq \left| \frac{x}{\sqrt{x^2-1}\ \operatorname{arccosh} x} \times \delta \right|.$$

That is the relative error in the argument is amplified by a factor at least $\dfrac{x}{\sqrt{x^2-1}\ \operatorname{arccosh} x}$ in the result. The equality should apply if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is simply a result of round-off in the machine representation it is possible that an extra figure may be lost in internal calculation and round-off. The behaviour of the amplification factor is shown in the following graph:



It should be noted that for $x > 2$ the factor is always less than 1.0. For large x we have the absolute error E in the result, in principle, given by

$$E \sim \delta.$$

This means that eventually accuracy is limited by ***machine precision***. More significantly for x close to 1, $x - 1 \sim \delta$, the above analysis becomes inapplicable due to the fact that both function and argument are bounded, $x \geq 1$, $\operatorname{arccosh} x \geq 0$. In this region we have

$$E \sim \sqrt{\delta}.$$

That is, there will be approximately half as many decimal places correct in the result as there were correct figures in the argument.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S11ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S11ACF
      EXTERNAL         S11ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S11ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X            Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S11ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S11ACF Example Program Data
             1.00
             2.0
             5.0
            10.0
            -0.5
```

9.3. Program Results

```
 S11ACF Example Program Results

      X            Y         IFAIL

   1.000E+00   0.000E+00       0
   2.000E+00   1.317E+00       0
   5.000E+00   2.292E+00       0
   1.000E+01   2.993E+00       0
  -5.000E-01   0.000E+00       1
```

S13AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S13AAF returns the value of the exponential integral $E_1(x)$, via the routine name.

2. Specification

```
real FUNCTION S13AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for

$$E_1(x) = \int_x^\infty \frac{e^{-u}}{u}\,du, \qquad x > 0.$$

For $0 < x \leq 4$, the approximation is based on the Chebyshev expansion

$$E_1(x) = y(t) - \ln x = \sum_r{}' a_r T_r(t) - \ln x,$$

where $t = \frac{1}{2}x - 1$.

For $x > 4$,

$$E_1(x) = \frac{e^{-x}}{x} y(t) = \frac{e^{-x}}{x} \sum_r{}' a_r T_r(t),$$

where $t = -1.0 + 14.5/(x+3.25) = \dfrac{11.25-x}{3.25+x}$.

In both cases, $-1 \leq t \leq +1$.

To guard against producing underflows, if $x > x_{hi}$ the result is set directly to zero. For the value of x_{hi} see the Users' Note for your implementation.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 5.1, p, 228, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument less than or equal to zero for which the function is not defined. The result returned is zero.

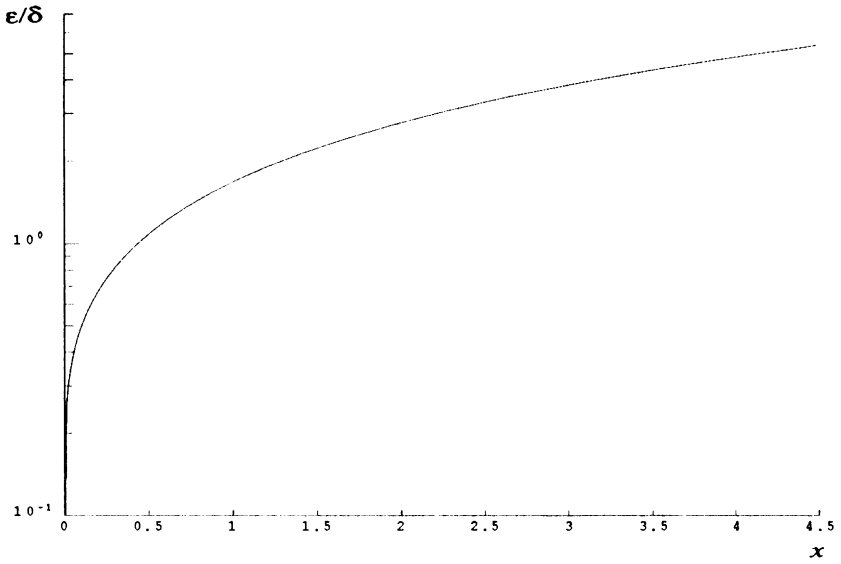
7. Accuracy

If δ and ε are the relative errors in argument and result respectively, then in principle,

$$|\varepsilon| \simeq \left| \frac{e^{-x}}{E_1(x)} \times \delta \right|$$

so the relative error in the argument is amplified in the result by at least a factor $e^{-x}/E_1(x)$. The equality should hold if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is simply a result of round-off in the machine representation, it is possible that an extra figure may be lost in internal calculation and round-off.

The behaviour of this amplification factor is shown in the following graph:



It should be noted that, for small x, the amplification factor tends to zero and eventually the error in the result will be limited by ***machine precision.***

For large x,

$$\varepsilon \sim x\delta = \Delta,$$

the absolute error in the argument.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S13AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S13AAF
      EXTERNAL         S13AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S13AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S13AAF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S13AAF Example Program Data
             2.0
            -1.0
```

9.3. Program Results

```
 S13AAF Example Program Results

      X           Y        IFAIL

   2.000E+00   4.890E-02       0
  -1.000E+00   0.000E+00       1
```

S13ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S13ACF returns the value of the cosine integral

$$\mathrm{Ci}(x) = \gamma + \ln x + \int_0^x \frac{\cos u - 1}{u}\, du, \qquad x > 0$$

via the routine name, where γ denotes Euler's constant.

2. Specification

```
real FUNCTION S13ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for $\mathrm{Ci}(x)$.

For $0 < x \leq 16$ it is based on the Chebyshev expansion

$$\mathrm{Ci}(x) = \ln x + \sum_{r=0}{}' a_r T_r(t), \qquad t = 2\left(\frac{x}{16}\right)^2 - 1.$$

For $16 < x < x_{hi}$ where the value of x_{hi} is given in the Users' Note for your implementation,

$$\mathrm{Ci}(x) = \frac{f(x)\,\sin x}{x} - \frac{g(x)\,\cos x}{x^2}$$

where $f(x) = \sum_{r=0}{}' f_r T_r(t)$ and $g(x) = \sum_{r=0}{}' g_r T_r(t)$, $\quad t = 2\left(\frac{16}{x}\right)^2 - 1.$

For $x \geq x_{hi}$, $\mathrm{Ci}(x) = 0$ to within the accuracy possible (see Section 7).

4. References

[1] ABRAMOWITZ, .M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 5.2, p. 231, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The routine has been called with an argument less than or equal to zero for which the function is not defined. The result returned is zero.

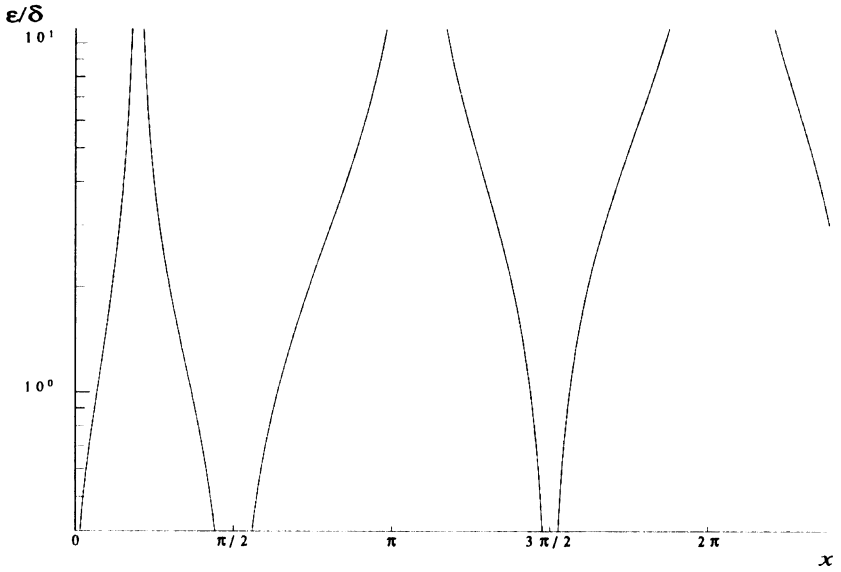
7. Accuracy

If E and ε are the absolute and relative errors in the result and δ is the relative error in the argument then in principle these are related by

$$|E| \simeq |\delta \cos x| \text{ and } |\varepsilon| \simeq \left|\frac{\delta \cos x}{\mathrm{Ci}(x)}\right|.$$

That is accuracy will be limited by ***machine precision*** near the origin and near the zeros of $\cos x$, but near the zeros of $\mathrm{Ci}(x)$ only absolute accuracy can be maintained.

The behaviour of this amplification is shown in the following graph:



For large values of x, $\mathrm{Ci}(x) \sim \frac{\sin x}{x}$ therefore $\varepsilon \sim \delta\, x \cot x$ and since δ is limited by the finite precision of the machine it becomes impossible to return results which have any relative accuracy. That is, when $x \geq 1/\delta$ we have that $|\mathrm{Ci}(x)| \leq 1/x \sim E$ and hence is not significantly different from zero.

Hence x_{hi} is chosen such that for values of $x \geq x_{hi}$, $\mathrm{Ci}(x)$ in principle would have values less than the ***machine precision*** and so is essentially zero.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S13ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
```

```
*     .. External Functions ..
      real                 S13ACF
      EXTERNAL             S13ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S13ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S13ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S13ACF Example Program Data
             0.2
             0.4
             0.6
             0.8
             1.0
```

9.3. Program Results

```
 S13ACF Example Program Results

      X           Y         IFAIL

   2.000E-01  -1.042E+00       0
   4.000E-01  -3.788E-01       0
   6.000E-01  -2.227E-02       0
   8.000E-01   1.983E-01       0
   1.000E+00   3.374E-01       0
```

S13ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S13ADF returns the value of the sine integral

$$\mathrm{Si}(x) = \int_0^x \frac{\sin u}{u}\, du,$$

via the routine name.

2. Specification

```
real FUNCTION S13ADF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for $\mathrm{Si}(x)$.

For $|x| \leq 16.0$ it is based on the Chebyshev expansion

$$\mathrm{Si}(x) = x\sum_{r=0}{}' a_r T_r(t), \qquad t = 2\left(\frac{x}{16}\right)^2 - 1.$$

For $16 < |x| < x_{hi}$, where x_{hi} is an implementation dependent number,

$$\mathrm{Si}(x) = \mathrm{sign}\left\{\frac{\pi}{2} - \frac{f(x)\cos x}{x} - \frac{g(x)\sin x}{x^2}\right\}$$

where $f(x) = \sum_{r=0}{}' f_r T_r(t)$ and $g(x) = \sum_{r=0}{}' g_r T_r(t)$, $\qquad t = 2\left(\frac{16}{x}\right)^2 - 1.$

For $|x| \geq x_{hi}$, $\mathrm{Si}(x) = \frac{1}{2}\pi \,\mathrm{sign}\, x$ to within ***machine precision***.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 5.2, p. 231, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no failure exits from this routine. The parameter IFAIL has been included for consistency with other routines in this chapter.

7. Accuracy

If δ and ϵ are the relative errors in the argument and result, respectively, then in principle

$$|\epsilon| \simeq \left| \frac{\delta \sin x}{\mathrm{Si}(x)} \right|.$$

The equality may hold if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is simply due to round-off in the machine representation, then since the factor relating δ to ϵ is always less than one, the accuracy will be limited by ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S13ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S13ADF
      EXTERNAL         S13ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S13ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S13ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S13ADF Example Program Data
             0.0
             0.2
             0.4
             0.6
             0.8
             1.0
```

9.3. Program Results

```
S13ADF Example Program Results

     X            Y         IFAIL

0.000E+00    0.000E+00         0
2.000E-01    1.996E-01         0
4.000E-01    3.965E-01         0
6.000E-01    5.881E-01         0
8.000E-01    7.721E-01         0
1.000E+00    9.461E-01         0
```

S14AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S14AAF returns the value of the Gamma function $\Gamma(x)$, via the routine name.

2. Specification

```
real FUNCTION S14AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Gamma function $\Gamma(x)$. The routine is based on the Chebyshev expansion:

$$\Gamma(1+u) = \sum_{r=0}{}' a_r T_r(t), \qquad \text{where } 0 \leq u < 1, \quad t = 2u - 1,$$

and uses the property $\Gamma(1+x) = x\Gamma(x)$. If $x = N + 1 + u$ where N is integral and $0 \leq u < 1$ then it follows that:

for $N > 0$ $\Gamma(x) = (x-1)(x-2) \ldots (x-N)\Gamma(1+u)$,

for $N = 0$ $\Gamma(x) = \Gamma(1+u)$,

for $N < 0$ $\Gamma(x) = \dfrac{\Gamma(1+u)}{x(x+1)(x+2) \ldots (x-N-1)}$.

There are four possible failures for this routine:

(i) if x is too large, there is a danger of overflow since $\Gamma(x)$ could become too large to be represented in the machine;

(ii) if x is too large and negative, there is a danger of underflow;

(iii) if x is equal to a negative integer, $\Gamma(x)$ would overflow since it has poles at such points;

(iv) if x is too near zero, there is again the danger of overflow on some machines. For small x, $\Gamma(x) \simeq \dfrac{1}{x}$, and on some machines there exists a range of non-zero but small values of x for which $1/x$ is larger than the greatest representable value.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 6, p. 255, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X must not be zero or a negative integer.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The argument is too large. On soft failure the routine returns the approximate value of $\Gamma(x)$ at the nearest valid argument.

IFAIL = 2

The argument is too large and negative. On soft failure the routine returns zero.

IFAIL = 3

The argument is too close to zero. On soft failure the routine returns the approximate value of $\Gamma(x)$ at the nearest valid argument.

IFAIL = 4

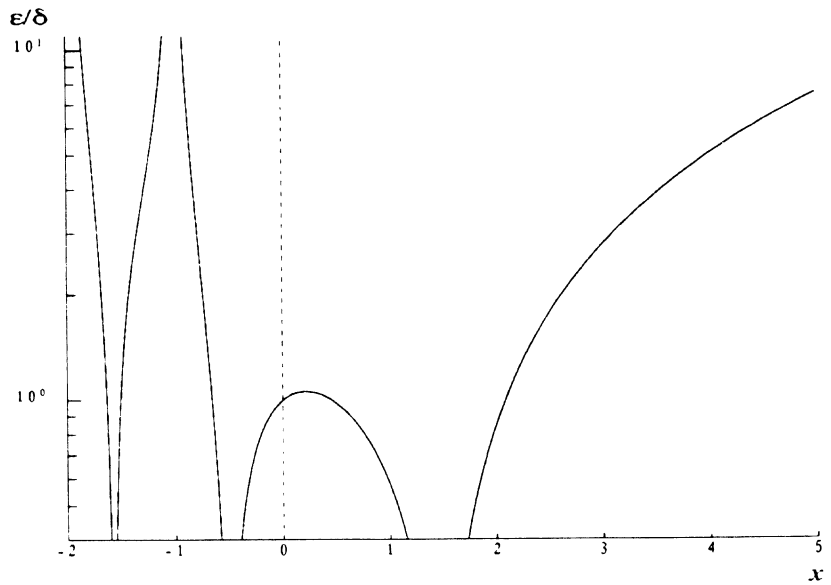
The argument is a negative integer, at which value $\Gamma(x)$ is infinite. On soft failure the routine returns a large positive value.

7. Accuracy

Let δ and ε be the relative errors in the argument and the result respectively. If δ is somewhat larger than the ***machine precision*** (i.e. is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq |x\Psi(x)|\ \delta$$

(provided ε is also greater than the representation error). Here $\Psi(x)$ is the digamma function $\frac{\Gamma'(x)}{\Gamma(x)}$. The following graph shows the behaviour of the error amplification factor $|x\Psi(x)|$.



If δ is of the same order as ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

There is clearly a severe, but unavoidable, loss of accuracy for arguments close to the poles of $\Gamma(x)$ at negative integers. However relative accuracy is preserved near the pole at $x = 0$ right up to the point of failure arising from the danger of overflow.

Also accuracy will necessarily be lost as x becomes large since in this region

$$\varepsilon \simeq \delta x \ln x.$$

However since $\Gamma(x)$ increases rapidly with x, the routine must fail due to the danger of setting overflow before this loss of accuracy is too great. (E.g. for $x = 20$, the amplification factor $\simeq 60$.)

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S14AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S14AAF
      EXTERNAL         S14AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S14AAF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S14AAF Example Program Data
             1.0
             1.25
             1.5
             1.75
             2.0
             5.0
             10.0
             -1.5
```

9.3. Program Results

```
S14AAF Example Program Results

      X             Y          IFAIL

  1.000E+00   1.000E+00          0
  1.250E+00   9.064E-01          0
  1.500E+00   8.862E-01          0
  1.750E+00   9.191E-01          0
  2.000E+00   1.000E+00          0
  5.000E+00   2.400E+01          0
  1.000E+01   3.629E+05          0
 -1.500E+00   2.363E+00          0
```

S14ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S14ABF returns a value for the logarithm of the Gamma function, $\ln \Gamma(x)$, via the routine name.

2. Specification

```
real FUNCTION S14ABF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to $\ln \Gamma(x)$. It is based on two Chebyshev expansions.

For $0 < x \leq x_{small}$, $\ln \Gamma(x) = -\ln x$ to within machine accuracy.

For $x_{small} < x \leq 15.0$, the recursive relation $\Gamma(1+x) = x\Gamma(x)$ is used to reduce the calculation to one involving $\Gamma(1+u)$, $0 \leq u < 1$ which is evaluated as:

$$\Gamma(1+u) = {\sum_{r=0}}' a_r T_r(t), \qquad t = 2u - 1.$$

Once $\Gamma(x)$ has been calculated, the required result is produced by taking the logarithm.

For $15.0 < x \leq x_{big}$,

$$\ln \Gamma(x) = (x-\tfrac{1}{2})\ln x - x + \tfrac{1}{2}\ln 2\pi + y(x)/x$$

where $y(x) = {\sum_{r=0}}' b_r T_r(t), \qquad t = 2\left(\frac{15}{x}\right)^2 - 1.$

For $x_{big} < x \leq x_{vbig}$ the term $y(x)/x$ is negligible and so its calculation is omitted.

For $x > x_{vbig}$ there is a danger of setting overflow so the routine must fail.

For $x \leq 0.0$ the function is not defined and the routine fails.

Note: x_{small} is calculated so that if $x < x_{small}$, $\Gamma(x) = 1/x$ to within machine accuracy.

x_{big} is calculated so that if $x > x_{big}$,

$$\ln \Gamma(x) = (x-\tfrac{1}{2})\ln x - x + \tfrac{1}{2}\ln 2\pi$$

to within machine accuracy.

x_{vbig} is calculated so that $\ln \Gamma(x_{vbig})$ is close to the value returned by X02ALF.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 6, pp. 255, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X ≤ 0.0, the function is undefined. On soft failure, the routine returns zero.

IFAIL = 2

X is too large, the function would overflow. On soft failure, the routine returns the value of the function at the largest permissible argument.

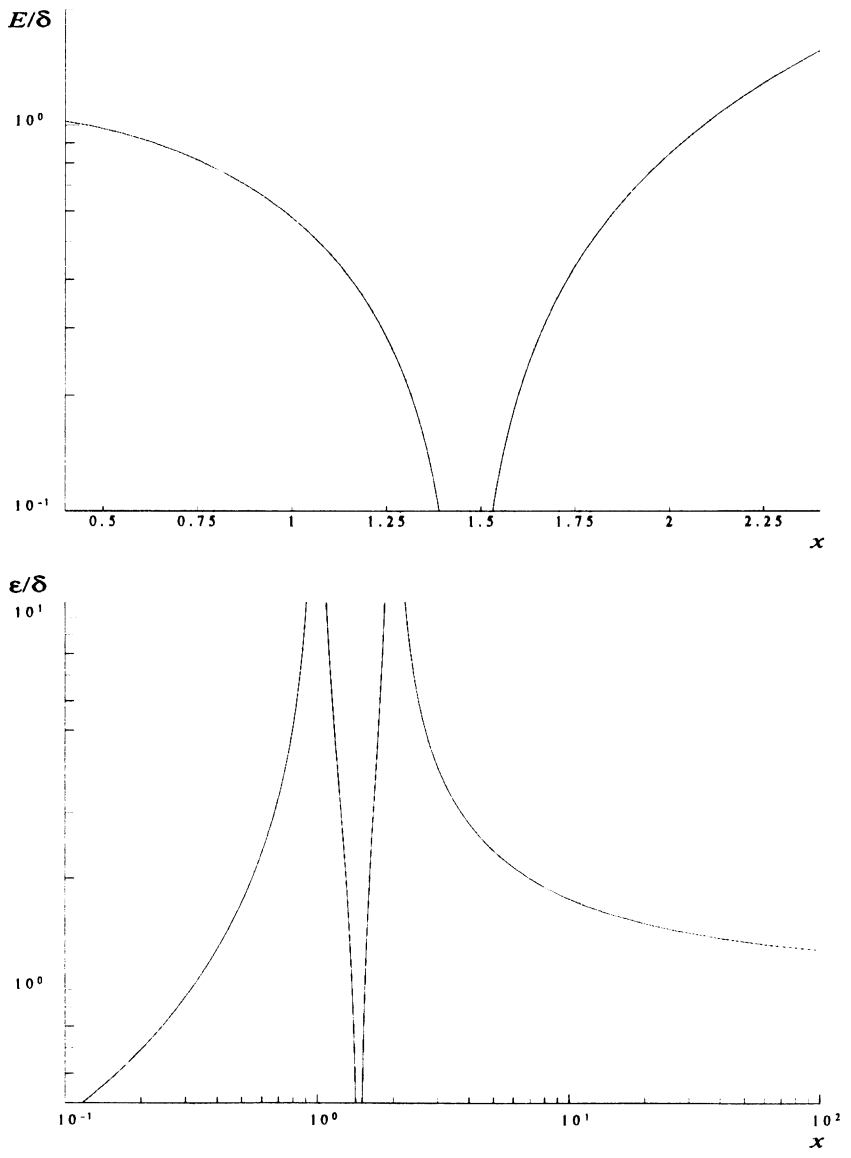
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively, and E be the absolute error in the result.

If δ is somewhat larger than the relative ***machine precision***, then

$$E \simeq |x \times \Psi(x)|\delta \text{ and } \varepsilon \simeq \left|\frac{x \times \Psi(x)}{\ln \Gamma(x)}\right|\delta$$

where $\Psi(x)$ is the digamma function $\dfrac{\Gamma'(x)}{\Gamma(x)}$. The following graphs show the behaviour of these error amplification factors:



These show that relative error can be controlled, since except near $x = 1$ or 2 relative error is attenuated by the function or at least is not greatly amplified.

For large x, $\varepsilon \simeq \left(1+\frac{1}{\ln x}\right)\delta$ and for small x, $\varepsilon \simeq \frac{1}{\ln x}\delta$.

The function $\ln \Gamma(x)$ has zeros at $x = 1$ and 2 and hence relative accuracy is not maintainable near those points. However absolute accuracy can still be provided near those zeros as is shown above.

If however, δ is of the order of the ***machine precision***, then rounding errors in the routine's internal arithmetic may result in errors which are slightly larger than those predicted by the equalities. It should be noted that even in areas where strong attenuation of errors is predicted the relative precision is bounded by the effective ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S14ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S14ABF
      EXTERNAL         S14ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S14ABF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S14ABF Example Program Data
             1.0
             1.25
             1.5
             1.75
             2.0
             5.0
             10.0
             20.0
             1000.0
             0.0
             -5.0
```

9.3. Program Results

```
 S14ABF Example Program Results

      X            Y         IFAIL

   1.000E+00   0.000E+00        0
   1.250E+00  -9.827E-02        0
   1.500E+00  -1.208E-01        0
   1.750E+00  -8.440E-02        0
   2.000E+00   0.000E+00        0
   5.000E+00   3.178E+00        0
   1.000E+01   1.280E+01        0
   2.000E+01   3.934E+01        0
   1.000E+03   5.905E+03        0
   0.000E+00   0.000E+00        1
  -5.000E+00   0.000E+00        1
```

S14ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S14ACF returns a value of the function $\psi(x) - \ln x$, where ψ is the psi function $\psi(x) = \dfrac{d}{dx}\ln\Gamma(x) = \dfrac{\Gamma'(x)}{\Gamma(x)}$.

2. Specification

```
real FUNCTION S14ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine returns a value of the function $\psi(x) - \ln x$. The psi function is computed without the logarithmic term so that when x is large, sums or differences of psi functions may be computed without unnecessary loss of precision, by analytically combining the logarithmic terms. For example, the difference $d = \Psi(x+\frac{1}{2}) - \psi(x)$ has an asymptotic behaviour for large x given by $d \sim \ln(x+\frac{1}{2}) - \ln x + O\left(\dfrac{1}{x^2}\right) \sim \ln\left(1+\dfrac{1}{2x}\right) \sim \dfrac{1}{2x}$.

Computing d directly would amount to subtracting two large numbers which are close to $\ln(x+\frac{1}{2})$ and $\ln x$ to produce a small number close to $\dfrac{1}{2x}$, resulting in a loss of significant digits. However, using this routine to compute $f(x) = \psi(x) - \ln x$, we can compute $d = f(x+\frac{1}{2}) - f(x) + \ln\left(1+\dfrac{1}{2x}\right)$, and the dominant logarithmic term may be computed accurately from its power series when x is large. Thus we avoid the unnecessary loss of precision.

The routine is derived from the routine PSIFN in Amos [1].

4. References

[1] AMOS, D.E.
Algorithm 610: A Portable FORTRAN Subroutine for Derivatives of the Psi Function.
ACM Trans. Math. Software 9, pp. 494-502, 1983.

[2] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions, Ch. 6, pp. 258-260.
Dover Publications, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, X ≤ 0.0. S14ACF returns the value zero.

IFAIL = 2

No result is computed because underflow is likely. The value of X is too large. S14ACF returns the value zero.

IFAIL = 3

No result is computed because overflow is likely. The value of X is too small. S14ACF returns the value zero.

7. Accuracy

All constants in subroutine S14ACF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$.

With the above proviso, results returned by this routine should be accurate almost to full precision, except at points close to the zero of $\psi(x)$, $x \simeq 1.461632$, where only absolute rather than relative accuracy can be obtained.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S14ACF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             F, X
      INTEGER          IFAIL
*     .. External Functions ..
      real             S14ACF
      EXTERNAL         S14ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '       X        psi(X)-log(X)'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 0
*
      F = S14ACF(X,IFAIL)
*
```

```
      WRITE (NOUT,99999) X, F
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,F12.4,F15.4)
      END
```

9.2. Program Data

```
S14ACF Example Program Data
0.1
0.5
3.6
8.0
```

9.3. Program Results

```
 S14ACF Example Program Results

        X         psi(X)-log(X)

      0.1000          -8.1212
      0.5000          -1.2704
      3.6000          -0.1453
      8.0000          -0.0638
```

S14ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S14ADF returns a sequence of values of scaled derivatives of the psi function $\psi(x)$.

2. Specification

```
SUBROUTINE S14ADF (X, N, M, ANS, IFAIL)
INTEGER          N, M, IFAIL
real             X, ANS(M)
```

3. Description

This routine computes m values of the function

$$w(k,x) = \frac{(-1)^{k+1}\psi^{(k)}(x)}{k!},$$

for $x > 0$, $k = n, n+1,\ldots,n+m-1$, where ψ is the psi function

$$\psi(x) = \frac{d}{dx}\ln\Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)},$$

and $\psi^{(k)}$ denotes the kth derivative of ψ.

The routine is derived from the routine PSIFN in Amos [1]. The basic method of evaluation of $w(k,x)$ is the asymptotic series

$$w(k,x) \sim \epsilon(k,x) + \frac{1}{2x^{k+1}} + \frac{1}{x^k}\sum_{j=1}^{\infty} B_{2j}\frac{(2j+k-1)!}{(2j)!\ k!\ x^{2j}}$$

for large x greater than a machine dependent value $x_{\min}$, followed by backward recurrence using

$$w(k,x) = w(k,x+1) + x^{-k-1}$$

for smaller values of x, where $\epsilon(k,x) = -\ln x$ when $k = 0$, $\epsilon(k,x) = \frac{1}{kx^k}$ when $k > 0$, and B_{2j}, $j = 1,2,\ldots$, are the Bernoulli numbers.

When k is large, the above procedure may be inefficient, and the expansion

$$w(k,x) = \sum_{j=1}^{\infty}\frac{1}{(x+j)^{k+1}},$$

which converges rapidly for large k, is used instead.

4. References

[1] AMOS, D.E.
Algorithm 610: A Portable FORTRAN Subroutine for Derivatives of the Psi Function.
ACM Trans. Math. Software 9, pp. 494-502, 1983.

[2] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions, Ch. 6, pp. 258-260.
Dover Publications, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: N – INTEGER. *Input*

On entry: the first member n of the sequence of functions.

Constraint: N $\geq$ 0.

3: M – INTEGER. *Input*

On entry: the number of members m required in the sequence $w(k,x)$, for $k = n,n+1,...,n+m-1$.

Constraint: M $\geq$ 1.

4: ANS(M) – ***real*** array. *Output*

On exit: the first m elements of ANS contain the required values $w(k,x)$, for $k = n,n+1,...,n+m-1$.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, X $\leq$ 0.0.

IFAIL = 2

On entry, N < 0.

IFAIL = 3

On entry, M < 1.

IFAIL = 4

No results are returned because underflow is likely. Either X or N + M – 1 is too large. If possible, reduce the value of M and call S14ADF again.

IFAIL = 5

No results are returned because overflow is likely. Either X is too small, or N + M – 1 is too large. If possible, reduce the value of M and call S14ADF again.

IFAIL = 6

No results are returned because there is not enough internal workspace to continue computation. N + M – 1 may be too large. If possible, reduce the value of M and call S14ADF again.

7. Accuracy

All constants in subroutine S14ADF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Empirical tests of S14ADF, taking values of x in the range $0.0 < x < 50.0$, and n in the range $1 \leq n \leq 50$, have shown that the maximum relative error is a loss of approximately two decimal places of precision. Tests with $n = 0$, i.e. testing the function $-\psi(x)$, have shown somewhat better accuracy, except at points close to the zero of $\psi(x)$, $x \simeq 1.461632$, where only absolute accuracy can be obtained.

8. Further Comments

The time taken for a call of S14ADF is approximately proportional to m, plus a constant. In general, it is much cheaper to call S14ADF with m greater than 1 to evaluate the function $w(k,x)$, for $k = n,n+1,...,n+m-1$, rather than to make m separate calls of S14ADF.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S14ADF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX
      PARAMETER        (MMAX=4)
*     .. Local Scalars ..
      real             X
      INTEGER          I, IFAIL, M, N
*     .. Local Arrays ..
      real             W(MMAX)
*     .. External Subroutines ..
      EXTERNAL         S14ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'       X           W(1)          W(2)          W(3)          W(4)'
      WRITE (NOUT,*)
      N = 0
      M = 4
   20 READ (NIN,*,END=40) X
*
      CALL S14ADF(X,N,M,W,IFAIL)
*
      WRITE (NOUT,99999) X, (W(I),I=1,M)
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,5(e12.4,2X))
      END
```

9.2. Program Data

```
S14ADF Example Program Data
0.1
0.5
3.6
8.0
```

9.3. Program Results

```
S14ADF Example Program Results

      X          W(1)          W(2)          W(3)          W(4)

 1.0000E-01    1.0424E+01    1.0143E+02    1.0009E+03    1.0001E+04
 5.0000E-01    1.9635E+00    4.9348E+00    8.4144E+00    1.6235E+01
 3.6000E+00   -1.1357E+00    3.1988E-01    5.0750E-02    1.0653E-02
 8.0000E+00   -2.0156E+00    1.3314E-01    8.8498E-03    7.8321E-04
```

S14BAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S14BAF computes values for the incomplete gamma functions $P(a,x)$ and $Q(a,x)$.

2. Specification

```
SUBROUTINE S14BAF (A, X, TOL, P, Q, IFAIL)
INTEGER          IFAIL
real             A, X, TOL, P, Q
```

3. Description

This subroutine evaluates the incomplete gamma functions in the normalised form

$$P(a,x) = \frac{1}{\Gamma(a)}\int_0^x t^{a-1}e^{-t}dt,$$

$$Q(a,x) = \frac{1}{\Gamma(a)}\int_x^\infty t^{a-1}e^{-t}dt,$$

with $x \geq 0$ and $a > 0$, to a user-specified accuracy. With this normalisation, $P(a,x) + Q(a,x) = 1$.

Several methods are used to evaluate the functions depending on the arguments a and x, the methods including Taylor expansion for $P(a,x)$, Legendre's continued fraction for $Q(a,x)$, and power series for $Q(a,x)$. When both a and x are large, and $a \simeq x$, the uniform asymptotic expansion of Temme [3] is employed for greater efficiency – specifically, this expansion is used when $a \geq 20$ and $0.7a \leq x \leq 1.4a$.

Once either of P or Q is computed, the other is obtained by subtraction from 1. In order to avoid loss of relative precision in this subtraction, the smaller of P and Q is computed first.

This routine is derived from subroutine GAM in Gautschi [2].

4. References

[1] GAUTSCHI, W.
A Computational Procedure for Incomplete Gamma Functions.
ACM Trans. Math. Software 5, pp. 466-481, 1979.

[2] GAUTSCHI, W.
Algorithm 542: Incomplete Gamma Functions.
ACM Trans. Math. Software 5, pp. 482-489, 1979.

[3] TEMME, N.M.
On the computation of the incomplete gamma functions for large values of the parameters.
In: 'Algorithms for Approximation', J.C. Mason and M.G. Cox. (ed).
Oxford University Press, 1987.

5. Parameters

1: A – ***real***. *Input*

On entry: the argument a of the functions.

Constraint: A > 0.0.

2: X – ***real.*** *Input*

On entry: the argument x of the functions.

Constraint: X ≥ 0.0.

3: TOL – ***real.*** *Input*

On entry: the relative accuracy required by the user in the results. If S14BAF is entered with TOL greater than 1.0 or less than ***machine precision***, then the value of ***machine precision*** is used instead.

4: P – ***real.*** *Output*

5: Q – ***real.*** *Output*

On exit: the values of the functions $P(a,x)$ and $Q(a,x)$ respectively.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

If, on exit, IFAIL ≠ 0 then S14BAF returns with a value of 0.0 for P and Q.

IFAIL = 1

On entry, A ≤ 0.0.

IFAIL = 2

On entry, X < 0.0.

IFAIL = 3

Convergence of the Taylor series or Legendre continued fraction fails within 600 iterations. This error is extremely unlikely to occur; if it does, contact NAG.

7. Accuracy

There are rare occasions when the relative accuracy attained is somewhat less than that specified by parameter TOL. However, the error should never exceed more than one or two decimal places. Note also that there is a limit of 18 decimal places on the achievable accuracy, because constants in the routine are given to this precision.

8. Further Comments

The time taken for a call of S14BAF depends on the precision requested through TOL, and also varies slightly with the input arguments a and x.

9. Example

The following program reads values of the argument a and x from a file, evaluates the function and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S14BAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             A, P, Q, TOL, X
      INTEGER          IFAIL
*     .. External Functions ..
      real             X02AJF
      EXTERNAL         X02AJF
*     .. External Subroutines ..
      EXTERNAL         S14BAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14BAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      TOL = X02AJF()
      WRITE (NOUT,*)
      WRITE (NOUT,*) '          A           X           P           Q'
   20 READ (NIN,*,END=40) A, X
      IFAIL = 0
*
      CALL S14BAF(A,X,TOL,P,Q,IFAIL)
*
      WRITE (NOUT,99999) A, X, P, Q
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,4F12.4)
      END
```

9.2. Program Data

```
S14BAF Example Program Data
  2.0   3.0
  7.0   1.0
  0.5  99.0
 20.0  21.0
 21.0  20.0
```

9.3. Program Results

```
S14BAF Example Program Results

         A           X           P           Q
    2.0000      3.0000      0.8009      0.1991
    7.0000      1.0000      0.0001      0.9999
    0.5000     99.0000      1.0000      0.0000
   20.0000     21.0000      0.6157      0.3843
   21.0000     20.0000      0.4409      0.5591
```

S15ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S15ABF returns the value of the cumulative Normal distribution function, $P(x)$, via the routine name.

2. Specification

```
real FUNCTION S15ABF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine evaluates an approximate value for the cumulative Normal distribution function

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

The routine is based on the fact that

$$P(x) = \tfrac{1}{2}\mathrm{erfc}\left(\frac{-x}{\sqrt{2}}\right)$$

and it calls S15ADF to obtain a value of erfc for the appropriate argument.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7.1, p. 297 and Ch. 26.2, p. 931, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no failure exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

7. Accuracy

Because of its close relationship with erfc, the accuracy of this routine is very similar to that in S15ADF. If ε and δ are the relative errors in result and argument, respectively, they are in principle related by

$$|\varepsilon| \simeq \left| \frac{xe^{-\frac{1}{2}x^2}}{\sqrt{2\pi}\, P(x)} \delta \right|$$

so that the relative error in the argument, x, is amplified by a factor, $\frac{xe^{-\frac{1}{2}x^2}}{\sqrt{2\pi}\,P(x)}$, in the result.

For x small and for x positive this factor is always less than one and accuracy is mainly limited by ***machine precision***.

For large negative x the factor behaves like $\sim x^2$ and hence to a certain extent relative accuracy is unavoidably lost.

However the absolute error in the result, E, is given by

$$|E| \simeq \left|\frac{xe^{-\frac{1}{2}x^2}}{\sqrt{2\pi}}\delta\right|$$

so absolute accuracy can be guaranteed for all x.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15ABF
      EXTERNAL         S15ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S15ABF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S15ABF Example Program Data
          -20.0
           -1.0
            0.0
            1.0
            2.0
           20.0
```

9.3. Program Results

```
S15ABF Example Program Results

     X           Y         IFAIL

-2.000E+01   0.000E+00       0
-1.000E+00   1.587E-01       0
 0.000E+00   5.000E-01       0
 1.000E+00   8.413E-01       0
 2.000E+00   9.772E-01       0
 2.000E+01   1.000E+00       0
```

S15ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S15ACF returns the value of the complement of the cumulative normal distribution function, $Q(x)$, via the routine name.

2. Specification

```
real FUNCTION S15ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine evaluates an approximate value for the complement of the cumulative normal distribution function

$$Q(x) = \frac{1}{\sqrt{2\pi}} \int_x^\infty e^{-u^2/2}\, du.$$

The routine is based on the fact that

$$Q(x) = \tfrac{1}{2}\operatorname{erfc}\left(\frac{x}{\sqrt{2}}\right)$$

and it calls S15ADF to obtain the necessary value of erfc, the complementary error function.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7.1, p. 297, Ch. 26.2, p. 931, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no failure exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

7. Accuracy

Because of its close relationship with erfc the accuracy of this routine is very similar to that in S15ADF. If ε and δ are the relative errors in result and argument, respectively, then in principle they are related by

$$|\varepsilon| \simeq \left| \frac{xe^{-x^2/2}}{\sqrt{2\pi}Q(x)}\,\delta \right|.$$

For x negative or small positive this factor is always less than one and accuracy is mainly limited by ***machine precision***. For large positive x we find $\epsilon \sim x^2\delta$ and hence to a certain extent relative accuracy is unavoidably lost. However the absolute error in the result, E, is given by

$$|E| \simeq \left| \frac{xe^{-x^2/2}}{\sqrt{2\pi}} \delta \right|$$

and since this factor is always less than one absolute accuracy can be guaranteed for all x.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15ACF
      EXTERNAL         S15ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S15ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S15ACF Example Program Data
          -20.0
           -1.0
            0.0
            1.0
            2.0
           20.0
```

9.3. Program Results

```
S15ACF Example Program Results

     X            Y         IFAIL

-2.000E+01   1.000E+00         0
-1.000E+00   8.413E-01         0
 0.000E+00   5.000E-01         0
 1.000E+00   1.587E-01         0
 2.000E+00   2.275E-02         0
 2.000E+00   0.000E+00         0
```

S15ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S15ADF returns the value of the complementary error function, erfc x, via the routine name.

2. Specification

```
real FUNCTION S15ADF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

The routine calculates an approximate value for the complement of the error function

$$\text{erfc}\, x = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-u^2}\, du = 1 - \text{erf}\, x.$$

For $x \geq 0$, it is based on the Chebyshev expansion

$$\text{erfc}\, x = e^{-x^2} y(x),$$

where $y(x) = \sum_{r=0}' a_r T_r(t)$ and $t = (x-3.75)/(x+3.75)$, $\quad -1 \leq t \leq +1$.

For $x \geq x_{hi}$, where there is a danger of setting underflow, the result is returned as zero.

For $x < 0$, $\text{erfc}\, x = 2 - e^{-x^2} y(|x|)$.

For $x < x_{low} < 0$, the result is returned as 2.0 which is correct to within ***machine precision***. The values of x_{hi} and x_{low} are given in the Users' Note for your implementation.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7, p. 297, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

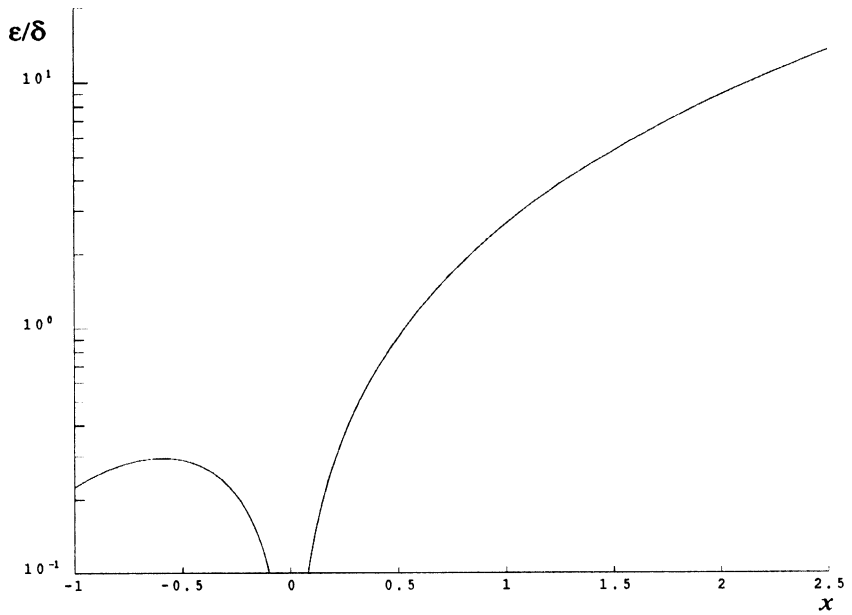
7. Accuracy

If δ and ε are relative errors in the argument and result, respectively, then in principle

$$|\varepsilon| \simeq \left| \frac{2xe^{-x^2}}{\sqrt{\pi}\ \mathrm{erfc}\, x} \delta \right|.$$

That is, the relative error in the argument, x, is amplified by a factor $\dfrac{2xe^{-x^2}}{\sqrt{\pi}\ \mathrm{erfc}\, x}$ in the result.

The behaviour of this factor is shown in the following graph:



It should be noted that near $x = 0$ this factor behaves as $\dfrac{2x}{\sqrt{\pi}}$ and hence the accuracy is largely determined by the ***machine precision***. Also for large negative x, where the factor is ~ $\dfrac{xe^{-x^2}}{\sqrt{\pi}}$, accuracy is mainly limited by ***machine precision***. However, for large positive x, the factor becomes ~ $2x^2$ and to an extent relative accuracy is necessarily lost. The absolute accuracy E is given by

$$E \simeq \frac{2xe^{-x^2}}{\sqrt{\pi}} \delta$$

so absolute accuracy is guaranteed for all x.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15ADF
      EXTERNAL         S15ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S15ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S15ADF Example Program Data
          -10.0
           -1.0
            0.0
            1.0
           15.0
```

9.3. Program Results

```
 S15ADF Example Program Results

      X           Y         IFAIL

  -1.000E+01   2.000E+00       0
  -1.000E+00   1.843E+00       0
   0.000E+00   1.000E+00       0
   1.000E+00   1.573E-01       0
   1.500E+01   0.000E+00       0
```

S15AEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S15AEF returns the value of the error function $\mathrm{erf}\, x$, via the routine name.

2. Specification

```
real FUNCTION S15AEF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

Evaluates the error function,

$$\mathrm{erf}\, x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt.$$

For $|x| \leq 2$,

$$\mathrm{erf}\, x = x \sum_{r=0}{}' a_r T_r(t), \qquad \text{where } t = \frac{1}{2}x^2 - 1.$$

For $2 < |x| < x_{hi}$,

$$\mathrm{erf}\, x = \mathrm{sign}\, x \left\{ 1 - \frac{e^{-x^2}}{|x|\sqrt{\pi}} \sum_{r=0}{}' b_r T_r(t) \right\}, \qquad \text{where } t = \frac{x-7}{x+3}.$$

For $|x| \geq x_{hi}$,

$$\mathrm{erf}\, x = \mathrm{sign}\, x.$$

x_{hi} is the value above which $\mathrm{erf}\, x = \pm 1$ within ***machine precision***. Its value is given in the Users' Note for your implementation.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7.1, p. 297, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

7. Accuracy

On a machine with approximately 11 significant figures the routine agrees with available tables to 10 figures and consistency checking with S15ADF of the relation

$$\text{erf}\, x + \text{erfc}\, x = 1.0$$

shows errors in at worst the 11th figure.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15AEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15AEF
      EXTERNAL         S15AEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15AEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S15AEF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S15AEF Example Program Data
           -6.0
           -4.5
           -1.0
            1.0
            4.5
            6.0
```

9.3. Program Results

```
S15AEF Example Program Results

     X           Y         IFAIL

-6.000E+00  -1.000E+00       0
-4.500E+00  -1.000E+00       0
-1.000E+00  -8.427E-01       0
 1.000E+00   8.427E-01       0
 4.500E+00   1.000E+00       0
 6.000E+00   1.000E+00       0
```

S15AFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S15AFF returns a value for Dawson's Integral, $F(x)$, via the routine name.

2. Specification

```
real FUNCTION S15AFF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation for Dawson's Integral

$$F(x) = e^{-x^2} \int_0^x e^{t^2}\, dt.$$

The routine is based on two Chebyshev expansions:

For $0 < |x| \leq 4$,

$$F(x) = x \sum_{r=0}{}' a_r T_r(t), \qquad \text{where } t = 2\left(\frac{x}{4}\right)^2 - 1.$$

For $|x| > 4$,

$$F(x) = \frac{1}{x} \sum_{r=0}{}' b_r T_r(t), \qquad \text{where } t = 2\left(\frac{4}{x}\right)^2 - 1.$$

For $|x|$ near zero, $F(x) \simeq x$, and for $|x|$ large, $F(x) \simeq \frac{1}{2x}$. These approximations are used for those values of x for which the result is correct to ***machine precision***. For very large x on some machines, $F(x)$ may underflow and then the result is set exactly to zero (see the Users' Note for your implementation for details).

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7, p. 298, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

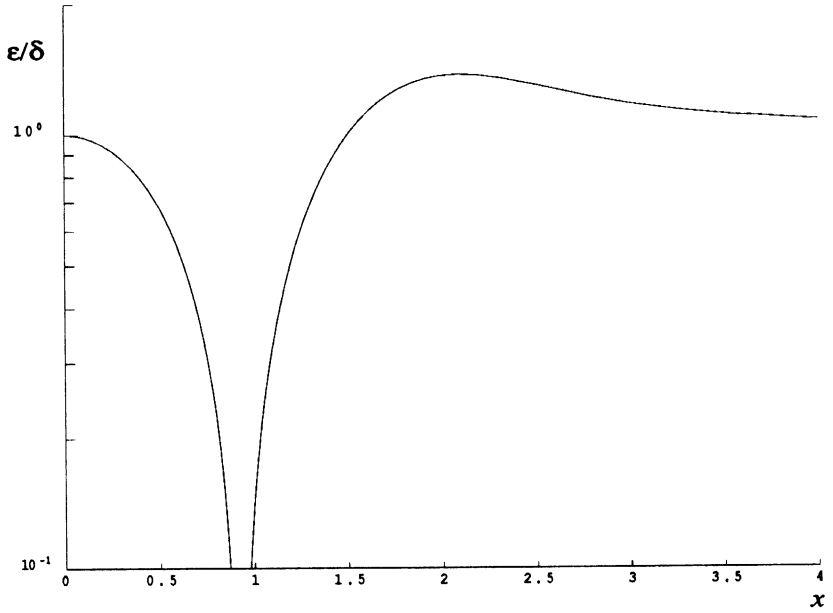
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is considerably greater than the ***machine precision*** (i.e. if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{x(1-2xF(x))}{F(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{x(1-2xF(x))}{F(x)} \right|$:



However if δ is of the same order as ***machine precision***, then rounding errors could make ε somewhat larger than the above relation indicates. In fact ε will be largely independent of x or δ, but will be of the order of a few times the machine precision.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15AFF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15AFF
      EXTERNAL         S15AFF
```

```
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15AFF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S15AFF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S15AFF Example Program Data
            -2.0
            -0.5
             1.0
             1.5
             2.0
             5.0
            10.0
```

9.3. Program Results

```
 S15AFF Example Program Results

      X           Y         IFAIL

  -2.000E+00  -3.013E-01       0
  -5.000E-01  -4.244E-01       0
   1.000E+00   5.381E-01       0
   1.500E+00   4.282E-01       0
   2.000E+00   3.013E-01       0
   5.000E+00   1.021E-01       0
   1.000E+01   5.025E-02       0
```

S15DDF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S15DDF computes values of the function $w(z) = e^{-z^2}erfc(-iz)$, for ***complex*** z.

2. Specification

```
complex FUNCTION S15DDF (Z, IFAIL)
INTEGER          IFAIL
complex          Z
```

3. Description

This routine computes values of the function $w(z) = e^{-z^2}erfc(-iz)$, where erfc z is the complementary error function

$$\text{erfc } z = \frac{2}{\sqrt{\pi}}\int_z^\infty e^{-t^2}dt,$$

for complex z. The method used is that in Gautschi [1] for z in the first quadrant of the complex plane, and is extended for z in other quadrants via the relations $w(-z) = 2e^{-z^2} - w(z)$ and $w(\bar{z}) = \overline{w(-z)}$. Following advice in Gautschi [1], and Van Der Laan and Temme [3], the code in Gautschi [2] has been adapted to work in various precisions up to 18 decimal places. The real part of $w(z)$ is sometimes known as the Voigt function.

4. References

[1] GAUTSCHI, W.
Efficient Computation of the Complex Error Function.
SIAM J. Numer. Anal. 7, pp. 187-198, 1970.

[2] GAUTSCHI, W.
Algorithm 363: Complex Error Function.
Comm. ACM 12, p. 635, 1969.

[3] VAN DER LAAN, C.G. and TEMME, N.M.
Calculation of special functions: the gamma function, the exponential integrals and error-like functions.
CWI Tract 10, Ch. 5, Centre for Mathematics and Computer Science, Amsterdam, 1984.

5. Parameters

1: Z – ***complex***. *Input*

On entry: the argument z of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

The real part of the result overflows, and is set to the largest safe number with the correct sign. The imaginary part of the result is meaningful.

IFAIL = 2

The imaginary part of the result overflows, and is set to the largest safe number with the correct sign. The real part of the result is meaningful.

IFAIL = 3

Both real and imaginary parts of the result overflow, and are set to the largest safe number with the correct signs.

IFAIL = 4

The result returned is accurate to less than half precision, due to the size of an intermediate result.

IFAIL = 5

The result returned has no precision, due to the size of an intermediate result, and is set to zero.

7. Accuracy

The accuracy of the returned result depends on the argument z. If z lies in the first or second quadrant of the complex plane (i.e. Im z is greater than or equal to zero), the result should be accurate almost to ***machine precision***, except that there is a limit of about 18 decimal places on the achievable accuracy because constants in the routine are given to this precision. With such arguments, IFAIL can only return as zero.

If however Im z is less than zero, accuracy may be lost in two ways; firstly, in the evaluation of e^{-z^2}, if $\mathrm{Im}(-z^2)$ is large, in which case a warning will be issued through IFAIL = 4 or 5; and secondly, near the zeros of the required function, where precision is lost due to cancellation, in which case no warning is given – the result has absolute accuracy rather than relative accuracy. Note also that in this half-plane, one or both parts of the result may overflow – this is signalled through IFAIL = 1, 2 or 3.

8. Further Comments

The time taken for a call of S15DDF depends on the argument z, the time increasing as $|z| \rightarrow 0.0$.

This routine may be used to compute values of erfc z and erf z for ***complex*** z by the relations $\mathrm{erfc}\, z = e^{-z^2} w(iz)$, $\mathrm{erf}\, z = 1 - \mathrm{erfc}\, z$. (For ***real*** arguments, S15ADF and S15AEF should be used).

9. Example

The following program reads values of the argument z from a file, evaluates the function at each value of z and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15DDF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          W, Z
      INTEGER          IFAIL
*     .. External Functions ..
      complex          S15DDF
      EXTERNAL         S15DDF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15DDF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '              Z                                  W'
   20 READ (NIN,*,END=40) Z
      IFAIL = 0
*
      W = S15DDF(Z,IFAIL)
*
      WRITE (NOUT,99999) Z, W
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,'(',F12.4,',',F12.4,')      (',F12.4,',',F12.4,')')
      END
```

9.2. Program Data

```
S15DDF Example Program Data
 ( 1.00E0,   0.00E0)       - Values for Z.
 (-3.01E0,   0.75E0)
 ( 2.75E0,  -1.52E0)
 (-1.33E0,  -0.54E0)
```

9.3. Program Results

```
 S15DDF Example Program Results

              Z                                  W
(      1.0000,       0.0000)      (      0.3679,       0.6072)
(     -3.0100,       0.7500)      (      0.0522,      -0.1838)
(      2.7500,      -1.5200)      (     -0.1015,       0.1654)
(     -1.3300,      -0.5400)      (     -0.1839,      -0.7891)
```

S17ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17ACF returns the value of the Bessel function $Y_0(x)$, via the routine name.

2. Specification

```
real FUNCTION S17ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Bessel function of the second kind $Y_0(x)$.

Note: $Y_0(x)$ is undefined for $x \leq 0$ and the routine will fail for such arguments.

The routine is based on four Chebyshev expansions:

For $0 < x \leq 8$,

$$Y_0(x) = \frac{2}{\pi} \ln x \sum_{r=0}{}' a_r T_r(t) + \sum_{r=0}{}' b_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{8}\right)^2 - 1$$

For $x > 8$,

$$Y_0(x) = \sqrt{\frac{2}{\pi x}}\left\{P_0(x)\sin\left(x-\frac{\pi}{4}\right) + Q_0(x)\cos\left(x-\frac{\pi}{4}\right)\right\}$$

where $P_0(x) = \sum_{r=0}{}' c_r T_r(t)$,

and $Q_0(x) = \frac{8}{x} \sum_{r=0}{}' d_r T_r(t), \quad$ with $t = 2\left(\frac{8}{x}\right)^2 - 1.$

For x near zero, $Y_0(x) \simeq \frac{2}{\pi}\left(\ln\left(\frac{x}{2}\right)+\gamma\right)$, where γ denotes Euler's constant. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For very large x, it becomes impossible to provide results with any reasonable accuracy (see Section 7), hence the routine fails. Such arguments contain insufficient information to determine the phase of oscillation of $Y_0(x)$; only the amplitude, $\sqrt{\frac{2}{\pi x}}$, can be determined and this is returned on soft failure. The range for which this occurs is roughly related to the ***machine precision***: the routine will fail if $x \gtrsim 1/$***machine precision*** (see the Users' Note for your implementation for details).

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] CLENSHAW, C.W.
Mathematical Tables.
Chebyshev Series for Mathematical Functions.
National Physical Laboratory, HMSO, 5, 1962.

5. Parameters

1: X – *real*. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large. On soft failure the routine returns the amplitude of the Y_0 oscillation, $\sqrt{\frac{2}{\pi x}}$.

IFAIL = 2

X ≤ 0.0, Y_0 is undefined. On soft failure the routine returns zero.

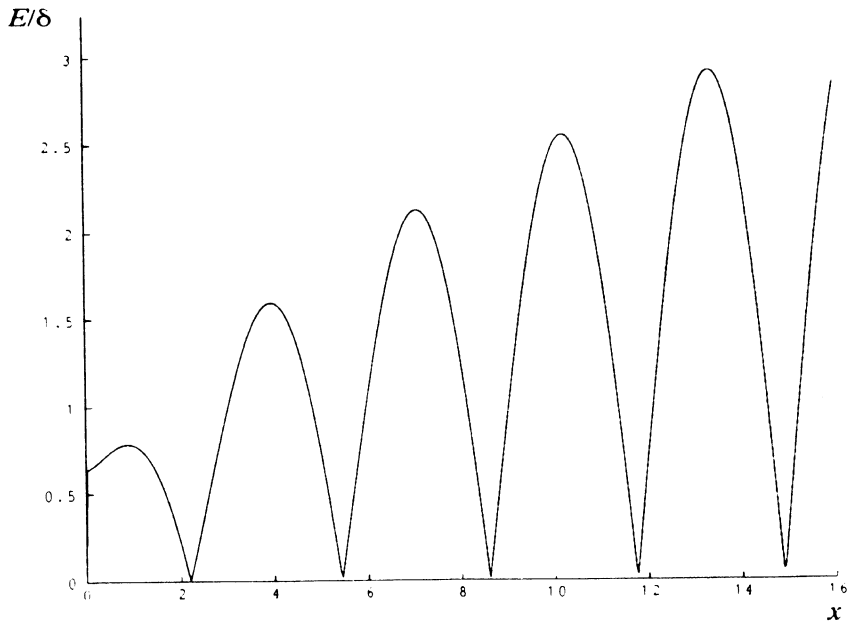
7. Accuracy

Let δ be the relative error in the argument and E be the absolute error in the result. (Since $Y_0(x)$ oscillates about zero, absolute error and not relative error is significant, except for very small x.)

If δ is somewhat larger than the machine representation error (e.g. if δ is due to data errors etc.), then E and δ are approximately related by

$$E \simeq |xY_1(x)|\ \delta$$

(provided E is also within machine bounds). The following graph displays the behaviour of the amplification factor $|xY_1(x)|$:



However, if δ is of the same order as the machine representation errors, then rounding errors could make E slightly larger than the above relation predicts.

For very small x, the errors are essentially independent of δ and the routine should provide relative accuracy bounded by the ***machine precision***.

For very large x, the above relation ceases to apply. In this region, $Y_0(x) \simeq \sqrt{\frac{2}{\pi x}}\sin\left(x-\frac{\pi}{4}\right)$. The amplitude $\sqrt{\frac{2}{\pi x}}$ can be calculated with reasonable accuracy for all x, but $\sin\left(x-\frac{\pi}{4}\right)$ cannot. If $x - \frac{\pi}{4}$ is written as $2N\pi + \theta$ where N is an integer and $0 \leq \theta < 2\pi$, then $\sin\left(x-\frac{\pi}{4}\right)$ is determined by θ only. If $x \geq \delta^{-1}$, θ cannot be determined with any accuracy at all. Thus if x is greater than, or of the order of the inverse of ***machine precision***, it is impossible to calculate the phase of $Y_0(x)$ and the routine must fail.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17ACF
      EXTERNAL         S17ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17ACF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
S17ACF Example Program Results

      X             Y         IFAIL

 0.000E+00    0.000E+00         2
 5.000E-01   -4.445E-01         0
 1.000E+00    8.826E-02         0
 3.000E+00    3.769E-01         0
 6.000E+00   -2.882E-01         0
 8.000E+00    2.235E-01         0
 1.000E+01    5.567E-02         0
-1.000E+00    0.000E+00         2
 1.000E+03    4.716E-03         0
```

S17ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17ADF returns the value of the Bessel Function $Y_1(x)$, via the routine name.

2. Specification

```
real FUNCTION S17ADF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Bessel Function of the second kind $Y_1(x)$.

Note: $Y_1(x)$ is undefined for $x \leq 0$ and the routine will fail for such arguments.

The routine is based on four Chebyshev expansions:

For $0 < x \leq 8$,

$$Y_1(x) = \frac{2}{\pi} \ln x \frac{x}{8} \sum_{r=0}{}' a_r T_r(t) - \frac{2}{\pi x} + \frac{x}{8} \sum_{r=0}{}' b_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{8}\right)^2 - 1;$$

For $x > 8$,

$$Y_1(x) = \sqrt{\frac{2}{\pi x}} \left\{ P_1(x) \sin\left(x - \frac{3\pi}{4}\right) + Q_1(x) \cos\left(x - \frac{3\pi}{4}\right) \right\}$$

where $P_1(x) = \sum_{r=0}{}' c_r T_r(t)$,

and $Q_1(x) = \frac{8}{x} \sum_{r=0}{}' d_r T_r(t), \qquad \text{with } t = 2\left(\frac{8}{x}\right)^2 - 1.$

For x near zero, $Y_1(x) \simeq -\frac{2}{\pi x}$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***. For extremely small x, there is a danger of overflow in calculating $-\frac{2}{\pi x}$ and for such arguments the routine will fail.

For very large x, it becomes impossible to provide results with any reasonable accuracy (see Section 7), hence the routine fails. Such arguments contain insufficient information to determine the phase of oscillation of $Y_1(x)$, only the amplitude, $\sqrt{\frac{2}{\pi x}}$, can be determined and this is returned on soft failure. The range for which this occurs is roughly related to ***machine precision***; the routine will fail if $x \geq 1/$***machine precision*** (see the Users' Note for your implementation for details).

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] CLENSHAW, C.W.
Mathematical Tables.
Chebyshev series for mathematical functions.
National Physical Laboratory, H.M.S.O., 5, 1962.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large. On soft failure the routine returns the amplitude of the Y_1 oscillation, $\sqrt{\frac{2}{\pi x}}$.

IFAIL = 2

X ≤ 0.0, Y_1 is undefined. On soft failure the routine returns zero.

IFAIL = 3

X is too close to zero, there is a danger of overflow. On soft failure, the routine returns the value of $Y_1(x)$ at the smallest valid argument.

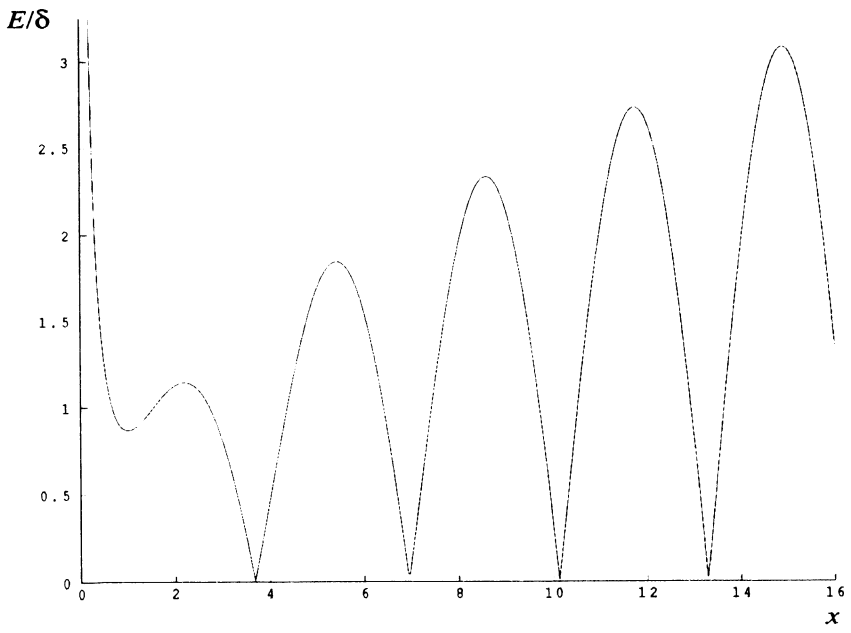
7. Accuracy

Let δ be the relative error in the argument and E be the absolute error in the result. (Since $Y_1(x)$ oscillates about zero, absolute error and not relative error is significant, except for very small x.)

If δ is somewhat larger than the ***machine precision*** (e.g. if δ is due to data errors etc.), then E and δ are approximately related by:

$$E \simeq |xY_0(x) - Y_1(x)|\ \delta$$

(provided E is also within machine bounds). The following graph displays the behaviour of the amplification factor $|xY_0(x) - Y_1(x)|$:



However, if δ is of the same order as ***machine precision***, then rounding errors could make E slightly larger than the above relation predicts.

For very small x, absolute error becomes large, but the relative error in the result is of the same order as δ.

For very large x, the above relation ceases to apply. In this region, $Y_1(x) \simeq \frac{2}{\pi x}\sin\left(x-\frac{3\pi}{4}\right)$. The amplitude $\frac{2}{\pi x}$ can be calculated with reasonable accuracy for all x, but $\sin\left(x-\frac{3\pi}{4}\right)$ cannot. If $x - \frac{3\pi}{4}$ is written as $2N\pi + \theta$ where N is an integer and $0 \leq \theta < 2\pi$, then $\sin\left(x-\frac{3\pi}{4}\right)$ is determined by θ only. If $x > \delta^{-1}$, θ cannot be determined with any accuracy at all. Thus if x is greater than, or of the order of, the inverse of the ***machine precision***, it is impossible to calculate the phase of $Y_1(x)$ and the routine must fail.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17ADF
      EXTERNAL         S17ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17ADF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
S17ADF Example Program Results

     X            Y         IFAIL

 0.000E+00    0.000E+00        2
 5.000E-01   -1.471E+00        0
 1.000E+00   -7.812E-01        0
 3.000E+00    3.247E-01        0
 6.000E+00   -1.750E-01        0
 8.000E+00   -1.581E-01        0
 1.000E+01    2.490E-01        0
-1.000E+00    0.000E+00        2
 1.000E+03   -2.478E-02        0
```

S17AEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17AEF returns the value of the Bessel Function $J_0(x)$, via the routine name.

2. Specification

```
real FUNCTION S17AEF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Bessel Function of the first kind $J_0(x)$.

Note: $J_0(-x) = J_0(x)$, so the approximation need only consider $x \geq 0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 8$,

$$J_0(x) = \sum_{r=0}{}' a_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{8}\right)^2 - 1.$$

For $x > 8$,

$$J_0(x) = \sqrt{\frac{2}{\pi x}}\left\{P_0(x)\cos\left(x-\frac{\pi}{4}\right) - Q_0(x)\sin\left(x-\frac{\pi}{4}\right)\right\}$$

where $P_0(x) = \sum_{r=0}{}' b_r T_r(t)$,

and $Q_0(x) = \frac{8}{x}\sum_{r=0}{}' c_r T_r(t), \qquad \text{with } t = 2\left(\frac{8}{x}\right)^2 - 1.$

For x near zero, $J_0(x) \simeq 1$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For very large x, it becomes impossible to provide results with any reasonable accuracy (see Section 7), hence the routine fails. Such arguments contain insufficient information to determine the phase of oscillation of $J_0(x)$; only the amplitude, $\sqrt{\frac{2}{\pi|x|}}$, can be determined and this is returned on soft failure. The range for which this occurs is roughly related to the ***machine precision***; the routine will fail if $|x| \geq 1/$***machine precision*** (see the Users' Note for your implementation).

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] CLENSHAW, C.W.
Mathematical Tables.
Chebyshev Series for Mathematical Functions.
National Physical Laboratory, HMSO, 5, 1962.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large. On soft failure the routine returns the amplitude of the J_0 oscillation, $\sqrt{\frac{2}{\pi|x|}}$.

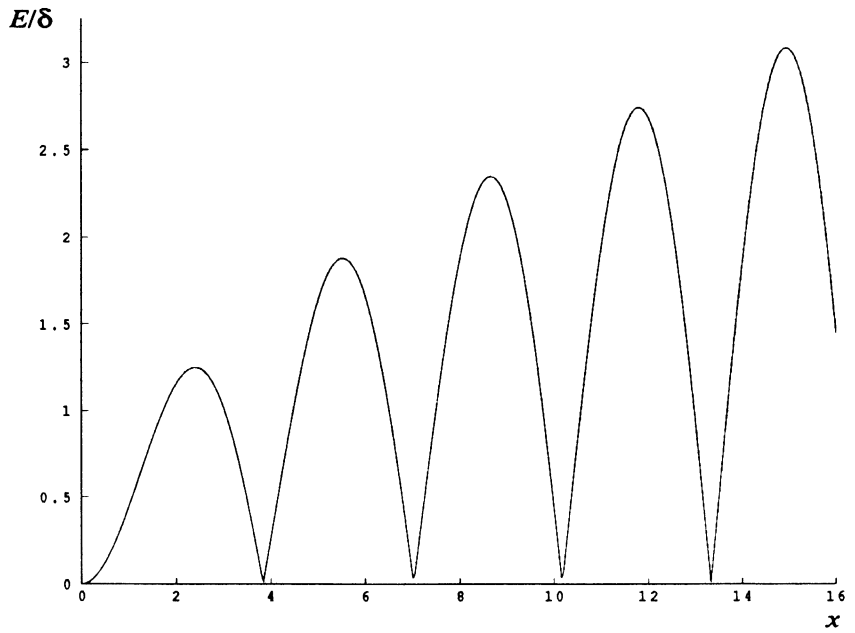
7. Accuracy

Let δ be the relative error in the argument and E be the absolute error in the result. (Since $J_0(x)$ oscillates about zero, absolute error and not relative error is significant.)

If δ is somewhat larger than the ***machine precision*** (e.g. if δ is due to data errors etc.), then E and δ are approximately related by:

$$E \simeq |xJ_1(x)|\ \delta$$

(provided E is also within machine bounds). The following graph displays the behaviour of the amplification factor $|xJ_1(x)|$:



However, if δ is of the same order as ***machine precision***, then rounding errors could make E slightly larger than the above relation predicts.

For very large x, the above relation ceases to apply. In this region, $J_0(x) \simeq \sqrt{\frac{2}{\pi|x|}}\cos\left(x-\frac{\pi}{4}\right)$. The amplitude $\sqrt{\frac{2}{\pi|x|}}$ can be calculated with reasonable accuracy for all x, but $\cos\left(x-\frac{\pi}{4}\right)$ cannot. If $x - \frac{\pi}{4}$ is written as $2N\pi + \theta$ where N is an integer and $0 \leq \theta < 2\pi$, then $\cos\left(x-\frac{\pi}{4}\right)$ is

determined by θ only. If $x \geq \delta^{-1}$, θ cannot be determined with any accuracy at all. Thus if x is greater than, or of the order of, the inverse of the ***machine precision***, it is impossible to calculate the phase of $J_0(x)$ and the routine must fail.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17AEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17AEF
      EXTERNAL         S17AEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17AEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17AEF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17AEF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
S17AEF Example Program Results

      X             Y         IFAIL

  0.000E+00   1.000E+00         0
  5.000E-01   9.385E-01         0
  1.000E+00   7.652E-01         0
  3.000E+00  -2.601E-01         0
  6.000E+00   1.506E-01         0
  8.000E+00   1.717E-01         0
  1.000E+01  -2.459E-01         0
 -1.000E+00   7.652E-01         0
  1.000E+03   2.479E-02         0
```

S17AFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17AFF returns the value of the Bessel function $J_1(x)$, via the routine name.

2. Specification

```
real FUNCTION S17AFF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Bessel function of the first kind $J_1(x)$.

Note: $J_1(-x) = -J_1(x)$, so the approximation need only consider $x \geq 0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 8$,

$$J_1(x) = \frac{x}{8} \sum_{r=0}{}' a_r T_r(t), \quad \text{with } t = 2\left(\frac{x}{8}\right)^2 - 1.$$

For $x > 8$,

$$J_1(x) = \sqrt{\frac{2}{\pi x}} \left\{ P_1(x)\cos\left(x - \frac{3\pi}{4}\right) - Q_1(x)\sin\left(x - \frac{3\pi}{4}\right) \right\}$$

where $P_1(x) = \sum_{r=0}{}' b_r T_r(t)$,

and $Q_1(x) = \frac{8}{x} \sum_{r=0}{}' c_r T_r(t), \quad \text{with } t = 2\left(\frac{8}{x}\right)^2 - 1.$

For x near zero, $J_1(x) \simeq \frac{x}{2}$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For very large x, it becomes impossible to provide results with any reasonable accuracy (see Section 7), hence the routine fails. Such arguments contain insufficient information to determine the phase of oscillation of $J_1(x)$; only the amplitude, $\sqrt{\frac{2}{\pi|x|}}$, can be determined and this is returned on soft failure. The range for which this occurs is roughly related to the ***machine precision***; the routine will fail if $|x| \geq 1/$***machine precision*** (see the Users' Note for your implementation for details).

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] CLENSHAW, C.W.
Mathematical Tables.
Chebyshev Series for Mathematical Functions.
National Physical Laboratory, HMSO, 5, 1962.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large. On soft failure the routine returns the amplitude of the J_1 oscillation, $\sqrt{\frac{2}{\pi|x|}}$.

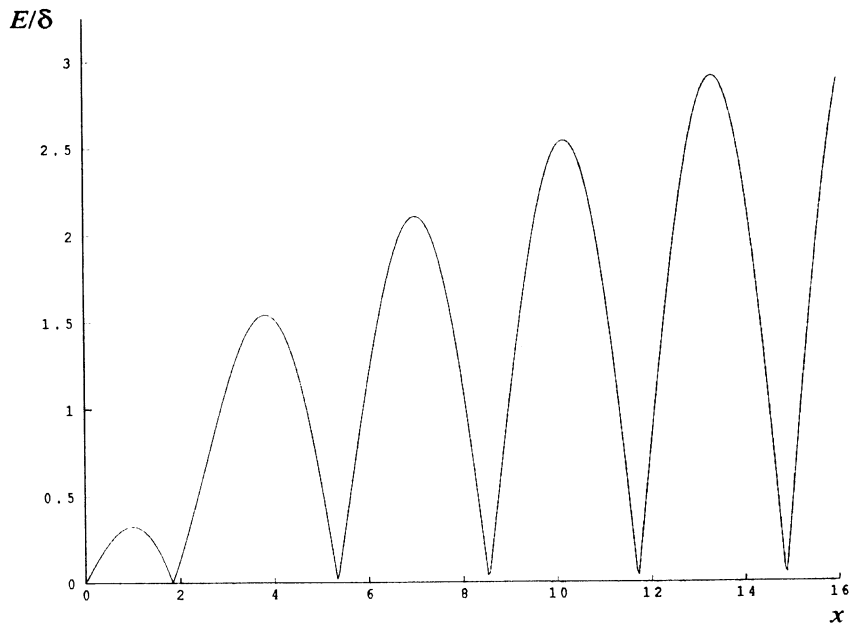
7. Accuracy

Let δ be the relative error in the argument and E be the absolute error in the result. (Since $J_1(x)$ oscillates about zero, absolute error and not relative error is significant.)

If δ is somewhat larger than ***machine precision*** (e.g. if δ is due to data errors etc.), then E and δ are approximately related by:

$$E \simeq |xJ_0(x)-J_1(x)|\ \delta$$

(provided E is also within machine bounds). The following graph displays the behaviour of the amplification factor $|xJ_0(x)-J_1(x)|$:



However, if δ is of the same order as ***machine precision***, then rounding errors could make E slightly larger than the above relation predicts.

For very large x, the above relation ceases to apply. In this region, $J_1(x) \simeq \sqrt{\frac{2}{\pi|x|}}\cos\left(x-\frac{3\pi}{4}\right)$. The amplitude $\sqrt{\frac{2}{\pi|x|}}$ can be calculated with reasonable accuracy for all x, but $\cos\left(x-\frac{3\pi}{4}\right)$ cannot. If $x - \frac{3\pi}{4}$ is written as $2N\pi + \theta$ where N is an integer and $0 \le \theta < 2\pi$, then $\cos\left(x-\frac{3\pi}{4}\right)$ is determined by θ only. If $x \ge \delta^{-1}$, θ cannot be determined with any accuracy at all. Thus if x is greater than, or of the order of the reciprocal of ***machine precision***, it is impossible to calculate the phase of $J_1(x)$ and the routine must fail.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17AFF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17AFF
      EXTERNAL         S17AFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17AFF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17AFF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17AFF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
S17AFF Example Program Results

     X            Y         IFAIL

 0.000E+00   0.000E+00         0
 5.000E-01   2.423E-01         0
 1.000E+00   4.401E-01         0
 3.000E+00   3.391E-01         0
 6.000E+00  -2.767E-01         0
 8.000E+00   2.346E-01         0
 1.000E+01   4.347E-02         0
-1.000E+00  -4.401E-01         0
 1.000E+03   4.728E-03         0
```

S17AGF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17AGF returns a value for the Airy function, $\mathrm{Ai}(x)$, via the routine name.

2. Specification

```
real FUNCTION S17AGF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Airy function, $\mathrm{Ai}(x)$. It is based on a number of Chebyshev expansions:

For $x < -5$,

$$\mathrm{Ai}(x) = \frac{a(t)\ \sin z - b(t)\ \cos z}{(-x)^{\frac{1}{4}}}$$

where $z = \frac{\pi}{4} + \frac{2}{3}\sqrt{-x^3}$, and $a(t)$ and $b(t)$ are expansions in the variable $t = -2\left(\frac{5}{x}\right)^3 - 1$.

For $-5 \leq x \leq 0$,

$$\mathrm{Ai}(x) = f(t) - x\ g(t),$$

where f and g are expansions in $t = -2\left(\frac{x}{5}\right)^3 - 1$.

For $0 < x < 4.5$,

$$\mathrm{Ai}(x) = e^{-3x/2}y(t),$$

where y is an expansion in $t = 4x/9 - 1$.

For $4.5 \leq x < 9$,

$$\mathrm{Ai}(x) = e^{-5x/2}u(t),$$

where u is an expansion in $t = 4x/9 - 3$.

For $x \geq 9$,

$$\mathrm{Ai}(x) = \frac{e^{-z}v(t)}{x^{\frac{1}{4}}},$$

where $z = \frac{2}{3}\sqrt{x^3}$ and v is an expansion in $t = 2\left(\frac{18}{z}\right) - 1$.

For $|x|$ < the ***machine precision***, the result is set directly to $\mathrm{Ai}(0)$. This both saves time and guards against underflow in intermediate calculations.

For large negative arguments, it becomes impossible to calculate the phase of the oscillatory function with any precision and so the routine must fail. This occurs if $x < -\left(\frac{3}{2\varepsilon}\right)^{\frac{1}{3}}$, where ε is the ***machine precision***.

For large positive arguments, where Ai decays in an essentially exponential manner, there is a danger of underflow so the routine must fail.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 10.4, p. 446., 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large and positive. On soft failure, the routine returns zero.

IFAIL = 2

X is too large and negative. On soft failure, the routine returns zero.

7. Accuracy

For negative arguments the function is oscillatory and hence absolute error is the appropriate measure. In the positive region the function is essentially exponential-like and here relative error is appropriate. The absolute error, E, and the relative error, ε, are related in principle to the relative error in the argument, δ, by

$$E \simeq |x\ \mathrm{Ai}'(x)|\delta, \qquad \varepsilon \simeq \left|\frac{x\ \mathrm{Ai}'(x)}{\mathrm{Ai}(x)}\right|\delta.$$

In practice, approximate equality is the best that can be expected. When δ, ε or E is of the order of the ***machine precision***, the errors in the result will be somewhat larger.

For small x, errors are strongly damped by the function and hence will be bounded by the ***machine precision***.

For moderate negative x, the error behaviour is oscillatory but the amplitude of the error grows like

$$\text{amplitude}\left(\frac{E}{\delta}\right) \sim \frac{|x|^{\frac{1}{4}}}{\sqrt{\pi}}.$$

However the phase error will be growing roughly like $\frac{2}{3}\sqrt{|x|^3}$ and hence all accuracy will be lost for large negative arguments due to the impossibility of calculating sin and cos to any accuracy if $\frac{2}{3}\sqrt{|x|^3} > \frac{1}{\delta}$.

For large positive arguments, the relative error amplification is considerable:

$$\frac{\varepsilon}{\delta} \sim \sqrt{x^3}.$$

This means a loss of roughly two decimal places accuracy for arguments in the region of 20. However very large arguments are not possible due to the danger of setting underflow and so the errors are limited in practice.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17AGF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17AGF
      EXTERNAL         S17AGF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17AGF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17AGF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17AGF Example Program Data
             -10.0
             -1.0
             0.0
             1.0
             5.0
             10.0
             20.0
```

9.3. Program Results

```
 S17AGF Example Program Results

      X           Y        IFAIL

  -1.000E+01   4.024E-02       0
  -1.000E+00   5.356E-01       0
   0.000E+00   3.550E-01       0
   1.000E+00   1.353E-01       0
   5.000E+00   1.083E-04       0
   1.000E+01   1.105E-10       0
   2.000E+01   1.692E-27       0
```

S17AHF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17AHF returns a value of the Airy function, $\mathrm{Bi}(x)$, via the routine name.

2. Specification

```
real FUNCTION S17AHF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Airy function $\mathrm{Bi}(x)$. It is based on a number of Chebyshev expansions.

For $x < -5$,

$$\mathrm{Bi}(x) = \frac{a(t)\cos z + b(t)\sin z}{(-x)^{\frac{1}{4}}},$$

where $z = \frac{\pi}{4} + \frac{2}{3}\sqrt{-x^3}$ and $a(t)$ and $b(t)$ are expansions in the variable $t = -2\left(\frac{5}{x}\right)^3 - 1$.

For $-5 \leq x \leq 0$,

$$\mathrm{Bi}(x) = \sqrt{3}\ (f(t)+xg(t)),$$

where f and g are expansions in $t = -2\left(\frac{x}{5}\right)^3 - 1$.

For $0 < x < 4.5$,

$$\mathrm{Bi}(x) = e^{11x/8}y(t),$$

where y is an expansion in $t = 4x/9 - 1$.

For $4.5 \leq x \leq 9$,

$$\mathrm{Bi}(x) = e^{5x/2}v(t),$$

where v is an expansion in $t = 4x/9 - 3$.

For $x \geq 9$,

$$\mathrm{Bi}(x) = \frac{e^z u(t)}{x^{\frac{1}{4}}},$$

where $z = \frac{2}{3}\sqrt{x^3}$ and u is an expansion in $t = 2\left(\frac{18}{z}\right) - 1$.

For $|x|$ < the ***machine precision***, the result is set directly to $\mathrm{Bi}(0)$. This both saves time and avoids possible intermediate underflows.

For large negative arguments, it becomes impossible to calculate the phase of the oscillating function with any accuracy so the routine must fail. This occurs if $x < -\left(\frac{3}{2\varepsilon}\right)^{\frac{1}{3}}$, where ε is the ***machine precision***.

For large positive arguments, there is a danger of causing overflow since Bi grows in an essentially exponential manner, so the routine must fail.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 10.4, p. 446, 1968.

5. Parameters

1: X – *real.* *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large and positive. On soft failure, the routine returns zero.

IFAIL = 2

X is too large and negative. On soft failure, the routine returns zero.

7. Accuracy

For negative arguments the function is oscillatory and hence absolute error is the appropriate measure. In the positive region the function is essentially exponential-like and here relative error is appropriate. The absolute error, E, and the relative error, ε, are related in principle to the relative error in the argument, δ, by

$$E \simeq |x\mathrm{Bi}'(x)|\delta, \qquad \varepsilon \simeq \left|\frac{x\mathrm{Bi}'(x)}{\mathrm{Bi}(x)}\right|\delta.$$

In practice, approximate equality is the best that can be expected. When δ, ε or E is of the order of the ***machine precision***, the errors in the result will be somewhat larger.

For small x, errors are strongly damped and hence will be bounded essentially by the ***machine precision***.

For moderate to large negative x, the error behaviour is clearly oscillatory but the amplitude of the error grows like

$$\text{amplitude}\left(\frac{E}{\delta}\right) \sim \frac{|x|^{\frac{1}{4}}}{\sqrt{\pi}}.$$

However the phase error will be growing roughly as $\frac{2}{3}\sqrt{|x|^3}$ and hence all accuracy will be lost for large negative arguments. This is due to the impossibility of calculating sin and cos to any accuracy if $\frac{2}{3}\sqrt{|x|^3} > \frac{1}{\delta}$.

For large positive arguments, the relative error amplification is considerable:

$$\frac{\varepsilon}{\delta} \sim \sqrt{x^3}.$$

This means a loss of roughly two decimal places accuracy for arguments in the region of 20. However very large arguments are not possible due to the danger of causing overflow and errors are therefore limited in practice.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17AHF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17AHF
      EXTERNAL         S17AHF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17AHF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17AHF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17AHF Example Program Data
             -10.0
             -1.0
             0.0
             1.0
             5.0
             10.0
             20.0
```

9.3. Program Results

```
S17AHF Example Program Results

      X             Y         IFAIL

 -1.000E+01  -3.147E-01         0
 -1.000E+00   1.040E-01         0
  0.000E+00   6.149E-01         0
  1.000E+00   1.207E+00         0
  5.000E+00   6.578E+02         0
  1.000E+01   4.556E+08         0
  2.000E+01   2.104E+25         0
```

S17AJF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17AJF returns a value of the derivative of the Airy function $\mathrm{Ai}(x)$, via the routine name.

2. Specification

```
real FUNCTION S17AJF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the derivative of the Airy function $\mathrm{Ai}(x)$. It is based on a number of Chebyshev expansions.

For $x < -5$,

$$\mathrm{Ai}'(x) = \sqrt[4]{-x}\left[a(t)\cos z + \frac{b(t)}{\zeta}\sin z\right],$$

where $z = \frac{\pi}{4} + \zeta$, $\zeta = \frac{2}{3}\sqrt{-x^3}$ and $a(t)$ and $b(t)$ are expansions in variable $t = -2\left(\frac{5}{x}\right)^3 - 1$.

For $-5 \leq x \leq 0$,

$$\mathrm{Ai}'(x) = x^2 f(t) - g(t),$$

where f and g are expansions in $t = -2\left(\frac{x}{5}\right)^3 - 1$.

For $0 < x < 4.5$,

$$\mathrm{Ai}'(x) = e^{-11x/8} y(t),$$

where $y(t)$ is an expansion in $t = 4\left(\frac{x}{9}\right) - 1$.

For $4.5 \leq x < 9$,

$$\mathrm{Ai}'(x) = e^{-5x/2} v(t),$$

where $v(t)$ is an expansion in $t = 4\left(\frac{x}{9}\right) - 3$.

For $x \geq 9$,

$$\mathrm{Ai}'(x) = \sqrt[4]{-x}\, e^{-z} u(t),$$

where $z = \frac{2}{3}\sqrt{x^3}$ and $u(t)$ is an expansion in $t = 2\left(\frac{18}{z}\right) - 1$.

For $|x|$ < the square of the ***machine precision***, the result is set directly to $\mathrm{Ai}'(0)$. This both saves time and avoids possible intermediate underflows.

For large negative arguments, it becomes impossible to calculate a result for the oscillating function with any accuracy and so the routine must fail. This occurs for $x < -\left(\frac{\sqrt{\pi}}{\varepsilon}\right)^{4/7}$, where ε is the ***machine precision***.

For large positive arguments, where Ai' decays in an essentially exponential manner, there is a danger of underflow so the routine must fail.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 10.4, p. 446, 1968.

5. Parameters

1: X – *real.* *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large and positive. On soft failure, the routine returns zero.

IFAIL = 2

X is too large and negative. On soft failure, the routine returns zero.

7. Accuracy

For negative arguments the function is oscillatory and hence absolute error is the appropriate measure. In the positive region the function is essentially exponential in character and here relative error is needed. The absolute error, E, and the relative error, ε, are related in principle to the relative error in the argument, δ, by

$$E \simeq |x^2 \mathrm{Ai}(x)|\delta \qquad \varepsilon \simeq \left|\frac{x^2 \mathrm{Ai}(x)}{\mathrm{Ai}'(x)}\right|\delta.$$

In practice, approximate equality is the best that can be expected. When δ, ε or E is of the order of the ***machine precision***, the errors in the result will be somewhat larger.

For small x, positive or negative, errors are strongly attenuated by the function and hence will be roughly bounded by the ***machine precision.***

For moderate to large negative x, the error, like the function, is oscillatory; however the amplitude of the error grows like

$$\frac{|x|^{7/4}}{\sqrt{\pi}}.$$

Therefore it becomes impossible to calculate the function with any accuracy if $|x|^{7/4} > \frac{\sqrt{\pi}}{\delta}$.

For large positive x, the relative error amplification is considerable:

$$\frac{\varepsilon}{\delta} \simeq \sqrt{x^3}.$$

However, very large arguments are not possible due to the danger of underflow. Thus in practice error amplification is limited.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17AJF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17AJF
      EXTERNAL         S17AJF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17AJF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17AJF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17AJF Example Program Data
             -10.0
             -1.0
             0.0
             1.0
             5.0
             10.0
             20.0
```

9.3. Program Results

```
 S17AJF Example Program Results

      X           Y         IFAIL

  -1.000E+01   9.963E-01       0
  -1.000E+00  -1.016E-02       0
   0.000E+00  -2.588E-01       0
   1.000E+00  -1.591E-01       0
   5.000E+00  -2.474E-04       0
   1.000E+01  -3.521E-10       0
   2.000E+01  -7.586E-27       0
```

S17AKF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17AKF returns a value for the derivative of the Airy function $\mathrm{Bi}(x)$, via the routine name.

2. Specification

```
real FUNCTION S17AKF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine calculates an approximate value for the derivative of the Airy function $\mathrm{Bi}(x)$. It is based on a number of Chebyshev expansions.

For $x < -5$,

$$\mathrm{Bi}'(x) = \sqrt[4]{-x}\left[-a(t)\,\sin z + \frac{b(t)}{\zeta}\,\cos z\right],$$

where $z = \frac{\pi}{4} + \zeta$, $\zeta = \frac{2}{3}\sqrt{-x^3}$ and $a(t)$ and $b(t)$ are expansions in the variable $t = -2\left(\frac{5}{x}\right)^3 - 1$.

For $-5 \leq x \leq 0$,

$$\mathrm{Bi}'(x) = \sqrt{3}(x^2 f(t) + g(t)),$$

where f and g are expansions in $t = -2\left(\frac{x}{5}\right)^3 - 1$.

For $0 < x < 4.5$,

$$\mathrm{Bi}'(x) = e^{3x/2} y(t),$$

where $y(t)$ is an expansion in $t = 4x/9 - 1$.

For $4.5 \leq x < 9$,

$$\mathrm{Bi}'(x) = e^{21x/8} u(t),$$

where $u(t)$ is an expansion in $t = 4x/9 - 3$.

For $x \geq 9$,

$$\mathrm{Bi}'(x) = \sqrt[4]{x} e^{z} v(t),$$

where $z = \frac{2}{3}\sqrt{x^3}$ and $v(t)$ is an expansion in $t = 2\left(\frac{18}{z}\right) - 1$.

For $|x|$ < the square of the ***machine precision***, the result is set directly to $\mathrm{Bi}'(0)$. This saves time and avoids possible underflows in calculation.

For large negative arguments, it becomes impossible to calculate a result for the oscillating function with any accuracy so the routine must fail. This occurs for $x < -\left(\frac{\sqrt{\pi}}{\varepsilon}\right)^{\frac{4}{3}}$, where ε is the ***machine precision***.

For large positive arguments, where Bi′ grows in an essentially exponential manner, there is a danger of overflow so the routine must fail.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 10.4, p. 446, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large and positive. On soft failure the routine returns zero.

IFAIL = 2

X is too large and negative. On soft failure the routine returns zero.

7. Accuracy

For negative arguments the function is oscillatory and hence absolute error is appropriate. In the positive region the function has essentially exponential behaviour and hence relative error is needed. The absolute error, E, and the relative error ε, are related in principle to the relative error in the argument δ, by

$$E \simeq |x^2 \mathrm{Bi}(x)|\delta \qquad \varepsilon \simeq \left|\frac{x^2 \mathrm{Bi}(x)}{\mathrm{Bi}'(x)}\right|\delta.$$

In practice, approximate equality is the best that can be expected. When δ, ε or E is of the order of the ***machine precision***, the errors in the result will be somewhat larger.

For small x, positive or negative, errors are strongly attenuated by the function and hence will effectively be bounded by the ***machine precision.***

For moderate to large negative x, the error is, like the function, oscillatory. However, the amplitude of the absolute error grows like $\frac{|x|^{\frac{1}{4}}}{\sqrt{\pi}}$. Therefore it becomes impossible to calculate the function with any accuracy if $|x|^{\frac{1}{4}} > \frac{\sqrt{\pi}}{\delta}$.

For large positive x, the relative error amplification is considerable: $\frac{\varepsilon}{\delta} \sim \sqrt{x^3}$. However, very large arguments are not possible due to the danger of overflow. Thus in practice the actual amplification that occurs is limited.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17AKF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S17AKF
      EXTERNAL         S17AKF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17AKF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S17AKF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S17AKF Example Program Data
             -10.0
             -1.0
             0.0
             1.0
             5.0
             10.0
             20.0
```

9.3. Program Results

```
 S17AKF Example Program Results

      X           Y        IFAIL

  -1.000E+01   1.194E-01       0
  -1.000E+00   5.924E-01       0
   0.000E+00   4.483E-01       0
   1.000E+00   9.324E-01       0
   5.000E+00   1.436E+03       0
   1.000E+01   1.429E+09       0
   2.000E+01   9.382E+25       0
```

S17DCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17DCF returns a sequence of values for the Bessel functions $Y_{\nu+n}(z)$ for complex z, non-negative ν and $n = 0,1,...,N-1$, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S17DCF (FNU, Z, N, SCALE, CY, NZ, CWRK, IFAIL)
INTEGER          N, NZ, IFAIL
real             FNU
complex          Z, CY(N), CWRK(N)
CHARACTER*1      SCALE
```

3. Description

This subroutine evaluates a sequence of values for the Bessel function $Y_\nu(z)$, where z is complex, $-\pi < \arg z \leq \pi$, and ν is the real, non-negative order. The N-member sequence is generated for orders $\nu, \nu+1,...,\nu+N-1$. Optionally, the sequence is scaled by the factor $e^{-|\mathrm{Im}\, z|}$.

Note: although the routine may not be called with ν less than zero, for negative orders the formula $Y_{-\nu}(z) = Y_\nu(z)\cos(\pi\nu) + J_\nu(z)\sin(\pi\nu)$ may be used (for the Bessel function $J_\nu(z)$, see S17DEF).

The routine is derived from the routine CBESY in Amos [2]. It is based on the relation $Y_\nu(z) = \dfrac{H_\nu^{(1)}(z) - H_\nu^{(2)}(z)}{2i}$, where $H_\nu^{(1)}(z)$ and $H_\nu^{(2)}(z)$ are the Hankel functions of the first and second kinds respectively (see S17DLF).

When N is greater than 1, extra values of $Y_\nu(z)$ are computed using recurrence relations.

For very large $|z|$ or $(\nu+N-1)$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$ or $(\nu+N-1)$, the computation is performed but results are accurate to less than half of ***machine precision***. If $|z|$ is very small, near the machine underflow threshold, or $(\nu+N-1)$ is too large, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions, Ch. 9, p. 358.
Dover Publications, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software, 12, pp. 265-273, 1986.

5. Parameters

1: FNU – ***real***. *Input*

On entry: the order, ν, of the first member of the sequence of functions.

Constraint: FNU $\geq$ 0.0.

2: Z – ***complex***. *Input*

On entry: the argument, z, of the functions.

Constraint: Z $\neq$ (0.0, 0.0).

3: N – INTEGER. *Input*

On entry: the number, N, of members required in the sequence $Y_\nu(z), Y_{\nu+1}(z),...,Y_{\nu+N-1}(z)$.

Constraint: N ≥ 1.

4: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the results are returned unscaled.

If SCALE = 'S' or 's', the results are returned scaled by the factor $e^{-|\mathrm{Im}\, z|}$.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

5: CY(N) – ***complex*** array. *Output*

On exit: the N required function values: CY(i) contains $Y_{\nu+i-1}(z)$, for i = 1,2,...,N.

6: NZ – INTEGER. *Output*

On exit: the number of components of CY that are set to zero due to underflow. The positions of such components in the array CY are arbitrary.

7: CWRK(N) – ***complex*** array. *Workspace*

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, FNU < 0.0,
or Z = (0.0, 0.0),
or N < 1,
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because ABS(Z) is less than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 3

No computation has been performed due to the likelihood of overflow, because FNU + N – 1 is too large – how large depends on Z as well as the overflow threshold of the machine.

IFAIL = 4

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the results returned by S17DCF are accurate to less than half of ***machine precision***. This error exit may occur if either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in results returned by S17DCF would be lost. This error exit may occur if either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 6

No results are returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S17DCF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S17DCF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S17DCF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||,|\log_{10}v|)$ represents the number of digits lost due to the argument reduction. Thus the larger the values of $|z|$ and v, the less the precision in the result. If S17DCF is called with $N > 1$, then computation of function values via recurrence may lead to some further small loss of accuracy.

If function values which should nominally be identical are computed by calls to S17DCF with different base values of v and different N, the computed values may not agree exactly. Empirical tests with modest values of v and z have shown that the discrepancy is limited to the least significant 3-4 digits of precision.

8. Further Comments

The time taken by the routine for a call of S17DCF is approximately proportional to the value of N, plus a constant. In general it is much cheaper to call S17DCF with N greater than 1, rather than to make N separate calls to S17DCF.

Paradoxically, for some values of z and v, it is cheaper to call S17DCF with a larger value of N than is required, and then discard the extra function values returned. However, it is not possible to state the precise circumstances in which this is likely to occur. It is due to the fact that the base value used to start recurrence may be calculated in different regions for different N, and the costs in each region may differ greatly.

Note that if the function required is $Y_0(x)$ or $Y_1(x)$, i.e. $v = 0.0$ or 1.0, where x is real and positive, and only a single unscaled function value is required, then it may be much cheaper to call S17ACF or S17ADF respectively.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the order FNU, the second is a complex value for the argument, Z, and the third is a value for the parameter SCALE. The program calls the routine with N = 2 to evaluate the function for orders FNU and FNU + 1, and it prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17DCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          N
      PARAMETER        (N=2)
*     .. Local Scalars ..
      complex          Z
      real             FNU
      INTEGER          IFAIL, NZ
      CHARACTER*1      SCALE
*     .. Local Arrays ..
      complex          CWRK(N), CY(N)
*     .. External Subroutines ..
      EXTERNAL         S17DCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17DCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Calling with N =', N
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'   FNU             Z         SCALE       CY(1)                CY(2)
     +   NZ IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) FNU, Z, SCALE
      IFAIL = 0
*
      CALL S17DCF(FNU,Z,N,SCALE,CY,NZ,CWRK,IFAIL)
*
      WRITE (NOUT,99998) FNU, Z, SCALE, CY(1), CY(2), NZ, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,A,I2)
99998 FORMAT (1X,F7.4,'  (',F7.3,',',F7.3,')   ',A,
     +       2('  (',F7.3,',',F7.3,')'),I4,I4)
      END
```

9.2. Program Data

```
S17DCF Example Program Data
 0.00     ( 0.3,  0.4)     'U'
 2.30     ( 2.0,  0.0)     'U'
 2.12     (-1.0,  0.0)     'U'
 1.58     (-2.3,  5.6)     'U'
 1.58     (-2.3,  5.6)     'S'
```

9.3. Program Results

```
S17DCF Example Program Results

Calling with N = 2

   FNU             Z         SCALE       CY(1)                CY(2)      NZ IFAIL

 0.0000  (  0.300,  0.400)   U  ( -0.498,  0.670)  ( -1.015,  0.949)   0   0
 2.3000  (  2.000,  0.000)   U  ( -0.740,  0.000)  ( -1.412,  0.000)   0   0
 2.1200  ( -1.000,  0.000)   U  ( -1.728,  0.860)  (  6.533, -2.615)   0   0
 1.5800  ( -2.300,  5.600)   U  ( 36.476, -1.552)  ( -2.679, 25.911)   0   0
 1.5800  ( -2.300,  5.600)   S  (  0.135, -0.006)  ( -0.010,  0.096)   0   0
```

S17DEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17DEF returns a sequence of values for the Bessel functions $J_{\nu+n}(z)$ for complex z, non-negative ν and $n = 0,1,...,N-1$, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S17DEF (FNU, Z, N, SCALE, CY, NZ, IFAIL)
INTEGER          N, NZ, IFAIL
real             FNU
complex          Z, CY(N)
CHARACTER*1      SCALE
```

3. Description

This subroutine evaluates a sequence of values for the Bessel function $J_\nu(z)$, where z is complex, $-\pi < \arg z \leq \pi$, and ν is the real, non-negative order. The N-member sequence is generated for orders $\nu, \nu+1,...,\nu+N-1$. Optionally, the sequence is scaled by the factor $e^{-|\mathrm{Im}\, z|}$.

Note: although the routine may not be called with ν less than zero, for negative orders the formula $J_{-\nu}(z) = J_\nu(z)\cos(\pi\nu) - Y_\nu(z)\sin(\pi\nu)$ may be used (for the Bessel function $Y_\nu(z)$, see S17DCF).

The routine is derived from the routine CBESJ in Amos [2]. It is based on the relations $J_\nu(z) = e^{\nu\pi i/2} I_\nu(-iz)$, $\mathrm{Im}\, z \geq 0.0$, and $J_\nu(z) = e^{-\nu\pi i/2} I_\nu(iz)$, $\mathrm{Im}\, z < 0.0$.

The Bessel function $I_\nu(z)$ is computed using a variety of techniques depending on the region under consideration.

When N is greater than 1, extra values of $J_\nu(z)$ are computed using recurrence relations.

For very large $|z|$ or $(\nu+N-1)$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$ or $(\nu+N-1)$, the computation is performed but results are accurate to less than half of ***machine precision***. If $\mathrm{Im}\, z$ is large, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software, 12, pp. 265-273, 1986.

5. Parameters

1: FNU – ***real***. *Input*

On entry: the order, ν, of the first member of the sequence of functions.

Constraint: FNU $\geq$ 0.0.

2: Z – ***complex***. *Input*

On entry: the argument z of the functions.

3: N – INTEGER. *Input*

On entry: the number, N, of members required in the sequence $J_\nu(z), J_{\nu+1}(z), \ldots, J_{\nu+N-1}(z)$.

Constraint: N ≥ 1.

4: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the results are returned unscaled.

If SCALE = 'S' or 's', the results are returned scaled by the factor $e^{-|\mathrm{Im}\, z|}$.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

5: CY(N) – ***complex*** array. *Output*

On exit: the N required function values: CY(i) contains $J_{\nu+i-1}(z)$, for i = 1,2,...,N.

6: NZ – INTEGER. *Output*

On exit: the number of components of CY that are set to zero due to underflow. If NZ > 0, then elements CY(N–NZ+1), CY(N–NZ+2),...,CY(N) are set to zero.

7: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, FNU < 0.0,
or N < 1,
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because Im Z is larger than a machine-dependent threshold value (given in the Users' Note for your implementation). This error exit can only occur when SCALE = 'U' or 'u'.

IFAIL = 3

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the results returned by S17DEF are accurate to less than half of ***machine precision***. This error exit may occur if either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 4

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in results returned by S17DEF would be lost. This error exit may occur when either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No results are returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S17DEF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S17DEF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S17DEF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||,|\log_{10}\nu|)$ represents the number of digits lost due to the argument reduction. Thus the larger the values of $|z|$ and ν, the less the precision in the result. If S17DEF is called with $N > 1$, then computation of function values via recurrence may lead to some further small loss of accuracy.

If function values which should nominally be identical are computed by calls to S17DEF with different base values of ν and different N, the computed values may not agree exactly. Empirical tests with modest values of ν and z have shown that the discrepancy is limited to the least significant 3-4 digits of precision.

8. Further Comments

The time taken by the routine for a call of S17DEF is approximately proportional to the value of N, plus a constant. In general it is much cheaper to call S17DEF with N greater than 1, rather than to make N separate calls to S17DEF.

Paradoxically, for some values of z and ν, it is cheaper to call S17DEF with a larger value of N than is required, and then discard the extra function values returned. However, it is not possible to state the precise circumstances in which this is likely to occur. It is due to the fact that the base value used to start recurrence may be calculated in different regions for different N, and the costs in each region may differ greatly.

Note that if the function required is $J_0(x)$ or $J_1(x)$, i.e. $\nu = 0.0$ or 1.0, where x is real and positive, and only a single unscaled function value is required, then it may be much cheaper to call S17AEF or S17AFF respectively.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the order FNU, the second is a complex value for the argument, Z, and the third is a value for the parameter SCALE. The program calls the routine with N = 2 to evaluate the function for orders FNU and FNU + 1, and it prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17DEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          N
      PARAMETER        (N=2)
*     .. Local Scalars ..
      complex          Z
      real             FNU
      INTEGER          IFAIL, NZ
      CHARACTER*1      SCALE
*     .. Local Arrays ..
      complex          CY(N)
*     .. External Subroutines ..
      EXTERNAL         S17DEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17DEF Example Program Results'
```

```
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Calling with N =', N
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'    FNU             Z         SCALE        CY(1)                CY(2)
     +    NZ IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) FNU, Z, SCALE
      IFAIL = 0
*
      CALL S17DEF(FNU,Z,N,SCALE,CY,NZ,IFAIL)
*
      WRITE (NOUT,99998) FNU, Z, SCALE, CY(1), CY(2), NZ, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,A,I2)
99998 FORMAT (1X,F7.4,'  (',F7.3,',',F7.3,')   ',A,
     +       2('  (',F7.3,',',F7.3,')'),I4,I4)
      END
```

9.2. Program Data

```
S17DEF Example Program Data
 0.00     ( 0.3,  0.4)     'U'
 2.30     ( 2.0,  0.0)     'U'
 2.12     (-1.0,  0.0)     'U'
 1.58     (-2.3,  5.6)     'U'
 1.58     (-2.3,  5.6)     'S'
```

9.3. Program Results

```
 S17DEF Example Program Results

 Calling with N = 2

    FNU             Z         SCALE       CY(1)                CY(2)      NZ IFAIL

  0.0000  (  0.300,  0.400)   U  (  1.017, -0.061)  (  0.157,  0.197)    0    0
  2.3000  (  2.000,  0.000)   U  (  0.272,  0.000)  (  0.089,  0.000)    0    0
  2.1200  ( -1.000,  0.000)   U  (  0.088,  0.035)  ( -0.014, -0.006)    0    0
  1.5800  ( -2.300,  5.600)   U  ( -1.551,-36.476)  ( 25.910,  2.677)    0    0
  1.5800  ( -2.300,  5.600)   S  ( -0.006, -0.135)  (  0.096,  0.010)    0    0
```

S17DGF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17DGF returns the value of the Airy function $\mathrm{Ai}(z)$ or its derivative $\mathrm{Ai}'(z)$ for complex z, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S17DGF (DERIV, Z, SCALE, AI, NZ, IFAIL)
INTEGER          NZ, IFAIL
complex          Z, AI
CHARACTER*1      DERIV, SCALE
```

3. Description

This subroutine returns a value for the Airy function $\mathrm{Ai}(z)$ or its derivative $\mathrm{Ai}'(z)$, where z is complex, $-\pi < \arg z \leq \pi$. Optionally, the value is scaled by the factor $e^{2z\sqrt{z}/3}$.

The routine is derived from the routine CAIRY in Amos [2]. It is based on the relations $\mathrm{Ai}(z) = \dfrac{\sqrt{z}K_{1/3}(w)}{\pi\sqrt{3}}$, and $\mathrm{Ai}'(z) = \dfrac{-zK_{2/3}(w)}{\pi\sqrt{3}}$, where K_ν is the modified Bessel function and $w = 2z\sqrt{z}/3$.

For very large $|z|$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$, the computation is performed but results are accurate to less than half of ***machine precision***. If Re w is too large, and the unscaled function is required, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software 12, pp. 265-273, 1986.

5. Parameters

1: DERIV – CHARACTER*1. *Input*

On entry: specifies whether the function or its derivative is required.

If DERIV = 'F' or 'f', $\mathrm{Ai}(z)$ is returned.

If DERIV = 'D' or 'd', $\mathrm{Ai}'(z)$ is returned.

Constraint: DERIV = 'F', 'f', 'D' or 'd'.

2: Z – ***complex***. *Input*

On entry: the argument z of the function.

3: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the result is returned unscaled.

If SCALE = 'S' or 's', the result is returned scaled by the factor $e^{2z\sqrt{z}/3}$.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

4: AI – ***complex***. *Output*

On exit: the required function or derivative value.

5: NZ – INTEGER. *Output*

On exit: NZ indicates whether or not AI is set to zero due to underflow. This can only occur when SCALE = 'U' or 'u'.

If NZ = 0, AI is not set to zero.

If NZ = 1, AI is set to zero.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, DERIV ≠ 'F', 'f', 'D' or 'd',
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because Re w is too large, where $w = 2Z\sqrt{Z}/3$ – how large depends on Z and the overflow threshold of the machine. This error exit can only occur when SCALE = 'U' or 'u'.

IFAIL = 3

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the result returned by S17DGF is accurate to less than half of ***machine precision***. This error exit may occur if ABS(Z) is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 4

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in the result returned by S17DGF would be lost. This error exit may occur if ABS(Z) is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No result is returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S17DGF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S17DGF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S17DGF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||)$ represents the number of digits lost due to the argument reduction. Thus the larger the value of $|z|$, the less the precision in the result.

Empirical tests with modest values of z, checking relations between Airy functions $\mathrm{Ai}(z)$, $\mathrm{Ai}'(z)$, $\mathrm{Bi}(z)$ and $\mathrm{Bi}'(z)$, have shown errors limited to the least significant 3-4 digits of precision.

8. Further Comments

Note that if the function is required to operate on a real argument only, then it may be much cheaper to call S17AGF or S17AJF.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the parameter DERIV, the second is a complex value for the argument, Z, and the third is a value for the parameter SCALE. The program calls the routine and prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17DGF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          AI, Z
      INTEGER          IFAIL, NZ
      CHARACTER*1      DERIV, SCALE
*     .. External Subroutines ..
      EXTERNAL         S17DGF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17DGF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +  'DERIV           Z          SCALE           AI          NZ  IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) DERIV, Z, SCALE
      IFAIL = 0
*
      CALL S17DGF(DERIV,Z,SCALE,AI,NZ,IFAIL)
*
      WRITE (NOUT,99999) DERIV, Z, SCALE, AI, NZ, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (3X,A,'   (',F8.4,',',F8.4,')   ',A,'   (',F8.4,',',F8.4,
     +       ')',I4,I5)
      END
```

9.2. Program Data

```
S17DGF Example Program Data
 'F'    ( 0.3,  0.4)    'U'
 'F'    ( 0.2,  0.0)    'U'
 'F'    ( 1.1, -6.6)    'U'
 'F'    ( 1.1, -6.6)    'S'
 'D'    (-1.0,  0.0)    'U'
```

9.3. Program Results

```
S17DGF Example Program Results

DERIV          Z          SCALE          AI          NZ  IFAIL

  F   (  0.3000,  0.4000)   U   (  0.2716, -0.1002)   0     0
  F   (  0.2000,  0.0000)   U   (  0.3037,  0.0000)   0     0
  F   (  1.1000, -6.6000)   U   (-43.6632,-47.9030)   0     0
  F   (  1.1000, -6.6000)   S   (  0.1655,  0.0597)   0     0
  D   ( -1.0000,  0.0000)   U   ( -0.0102,  0.0000)   0     0
```

S17DHF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17DHF returns the value of the Airy function $\mathrm{Bi}(z)$ or its derivative $\mathrm{Bi}'(z)$ for complex z, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S17DHF (DERIV, Z, SCALE, BI, IFAIL)
INTEGER          IFAIL
complex          Z, BI
CHARACTER*1      DERIV, SCALE
```

3. Description

This subroutine returns a value for the Airy function $\mathrm{Bi}(z)$ or its derivative $\mathrm{Bi}'(z)$, where z is complex, $-\pi < \arg z \leq \pi$. Optionally, the value is scaled by the factor $e^{|\mathrm{Re}(2z\sqrt{z}/3)|}$.

The routine is derived from the routine CBIRY in Amos [2]. It is based on the relations $\mathrm{Bi}(z) = \frac{\sqrt{z}}{\sqrt{3}}(I_{-1/3}(w)+I_{1/3}(w))$, and $\mathrm{Bi}'(z) = \frac{z}{\sqrt{3}}(I_{-2/3}(w)+I_{2/3}(w))$, where I_ν is the modified Bessel function and $w = 2z\sqrt{z}/3$.

For very large $|z|$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$, the computation is performed but results are accurate to less than half of ***machine precision***. If $\mathrm{Re}\, z$ is too large, and the unscaled function is required, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software, 12, pp. 265-273, 1986.

5. Parameters

1: DERIV – CHARACTER*1. *Input*

On entry: specifies whether the function or its derivative is required.

If DERIV = 'F' or 'f', $\mathrm{Bi}(z)$ is returned.

If DERIV = 'D' or 'd', $\mathrm{Bi}'(z)$ is returned.

Constraint: DERIV = 'F', 'f', 'D' or 'd'.

2: Z – ***complex***. *Input*

On entry: the argument z of the function.

3: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the result is returned unscaled.

If SCALE = 'S' or 's', the result is returned scaled by the factor $e^{|\mathrm{Re}(2z\sqrt{z}/3)|}$.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

4: BI – ***complex***. *Output*

On exit: the required function or derivative value.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, DERIV ≠ 'F', 'f', 'D' or 'd',
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because real(Z) is too large – how large depends on the overflow threshold of the machine. This error exit can only occur when SCALE = 'U' or 'u'.

IFAIL = 3

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the result returned by S17DHF is accurate to less than half of ***machine precision***. This error exit may occur if ABS(Z) is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 4

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in the result returned by S17DHF would be lost. This error exit may occur if ABS(Z) is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No result is returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S17DHF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S17DHF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S17DHF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||)$ represents the number of digits lost due to the argument reduction. Thus the larger the value of $|z|$, the less the precision in the result.

Empirical tests with modest values of z, checking relations between Airy functions $\mathrm{Ai}(z)$, $\mathrm{Ai}'(z)$, $\mathrm{Bi}(z)$ and $\mathrm{Bi}'(z)$, have shown errors limited to the least significant 3-4 digits of precision.

8. Further Comments

Note that if the function is required to operate on a real argument only, then it may be much cheaper to call S17AHF or S17AKF.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the parameter DERIV, the second is a complex value for the argument, Z, and the third is a value for the parameter SCALE. The program calls the routine and prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17DHF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          BI, Z
      INTEGER          IFAIL
      CHARACTER*1      DERIV, SCALE
*     .. External Subroutines ..
      EXTERNAL         S17DHF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17DHF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +  'DERIV           Z          SCALE           BI          IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) DERIV, Z, SCALE
      IFAIL = 0
*
      CALL S17DHF(DERIV,Z,SCALE,BI,IFAIL)
*
      WRITE (NOUT,99999) DERIV, Z, SCALE, BI, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (3X,A,'   (',F8.4,',',F8.4,')   ',A,'   (',F8.4,',',F8.4,
     +       ')',I5)
      END
```

9.2. Program Data

```
S17DHF Example Program Data
 'F'   ( 0.3,  0.4)    'U'
 'F'   ( 0.2,  0.0)    'U'
 'F'   ( 1.1, -6.6)    'U'
 'F'   ( 1.1, -6.6)    'S'
 'D'   (-1.0,  0.0)    'U'
```

9.3. Program Results

```
S17DHF Example Program Results

DERIV            Z            SCALE            BI          IFAIL

  F    (  0.3000,  0.4000)     U    (  0.7355,  0.1825)     0
  F    (  0.2000,  0.0000)     U    (  0.7055,  0.0000)     0
  F    (  1.1000, -6.6000)     U    (-47.9039, 43.6634)     0
  F    (  1.1000, -6.6000)     S    ( -0.1300,  0.1185)     0
  D    ( -1.0000,  0.0000)     U    (  0.5924,  0.0000)     0
```

S17DLF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S17DLF returns a sequence of values for the Hankel functions $H_{\nu+n}^{(1)}(z)$ or $H_{\nu+n}^{(2)}(z)$ for complex z, non-negative ν and $n = 0,1,...,N-1$, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S17DLF (M, FNU, Z, N, SCALE, CY, NZ, IFAIL)
INTEGER          M, N, NZ, IFAIL
real             FNU
complex          Z, CY(N)
CHARACTER*1      SCALE
```

3. Description

This subroutine evaluates a sequence of values for the Hankel function $H_\nu^{(1)}(z)$ or $H_\nu^{(2)}(z)$, where z is complex, $-\pi < \arg z \leq \pi$, and ν is the real, non-negative order. The N-member sequence is generated for orders ν, $\nu+1,...,\nu+N-1$. Optionally, the sequence is scaled by the factor e^{-iz} if the function is $H_\nu^{(1)}(z)$ or by the factor e^{iz} if the function is $H_\nu^{(2)}(z)$.

Note: although the routine may not be called with ν less than zero, for negative orders the formulae $H_{-\nu}^{(1)}(z) = e^{\nu\pi i}H_\nu^{(1)}(z)$, and $H_{-\nu}^{(2)}(z) = e^{-\nu\pi i}H_\nu^{(2)}(z)$ may be used.

The routine is derived from the routine CBESH in Amos [2]. It is based on the relation

$$H_\nu^{(m)}(z) = \frac{1}{p}e^{-p\nu}K_\nu(ze^{-p}),$$

where $p = \frac{i\pi}{2}$ if $m = 1$ and $p = \frac{-i\pi}{2}$ if $m = 2$, and the Bessel function $K_\nu(z)$ is computed in the right half-plane only. Continuation of $K_\nu(z)$ to the left half-plane is computed in terms of the Bessel function $I_\nu(z)$. These functions are evaluated using a variety of different techniques, depending on the region under consideration.

When N is greater than 1, extra values of $H_\nu^{(m)}(z)$ are computed using recurrence relations.

For very large $|z|$ or $(\nu+N-1)$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$ or $(\nu+N-1)$, the computation is performed but results are accurate to less than half of ***machine precision***. If $|z|$ is very small, near the machine underflow threshold, or $(\nu+N-1)$ is too large, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software, 12, pp. 265-273, 1986.

5. Parameters

1: M – INTEGER. *Input*

On entry: the kind of functions required.

If M = 1, the functions are $H_\nu^{(1)}(z)$.

If M = 2, the functions are $H_\nu^{(2)}(z)$.

Constraint: M = 1 or 2.

2: FNU – ***real***. *Input*

On entry: the order, ν, of the first member of the sequence of functions.

Constraint: FNU ≥ 0.0.

3: Z – ***complex***. *Input*

On entry: the argument z of the functions.

Constraint: Z ≠ (0.0, 0.0).

4: N – INTEGER. *Input*

On entry: the number, N, of members required in the sequence $H_\nu^{(M)}(z)$, $H_{\nu+1}^{(M)}(z)$,..., $H_{\nu+N-1}^{(M)}(z)$.

Constraint: N ≥ 1.

5: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the results are returned unscaled.

If SCALE = 'S' or 's', the results are returned scaled by the factor e^{-iz} when M = 1, or by the factor e^{iz} when M = 2.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

6: CY(N) – ***complex*** array. *Output*

On exit: the N required function values: CY(i) contains $H_{\nu+i-1}^{(M)}(z)$, for i = 1,2,...,N.

7: NZ – INTEGER. *Output*

On exit: the number of components of CY that are set to zero due to underflow. If NZ > 0, then if Im z > 0.0 and M = 1, or Im z < 0.0 and M = 2, elements CY(1), CY(2),...,CY(NZ) are set to zero. In the complementary half-planes, NZ simply states the number of underflows, and not which elements they are.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, M ≠ 1 and M ≠ 2,
or FNU < 0.0,
or Z = (0.0, 0.0),

or N < 1,
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because ABS(Z) is less than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 3

No computation has been performed due to the likelihood of overflow, because FNU + N – 1 is too large – how large depends on Z and the overflow threshold of the machine.

IFAIL = 4

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the results returned by S17DLF are accurate to less than half of ***machine precision***. This error exit may occur if either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in results returned by S17DLF would be lost. This error exit may occur when either of ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 6

No results are returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S17DLF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S17DLF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S17DLF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||,|\log_{10}v|)$ represents the number of digits lost due to the argument reduction. Thus the larger the values of $|z|$ and v, the less the precision in the result. If S17DLF is called with $N > 1$, then computation of function values via recurrence may lead to some further small loss of accuracy.

If function values which should nominally be identical are computed by calls to S17DLF with different base values of v and different N, the computed values may not agree exactly. Empirical tests with modest values of v and z have shown that the discrepancy is limited to the least significant 3-4 digits of precision.

8. Further Comments

The time taken by the routine for a call of S17DLF is approximately proportional to the value of N, plus a constant. In general it is much cheaper to call S17DLF with N greater than 1, rather than to make N separate calls to S17DLF.

Paradoxically, for some values of z and v, it is cheaper to call S17DLF with a larger value of N than is required, and then discard the extra function values returned. However, it is not possible to state the precise circumstances in which this is likely to occur. It is due to the fact that the base value used to start recurrence may be calculated in different regions for different N, and the costs in each region may differ greatly.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the kind of function, M, the second is a value for the order FNU, the third is a complex value for the argument, Z, and the fourth is a value for the parameter SCALE. The program calls the routine with N = 2 to evaluate the function for orders FNU and FNU + 1, and it prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S17DLF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          N
      PARAMETER        (N=2)
*     .. Local Scalars ..
      complex          Z
      real             FNU
      INTEGER          IFAIL, M, NZ
      CHARACTER*1      SCALE
*     .. Local Arrays ..
      complex          CY(N)
*     .. External Subroutines ..
      EXTERNAL         S17DLF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S17DLF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Calling with N =', N
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'M    FNU            Z       SCALE       CY(1)              CY(2)
     +     NZ IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) M, FNU, Z, SCALE
      IFAIL = 0
*
      CALL S17DLF(M,FNU,Z,N,SCALE,CY,NZ,IFAIL)
*
      WRITE (NOUT,99998) M, FNU, Z, SCALE, CY(1), CY(2), NZ, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,A,I2)
99998 FORMAT (1X,I1,1X,F7.4,'  (',F7.3,',',F7.3,')  ',A,
     +       2('  (',F7.3,',',F7.3,')'),I4,I4)
      END
```

9.2. Program Data

```
S17DLF Example Program Data
 1    0.00    ( 0.3,  0.4)    'U'
 1    2.30    ( 2.0,  0.0)    'U'
 1    2.12    (-1.0,  0.0)    'U'
 2    6.00    ( 3.1, -1.6)    'U'
 2    6.00    ( 3.1, -1.6)    'S'
```

9.3. Program Results

```
S17DLF Example Program Results

Calling with N = 2

 M    FNU            Z          SCALE       CY(1)                CY(2)          NZ IFAIL
 1  0.0000  (  0.300,  0.400)    U   (  0.347, -0.559)  ( -0.791, -0.818)    0    0
 1  2.3000  (  2.000,  0.000)    U   (  0.272, -0.740)  (  0.089, -1.412)    0    0
 1  2.1200  ( -1.000,  0.000)    U   ( -0.772, -1.693)  (  2.601,  6.527)    0    0
 2  6.0000  (  3.100, -1.600)    U   ( -1.371, -1.280)  ( -1.491, -5.993)    0    0
 2  6.0000  (  3.100, -1.600)    S   (  7.050,  6.052)  (  8.614, 29.352)    0    0
```

S18ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18ACF returns the value of the modified Bessel Function $K_0(x)$, via the routine name.

2. Specification

```
real FUNCTION S18ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the modified Bessel Function of the second kind $K_0(x)$.

Note: $K_0(x)$ is undefined for $x \leq 0$ and the routine will fail for such arguments.

The routine is based on five Chebyshev expansions:

For $0 < x \leq 1$,

$$K_0(x) = -\ln x \sum_{r=0}{}' a_r T_r(t) + \sum_{r=0}{}' b_r T_r(t), \qquad \text{where } t = 2x^2 - 1;$$

For $1 < x \leq 2$,

$$K_0(x) = e^{-x} \sum_{r=0}{}' c_r T_r(t), \qquad \text{where } t = 2x - 3;$$

For $2 < x \leq 4$,

$$K_0(x) = e^{-x} \sum_{r=0}{}' d_r T_r(t), \qquad \text{where } t = x - 3;$$

For $x > 4$,

$$K_0(x) = \frac{e^{-x}}{\sqrt{x}} \sum_{r=0}{}' e_r T_r(t), \qquad \text{where } t = \frac{9 - x}{1 + x}.$$

For x near zero, $K_0(x) \simeq -\gamma - \ln\left(\frac{x}{2}\right)$, where γ denotes Euler's constant. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For large x, where there is a danger of underflow due to the smallness of K_0, the result is set exactly to zero.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X ≤ 0.0, K_0 is undefined. On soft failure the routine returns zero.

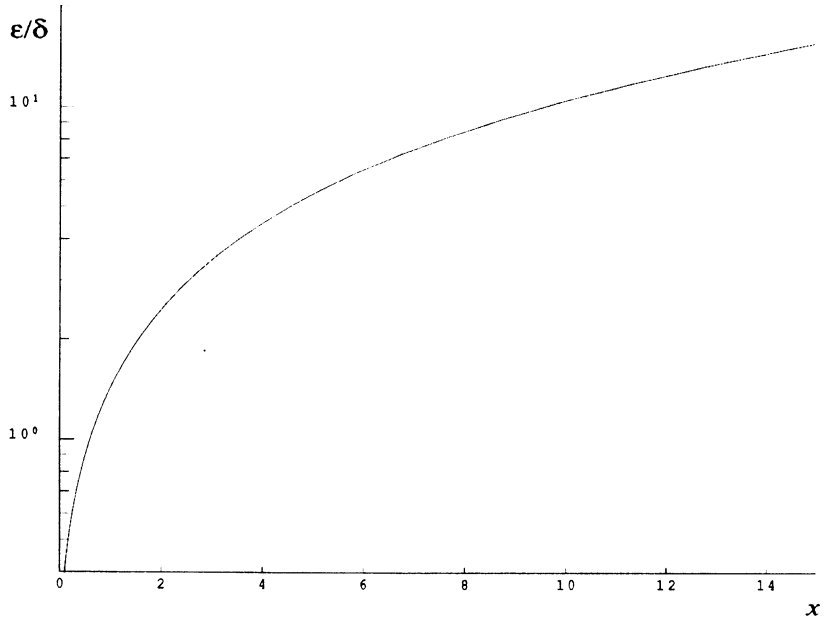
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e. if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{xK_1(x)}{K_0(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{xK_1(x)}{K_0(x)} \right|$:



However, if δ is of the same order as ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

For small x, the amplification factor is approximately $\left| \frac{1}{\ln x} \right|$, which implies strong attenuation of the error, but in general ε can never be less than the ***machine precision***.

For large x, $\varepsilon \simeq x\delta$ and we have strong amplification of the relative error. Eventually K_0, which is asymptotically given by $\frac{e^{-x}}{\sqrt{x}}$, becomes so small that it cannot be calculated without underflow and hence the routine will return zero. Note that for large x the errors will be dominated by those of the Fortran intrinsic function EXP.

8. Further Comments

For details of the time taken by the routine see the appropriate the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18ACF
      EXTERNAL         S18ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18ACF Example Program Data
             0.0
             0.4
             0.6
             1.4
             1.6
             2.5
             3.5
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
S18ACF Example Program Results

      X             Y          IFAIL

  0.000E+00    0.000E+00          1
  4.000E-01    1.115E+00          0
  6.000E-01    7.775E-01          0
  1.400E+00    2.437E-01          0
  1.600E+00    1.880E-01          0
  2.500E+00    6.235E-02          0
  3.500E+00    1.960E-02          0
  6.000E+00    1.244E-03          0
  8.000E+00    1.465E-04          0
  1.000E+01    1.778E-05          0
 -1.000E+00    0.000E+00          1
  1.000E+03    0.000E+00          0
```

S18ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18ADF returns the value of the modified Bessel Function $K_1(x)$, via the routine name.

2. Specification

```
real FUNCTION S18ADF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the modified Bessel Function of the second kind $K_1(x)$.

Note: $K_1(x)$ is undefined for $x \leq 0$ and the routine will fail for such arguments.

The routine is based on five Chebyshev expansions:

For $0 < x \leq 1$,

$$K_1(x) = \frac{1}{x} + x \ln x \sum_{r=0}{}' a_r T_r(t) - x \sum_{r=0}{}' b_r T_r(t), \qquad \text{where } t = 2x^2 - 1;$$

For $1 < x \leq 2$,

$$K_1(x) = e^{-x} \sum_{r=0}{}' c_r T_r(t), \qquad \text{where } t = 2x - 3;$$

For $2 < x \leq 4$,

$$K_1(x) = e^{-x} \sum_{r=0}{}' d_r T_r(t), \qquad \text{where } t = x - 3;$$

For $x > 4$,

$$K_1(x) = \frac{e^{-x}}{\sqrt{x}} \sum_{r=0}{}' e_r T_r(t), \qquad \text{where } t = \frac{9 - x}{1 + x}.$$

For x near zero, $K_1(x) \simeq \frac{1}{x}$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***. For very small x on some machines, it is impossible to calculate $\frac{1}{x}$ without overflow and the routine must fail.

For large x, where there is a danger of underflow due to the smallness of K_1, the result is set exactly to zero.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X ≤ 0.0, K_1 is undefined. On soft failure the routine returns zero.

IFAIL = 2

X is too small, there is a danger of overflow. On soft failure the routine returns approximately the largest representable value.

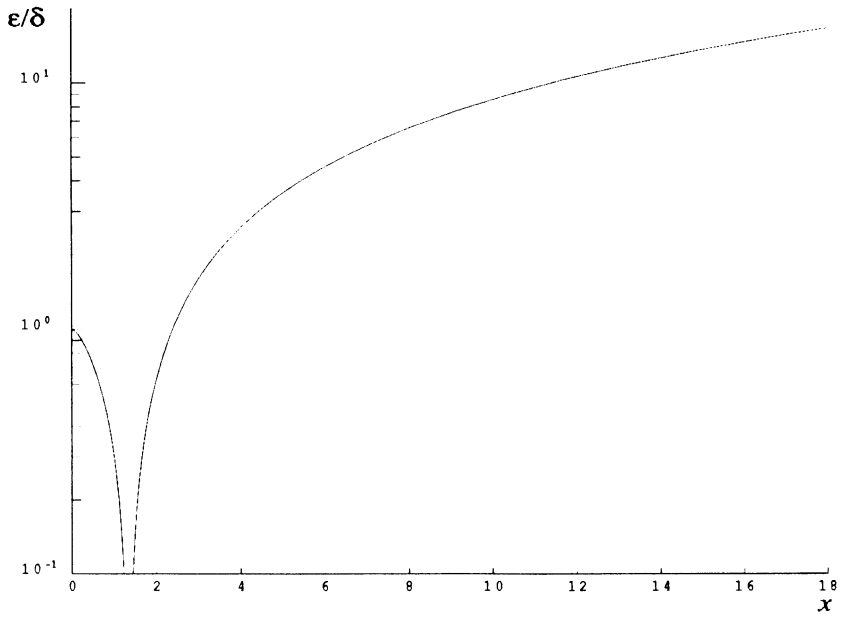
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e. if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{xK_0(x) - K_1(x)}{K_1(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{xK_0(x) - K_1(x)}{K_1(x)} \right|$:



However if δ is of the same order as the ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

For small x, $\varepsilon \simeq \delta$ and there is no amplification of errors.

For large x, $\varepsilon \simeq x\delta$ and we have strong amplification of the relative error. Eventually K_1, which is asymptotically given by $\frac{e^{-x}}{\sqrt{x}}$, becomes so small that it cannot be calculated without underflow and hence the routine will return zero. Note that for large x the errors will be dominated by those of the Fortran intrinsic function EXP.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18ADF
      EXTERNAL         S18ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18ADF Example Program Data
             0.0
             0.4
             0.6
             1.4
             1.6
             2.5
             3.5
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
S18ADF Example Program Results

      X             Y         IFAIL

 0.000E+00    0.000E+00          1
 4.000E-01    2.184E+00          0
 6.000E-01    1.303E+00          0
 1.400E+00    3.208E-01          0
 1.600E+00    2.406E-01          0
 2.500E+00    7.389E-02          0
 3.500E+00    2.224E-02          0
 6.000E+00    1.344E-03          0
 8.000E+00    1.554E-04          0
 1.000E+01    1.865E-05          0
-1.000E+00    0.000E+00          1
 1.000E+03    0.000E+00          0
```

S18AEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18AEF returns the value of the modified Bessel Function $I_0(x)$, via the routine name.

2. Specification

```
real FUNCTION S18AEF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the modified Bessel Function of the first kind $I_0(x)$.

Note: $I_0(-x) = I_0(x)$, so the approximation need only consider $x \geq 0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 4$,

$$I_0(x) = e^x \sum_{r=0}{}' a_r T_r(t), \qquad \text{where } t = 2\left(\frac{x}{4}\right) - 1;$$

For $4 < x \leq 12$,

$$I_0(x) = e^x \sum_{r=0}{}' b_r T_r(t), \qquad \text{where } t = \frac{x - 8}{4};$$

For $x > 12$,

$$I_0(x) = \frac{e^x}{\sqrt{x}} \sum_{r=0}{}' c_r T_r(t), \qquad \text{where } t = 2\left(\frac{12}{x}\right) - 1.$$

For small x, $I_0(x) \simeq 1$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For large x, the routine must fail because of the danger of overflow in calculating e^x.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large. On soft failure the routine returns the approximate value of $I_0(x)$ at the nearest valid argument.

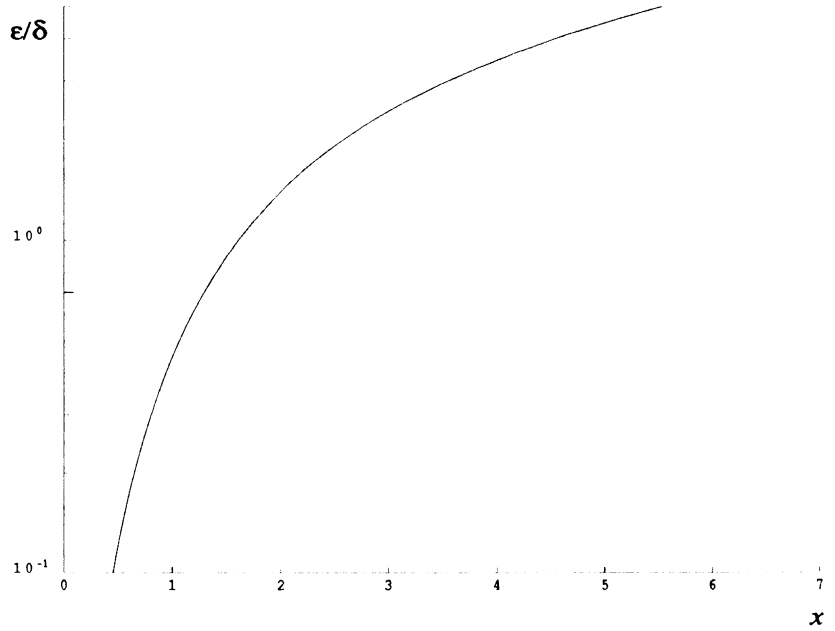
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e. if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{xI_1(x)}{I_0(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{xI_1(x)}{I_0(x)} \right|$:



However if δ is of the same order as ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

For small x the amplification factor is approximately $\frac{x^2}{2}$, which implies strong attenuation of the error, but in general ε can never be less than the ***machine precision***.

For large x, $\varepsilon \simeq x\delta$ and we have strong amplification of errors. However the routine must fail for quite moderate values of x, because $I_0(x)$ would overflow; hence in practice the loss of accuracy for large x is not excessive. Note that for large x the errors will be dominated by those of the Fortran intrinsic function EXP.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18AEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18AEF
      EXTERNAL         S18AEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18AEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18AEF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18AEF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             8.0
             10.0
             15.0
             20.0
             -1.0
```

9.3. Program Results

```
 S18AEF Example Program Results

      X           Y         IFAIL

   0.000E+00   1.000E+00       0
   5.000E-01   1.063E+00       0
   1.000E+00   1.266E+00       0
   3.000E+00   4.881E+00       0
   6.000E+00   6.723E+01       0
   8.000E+00   4.276E+02       0
   1.000E+01   2.816E+03       0
   1.500E+01   3.396E+05       0
   2.000E+01   4.356E+07       0
  -1.000E+00   1.266E+00       0
```

S18AFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18AFF returns a value for the modified Bessel Function $I_1(X)$, via the routine name.

2. Specification

```
real FUNCTION S18AFF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the modified Bessel Function of the first kind $I_1(x)$.

Note: $I_1(-x) = -I_1(x)$, so the approximation need only consider $x \geq 0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 4$,

$$I_1(x) = x \sum_{r=0}{}' a_r T_r(t), \qquad \text{where } t = 2\left(\frac{x}{4}\right)^2 - 1;$$

For $4 < x \leq 12$,

$$I_1(x) = e^x \sum_{r=0}{}' b_r T_r(t), \qquad \text{where } t = \frac{x - 8}{4};$$

For $x > 12$,

$$I_1(x) = \frac{e^x}{\sqrt{x}} \sum_{r=0}{}' c_r T_r(t), \qquad \text{where } t = 2\left(\frac{12}{x}\right) - 1.$$

For small x, $I_1(x) \simeq x$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For large x, the routine must fail because $I_1(x)$ cannot be represented without overflow.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

X is too large. On soft failure the routine returns the approximate value of $I_1(x)$ at the nearest valid argument.

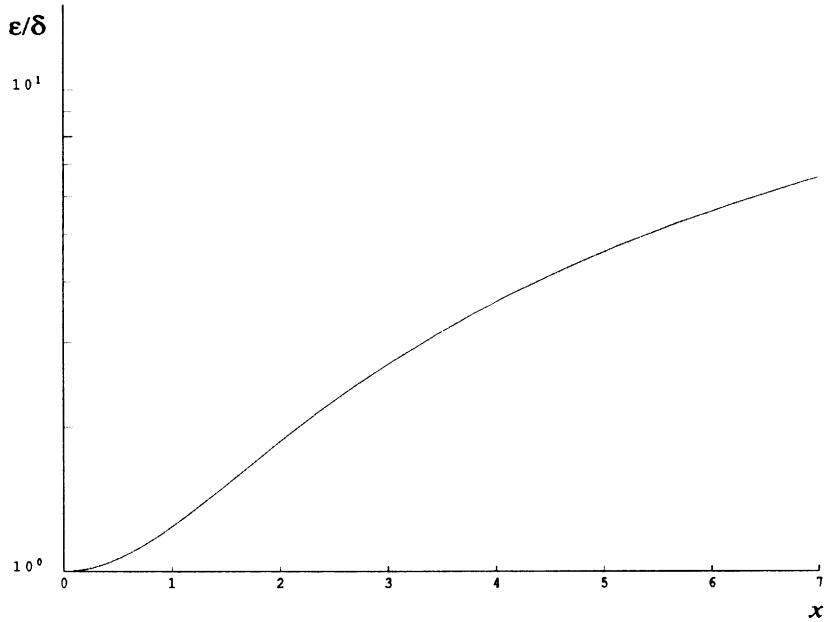
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e. if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{xI_0(x) - I_1(x)}{I_1(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{xI_0(x) - I_1(x)}{I_1(x)} \right|$:



However if δ is of the same order as ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

For small x, $\varepsilon \simeq \delta$ and there is no amplification of errors.

For large x, $\varepsilon \simeq x\delta$ and we have strong amplification of errors. However the routine must fail for quite moderate values of x because $I_1(x)$ would overflow; hence in practice the loss of accuracy for large x is not excessive. Note that for large x, the errors will be dominated by those of the Fortran intrinsic function EXP.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18AFF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18AFF
      EXTERNAL         S18AFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18AFF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18AFF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18AFF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             8.0
             10.0
             15.0
             20.0
             -1.0
```

9.3. Program Results

```
 S18AFF Example Program Results

      X           Y         IFAIL

   0.000E+00   0.000E+00       0
   5.000E-01   2.579E-01       0
   1.000E+00   5.652E-01       0
   3.000E+00   3.953E+00       0
   6.000E+00   6.134E+01       0
   8.000E+00   3.999E+02       0
   1.000E+01   2.671E+03       0
   1.500E+01   3.281E+05       0
   2.000E+01   4.245E+07       0
  -1.000E+00  -5.652E-01       0
```

S18CCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18CCF returns a value of the scaled modified Bessel function $e^x K_0(x)$ via the routine name.

2. Specification

```
real FUNCTION S18CCF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to $e^x K_0(x)$, where K_0 is a modified Bessel function of the second kind. The scaling factor e^x removes most of the variation in $K_0(x)$.

The routine uses the same Chebyshev expansions as S18ACF, which returns the unscaled value of $K_0(x)$.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry X ≤ 0.0, K_0 is undefined.

On soft failure, S18CCF returns zero.

7. Accuracy

Relative errors in the argument are attenuated when propagated into the function value. When the accuracy of the argument is essentially limited by the ***machine precision***, the accuracy of the function value will be similarly limited by at most a small multiple of the ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18CCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18CCF
      EXTERNAL         S18CCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18CCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18CCF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18CCF Example Program Data
             0.0
             0.4
             0.6
             1.4
             2.5
             10.0
             1000.0
             -1.0
```

9.3. Program Results

```
 S18CCF Example Program Results

      X           Y        IFAIL

   0.000E+00   0.000E+00       1
   4.000E-01   1.663E+00       0
   6.000E-01   1.417E+00       0
   1.400E+00   9.881E-01       0
   2.500E+00   7.595E-01       0
   1.000E+01   3.916E-01       0
   1.000E+03   3.963E-02       0
  -1.000E+00   0.000E+00       1
```

S18CDF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18CDF returns a value of the scaled modified Bessel function $e^x K_1(x)$ via the routine name.

2. Specification

```
real FUNCTION S18CDF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to $e^x K_1(x)$, where K_1 is a modified Bessel function of the second kind. The scaling factor e^x removes most of the variation in $K_1(x)$.

The routine uses the same Chebyshev expansions as S18ADF, which returns the unscaled value of $K_1(x)$.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

Constraint: X > 0.0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry X ≤ 0.0, K_1 is undefined. On soft failure S18CDF returns zero.

IFAIL = 2

On entry X is too close to zero, there is a danger of causing overflow. On soft failure, S18CDF returns the value of the function at the smallest permitted value of the argument.

7. Accuracy

Relative errors in the argument are attenuated when propagated into the function value. When the accuracy of the argument is essentially limited by the ***machine precision***, the accuracy of the function value will be similarly limited by at most a small multiple of the ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18CDF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18CDF
      EXTERNAL         S18CDF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18CDF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18CDF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18CDF Example Program Data
             0.0
             0.4
             0.6
             1.4
             2.5
             10.0
             1000.0
             -1.0
```

9.3. Program Results

```
 S18CDF Example Program Results

      X           Y         IFAIL

   0.000E+00   0.000E+00       1
   4.000E-01   3.259E+00       0
   6.000E-01   2.374E+00       0
   1.400E+00   1.301E+00       0
   2.500E+00   9.002E-01       0
   1.000E+01   4.108E-01       0
   1.000E+03   3.965E-02       0
  -1.000E+00   0.000E+00       1
```

S18CEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18CEF returns a value of the scaled modified Bessel function $e^{-|x|}I_0(x)$ via the routine name.

2. Specification

```
real FUNCTION S18CEF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to $e^{-|x|}I_0(x)$, where I_0 is a modified Bessel function of the first kind. The scaling factor $e^{-|x|}$ removes most of the variation in $I_0(x)$.

The routine uses the same Chebyshev expansions as S18AEF, which returns the unscaled value of $I_0(x)$.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no actual failure exits from this routine. IFAIL is always set to zero. This parameter is included for compatibility with other routines in this chapter.

7. Accuracy

Relative errors in the argument are attenuated when propagated into the function value. When the accuracy of the argument is essentially limited by the ***machine precision***, the accuracy of the function value will be similarly limited by at most a small multiple of the ***machine precision***.

8. Further Comments

For details of the time taken by the routine see appropriate the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18CEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18CEF
      EXTERNAL         S18CEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18CEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18CEF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18CEF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             10.0
             1000.0
             -1.0
```

9.3. Program Results

```
 S18CEF Example Program Results

      X           Y        IFAIL

   0.000E+00   1.000E+00       0
   5.000E-01   6.450E-01       0
   1.000E+00   4.658E-01       0
   3.000E+00   2.430E-01       0
   6.000E+00   1.667E-01       0
   1.000E+01   1.278E-01       0
   1.000E+03   1.262E-02       0
  -1.000E+00   4.658E-01       0
```

S18CFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18CFF returns a value of the scaled modified Bessel function $e^{-|x|}I_1(x)$ via the routine name.

2. Specification

```
real FUNCTION S18CFF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to $e^{-|x|}I_1(x)$, where I_1 is a modified Bessel function of the first kind. The scaling factor $e^{-|x|}$ removes most of the variation in $I_1(x)$.

The routine uses the same Chebyshev expansions as S18AFF, which returns the unscaled value of $I_1(x)$.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 374, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no actual failure exits from this routine. IFAIL is always set to zero. This parameter is included for compatibility with other routines in this chapter.

7. Accuracy

Relative errors in the argument are attenuated when propagated into the function value. When the accuracy of the argument is essentially limited by the ***machine precision***, the accuracy of the function value will be similarly limited by at most a small multiple of the ***machine precision***.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18CFF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S18CFF
      EXTERNAL         S18CFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18CFF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S18CFF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S18CFF Example Program Data
             0.0
             0.5
             1.0
             3.0
             6.0
             10.0
             1000.0
             -1.0
```

9.3. Program Results

```
 S18CFF Example Program Results

      X           Y        IFAIL

   0.000E+00   0.000E+00       0
   5.000E-01   1.564E-01       0
   1.000E+00   2.079E-01       0
   3.000E+00   1.968E-01       0
   6.000E+00   1.521E-01       0
   1.000E+01   1.213E-01       0
   1.000E+03   1.261E-02       0
  -1.000E+00  -2.079E-01       0
```

S18DCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18DCF returns a sequence of values for the modified Bessel functions $K_{\nu+n}(z)$ for complex z, non-negative ν and $n = 0,1,...,N-1$, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S18DCF (FNU, Z, N, SCALE, CY, NZ, IFAIL)
INTEGER          N, NZ, IFAIL
real             FNU
complex          Z, CY(N)
CHARACTER*1      SCALE
```

3. Description

This subroutine evaluates a sequence of values for the modified Bessel function $K_\nu(z)$, where z is complex, $-\pi < \arg z \leq \pi$, and ν is the real, non-negative order. The N–member sequence is generated for orders ν, $\nu+1,...,\nu+N-1$. Optionally, the sequence is scaled by the factor e^z.

The routine is derived from the routine CBESK in Amos [2].

Note: although the routine may not be called with ν less than zero, for negative orders the formula $K_{-\nu}(z) = K_\nu(z)$ may be used.

When N is greater than 1, extra values of $K_\nu(z)$ are computed using recurrence relations.

For very large $|z|$ or $(\nu+N-1)$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$ or $(\nu+N-1)$, the computation is performed but results are accurate to less than half of ***machine precision***. If $|z|$ is very small, near the machine underflow threshold, or $(\nu+N-1)$ is too large, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software 12, pp. 265-273, 1986.

5. Parameters

1: FNU – ***real***. *Input*

On entry: the order, ν, of the first member of the sequence of functions.

Constraint: FNU $\geq$ 0.0.

2: Z – ***complex***. *Input*

On entry: the argument z of the functions.

Constraint: Z $\neq$ (0.0, 0.0).

3: N – INTEGER. *Input*

On entry: the number, N, of members required in the sequence $K_\nu(z)$, $K_{\nu+1}(z)$, ..., $K_{\nu+N-1}(z)$.

Constraint: N ≥ 1.

4: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the results are returned unscaled.

If SCALE = 'S' or 's', the results are returned scaled by the factor e^z.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

5: CY(N) – ***complex*** array. *Output*

On exit: the N required function values: CY(i) contains $K_{\nu+i-1}(z)$, for i = 1,2,...,N.

6: NZ – INTEGER. *Output*

On exit: the number of components of CY that are set to zero due to underflow. If NZ > 0 and Re $z \geq 0.0$, elements CY(1),CY(2),...,CY(NZ) are set to zero. If Re $z < 0.0$, NZ simply states the number of underflows, and not which elements they are.

7: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, FNU < 0.0,
or Z = (0.0, 0.0),
or N < 1,
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because ABS(Z) is less than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 3

No computation has been performed due to the likelihood of overflow, because FNU + N – 1 is too large – how large depends on Z and the overflow threshold of the machine.

IFAIL = 4

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the results returned by S18DCF are accurate to less than half of ***machine precision***. This error exit may occur if either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in results returned by S18DCF would be lost. This error exit may occur when either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 6

No results are returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S18DCF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S18DCF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S18DCF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||,|\log_{10}v|)$ represents the number of digits lost due to the argument reduction. Thus the larger the values of $|z|$ and v, the less the precision in the result. If S18DCF is called with $N > 1$, then computation of function values via recurrence may lead to some further small loss of accuracy.

If function values which should nominally be identical are computed by calls to S18DCF with different base values of v and different N, the computed values may not agree exactly. Empirical tests with modest values of v and z have shown that the discrepancy is limited to the least significant 3-4 digits of precision.

8. Further Comments

The time taken by the routine for a call of S18DCF is approximately proportional to the value of N, plus a constant. In general it is much cheaper to call S18DCF with N greater than 1, rather than to make N separate calls to S18DCF.

Paradoxically, for some values of z and v, it is cheaper to call S18DCF with a larger value of N than is required, and then discard the extra function values returned. However, it is not possible to state the precise circumstances in which this is likely to occur. It is due to the fact that the base value used to start recurrence may be calculated in different regions for different N, and the costs in each region may differ greatly.

Note that if the function required is $K_0(x)$ or $K_1(x)$, i.e. $v = 0.0$ or 1.0, where x is real and positive, and only a single function value is required, then it may be much cheaper to call S18ACF, S18ADF, S18CCF or S18CDF, depending on whether a scaled result is required or not.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the order FNU, the second is a complex value for the argument, Z, and the third is a value for the parameter SCALE. The program calls the routine with N = 2 to evaluate the function for orders FNU and FNU + 1, and it prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18DCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          N
      PARAMETER        (N=2)
```

```
*     .. Local Scalars ..
      complex           Z
      real              FNU
      INTEGER           IFAIL, NZ
      CHARACTER*1       SCALE
*     .. Local Arrays ..
      complex           CY(N)
*     .. External Subroutines ..
      EXTERNAL          S18DCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18DCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Calling with N =', N
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'    FNU             Z         SCALE       CY(1)                CY(2)
     +    NZ IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) FNU, Z, SCALE
      IFAIL = 0
*
      CALL S18DCF(FNU,Z,N,SCALE,CY,NZ,IFAIL)
*
      WRITE (NOUT,99998) FNU, Z, SCALE, CY(1), CY(2), NZ, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,A,I2)
99998 FORMAT (1X,F7.4,'  (',F7.3,',',F7.3,')   ',A,
     +       2('  (',F7.3,',',F7.3,')'),I4,I4)
      END
```

9.2. Program Data

```
S18DCF Example Program Data
 0.00     ( 0.3,  0.4)    'U'
 2.30     ( 2.0,  0.0)    'U'
 2.12     (-1.0,  0.0)    'U'
 5.10     ( 3.0,  2.0)    'U'
 5.10     ( 3.0,  2.0)    'S'
```

9.3. Program Results

```
S18DCF Example Program Results

Calling with N =  2

    FNU             Z         SCALE       CY(1)                CY(2)      NZ IFAIL

  0.0000  (  0.300,  0.400)   U  (  0.831, -0.803)  (  0.831, -1.735)    0    0
  2.3000  (  2.000,  0.000)   U  (  0.325,  0.000)  (  0.909,  0.000)    0    0
  2.1200  ( -1.000,  0.000)   U  (  1.763, -1.047)  ( -8.087,  3.147)    0    0
  5.1000  (  3.000,  2.000)   U  ( -0.426,  0.243)  ( -0.810,  1.255)    0    0
  5.1000  (  3.000,  2.000)   S  ( -0.880, -9.803)  (-16.150,-25.293)    0    0
```

S18DEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S18DEF returns a sequence of values for the modified Bessel functions $I_{\nu+n}(z)$ for complex z, non-negative ν and $n = 0,1,...,N-1$, with an option for exponential scaling.

2. Specification

```
SUBROUTINE S18DEF (FNU, Z, N, SCALE, CY, NZ, IFAIL)
INTEGER          N, NZ, IFAIL
real             FNU
complex          Z, CY(N)
CHARACTER*1      SCALE
```

3. Description

This subroutine evaluates a sequence of values for the modified Bessel function $I_\nu(z)$, where z is complex, $-\pi < \arg z \leq \pi$, and ν is the real, non-negative order. The N-member sequence is generated for orders ν, $\nu+1,...,\nu+N-1$. Optionally, the sequence is scaled by the factor $e^{-|\mathrm{Re}\, z|}$.

The routine is derived from the routine CBESI in Amos [2].

Note: although the routine may not be called with ν less than zero, for negative orders the formula $I_{-\nu}(z) = I_\nu(z) + \frac{2}{\pi}\sin(\pi\nu)K_\nu(z)$ may be used (for the Bessel function $K_\nu(z)$, see S18DCF).

When N is greater than 1, extra values of $I_\nu(z)$ are computed using recurrence relations.

For very large $|z|$ or $(\nu+N-1)$, argument reduction will cause total loss of accuracy, and so no computation is performed. For slightly smaller $|z|$ or $(\nu+N-1)$, the computation is performed but results are accurate to less than half of ***machine precision***. If $\mathrm{real}(z)$ is too large and the unscaled function is required, there is a risk of overflow and so no computation is performed. In all the above cases, a warning is given by the routine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9, p. 358, 1968.

[2] AMOS, D.E.
Algorithm 644: A Portable Package for Bessel Functions of a Complex Argument and Nonnegative Order.
ACM Trans. Math. Software, 12, pp. 265-273, 1986.

5. Parameters

1: FNU – ***real.*** *Input*

On entry: the order, ν, of the first member of the sequence of functions.

Constraint: FNU $\geq$ 0.0.

2: Z – ***complex.*** *Input*

On entry: the argument z of the functions.

3: N – INTEGER. *Input*

On entry: the number, N, of members required in the sequence $I_\nu(z), I_{\nu+1}(z), \ldots, I_{\nu+N-1}(z)$.

Constraint: N ≥ 1.

4: SCALE – CHARACTER*1. *Input*

On entry: the scaling option.

If SCALE = 'U' or 'u', the results are returned unscaled.

If SCALE = 'S' or 's', the results are returned scaled by the factor $e^{-|\mathrm{Re}\, z|}$.

Constraint: SCALE = 'U', 'u', 'S' or 's'.

5: CY(N) – ***complex*** array. *Output*

On exit: the N required function values: CY(i) contains $I_{\nu+i-1}(z)$, for i = 1,2,...,N.

6: NZ – INTEGER. *Output*

On exit: the number of components of CY that are set to zero due to underflow.

If NZ > 0, then elements CY(N–NZ+1),CY(N–NZ+2),...,CY(N) are set to zero.

7: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, FNU < 0.0,
or N < 1,
or SCALE ≠ 'U', 'u', 'S' or 's'.

IFAIL = 2

No computation has been performed due to the likelihood of overflow, because real(Z) is greater than a machine-dependent threshold value (given in the Users' Note for your implementation). This error exit can only occur when SCALE = 'U' or 'u'.

IFAIL = 3

The computation has been performed, but the errors due to argument reduction in elementary functions make it likely that the results returned by S18DEF are accurate to less than half of ***machine precision***. This error exit may occur when either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 4

No computation has been performed because the errors due to argument reduction in elementary functions mean that all precision in results returned by S18DEF would be lost. This error exit may occur when either ABS(Z) or FNU + N – 1 is greater than a machine-dependent threshold value (given in the Users' Note for your implementation).

IFAIL = 5

No results are returned because the algorithm termination condition has not been met. This may occur because the parameters supplied to S18DEF would have caused overflow or underflow.

7. Accuracy

All constants in subroutine S18DEF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t, then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t,18)$. Because of errors in argument reduction when computing elementary functions inside S18DEF, the actual number of correct digits is limited, in general, by $p - s$, where $s \approx \max(1,|\log_{10}|z||,|\log_{10}\nu|)$ represents the number of digits lost due to the argument reduction. Thus the larger the values of $|z|$ and ν, the less the precision in the result. If S18DEF is called with $N > 1$, then computation of function values via recurrence may lead to some further small loss of accuracy.

If function values which should nominally be identical are computed by calls to S18DEF with different base values of ν and different N, the computed values may not agree exactly. Empirical tests with modest values of ν and z have shown that the discrepancy is limited to the least significant 3-4 digits of precision.

8. Further Comments

The time taken by the routine for a call of S18DEF is approximately proportional to the value of N, plus a constant. In general it is much cheaper to call S18DEF with N greater than 1, rather than to make N separate calls to S18DEF.

Paradoxically, for some values of z and ν, it is cheaper to call S18DEF with a larger value of N than is required, and then discard the extra function values returned. However, it is not possible to state the precise circumstances in which this is likely to occur. It is due to the fact that the base value used to start recurrence may be calculated in different regions for different N, and the costs in each region may differ greatly.

Note that if the function required is $I_0(x)$ or $I_1(x)$, i.e. $\nu = 0.0$ or 1.0, where x is real and positive, and only a single function value is required, then it may be much cheaper to call S18AEF, S18AFF, S18CEF or S18CFF, depending on whether a scaled result is required or not.

9. Example

The following example program prints a caption and then proceeds to read sets of data from the input data stream. The first datum is a value for the order FNU, the second is a complex value for the argument, Z, and the third is a value for the parameter SCALE. The program calls the routine with N = 2 to evaluate the function for orders FNU and FNU + 1, and it prints the results. The process is repeated until the end of the input data stream is encountered.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S18DEF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          N
      PARAMETER        (N=2)
*     .. Local Scalars ..
      complex          Z
      real             FNU
      INTEGER          IFAIL, NZ
      CHARACTER*1      SCALE
```

```
*     .. Local Arrays ..
      complex           CY(N)
*     .. External Subroutines ..
      EXTERNAL          S18DEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S18DEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Calling with N =', N
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'   FNU             Z         SCALE       CY(1)                CY(2)
     +   NZ IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) FNU, Z, SCALE
      IFAIL = 0
*
      CALL S18DEF(FNU,Z,N,SCALE,CY,NZ,IFAIL)
*
      WRITE (NOUT,99998) FNU, Z, SCALE, CY(1), CY(2), NZ, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,A,I2)
99998 FORMAT (1X,F7.4,'  (',F7.3,',',F7.3,')   ',A,
     +       2('  (',F7.3,',',F7.3,')'),I4,I4)
      END
```

9.2. Program Data

```
S18DEF Example Program Data
 0.00    ( 0.3, -0.4)    'U'
 2.30    ( 2.0,  0.0)    'U'
 2.12    (-1.0,  0.0)    'U'
 5.50    (-6.1,  9.8)    'U'
 5.50    (-6.1,  9.8)    'S'
```

9.3. Program Results

```
 S18DEF Example Program Results

 Calling with N = 2

    FNU            Z         SCALE       CY(1)              CY(2)      NZ IFAIL

  0.0000  (  0.300, -0.400)   U  (  0.982, -0.059)  (  0.143, -0.203)   0   0
  2.3000  (  2.000,  0.000)   U  (  0.500,  0.000)  (  0.142,  0.000)   0   0
  2.1200  ( -1.000,  0.000)   U  (  0.103,  0.041)  ( -0.016, -0.006)   0   0
  5.5000  ( -6.100,  9.800)   U  ( 22.534, 13.710)  (-19.635, -1.660)   0   0
  5.5000  ( -6.100,  9.800)   S  (  0.051,  0.031)  ( -0.044, -0.004)   0   0
```

S19AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S19AAF returns a value for the Kelvin function ber x via the routine name.

2. Specification

```
real FUNCTION S19AAF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Kelvin function ber x.

Note: $\text{ber}(-x) = \text{ber}\, x$, so the approximation need only consider $x \geq 0.0$.

The routine is based on several Chebyshev expansions:

For $0 \leq x \leq 5$,

$$\text{ber}\, x = \sum_{r=0}{}' a_r T_r(t) \text{ with } t = 2\left(\frac{x}{5}\right)^4 - 1;$$

for $x > 5$,

$$\text{ber}\, x = \frac{e^{\frac{x}{\sqrt{2}}}}{\sqrt{2\pi x}}\left|\left(1+\frac{1}{x}a(t)\right)\cos\alpha + \frac{1}{x}b(t)\sin\alpha\right| + \frac{e^{\frac{-x}{\sqrt{2}}}}{\sqrt{2\pi x}}\left|\left(1+\frac{1}{x}c(t)\right)\sin\beta + \frac{1}{x}d(t)\cos\beta\right|$$

where $\alpha = \dfrac{x}{\sqrt{2}} - \dfrac{\pi}{8}$, $\beta = \dfrac{x}{\sqrt{2}} + \dfrac{\pi}{8}$,

and $a(t)$, $b(t)$, $c(t)$, and $d(t)$ are expansions in the variable $t = \dfrac{10}{x} - 1$.

When x is sufficiently close to zero, the result is set directly to $\text{ber}\, 0 = 1.0$.

For large x, there is a danger of the result being totally inaccurate, as the error amplification factor grows in an essentially exponential manner; therefore the routine must fail.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9.9, p. 379, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry ABS(X) is too large for an accurate result to be returned. On soft failure, the routine returns zero.

7. Accuracy

Since the function is oscillatory, the absolute error rather than the relative error is important. Let E be the absolute error in the result and δ be the relative error in the argument. If δ is somewhat larger than the ***machine precision***, then we have:

$$E \simeq \left| \frac{x}{\sqrt{2}} (\mathrm{ber}_1 x + \mathrm{bei}_1 x) \right| \delta$$

(provided E is within machine bounds).

For small x the error amplification is insignificant and thus the absolute error is effectively bounded by the ***machine precision***.

For medium and large x, the error behaviour is oscillatory and its amplitude grows like $\sqrt{\frac{x}{2\pi}} e^{\frac{x}{\sqrt{2}}}$.

Therefore it is not possible to calculate the function with any accuracy when $\sqrt{x}\, e^{\frac{x}{\sqrt{2}}} > \frac{\sqrt{2\pi}}{\delta}$.

Note that this value of x is much smaller than the minimum value of x for which the function overflows.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S19AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S19AAF
      EXTERNAL         S19AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S19AAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S19AAF(X,IFAIL)
*
```

```
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S19AAF Example Program Data
             0.1
             1.0
             2.5
             5.0
             10.0
             15.0
             60.0
             -1.0
```

9.3. Program Results

```
 S19AAF Example Program Results

      X            Y         IFAIL

   1.000E-01   1.000E+00        0
   1.000E+00   9.844E-01        0
   2.500E+00   4.000E-01        0
   5.000E+00  -6.230E+00        0
   1.000E+01   1.388E+02        0
   1.500E+01  -2.967E+03        0
   6.000E+01   0.000E+00        1
  -1.000E+00   9.844E-01        0
```

S19ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S19ABF returns a value for the Kelvin function bei x via the routine name.

2. Specification

```
real FUNCTION S19ABF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Kelvin function bei x.

Note: bei $-x$ = bei x, so the approximation need only consider $x \geq 0.0$.

The routine is based on several Chebyshev expansions:

For $0 \leq x \leq 5$,

$$\text{bei}\, x = \frac{x^2}{4}{\sum_{r=0}}' a_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{5}\right)^4 - 1;$$

For $x > 5$,

$$\text{bei}\, x = \frac{e^{\frac{x}{\sqrt{2}}}}{\sqrt{2\pi x}}\left|\left(1+\frac{1}{x}a(t)\right)\sin\alpha - \frac{1}{x}b(t)\cos\alpha\right| + \frac{e^{\frac{x}{\sqrt{2}}}}{\sqrt{2\pi x}}\left|\left(1+\frac{1}{x}c(t)\right)\cos\beta - \frac{1}{x}d(t)\sin\beta\right|$$

where $\alpha = \frac{x}{\sqrt{2}} - \frac{\pi}{8}$, $\beta = \frac{x}{\sqrt{2}} + \frac{\pi}{8}$,

and $a(t)$, $b(t)$, $c(t)$, and $d(t)$ are expansions in the variable $t = \frac{10}{x} - 1$.

When x is sufficiently close to zero, the result is computed as bei $x = \frac{x^2}{4}$. If this result would underflow, the result returned is bei $x = 0.0$.

For large x, there is a danger of the result being totally inaccurate, as the error amplification factor grows in an essentially exponential manner; therefore the routine must fail.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9.9, p. 379, 1968.

5. Parameters

1: X – ***real***. *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry ABS(X) is too large for an accurate result to be returned. On soft failure, the routine returns zero.

7. Accuracy

Since the function is oscillatory, the absolute error rather than the relative error is important. Let E be the absolute error in the function, and δ be the relative error in the argument. If δ is somewhat larger than the ***machine precision***, then we have:

$$E \simeq \left| \frac{x}{\sqrt{2}}(-\mathrm{ber}_1 x + \mathrm{bei}_1 x) \right| \delta$$

(provided E is within machine bounds).

For small x the error amplification is insignificant and thus the absolute error is effectively bounded by the ***machine precision***.

For medium and large x, the error behaviour is oscillatory and its amplitude grows like $\sqrt{\frac{x}{2\pi}}\, e^{\frac{x}{\sqrt{2}}}$. Therefore it is impossible to calculate the functions with any accuracy when $\sqrt{x}\, e^{\frac{x}{\sqrt{2}}} > \frac{\sqrt{2\pi}}{\delta}$. Note that this value of x is much smaller than the minimum value of x for which the function overflows.

8. Further Comments

For details of the time taken by the routine see the Users' Note for your implementation.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S19ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S19ABF
      EXTERNAL         S19ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S19ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S19ABF(X,IFAIL)
*
```

```
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S19ABF Example Program Data
             0.1
             1.0
             2.5
             5.0
             10.0
             15.0
             60.0
             -1.0
```

9.3. Program Results

```
 S19ABF Example Program Results

      X            Y         IFAIL

   1.000E-01   2.500E-03       0
   1.000E+00   2.496E-01       0
   2.500E+00   1.457E+00       0
   5.000E+00   1.160E-01       0
   1.000E+01   5.637E+01       0
   1.500E+01  -2.953E+03       0
   6.000E+01   0.000E+00       1
  -1.000E+00   2.496E-01       0
```

S19ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S19ACF returns a value for the Kelvin function $\ker x$, via the routine name.

2. Specification

```
real FUNCTION S19ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Kelvin function $\ker x$.

Note: for $x < 0$ the function is undefined and at $x = 0$ it is infinite so we need only consider $x > 0$.

The routine is based on several Chebyshev expansions:

For $0 < x \leq 1$,

$$\ker x = -f(t)\log x + \frac{\pi}{16}x^2 g(t) + y(t)$$

where $f(t)$, $g(t)$ and $y(t)$ are expansions in the variable $t = 2x^4 - 1$;

For $1 < x \leq 3$,

$$\ker x = \exp\left(-\frac{11}{16}x\right)q(t)$$

where $q(t)$ is an expansion in the variable $t = x - 2$;

For $x > 3$,

$$\ker x = \sqrt{\frac{\pi}{2x}}e^{\frac{-x}{\sqrt{2}}}\left[\left(1+\frac{1}{x}c(t)\right)\cos\beta - \frac{1}{x}d(t)\sin\beta\right]$$

where $\beta = \frac{x}{\sqrt{2}} + \frac{\pi}{8}$, and $c(t)$ and $d(t)$ are expansions in the variable $t = \frac{6}{x} - 1$.

When x is sufficiently close to zero, the result is computed as

$$\ker x = -\gamma - \log\left(\frac{x}{2}\right) + \left(\pi - \frac{3}{8}x^2\right)\frac{x^2}{16}$$

and when x is even closer to zero, simply as

$$\ker x = -\gamma - \log\left(\frac{x}{2}\right).$$

For large x, $\ker x$ is asymptotically given by $\sqrt{\frac{\pi}{2x}}e^{\frac{-x}{\sqrt{2}}}$ and this becomes so small that it cannot be computed without underflow and the routine fails.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9.9, p. 379, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

Constraint: X > 0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry X is too large, the result underflows. On soft failure, the routine returns zero.

IFAIL = 2

On entry X ≤ 0, the function is undefined. On soft failure the routine returns zero.

7. Accuracy

Let E be the absolute error in the result, ε be the relative error in the result and δ be the relative error in the argument. If δ is somewhat larger than the ***machine precision***, then we have:

$$E \simeq \left| \frac{x}{\sqrt{2}} (\ker_1 x + \mathrm{kei}_1 x) \right| \delta,$$

$$\varepsilon \simeq \left| \frac{x \ \ker_1 x + \mathrm{kei}_1 x}{\sqrt{2} \qquad \ker x} \right| \delta.$$

For very small x, the relative error amplification factor is approximately given by $\frac{1}{|\log x|}$, which implies a strong attenuation of relative error. However, ε in general cannot be less than the ***machine precision***.

For small x, errors are damped by the function and hence are limited by the ***machine precision***.

For medium and large x, the error behaviour, like the function itself, is oscillatory, and hence only the absolute accuracy for the function can be maintained. For this range of x, the amplitude of the absolute error decays like $\sqrt{\frac{\pi x}{2}} e^{\frac{-x}{\sqrt{2}}}$ which implies a strong attenuation of error. Eventually, $\ker x$, which asymptotically behaves like $\sqrt{\frac{\pi}{2x}} e^{\frac{-x}{\sqrt{2}}}$, becomes so small that it cannot be calculated without causing underflow, and the routine returns zero. Note that for large x the errors are dominated by those of the Fortran intrinsic function EXP.

8. Further Comments

Underflow may occur for a few values of x close to the zeros of $\ker x$, below the limit which causes a failure with IFAIL = 1.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S19ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S19ACF
      EXTERNAL         S19ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S19ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S19ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S19ACF Example Program Data
             0.0
             0.1
             1.0
             2.5
             5.0
             10.0
             15.0
             1100.0
             -1.0
```

9.3. Program Results

```
 S19ACF Example Program Results

      X           Y        IFAIL

  0.000E+00   0.000E+00       2
  1.000E-01   2.420E+00       0
  1.000E+00   2.867E-01       0
  2.500E+00  -6.969E-02       0
  5.000E+00  -1.151E-02       0
  1.000E+01   1.295E-04       0
  1.500E+01  -1.514E-08       0
  1.100E+03   0.000E+00       1
 -1.000E+00   0.000E+00       2
```

S19ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S19ADF returns a value for the Kelvin function kei x via the routine name.

2. Specification

```
real FUNCTION S19ADF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Kelvin function kei x.

Note: for $x < 0$ the function is undefined, so we need only consider $x \geq 0$.

The routine is based on several Chebyshev expansions:

For $0 \leq x \leq 1$,

$$\text{kei}\, x = -\frac{\pi}{4} f(t) + \frac{x^2}{4}[-g(t)\log x + v(t)]$$

where $f(t)$, $g(t)$ and $v(t)$ are expansions in the variable $t = 2x^4 - 1$;

For $1 < x \leq 3$,

$$\text{kei}\, x = \exp\left(-\frac{9}{8}x\right) u(t)$$

where $u(t)$ is an expansion in the variable $t = x - 2$;

For $x > 3$,

$$\text{kei}\, x = \sqrt{\frac{\pi}{2x}} e^{\frac{-x}{\sqrt{2}}} \left[\left(1+\frac{1}{x}\right) c(t)\sin\beta + \frac{1}{x} d(t)\cos\beta\right]$$

where $\beta = \dfrac{x}{\sqrt{2}} + \dfrac{\pi}{8}$, and $c(t)$ and $d(t)$ are expansions in the variable $t = \dfrac{6}{x} - 1$.

For $x < 0$, the function is undefined, and hence the routine fails and returns zero.

When x is sufficiently close to zero, the result is computed as

$$\text{kei}\, x = -\frac{\pi}{4} + \left(1-\gamma-\log\left(\frac{x}{2}\right)\right)\frac{x^2}{4}$$

and when x is even closer to zero simply as

$$\text{kei}\, x = -\frac{\pi}{4}.$$

For large x, kei x is asymptotically given by $\sqrt{\dfrac{\pi}{2x}} e^{\frac{-x}{\sqrt{2}}}$ and this becomes so small that it cannot be computed without underflow and the routine fails.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 9.9, p. 379, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

Constraint: X $\geq$ 0.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry X is too large, the result underflows. On soft failure, the routine returns zero.

IFAIL = 2

On entry X < 0, the function is undefined. On soft failure the routine returns zero.

7. Accuracy

Let E be the absolute error in the result, and δ be the relative error in the argument. If δ is somewhat larger than the machine representation error, then we have:

$$E \simeq \left| \frac{x}{\sqrt{2}}(-\mathrm{ker}_1\, x + \mathrm{kei}_1\, x) \right| \delta.$$

For small x, errors are attenuated by the function and hence are limited by the ***machine precision.***

For medium and large x, the error behaviour, like the function itself, is oscillatory and hence only absolute accuracy of the function can be maintained. For this range of x, the amplitude of the absolute error decays like $\sqrt{\frac{\pi x}{2}} e^{\frac{-x}{\sqrt{2}}}$, which implies a strong attenuation of error. Eventually, kei x, which is asymptotically given by $\sqrt{\frac{\pi}{2x}} e^{\frac{-x}{\sqrt{2}}}$, becomes so small that it cannot be calculated without causing underflow and therefore the routine returns zero. Note that for large x, the errors are dominated by those of the Fortran intrinsic function EXP.

8. Further Comments

Underflow may occur for a few values of x close to the zeros of kei x, below the limit which causes a failure with IFAIL = 1.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S19ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
```

```
*     .. External Functions ..
      real                 S19ADF
      EXTERNAL             S19ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S19ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X            Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S19ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S19ADF Example Program Data
             0.0
             0.1
             1.0
             2.5
             5.0
             10.0
             15.0
             1100.0
             -1.0
```

9.3. Program Results

```
 S19ADF Example Program Results

      X            Y         IFAIL

   0.000E+00  -7.854E-01       0
   1.000E-01  -7.769E-01       0
   1.000E+00  -4.950E-01       0
   2.500E+00  -1.107E-01       0
   5.000E+00   1.119E-02       0
   1.000E+01  -3.075E-04       0
   1.500E+01   7.963E-06       0
   1.100E+03   0.000E+00       1
  -1.000E+00   0.000E+00       2
```

S20ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S20ACF returns a value for the Fresnel Integral $S(x)$, via the routine name.

2. Specification

```
real FUNCTION S20ACF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Fresnel Integral

$$S(x) = \int_0^x \sin\left(\frac{\pi}{2}t^2\right)\,dt.$$

Note: $S(x) = -S(-x)$, so the approximation need only consider $x \geq 0.0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 3$,

$$S(x) = x^3 \sum_{r=0}{}' a_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{3}\right)^4 - 1;$$

For $x > 3$,

$$S(x) = \frac{1}{2} - \frac{f(x)}{x}\cos\left(\frac{\pi}{2}x^2\right) - \frac{g(x)}{x^3}\sin\left(\frac{\pi}{2}x^2\right),$$

where $f(x) = \sum_{r=0}{}' b_r T_r(t)$,

and $g(x) = \sum_{r=0}{}' c_r T_r(t), \qquad \text{with } t = 2\left(\frac{3}{x}\right)^4 - 1.$

For small x, $S(x) \simeq \frac{\pi}{6}x^3$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***. For very small x, this approximation would underflow; the result is then set exactly to zero.

For large x, $f(x) \simeq \frac{1}{\pi}$ and $g(x) \simeq \frac{1}{\pi^2}$. Therefore for moderately large x, when $\frac{1}{\pi^2 x^3}$ is negligible compared with $\frac{1}{2}$, the second term in the approximation for $x > 3$ may be dropped. For very large x, when $\frac{1}{\pi x}$ becomes negligible, $S(x) \simeq \frac{1}{2}$. However there will be considerable difficulties in calculating $\cos\left(\frac{\pi}{2}x^2\right)$ accurately before this final limiting value can be used. Since $\cos\left(\frac{\pi}{2}x^2\right)$ is periodic, its value is essentially determined by the fractional part of x^2. If $x^2 = N + \theta$ where N is an integer and $0 \leq \theta < 1$, then $\cos\left(\frac{\pi}{2}x^2\right)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain significance in the calculation of $\cos\left(\frac{\pi}{2}x^2\right)$ either all the way to the very large x limit, or at least until the integer part of $\frac{x}{2}$ is equal to the maximum integer allowed on the machine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7, p. 300, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

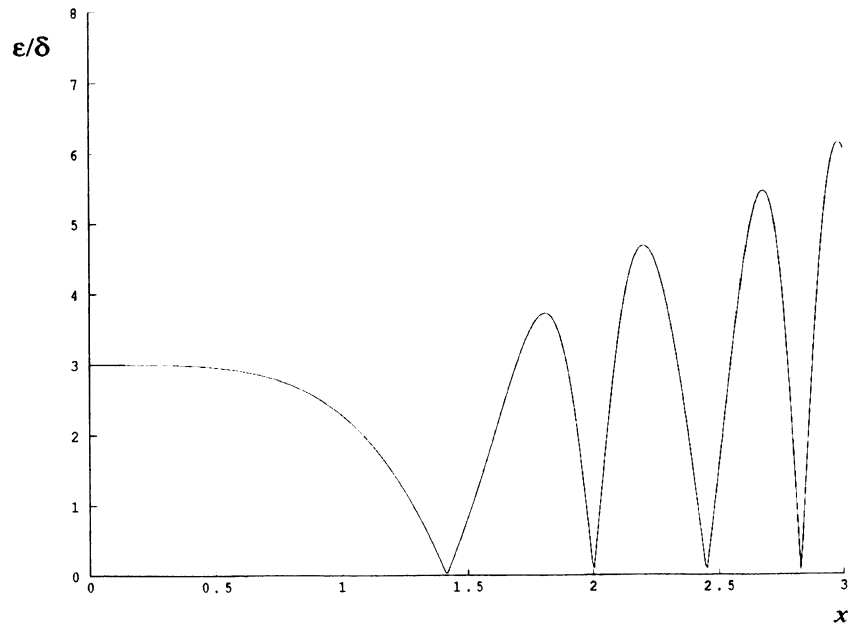
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e. if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{x \sin\left(\frac{\pi}{2}x^2\right)}{S(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{x \sin\left(\frac{\pi}{2}x^2\right)}{S(x)} \right|$:



However if δ is of the same order as the ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

For small x, $\varepsilon \simeq 3\delta$ and hence there is only moderate amplification of relative error. Of course for very small x where the correct result would underflow and exact zero is returned, relative error-control is lost.

For moderately large values of x,

$$|\varepsilon| \simeq \left|2x \sin\left(\frac{\pi}{2}x^2\right)\right| |\delta|$$

and the result will be subject to increasingly large amplification of errors. However the above relation breaks down for large values of x (i.e. when $\frac{1}{x^2}$ is of the order of the ***machine precision***); in this region the relative error in the result is essentially bounded by $\frac{2}{\pi x}$.

Hence the effects of error amplification are limited and at worst the relative error loss should not exceed half the possible number of significant figures.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S20ACF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S20ACF
      EXTERNAL         S20ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S20ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X          Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S20ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S20ACF Example Program Data
             0.0
             0.5
             1.0
             2.0
             4.0
             5.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
 S20ACF Example Program Results

      X           Y         IFAIL

   0.000E+00   0.000E+00       0
   5.000E-01   6.473E-02       0
   1.000E+00   4.383E-01       0
   2.000E+00   3.434E-01       0
   4.000E+00   4.205E-01       0
   5.000E+00   4.992E-01       0
   6.000E+00   4.470E-01       0
   8.000E+00   4.602E-01       0
   1.000E+01   4.682E-01       0
  -1.000E+00  -4.383E-01       0
   1.000E+03   4.997E-01       0
```

S20ADF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S20ADF returns a value for the Fresnel Integral $C(x)$, via the routine name.

2. Specification

```
real FUNCTION S20ADF (X, IFAIL)
INTEGER          IFAIL
real             X
```

3. Description

This routine evaluates an approximation to the Fresnel Integral

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right)dt.$$

Note: $C(x) = -C(-x)$, so the approximation need only consider $x \geq 0.0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 3$,

$$C(x) = x\sum_{r=0}{}' a_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{3}\right)^4 - 1;$$

For $x > 3$,

$$C(x) = \frac{1}{2} + \frac{f(x)}{x}\sin\left(\frac{\pi}{2}x^2\right) - \frac{g(x)}{x^3}\cos\left(\frac{\pi}{2}x^2\right),$$

where $f(x) = \sum_{r=0}{}' b_r T_r(t)$,

and $g(x) = \sum_{r=0}{}' c_r T_r(t), \qquad \text{with } t = 2\left(\frac{3}{x}\right)^4 - 1.$

For small x, $C(x) \simeq x$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For large x, $f(x) \simeq \frac{1}{\pi}$ and $g(x) \simeq \frac{1}{\pi^2}$. Therefore for moderately large x, when $\frac{1}{\pi^2 x^3}$ is negligible compared with $\frac{1}{2}$, the second term in the approximation for $x > 3$ may be dropped. For very large x, when $\frac{1}{\pi x}$ becomes negligible, $C(x) \simeq \frac{1}{2}$. However there will be considerable difficulties in calculating $\sin\left(\frac{\pi}{2}x^2\right)$ accurately before this final limiting value can be used. Since $\sin\left(\frac{\pi}{2}x^2\right)$ is periodic, its value is essentially determined by the fractional part of x^2. If $x^2 = N + \theta$, where N is an integer and $0 \leq \theta < 1$, then $\sin\left(\frac{\pi}{2}x^2\right)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain some significance in the calculation of $\sin\left(\frac{\pi}{2}x^2\right)$ either all the way to the very large x limit, or at least until the integer part of $\frac{x}{2}$ is equal to the maximum integer allowed on the machine.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 7, p. 300, 1968.

5. Parameters

1: X – ***real.*** *Input*

On entry: the argument x of the function.

2: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

There are no actual failure exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

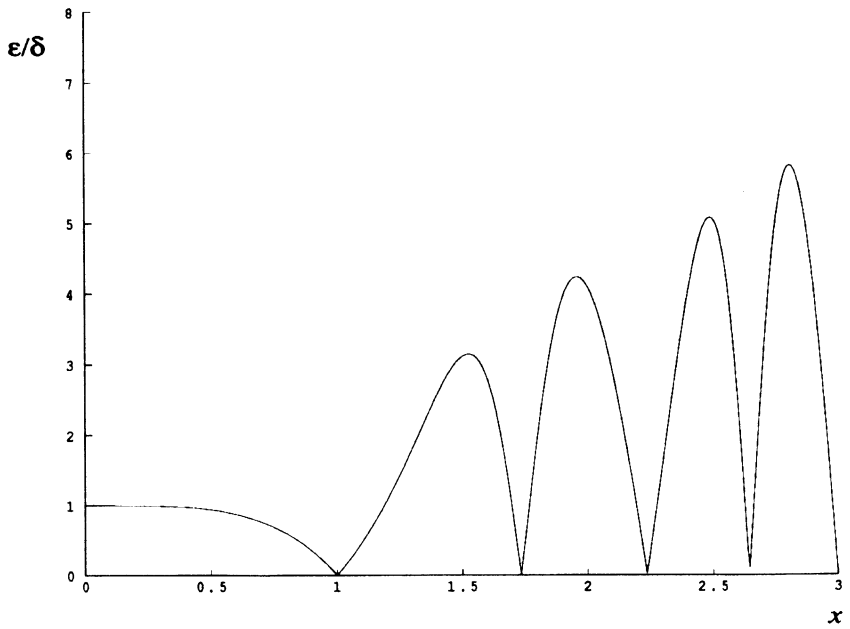
7. Accuracy

Let δ and ε be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq \left| \frac{x \cos\left(\frac{\pi}{2}x^2\right)}{C(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{x \cos\left(\frac{\pi}{2}x^2\right)}{C(x)} \right|$:



However if δ is of the same order as the ***machine precision***, then rounding errors could make ε slightly larger than the above relation predicts.

For small x, $\varepsilon \simeq \delta$ and there is no amplification of relative error.

For moderately large values of x,

$$|\varepsilon| \simeq \left|2x \cos\left(\frac{\pi}{2}x^2\right)\right| |\delta|$$

and the result will be subject to increasingly large amplification of errors. However the above relation breaks down for large values of x (i.e. when $\frac{1}{x^2}$ is of the order of the ***machine precision***); in this region the relative error in the result is essentially bounded by $\frac{2}{\pi x}$.

Hence the effects of error amplification are limited and at worst the relative error loss should not exceed half the possible number of significant figures.

8. Further Comments

None.

9. Example

The following program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S20ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S20ADF
      EXTERNAL         S20ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S20ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '      X           Y         IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S20ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2. Program Data

```
S20ADF Example Program Data
             0.0
             0.5
             1.0
             2.0
             4.0
             5.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3. Program Results

```
 S20ADF Example Program Results

      X            Y         IFAIL

  0.000E+00    0.000E+00        0
  5.000E-01    4.923E-01        0
  1.000E+00    7.799E-01        0
  2.000E+00    4.883E-01        0
  4.000E+00    4.984E-01        0
  5.000E+00    5.636E-01        0
  6.000E+00    4.995E-01        0
  8.000E+00    4.998E-01        0
  1.000E+01    4.999E-01        0
 -1.000E+00   -7.799E-01        0
  1.000E+03    5.000E-01        0
```

S21BAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S21BAF returns a value of an elementary integral, which occurs as a degenerate case of an elliptic integral of the first kind, via the routine name.

2. Specification

```
real FUNCTION S21BAF (X, Y, IFAIL)
INTEGER          IFAIL
real             X, Y
```

3. Description

This routine calculates an approximate value for the integral

$$R_C(x,y) = \tfrac{1}{2}\int_0^\infty \frac{dt}{\sqrt{t+x}\,(t+y)}$$

where $x \geq 0$ and $y \neq 0$.

This function, which is related to the logarithm or inverse hyperbolic functions for $y < x$ and to inverse circular functions if $x < y$, arises as a degenerate form of the elliptic integral of the first kind. If $y < 0$, the result computed is the Cauchy principal value of the integral.

The basic algorithm, which is due to Carlson [2] and [3], is to reduce the arguments recursively towards their mean by the system:

$$\begin{aligned} x_0 &= x, & y_0 &= y \\ \mu_n &= (x_n+2y_n)/3, & S_n &= (y_n-x_n)/3\mu_n \\ \lambda_n &= y_n + 2\sqrt{x_n y_n} & & \\ x_{n+1} &= (x_n+\lambda_n)/4, & y_{n+1} &= (y_n+\lambda_n)/4. \end{aligned}$$

The quantity $|S_n|$ for $n = 0,1,2,3,\ldots$ decreases with increasing n, eventually $|S_n| \sim 1/4^n$. For small enough S_n the required function value can be approximated by the first few terms of the Taylor series about the mean. That is

$$R_C(x,y) = \left(1 + \frac{3S_n^2}{10} + \frac{S_n^3}{7} + \frac{3S_n^4}{8} + \frac{9S_n^5}{22}\right)/\sqrt{\mu_n}.$$

The truncation error involved in using this approximation is bounded by $16|S_n|^6/(1-2|S_n|)$ and the recursive process is stopped when S_n is small enough for this truncation error to be negligible compared to the ***machine precision***.

Within the domain of definition, the function value is itself representable for all representable values of its arguments. However, for values of the arguments near the extremes the above algorithm must be modified so as to avoid causing underflows or overflows in intermediate steps. In extreme regions arguments are pre-scaled away from the extremes and compensating scaling of the result is done before returning to the calling program.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 17, 1968.

[2] CARLSON, B.C.
Computing Elliptic Integrals by Duplication.
Department of Physics, Iowa State University, Preprint 1978.

[3] CARLSON, B.C.
A Table of Elliptic Integrals of the Third Kind.
Math. Comp. 51, pp. 267-280, 1988.

5. Parameters

1: X – ***real.*** *Input*

2: Y – ***real.*** *Input*

On entry: the arguments x and y of the function, respectively.

Constraint: $X \geq 0.0$ and $Y \neq 0.0$.

3: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry $X < 0.0$; the function is undefined.

IFAIL = 2

On entry $Y = 0.0$; the function is undefined.
On soft failure the routine returns zero.

7. Accuracy

In principle the routine is capable of producing full ***machine precision***. However round off errors in internal arithmetic will result in slight loss of accuracy. This loss should never be excessive as the algorithm does not involve any significant amplification of round off error. It is reasonable to assume that the result is accurate to within a small multiple of the ***machine precision***.

8. Further Comments

Users should consult the Chapter Introduction which shows the relationship of this function to the classical definitions of the elliptic integrals.

9. Example

This example program simply generates a small set of non-extreme arguments which are used with the routine to produce the table of low accuracy results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21BAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Scalars ..
      real             RC, X, Y
      INTEGER          IFAIL, IX
*     .. External Functions ..
      real             S21BAF
      EXTERNAL         S21BAF
```

```
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21BAF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X       Y         S21BAF   IFAIL'
      WRITE (NOUT,*)
      DO 20 IX = 1, 3
         X = IX*0.5e0
         Y = 1.0e0
         IFAIL = 1
*
         RC = S21BAF(X,Y,IFAIL)
*
         WRITE (NOUT,99999) X, Y, RC, IFAIL
   20 CONTINUE
      STOP
*
99999 FORMAT (1X,2F7.2,F12.4,I5)
      END
```

9.2. Program Data

None.

9.3. Program Results

```
 S21BAF Example Program Results

     X       Y         S21BAF   IFAIL

  0.50    1.00       1.1107     0
  1.00    1.00       1.0000     0
  1.50    1.00       0.9312     0
```

S21BBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S21BBF returns a value of the symmetrised elliptic integral of the first kind, via the routine name.

2. Specification

```
real FUNCTION S21BBF (X, Y, Z, IFAIL)
INTEGER          IFAIL
real             X, Y, Z
```

3. Description

This routine calculates an approximation to the integral

$$R_F(x,y,z) = \tfrac{1}{2}\int_0^\infty \frac{dt}{\sqrt{(t+x)(t+y)(t+z)}}$$

where $x, y, z \geq 0$ and at most one is zero.

The basic algorithm, which is due to Carlson [2] and [3], is to reduce the arguments recursively towards their mean by the rule:

$x_0 = \min(x,y,z)$, $z_0 = \max(x,y,z)$,

$y_0 =$ remaining third intermediate value argument.

(This ordering, which is possible because of the symmetry of the function, is done for technical reasons related to the avoidance of overflow and underflow.)

$$\begin{aligned}
\mu_n &= (x_n+y_n+z_n)/3 \\
X_n &= 1 - x_n/\mu_n \\
Y_n &= 1 - y_n/\mu_n \\
Z_n &= 1 - z_n/\mu_n \\
\lambda_n &= \sqrt{x_n y_n} + \sqrt{y_n z_n} + \sqrt{z_n x_n} \\
x_{n+1} &= (x_n+\lambda_n)/4 \\
y_{n+1} &= (y_n+\lambda_n)/4 \\
z_{n+1} &= (z_n+\lambda_n)/4
\end{aligned}$$

$\varepsilon_n = \max(|X_n|,|Y_n|,|Z_n|)$ and the function may be approximated adequately by a 5th order power series:

$$R_F(x,y,z) = \frac{1}{\sqrt{\mu_n}}\left(1 - \frac{E_2}{10} + \frac{E_2^2}{24} - \frac{3E_2E_3}{44} + \frac{E_3}{14}\right)$$

where $E_2 = X_nY_n + Y_nZ_n + Z_nX_n$, $E_3 = X_nY_nZ_n$.

The truncation error involved in using this approximation is bounded by $\varepsilon_n^6/4(1-\varepsilon_n)$ and the recursive process is stopped when this truncation error is negligible compared with the ***machine precision***.

Within the domain of definition, the function value is itself representable for all representable values of its arguments. However, for values of the arguments near the extremes the above algorithm must be modified so as to avoid causing underflows or overflows in intermediate steps. In extreme regions arguments are pre-scaled away from the extremes and compensating scaling of the result is done before returning to the calling program.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 17, 1968.

[2] CARLSON, B.C.
Computing Elliptic Integrals by Duplication.
Department of Physics, Iowa State University, Preprint 1978.

[3] CARLSON, B.C.
A Table of Elliptic Integrals of the Third Kind.
Math. Comp. 51, pp. 267-280, 1988.

5. Parameters

1: X – ***real.*** *Input*
2: Y – ***real.*** *Input*
3: Z – ***real.*** *Input*

On entry: the arguments x, y and z of the function.

Constraint: X, Y, Z $\geq$ 0.0 and only one of X, Y and Z may be zero.

4: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry one or more of X, Y and Z is negative; the function is undefined.

IFAIL = 2

On entry two or more of X, Y and Z are zero; the function is undefined.
On soft failure, the routine returns zero.

7. Accuracy

In principle the routine is capable of producing full ***machine precision***. However round off errors in internal arithmetic will result in slight loss of accuracy. This loss should never be excessive as the algorithm does not involve any significant amplification of round off error. It is reasonable to assume that the result is accurate to within a small multiple of the ***machine precision***.

8. Further Comments

Users should consult the Chapter Introduction which shows the relationship of this function to the classical definitions of the elliptic integrals.

If two arguments are equal, the function reduces to the elementary integral R_C, computed by S21BAF.

9. Example

This example program simply generates a small set of non-extreme arguments which are used with the routine to produce the table of low accuracy results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21BBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Scalars ..
      real             RF, X, Y, Z
      INTEGER          IFAIL, IX
*     .. External Functions ..
      real             S21BBF
      EXTERNAL         S21BBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21BBF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X       Y       Z         S21BBF   IFAIL'
      WRITE (NOUT,*)
      DO 20 IX = 1, 3
         X = IX*0.5e0
         Y = (IX+1)*0.5e0
         Z = (IX+2)*0.5e0
         IFAIL = 1
*
         RF = S21BBF(X,Y,Z,IFAIL)
*
         WRITE (NOUT,99999) X, Y, Z, RF, IFAIL
   20 CONTINUE
      STOP
*
99999 FORMAT (1X,3F7.2,F12.4,I5)
      END
```

9.2. Program Data

None.

9.3. Program Results

```
 S21BBF Example Program Results

     X       Y       Z         S21BBF   IFAIL

  0.50    1.00    1.50       1.0281       0
  1.00    1.50    2.00       0.8260       0
  1.50    2.00    2.50       0.7116       0
```

S21BCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S21BCF returns a value of the symmetrised elliptic integral of the second kind, via the routine name.

2. Specification

```
real FUNCTION S21BCF (X, Y, Z, IFAIL)
INTEGER          IFAIL
real             X, Y, Z
```

3. Description

This routine calculates an approximate value for the integral

$$R_D(x,y,z) = \tfrac{3}{2}\int_0^\infty \frac{dt}{\sqrt{(t+x)\,(t+y)\,(t+z)^3}}$$

where $x, y \geq 0$, at most one of x and y is zero, and $z > 0$.

The basic algorithm, which is due to Carlson [2] and [3], is to reduce the arguments recursively towards their mean by the rule:

$$\begin{aligned}
x_0 &= x,\ y_0 = y,\ z_0 = z \\
\mu_n &= (x_n+y_n+3z_n)/5 \\
X_n &= 1 - x_n/\mu_n \\
Y_n &= 1 - y_n/\mu_n \\
Z_n &= 1 - z_n/\mu_n \\
\lambda_n &= \sqrt{x_n y_n} + \sqrt{y_n z_n} + \sqrt{z_n x_n} \\
x_{n+1} &= (x_n+\lambda_n)/4 \\
y_{n+1} &= (y_n+\lambda_n)/4 \\
z_{n+1} &= (z_n+\lambda_n)/4
\end{aligned}$$

For n sufficiently large,

$$\varepsilon_n = \max(|X_n|,\ |Y_n|,\ |Z_n|) \sim (\tfrac{1}{4})^n$$

and the function may be approximated adequately by a 5th order power series

$$R_D(x,y,z) = 3\sum_{m=0}^{n-1} \frac{4^{-m}}{(z_m+\lambda_n)\sqrt{z_m}} + \frac{4^{-n}}{\sqrt{\mu_n^3}}\left[1+\frac{3}{7}S_n^{(2)}+\frac{1}{3}S_n^{(3)}+\frac{3}{22}(S_n^{(2)})^2+\frac{3}{11}S_n^{(4)}+\frac{3}{13}S_n^{(2)}S_n^{(3)}+\frac{3}{13}S_n^{(5)}\right]$$

where

$$S_n^{(m)} = \left(X_n^m+Y_n^m+3Z_n^m\right)/2m.$$

The truncation error in this expansion is bounded by $\dfrac{3\varepsilon_n^6}{\sqrt{(1-\varepsilon_n)^3}}$ and the recursive process is terminated when this quantity is negligible compared with the ***machine precision***.

The routine may fail either because it has been called with arguments outside the domain of definition, or with arguments so extreme that there is an unavoidable danger of setting underflow or overflow.

Note: $R_D(x,x,x) = x^{-\frac{3}{2}}$, so there exists a region of extreme arguments for which the function value is not representable.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 17, 1968.

[2] CARLSON, B.C.
Computing Elliptic Integrals by Duplication.
Department of Physics, Iowa State University, Preprint 1978.

[3] CARLSON, B.C.
A Table of Elliptic Integrals of the Third Kind.
Math. Comput. 51, pp. 267-280, 1988.

5. Parameters

1: X – ***real***. *Input*
2: Y – ***real***. *Input*
3: Z – ***real***. *Input*

On entry: the arguments x, y and z of the function.

Constraint: X, Y $\geq$ 0.0, Z $>$ 0.0 and only one of X and Y may be zero.

4: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, either X or Y is negative, or both X and Y are zero; the function is undefined.

IFAIL = 2

On entry, Z $\leq$ 0.0; the function is undefined.

IFAIL = 3

On entry, either Z is too close to zero or both X and Y are too close to zero: there is a danger of setting overflow.

IFAIL = 4

On entry, at least one of X, Y and Z is too large: there is a danger of setting underflow.

On soft failure the routine returns zero.

7. Accuracy

In principle the routine is capable of producing full ***machine precision***. However round-off errors in internal arithmetic will result in slight loss of accuracy. This loss should never be excessive as the algorithm does not involve any significant amplification of round-off error. It is reasonable to assume that the result is accurate to within a small multiple of the ***machine precision***.

8. Further Comments

Users should consult the Chapter Introduction which shows the relationship of this function to the classical definitions of the elliptic integrals.

9. Example

This example program simply generates a small set of non-extreme arguments which are used with the routine to produce the table of low accuracy results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21BCF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Scalars ..
      real             RD, X, Y, Z
      INTEGER          IFAIL, IX, IY
*     .. External Functions ..
      real             S21BCF
      EXTERNAL         S21BCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21BCF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '    X      Y      Z        S21BCF  IFAIL'
      WRITE (NOUT,*)
      DO 40 IX = 1, 3
         X = IX*0.5e0
         DO 20 IY = IX, 3
            Y = IY*0.5e0
            Z = 1.0e0
            IFAIL = 1
*
            RD = S21BCF(X,Y,Z,IFAIL)
*
            WRITE (NOUT,99999) X, Y, Z, RD, IFAIL
   20    CONTINUE
   40 CONTINUE
      STOP
*
99999 FORMAT (1X,3F7.2,F12.4,I5)
      END
```

9.2. Program Data

None.

9.3. Program Results

```
S21BCF Example Program Results

     X      Y      Z        S21BCF  IFAIL

  0.50   0.50   1.00        1.4787      0
  0.50   1.00   1.00        1.2108      0
  0.50   1.50   1.00        1.0611      0
  1.00   1.00   1.00        1.0000      0
  1.00   1.50   1.00        0.8805      0
  1.50   1.50   1.00        0.7775      0
```

S21BDF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S21BDF returns a value of the symmetrised elliptic integral of the third kind, via the routine name.

2. Specification

```
real FUNCTION S21BDF (X, Y, Z, R, IFAIL)
INTEGER          IFAIL
real             X, Y, Z, R
```

3. Description

This routine calculates an approximation to the integral

$$R_J(x,y,z,\rho) = \tfrac{3}{2}\int_0^\infty \frac{dt}{(t+\rho)\sqrt{(t+x)(t+y)(t+z)}}$$

where $x, y, z \geq 0$, $\rho \neq 0$ and at most one of x, y and z is zero.

If $p < 0$, the result computed is the Cauchy principal value of the integral.

The basic algorithm, which is due to Carlson [2] and [3], is to reduce the arguments recursively towards their mean by the rule:

$$\begin{aligned}
x_0 &= x,\ y_0 = y,\ z_0 = z,\ \rho_0 = \rho \\
\mu_n &= (x_n+y_n+z_n+2\rho_n)/5 \\
X_n &= 1 - x_n/\mu_n \\
Y_n &= 1 - y_n/\mu_n \\
Z_n &= 1 - z_n/\mu_n \\
P_n &= 1 - \rho_n/\mu_n \\
\lambda_n &= \sqrt{x_n y_n} + \sqrt{y_n z_n} + \sqrt{z_n x_n} \\
x_{n+1} &= (x_n+\lambda_n)/4 \\
y_{n+1} &= (y_n+\lambda_n)/4 \\
z_{n+1} &= (z_n+\lambda_n)/4 \\
\rho_{n+1} &= (\rho_n+\lambda_n)/4 \\
\alpha_n &= \left[\rho_n\left(\sqrt{x_n}+\sqrt{y_n}+\sqrt{z_n}\right) + \sqrt{x_n y_n z_n}\right]^2 \\
\beta_n &= \rho_n(\rho_n+\lambda_n)^2.
\end{aligned}$$

For n sufficiently large,

$$\varepsilon_n = \max(|X_n|,|Y_n|,|Z_n|,|P_n|) \sim \frac{1}{4^n}$$

and the function may be approximated by a 5th order power series

$$\begin{aligned}
R_J(x,y,z,\rho) = {} & 3\sum_{m=0}^{n-1} 4^{-m} R_C(\alpha_m,\beta_m) \\
& + \frac{4^{-n}}{\sqrt{\mu_n^3}}\left[1 + \frac{3}{7}S_n^{(2)} + \frac{1}{3}S_n^{(3)} + \frac{3}{22}(S_n^{(2)})^2 + \frac{3}{11}S_n^{(4)} + \frac{3}{13}S_n^{(2)}S_n^{(3)} + \frac{3}{13}S_n^{(5)}\right]
\end{aligned}$$

where $S_n^{(m)} = (X_n^m+Y_n^m+Z_n^m+2P_n^m)/2m$.

The truncation error in this expansion is bounded by $3\varepsilon_n^6/\sqrt{(1-\varepsilon_n)^3}$ and the recursion process is terminated when this quantity is negligible compared with the ***machine precision***. The routine may fail either because it has been called with arguments outside the domain of definition or with arguments so extreme that there is an unavoidable danger of setting underflow or overflow.

Note: $R_J(x,x,x,x) = x^{-\frac{3}{2}}$, so there exists a region of extreme arguments for which the function value is not representable.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 17, 1968.

[2] CARLSON, B.C.
Computing Elliptic Integrals by Duplication.
Department of Physics, Iowa State University, Preprint 1978.

[3] CARLSON, B.C.
A Table of Elliptic Integrals of the Third Kind.
Math. Comp. 51, pp. 267-280, 1988.

5. Parameters

1: X – ***real***. *Input*

2: Y – ***real***. *Input*

3: Z – ***real***. *Input*

4: R – ***real***. *Input*

On entry: the arguments x, y, z and ρ of the function.

Constraint: X, Y, Z $\geq$ 0.0, R $\neq$ 0.0 and at most one of X, Y and Z may be zero.

5: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry at least one of X, Y and Z is negative, or at least two of them are zero; the function is undefined.

IFAIL = 2

On entry R = 0.0; the function is undefined.

IFAIL = 3

On entry either R is too close to zero, or any two of X, Y and Z are too close to zero; there is a danger of setting overflow.

IFAIL = 4

On entry at least one of X, Y, Z and R is too large; there is a danger of setting underflow.

7. Accuracy

In principle the routine is capable of producing full ***machine precision***. However round-off errors in internal arithmetic will result in slight loss of accuracy. This loss should never be excessive as the algorithm does not involve any significant amplification of round-off error. It is reasonable to assume that the result is accurate to within a small multiple of the ***machine precision***.

8. Further Comments

Users should consult the Chapter Introduction which shows the relationship of this function to the classical definitions of the elliptic integrals.

If the argument R is equal to any of the other arguments, the function reduces to the integral R_D, computed by S21BCF.

9. Example

This example program simply generates a small set of non-extreme arguments which are used with the routine to produce the table of low accuracy results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21BDF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Scalars ..
      real             R, RJ, X, Y, Z
      INTEGER          IFAIL, IX, IY, IZ
*     .. External Functions ..
      real             S21BDF
      EXTERNAL         S21BDF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21BDF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '    X      Y      Z      R        S21BDF  IFAIL'
      WRITE (NOUT,*)
      DO 60 IX = 1, 3
         X = IX*0.5e0
         DO 40 IY = IX, 3
            Y = IY*0.5e0
            DO 20 IZ = IY, 3
               Z = IZ*0.5e0
               R = 2.0e0
               IFAIL = 1
*
               RJ = S21BDF(X,Y,Z,R,IFAIL)
*
               WRITE (NOUT,99999) X, Y, Z, R, RJ, IFAIL
   20       CONTINUE
   40    CONTINUE
   60 CONTINUE
      STOP
*
99999 FORMAT (1X,4F7.2,F12.4,I5)
      END
```

9.2. Program Data

None.

9.3. Program Results

S21BDF Example Program Results

X	Y	Z	R	S21BDF	IFAIL
0.50	0.50	0.50	2.00	1.1184	0
0.50	0.50	1.00	2.00	0.9221	0
0.50	0.50	1.50	2.00	0.8115	0
0.50	1.00	1.00	2.00	0.7671	0
0.50	1.00	1.50	2.00	0.6784	0
0.50	1.50	1.50	2.00	0.6017	0
1.00	1.00	1.00	2.00	0.6438	0
1.00	1.00	1.50	2.00	0.5722	0
1.00	1.50	1.50	2.00	0.5101	0
1.50	1.50	1.50	2.00	0.4561	0

S21CAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

S21CAF evaluates the Jacobian elliptic functions sn, cn and dn.

2. Specification

```
SUBROUTINE S21CAF (U, M, SN, CN, DN, IFAIL)
INTEGER          IFAIL
real             U, M, SN, CN, DN
```

3. Description

This routine evaluates the Jacobian elliptic functions of argument u and parameter m,

$$\begin{aligned} \mathrm{sn}(u|m) &= \sin\phi, \\ \mathrm{cn}(u|m) &= \cos\phi, \\ \mathrm{dn}(u|m) &= \sqrt{1-m\sin^2\phi}\,, \end{aligned}$$

where ϕ, called the *amplitude* of u, is defined by the integral

$$u = \int_0^{\phi} \frac{d\theta}{\sqrt{1-m\sin^2\theta}}.$$

The elliptic functions are sometimes written simply as $\mathrm{sn}\,u$, $\mathrm{cn}\,u$ and $\mathrm{dn}\,u$, avoiding explicit reference to the parameter m.

Another nine elliptic functions may be computed via the formulae

$$\begin{aligned} \mathrm{cd}\,u &= \mathrm{cn}\,u/\mathrm{dn}\,u \\ \mathrm{sd}\,u &= \mathrm{sn}\,u/\mathrm{dn}\,u \\ \mathrm{nd}\,u &= 1/\mathrm{dn}\,u \\ \mathrm{dc}\,u &= \mathrm{dn}\,u/\mathrm{cn}\,u \\ \mathrm{nc}\,u &= 1/\mathrm{cn}\,u \\ \mathrm{sc}\,u &= \mathrm{sn}\,u/\mathrm{cn}\,u \\ \mathrm{ns}\,u &= 1/\mathrm{sn}\,u \\ \mathrm{ds}\,u &= \mathrm{dn}\,u/\mathrm{sn}\,u \\ \mathrm{cs}\,u &= \mathrm{cn}\,u/\mathrm{sn}\,u \end{aligned}$$

(see Abramowitz and Stegun [1]).

S21CAF is based on a procedure given by Bulirsch [2], and uses the process of the arithmetic-geometric mean ([1], 16.9). Constraints are placed on the values of u and m in order to avoid the possibility of machine overflow.

4. References

[1] ABRAMOWITZ, M. and STEGUN, I.A.
Handbook of Mathematical Functions.
Dover Publications, Ch. 16, 1968.

[2] BULIRSCH, R.
Numerical Calculation of Elliptic Integrals and Elliptic Functions.
Num. Math., 7, pp 76-90, 1965.

5. Parameters

1: U – ***real.*** *Input*

2: M – ***real.*** *Input*

On entry: the argument u and the parameter m of the functions, respectively.

Constraints: ABS(U) $\leq \sqrt{\lambda}$, where λ = 1/X02AMF,
ABS(M) $\leq \sqrt{\lambda}$ if ABS(U) $< 1/\sqrt{\lambda}$.

3: SN – ***real.*** *Output*

4: CN – ***real.*** *Output*

5: DN – ***real.*** *Output*

On exit: the values of the functions sn u, cn u and dn u, respectively.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

If, on exit, IFAIL $\neq$ 0, then S21CAF returns with the value 0.0 for sn, cn and dn.

IFAIL = 1

On entry, ABS(U) $> \sqrt{\lambda}$, where λ = 1/X02AMF.

IFAIL = 2

On entry, ABS(M) $> \sqrt{\lambda}$ and ABS(U) $< 1/\sqrt{\lambda}$.

7. Accuracy

In principle the routine is capable of achieving full relative precision in the computed values. However, the accuracy obtainable in practice depends on the accuracy of the Fortran intrinsic functions for elementary functions such as SIN and COS.

8. Further Comments

None.

9. Example

The following program reads values of the argument u and parameter m from a file, evaluates the function and prints the results.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21CAF Example Program Text
*     Mark 15 Release. NAG Copyright 1991
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             CN, DN, M, SN, U
      INTEGER          IFAIL
*     .. External Subroutines ..
      EXTERNAL         S21CAF
```

```
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21CAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     + '           U             M            SN            CN            DN'
   20 READ (NIN,*,END=40) U, M
*
      IFAIL = 0
      CALL S21CAF(U,M,SN,CN,DN,IFAIL)
*
      WRITE (NOUT,99999) U, M, SN, CN, DN
      GO TO 20
   40 STOP
*
99999 FORMAT (3X,5e13.4)
      END
```

9.2. Program Data

```
S21CAF Example Program Data
  0.2   0.3
  5.0  -1.0
 -0.5  -0.1
 10.0  11.0
```

9.3. Program Results

```
 S21CAF Example Program Results

          U             M             SN            CN            DN
     0.2000E+00    0.3000E+00    0.1983E+00    0.9801E+00    0.9941E+00
     0.5000E+01   -0.1000E+01   -0.2440E+00    0.9698E+00    0.1029E+01
    -0.5000E+00   -0.1000E+00   -0.4812E+00    0.8766E+00    0.1012E+01
     0.1000E+02    0.1100E+02    0.2512E+00    0.9679E+00    0.5528E+00
```

Chapter X01 – Mathematical Constants

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
X01AAF	5	Provides the mathematical constant π
X01ABF	5	Provides the mathematical constant γ (Euler's Constant)

Chapter X01

Mathematical Constants

Contents

1 Scope of the Chapter

This chapter is concerned with the provision of mathematical constants required by other routines within the Library.

It should be noted that because of the trivial nature of the routines individual routine documents are not provided.

2 Background to the Problems

Some Library routines require mathematical constants to maximum ***machine precision***. These routines call Chapter X01 and thus lessen the number of changes that have to be made between different implementations of the Library.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

Although these routines are primarily intended for use by other routines they may be accessed directly by the user:

Constant	**Fortran Specification**
π	***real*** `FUNCTION X01AAF(X)`
	real `X`
γ (Euler's constant)	***real*** `FUNCTION X01ABF(X)`
	real `X`

The parameter X of these routines is a dummy parameter.

Chapter X02 – Machine Constants

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
X02AHF	9	The largest permissable argument for sin and cos
X02AJF	12	The machine precision
X02AKF	12	The smallest positive model number
X02ALF	12	The largest positive model number
X02AMF	12	The safe range parameter
X02ANF	15	The safe range parameter for complex floating-point arithmetic
X02BBF	5	The largest representable integer
X02BEF	5	The maximum number of decimal digits that can be represented
X02BHF	12	The floating-point model parameter, b
X02BJF	12	The floating-point model parameter, p
X02BKF	12	The floating-point model parameter e_{min}
X02BLF	12	The floating-point model parameter e_{max}
X02DAF	8	Switch for taking precautions to avoid underflow
X02DJF	12	The floating-point model parameter ROUNDS

Chapter X02

Machine Constants

Contents

1 Scope of the Chapter

This chapter is concerned with **parameters** which characterise certain aspects of the **computing environment** in which the NAG Fortran Library is implemented. They relate primarily to floating-point arithmetic, but also to integer arithmetic, the elementary functions and exception handling. The values of the parameters vary from one implementation of the Library to another, but within the context of a single implementation they are constants.

The parameters are intended for use primarily by other routines in the Library, but users of the Library may sometimes need to refer to them directly.

Each parameter-value is returned by a separate Fortran function. Because of the trivial nature of the functions, individual routine documents are not provided; the necessary details are given in Section 3 of this Introduction.

2 Background to the Problems

2.1 Floating-Point Arithmetic

2.1.1 A model of floating-point arithmetic

In order to characterise the important properties of floating-point arithmetic by means of a small number of parameters, NAG uses a simplified **model** of floating-point arithmetic. The parameters of the model can be chosen to provide a sufficiently close description of the behaviour of actual implementations of floating-point arithmetic, but not, in general, an exact description; actual implementations vary too much in the details of how numbers are represented or arithmetic operations are performed.

The model is based on that developed by Brown [1], but differs in some respects. The essential features are summarised here.

The model is characterised by four integer parameters and one logical parameter. The four integer parameters are:

b: the base

p: the precision (i.e., the number of significant base-b digits)

$e_{\min}$: the minimum exponent

$e_{\max}$: the maximum exponent

These parameters define a set of numerical values of the form:

$$f \times b^e$$

where the exponent e must lie in the range $[e_{\min}, e_{\max}]$, and the fraction f (also called the mantissa or significand) lies in the range $[1/b, 1)$, and may be written:

$$f = 0.f_1 f_2 \ldots f_p$$

Thus f is a p-digit fraction to the base b; the f_i are the base-b digits of the fraction: they are integers in the range 0 to $b-1$, and the leading digit f_1 must not be zero.

The set of values so defined (together with zero) are called **model numbers.** For example, if $b = 10$, $p = 5$, $e_{\min} = -99$ and $e_{\max} = +99$, then a typical model number is 0.12345×10^{67}.

The model numbers must obey certain rules for the computed results of the following basic arithmetic operations: addition, subtraction, multiplication, negation, absolute value, and comparisons. The rules depend on the value of the logical parameter ROUNDS.

If ROUNDS is **true**, then the computed result must be the nearest model number to the exact result (assuming that overflow or underflow does not occur); if the exact result is midway between two model numbers, then it may be rounded either way.

If ROUNDS is **false**, then: if the exact result is a model number, the computed result must be equal to the exact result; otherwise, the computed result may be either of the adjacent model numbers on either side of the exact result.

For division and square root, this latter rule is further relaxed (regardless of the value of ROUNDS): the computed result may also be one of the next adjacent model numbers on either side of the permitted values just stated.

On some machines, the full set of representable floating-point numbers conforms to the rules of the model with appropriate values of b, p, $e_{\min}$, $e_{\max}$ and ROUNDS. For example, for DEC VAX machines in single precision:

$$\begin{aligned} b &= 2 \\ p &= 24 \\ e_{\min} &= -127 \\ e_{\max} &= 127 \end{aligned}$$ and ROUNDS is **true**.

For machines supporting IEEE binary double precision arithmetic:

$$\begin{aligned} b &= 2 \\ p &= 53 \\ e_{\min} &= -1021 \\ e_{\max} &= 1024 \end{aligned}$$ and ROUNDS is **true**.

For other machines, values of the model parameters must be chosen which define a large subset of the representable numbers; typically it may be necessary to decrease p by 1 (in which case ROUNDS is always set to **false**), or to increase $e_{\min}$ or decrease $e_{\max}$ by a little bit. There are additional rules to ensure that arithmetic operations on those representable numbers that are not model numbers are consistent with arithmetic on model numbers.

(**Note.** The model used here differs from that described in Brown [1] in the following respects: square-root is treated, like division, as a weakly supported operator; and the logical parameter ROUNDS has been introduced to take account of machines with good rounding.)

2.1.2 Derived parameters of floating-point arithmetic

Most numerical algorithms require access, not to the basic parameters of the model, but to certain derived values, of which the most important are:

the ***machine precision*** ϵ: $= \left(\frac{1}{2}\right) \times b^{1-p}$ if ROUNDS is **true**,
$= b^{1-p}$ otherwise (but see Note below).

the smallest positive model number: $= b^{e_{\min}-1}$

the largest positive model number: $= (1 - b^{-p}) \times b^{e_{\max}}$

Note. This value is increased very slightly in some implementations to ensure that the computed result of $1 + \epsilon$ or $1 - \epsilon$ differs from 1. For example in IEEE binary single precision arithmetic the value is set to $2^{-24} + 2^{-47}$.

Two additional derived values are used in the NAG Fortran Library. Their definitions depend not only on the properties of the basic arithmetic operations just considered, but also on properties of some of the elementary functions. We define the **safe range** parameter to be the smallest positive model number z such that for any x in the range $[z, 1/z]$ the following can be computed without undue loss of accuracy, overflow, underflow or other error:

$-x$

$1/x$

$-1/x$

SQRT(x)

LOG(x)

EXP(LOG(x))

y**(LOG(x)/LOG(y)) for any y

In a similar fashion we define the safe range parameter for complex arithmetic as the smallest positive model number z such that for any x in the range $[z, 1/z]$ the following can be computed without any undue loss of accuracy, overflow, underflow or other error:

$-w$
$1/w$
$-1/w$
SQRT(w)
LOG(w)
EXP(LOG(w))
y**(LOG(w)/LOG(y)) for any y
ABS(w)

where w is any of x, ix, $x+ix$, $1/x$, i/x, $1/x+i/x$, and i is the square root of -1.

This parameter was introduced to take account of the quality of complex arithmetic on the machine. On machines with well implemented complex arithmetic, its value will differ from that of the real safe range parameter by a small multiplying factor less than 10. For poorly implemented complex arithmetic this factor may be larger by many orders of magnitude.

2.2 Other Aspects of the Computing Environment

No attempt has been made to characterise comprehensively any other aspects of the computing environment. The other functions in this chapter provide specific information that is occasionally required by routines in the Library.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

3.1 Historical Note

At Mark 12 a new set of routines was introduced to return parameters of floating-point arithmetic. The new set of routines is more carefully defined, and they do not require a dummy parameter. They are listed in Section 3.2. The older routines have since been withdrawn (see Section 4).

3.2 Parameters of Floating-point Arithmetic

real FUNCTION X02AJF()	returns the **machine precision**, i.e., $(\frac{1}{2}) \times b^{1-p}$ if ROUNDS is **true** or b^{1-p} otherwise (or a value very slightly larger than this, see Section 2.1.2)
real FUNCTION X02AKF()	returns the smallest positive model number, i.e., $b^{e_{\min}-1}$
real FUNCTION X02ALF()	returns the largest positive model number, i.e., $(1-b^{-p}) \times b^{e_{\max}}$
real FUNCTION X02AMF()	returns the **safe range** parameter as defined in Section 2.1.2
real FUNCTION X02ANF()	returns the **safe range** parameter for complex arithmetic as defined in Section 2.1.2
INTEGER FUNCTION X02BHF()	returns the model parameter b
INTEGER FUNCTION X02BJF()	returns the model parameter p
INTEGER FUNCTION X02BKF()	returns the model parameter $e_{\min}$
INTEGER FUNCTION X02BLF()	returns the model parameter $e_{\max}$
LOGICAL FUNCTION X02DJF()	returns the model parameter ROUNDS

3.3 Parameters of Other Aspects of the Computing Environment

real FUNCTION X02AHF(X) ***real*** X	returns the largest positive **real** argument for which the intrinsic functions SIN and COS return a result with some meaningful accuracy
INTEGER FUNCTION X02BBF(X) ***real*** X	returns the largest positive integer value
INTEGER FUNCTION X02BEF(X) ***real*** X	returns the maximum number of decimal digits which can be accurately represented over the whole range of floating-point numbers
LOGICAL FUNCTION X02DAF(X) ***real*** X	returns **false** if the system sets underflowing quantities to zero, without any error indication or undesirable warning or system overhead

The parameter X in these routines is a dummy parameter.

4 Routines Withdrawn or Scheduled for Withdrawal

Since Mark 13 the following routines have been withdrawn. Advice on replacing calls to these routines is given in the document 'Advice on Replacement Calls for Withdrawn/Superseded Routines'.

X02AAF	X02ABF	X02ACF	X02ADF	X02AEF	X02AFF
X02AGF	X02BAF	X02BCF	X02BDF	X02CAF	

5 References

[1] Brown W S (1981) A simple but realistic model of floating-point computation *ACM Trans. Math. Software* **7** 445–480

6 Example Program

The example program listed below simply prints the values of all the functions in Chapter X02. Obviously the results will vary from one implementation of the Library to another. The results listed in Section 6.3 are those from a double precision implementation on a Silicon Graphics workstation.

6.1 Example Text

```
*     X02AJF Example Program Text
*     Mark 17 Revised.  NAG Copyright 1995.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. External Functions ..
      real             X02AHF, X02AJF, X02AKF, X02ALF, X02AMF, X02ANF
      INTEGER          X02BBF, X02BEF, X02BHF, X02BJF, X02BKF, X02BLF
      LOGICAL          X02DAF, X02DJF
      EXTERNAL         X02AHF, X02AJF, X02AKF, X02ALF, X02AMF, X02ANF,
     +                 X02BBF, X02BEF, X02BHF, X02BJF, X02BKF, X02BLF,
     +                 X02DAF, X02DJF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X02AJF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '(results are machine-dependent)'
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'The basic parameters of the model'
      WRITE (NOUT,*)
      WRITE (NOUT,99999) ' X02BHF = ', X02BHF(),
```

```
     +  '  (the model parameter B)'
        WRITE (NOUT,99999) ' X02BJF = ', X02BJF(),
     +  '  (the model parameter P)'
        WRITE (NOUT,99999) ' X02BKF = ', X02BKF(),
     +  '  (the model parameter EMIN)'
        WRITE (NOUT,99999) ' X02BLF = ', X02BLF(),
     +  '  (the model parameter EMAX)'
        WRITE (NOUT,99998) ' X02DJF = ', X02DJF(),
     +  '  (the model parameter ROUNDS)'
        WRITE (NOUT,*)
        WRITE (NOUT,*) 'Derived parameters of floating-point arithmetic'
        WRITE (NOUT,*)
        WRITE (NOUT,*) ' X02AJF = ', X02AJF(), '  (the machine precision)'
        WRITE (NOUT,*) ' X02AKF = ', X02AKF(),
     +  '  (the smallest positive model number)'
        WRITE (NOUT,*) ' X02ALF = ', X02ALF(),
     +  '  (the largest positive model number)'
        WRITE (NOUT,*) ' X02AMF = ', X02AMF(),
     +  '  (the real safe range parameter)'
        WRITE (NOUT,*) ' X02ANF = ', X02ANF(),
     +  '  (the complex safe range parameter)'
        WRITE (NOUT,*)
        WRITE (NOUT,*)
     +  'Parameters of other aspects of the computing environment'
        WRITE (NOUT,*)
        WRITE (NOUT,*) ' X02AHF = ', X02AHF(0.0e0),
     +  '  (largest argument for SIN and COS)'
        WRITE (NOUT,99997) ' X02BBF = ', X02BBF(0.0e0),
     +  '  (largest positive integer)'
        WRITE (NOUT,99997) ' X02BEF = ', X02BEF(0.0e0),
     +  '  (precision in decimal digits)'
        WRITE (NOUT,99996) ' X02DAF = ', X02DAF(0.0e0),
     +  '  (indicates how underflow is handled)'
        STOP
*
99999 FORMAT (1X,A,I7,A)
99998 FORMAT (1X,A,L7,A)
99997 FORMAT (1X,A,I20,A)
99996 FORMAT (1X,A,L20,A)
      END
```

6.2 Example Data

None.

6.3 Example Results

```
X02AJF Example Program Results

(results are machine-dependent)

The basic parameters of the model

 X02BHF =       2  (the model parameter B)
 X02BJF =      53  (the model parameter P)
 X02BKF =   -1021  (the model parameter EMIN)
 X02BLF =    1024  (the model parameter EMAX)
 X02DJF =       T  (the model parameter ROUNDS)
```

```
Derived parameters of floating-point arithmetic

 X02AJF =   1.1102230246251600E-16  (the machine precision)
 X02AKF =   2.2250738585072107-308  (the smallest positive model number)
 X02ALF =   1.7976931348623093+308  (the largest positive model number)
 X02AMF =   2.2250738585072107-308  (the real safe range parameter)
 X02ANF =   2.2250738585072107-308  (the complex safe range parameter)

Parameters of other aspects of the computing environment

 X02AHF =   1.8014398509481900E+16  (largest argument for SIN and COS)
 X02BBF =           2147483647  (largest positive integer)
 X02BEF =                   15  (precision in decimal digits)
 X02DAF =                    F  (indicates how underflow is handled)
```

Chapter X03 – Inner Products

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
X03AAF	5	Real inner product added to initial value, basic/additional precision
X03ABF	5	Complex inner product added to initial value, basic/additional precision

Chapter X03

Inner Products

Contents

1 Scope of the Chapter

This chapter is concerned with the calculation of innerproducts required by other routines within the Library.

2 Background to the Problems

Some Library routines require to calculate the innerproduct

$$c + \sum_i x_i y_i,$$

preferably in additional precision, but, if this is unavailable or prohibitively expensive, then in basic precision. These routines call Chapter X03 so that machine dependencies of this type can be isolated to this chapter.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

Although these routines are primarily intended for use by other Library routines they may be accessed directly by the user:

X03AAF Calculates the innerproduct for real values c, x_i and y_i,

X03ABF Calculates the innerproduct for complex values c, x_i and y_i,

X03AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X03AAF calculates the value of a scalar product using ***basic*** or ***additional precision*** and adds it to a ***basic*** or ***additional precision*** initial value.

2. Specification

```
      SUBROUTINE X03AAF (A, ISIZEA, B, ISIZEB, N, ISTEPA, ISTEPB, C1, C2,
     1                   D1, D2, SW, IFAIL)
      INTEGER          ISIZEA, ISIZEB, N, ISTEPA, ISTEPB, IFAIL
      real             A(ISIZEA), B(ISIZEB), C1, C2, D1, D2
      LOGICAL          SW
```

3. Description

The routine calculates the scalar product of two ***real*** vectors and adds it to an initial value c to give a correctly rounded result d:

$$d = c + \sum_{i=1}^{n} a_i b_i.$$

If $n < 1$, $d = c$.

The vector elements a_i and b_i are stored in selected elements of the one-dimensional array parameters A and B, which in the (sub)program from which X03AAF is called may be identified with parts of possibly multi-dimensional arrays according to the standard Fortran rules. For example, the vectors may be parts of a row or column of a matrix. See Section 5 for details, and Section 9 for an example.

Both the initial value c and the result d are defined by a pair of ***real*** variables, so that they may take either ***basic*** or ***additional precision*** values.

(a) If SW = .TRUE., the products are accumulated in ***additional precision***, and on exit the result is available either in ***basic precision***, correctly rounded, or in ***additional precision***.

(b) If SW = .FALSE., the products are accumulated in ***basic precision***, and the result is returned in ***basic precision***.

This routine is designed primarily for use as an auxiliary routine by other routines in the NAG Fortran Library, especially those in the chapters on Linear Algebra.

4. References

None.

5. Parameters

1: A(ISIZEA) – ***real*** array. *Input*

On entry: the elements of the first vector.

The ith vector element is stored in the array element A($(i-1)\times$ISTEPA+1). In the user's (sub)program from which X03AAF is called, A can be part of a multi-dimensional array and the actual argument must be the array element containing the first vector element.

2: ISIZEA – INTEGER. *Input*

On entry: the dimension of array A inside the routine.

The upper bound for ISIZEA is found by multiplying together the dimensions of A as declared in the user's (sub)program from which X03AAF is called, subtracting the starting position and adding 1.

Constraint: ISIZEA ≥ (N−1)×ISTEPA + 1.

3: B(ISIZEB) – ***real*** array. *Input*

On entry: the elements of the second vector.

The ith vector element is stored in the array element B((*i*−1)×ISTEPB+1). In the user's (sub)program from which X03AAF is called, B can be part of a multi-dimensional array and the actual argument must be the array element containing the first vector element.

4: ISIZEB – INTEGER. *Input*

On entry: the dimension of array B inside the routine.

The upper bound for ISIZEB is found by multiplying together the dimensions of B as declared in the (sub)program from which X03AAF is called, subtracting the starting position and adding 1.

Constraint: ISIZEB ≥ (N−1)×ISTEPB + 1.

5: N – INTEGER. *Input*

On entry: the number of elements in the scalar product, n.

6: ISTEPA – INTEGER. *Input*

On entry: the step length between elements of the first vector in array A.

Constraint: ISTEPA > 0.

7: ISTEPB – INTEGER. *Input*

On entry: the step length between elements of the second vector in array B.

Constraint: ISTEPB > 0.

8: C1 – ***real***. *Input*

9: C2 – ***real***. *Input*

On entry: C1 and C2 must specify the initial value c: c = C1 + C2. Normally, if c is in ***additional precision***, C1 specifies the most significant part and C2 the least significant part; if c is in ***basic precision***, then C1 specifies c and C2 must have the value 0.0. Both C1 and C2 must be defined on entry.

10: D1 – ***real***. *Output*

11: D2 – ***real***. *Output*

On exit: the result d.

If the calculation is in ***additional precision*** (SW = .TRUE.),

D1 = d rounded to ***basic precision***,

D2 = d − D1;

thus D1 holds the correctly rounded ***basic precision*** result and the sum D1 + D2 gives the result in ***additional precision***. D2 may have the opposite sign to D1.

If the calculation is in ***basic precision*** (SW = .FALSE.),

D1 = d,
D2 = 0.0.

12: SW – LOGICAL. *Input*

On entry: the precision to be used in the calculation.

SW = .TRUE., – ***additional precision***;
SW = .FALSE., – ***basic precision***.

13: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry, ISTEPA ≤ 0,
or ISTEPB ≤ 0.

IFAIL = 2

On entry, ISIZEA < (N–1)×ISTEPA + 1,
or ISIZEB < (N–1)×ISTEPB + 1.

7. Accuracy

If the calculation is an ***additional precision***, the rounded ***basic precision*** result D1 is correct to full implementation accuracy, provided that exceptionally severe cancellation does not occur in the summation. If the calculation is in ***basic precision***, such accuracy cannot be guaranteed.

8. Further Comments

The time taken by the routine is approximately proportional to n and also depends on whether ***basic*** or ***additional precision*** is used.

On exit the variables D1 and D2 may be used directly to supply a ***basic*** or ***additional precision*** initial value for a subsequent call of X03AAF.

9. Example

To calculate the scalar product of the second column of the matrix A and the vector B, and add it to an initial value 1.0 where

$$A = \begin{pmatrix} -2 & -3 & 7 \\ 2 & -5 & 3 \\ -9 & 1 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 8 \\ -4 \\ -2 \end{pmatrix}.$$

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X03AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          N
      PARAMETER        (N=3)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             C1, C2, D1, D2
      INTEGER          I, IFAIL, ISIZEA, ISIZEB, ISTEPA, ISTEPB, J
      LOGICAL          SW
*     .. Local Arrays ..
      real             A(N,N), B(N)
*     .. External Subroutines ..
      EXTERNAL         X03AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X03AAF Example Program Results'
```

```
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) ((A(I,J),J=1,N),I=1,N), (B(I),I=1,N)
      C1 = 1.0e0
      C2 = 0.0e0
      ISIZEA = N
      ISIZEB = N
      ISTEPA = 1
      ISTEPB = 1
      SW = .TRUE.
      IFAIL = 0
*
      CALL X03AAF(A(1,2),ISIZEA,B,ISIZEB,N,ISTEPA,ISTEPB,C1,C2,D1,D2,SW,
     +            IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'D1 = ', D1, ' D2 = ', D2
      STOP
*
99999 FORMAT (1X,A,F4.1,A,F4.1)
      END
```

9.2. Program Data

```
X03AAF Example Program Data
   -2   -3    7
    2   -5    3
   -9    1    0
    8   -4   -2
```

9.3. Program Results

```
 X03AAF Example Program Results

 D1 = -5.0 D2 =  0.0
```

X03ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X03ABF calculates the value of a ***complex*** scalar product using ***basic*** or ***additional precision*** and adds it to a ***complex*** initial value.

2. Specification

```
      SUBROUTINE X03ABF (A, ISIZEA, B, ISIZEB, N, ISTEPA, ISTEPB, CX, DX,
     1                   SW, IFAIL)
      INTEGER          ISIZEA, ISIZEB, N, ISTEPA, ISTEPB, IFAIL
      complex          A(ISIZEA), B(ISIZEB), CX, DX
      LOGICAL          SW
```

3. Description

The routine calculates the scalar product of two ***complex*** vectors and adds it to an initial value c to give a correctly rounded result d:

$$d = c + \sum_{i=1}^{n} a_i b_i.$$

If $n < 1$, $d = c$.

The vector elements a_i and b_i are stored in selected elements of the one-dimensional array parameters A and B, which in the (sub)program from which X03ABF is called may be identified with parts of possibly multi-dimensional arrays according to the standard Fortran rules. For example, the vectors may be parts of a row or column of a matrix. See Section 5 for details, and Section 9 for an example.

The products are accumulated in ***basic*** and ***additional precision*** depending on the parameter SW.

This routine has been designed primarily for use as an auxiliary routine by other routines in the NAG Fortran Library, especially those in the chapters on Linear Algebra.

4. References

None.

5. Parameters

1: A(ISIZEA) – ***complex*** array. *Input*

On entry: the elements of the first vector.

The ith vector element is stored in the array element A($(i-1)\times$ISTEPA+1). In the user's (sub)program from which X03ABF is called, A can be part of a multi-dimensional array and the actual argument must be the array element containing the first vector element.

2: ISIZEA – INTEGER. *Input*

On entry: the dimension of array A inside the routine.

The upper bound for ISIZEA is found by multiplying together the dimensions of A as declared in the (sub)program from which X03ABF is called, subtracting the starting position and adding 1.

Constraint: ISIZEA $\geq$ (N−1)$\times$ISTEPA + 1.

3: B(ISIZEB) – ***complex*** array. *Input*

On entry: the elements of the second vector.

The ith vector element is stored in the array element B($(i-1)\times$ISTEPB+1). In the (sub)program from which X03ABF is called, B can be part of a multi-dimensional array and the actual argument must be the array element containing the first vector element.

4: ISIZEB – INTEGER. *Input*

On entry: the dimension of array B inside the routine.

The upper bound for ISIZEB is found by multiplying together the dimensions of B as declared in the user's (sub)program from which X03ABF is called, subtracting the starting position and adding 1.

Constraint: ISIZEB $\geq$ (N−1)$\times$ISTEPB + 1.

5: N – INTEGER. *Input*

On entry: the number of elements in the scalar product, n.

6: ISTEPA – INTEGER. *Input*

On entry: the step length between elements of the first vector in array A.

Constraint: ISTEPA > 0.

7: ISTEPB – INTEGER. *Input*

On entry: the step length between elements of the second vector in array B.

Constraint: ISTEPB > 0.

8: CX – ***complex***. *Input*

On entry: the initial value c.

9: DX – ***complex***. *Output*

On exit: the result d.

10: SW – LOGICAL. *Input*

On entry: the precision to be used.

If SW = .TRUE., ***additional precision***.
If SW = .FALSE., ***basic precision***.

11: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry, ISTEPA $\leq$ 0,
or ISTEPB $\leq$ 0.

IFAIL = 2

On entry, ISIZEA < (N−1)$\times$ISTEPA + 1,
or ISIZEB < (N−1)$\times$ISTEPB + 1.

7. Accuracy

If the calculation is in ***additional precision***, the result is correct to full implementation accuracy provided that exceptionally severe cancellation does not occur in the summation. If the calculation is in ***basic precision***, such accuracy cannot be guaranteed.

8. Further Comments

The time taken by the routine is approximately proportional to n and also depends on whether ***basic*** or ***additional precision*** is used.

9. Example

To calculate the scalar product of the second column of the matrix A and the vector B, and add it to an initial value of $1 + i$, where

$$A = \begin{pmatrix} -1 & -i & 1 \\ 2+3i & i & 2i \\ 0 & -1-i & 1-2i \end{pmatrix} \quad B = \begin{pmatrix} i \\ 1-i \\ -i \end{pmatrix}.$$

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X03ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          N
      PARAMETER        (N=3)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          CX, DX
      INTEGER          I, IFAIL, ISIZEA, ISIZEB, ISTEPA, ISTEPB, J
      LOGICAL          SW
*     .. Local Arrays ..
      complex          A(N,N), B(N)
*     .. External Subroutines ..
      EXTERNAL         X03ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X03ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) ((A(I,J),J=1,N),I=1,N), (B(I),I=1,N)
      CX = (1.0e0,1.0e0)
      ISIZEA = N
      ISIZEB = N
      ISTEPA = 1
      ISTEPB = 1
      SW = .TRUE.
      IFAIL = 0
*
      CALL X03ABF(A(1,2),ISIZEA,B,ISIZEB,N,ISTEPA,ISTEPB,CX,DX,SW,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Result = ', DX
      STOP
*
99999 FORMAT (1X,A,'(',F3.0,',',F3.0,')')
      END
```

9.2. Program Data

```
X03ABF Example Program Data
 (-1.0, 0.0) ( 0.0, -1.0) (1.0,  0.0)
 ( 2.0, 3.0) ( 0.0,  1.0) (0.0,  2.0)
 ( 0.0, 0.0) (-1.0, -1.0) (1.0, -2.0)
 ( 0.0, 1.0) ( 1.0, -1.0) (0.0, -1.0)
```

9.3. Program Results

```
 X03ABF Example Program Results

 Result = ( 2., 3.)
```

Chapter X04 – Input/Output Utilities

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
X04AAF	7	Return or set unit number for error messages
X04ABF	7	Return or set unit number for advisory messages
X04ACF	19	Open unit number for reading, writing or appending, and associate unit with named file
X04ADF	19	Close file associated with given unit number
X04BAF	12	Write formatted record to external file
X04BBF	12	Read formatted record from external file
X04CAF	14	Print real general matrix (easy-to-use)
X04CBF	14	Print real general matrix (comprehensive)
X04CCF	14	Print real packed triangular matrix (easy-to-use)
X04CDF	14	Print real packed triangular matrix (comprehensive)
X04CEF	14	Print real packed banded matrix (easy-to-use)
X04CFF	14	Print real packed banded matrix (comprehensive)
X04DAF	14	Print complex general matrix (easy-to-use)
X04DBF	14	Print complex general matrix (comprehensive)
X04DCF	14	Print complex packed triangular matrix (easy-to-use)
X04DDF	14	Print complex packed triangular matrix (comprehensive)
X04DEF	14	Print complex packed banded matrix (easy-to-use)
X04DFF	14	Print complex packed banded matrix (comprehensive)
X04EAF	14	Print integer matrix (easy-to-use)
X04EBF	14	Print integer matrix (comprehensive)

Chapter X04

Input/Output Utilities

Contents

1 Scope of the Chapter

This chapter contains utility routines concerned with input and output to or from an external file.

2 Background to the Problems

2.1 Output from NAG Library Routines

Output from NAG library routines to an external file falls into two categories.

(a) **Error messages**
which are always associated with an error exit from a routine, that is, with a non-zero value of IFAIL as specified in Section 6 of the routine document.

(b) **Advisory messages**
which include output of final results, output of intermediate results to monitor the course of a computation, and various warning or informative messages.

Each category of output is written to its own Fortran output unit – the **error message unit** or the **advisory message unit**. In practice these may be the same unit number. Default unit numbers are provided for each implementation of the Library (see the Users' Note for your implementation); they may be changed by users. Output of error messages may be controlled by the setting of IFAIL (see the Essential Introduction or Chapter P01). Output of advisory messages may usually be controlled by the setting of some other parameter (e.g. MSGLVL) (or in some routines also by IFAIL). An alternative mechanism for completely suppressing output is to set the relevant unit number < 0.

At present only formatted records are output from the Library. All formatted output to an external file from within the Library is performed by X04BAF. Similarly, all formatted input from an external file is performed by X04BBF.

For further information about error and advisory messages, see Chapter P01.

When the library is being called from another language, such as C or Visual Basic, the routines X04ACF and X04ADF may be especially useful. X04ACF connects a file to a FORTRAN unit and X04ADF disconnects a file from a FORTRAN unit.

2.2 Matrix Printing Routines

Routines are provided to allow formatted output of

(a) general matrices stored in a two-dimensional array (real, complex and integer data types);

(b) triangular matrices stored in a packed one-dimensional array (real and complex data types);

(c) band matrices stored in a packed two-dimensional array (real and complex data types).

Routines in (b) and (c) allow printing of matrices stored in formats used in particular by Chapter F06 and Chapter F07 of the Library.

By appropriate choice of arguments the user can specify titles, labels, maximum output record length, and the format of individual matrix elements. All output is directed to the unit number for output of advisory messages, which may be altered by a call to X04ABF.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

Apart from the obvious utility of the matrix printing routines, users of the Library may need to call routines in Chapter X04 for the following purposes.

If the default unit number for error messages (given in the Users' Note for your implementation) is not satisfactory, it may be changed to a new value NERR by the statement

```
CALL X04AAF(1,NERR)
```

Similarly the unit number for advisory messages may be changed to a new value NADV by the statement

```
CALL X04ABF(1,NADV)
```

4 Index

X04AAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04AAF returns the value of the current error message unit number, or sets the current error message unit number to a new value.

2. Specification

```
SUBROUTINE X04AAF (IFLAG, NERR)
INTEGER          IFLAG, NERR
```

3. Description

This routine enables those library routines which output error messages, to determine the number of the output unit to which the error messages are to be sent; in this case X04AAF is called with IFLAG = 0. X04AAF may also be called with IFLAG = 1 to set the unit number to a specified value. Otherwise a default value (stated in the Users' Note for your implementation) is returned.

Records written to this output unit by other library routines are at most 80 characters long (including a line-printer carriage control character).

Note that if the unit number is set < 0, no messages will be output.

4. References

None.

5. Parameters

1: IFLAG – INTEGER. *Input*

On entry: the action to be taken (see NERR).

Constraint: IFLAG = 0 or 1.

2: NERR – INTEGER. *Input/Output*

On entry:

if IFLAG = 0, NERR need not be set;
if IFLAG = 1, NERR must specify the new error message unit number.

On exit:

if IFLAG = 0, NERR is set to the current error message unit number,
if IFLAG = 1, NERR is unchanged.

Note that Fortran unit numbers must be positive or zero. If NERR is set < 0, output of error messages is totally suppressed.

6. Error Indicators and Warnings

None.

7. Accuracy

Not applicable.

8. Further Comments

The time taken by the routine is negligible.

9. Example

In this example X04AAF is called by the user's main program to make the error message from the routine DUMMY appear on the same unit as the rest of the output (unit 6). Normally a NAG Fortran Library routine with an IFAIL parameter (see Chapter P01) would take the place of DUMMY.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04AAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. External Subroutines ..
      EXTERNAL         DUMMY, X04AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04AAF Example Program Results'
*
      CALL X04AAF(1,NOUT)
      CALL DUMMY
*
      STOP
      END
*
      SUBROUTINE DUMMY
*     .. Local Scalars ..
      INTEGER          NERR
*     .. External Subroutines ..
      EXTERNAL         X04AAF
*     .. Executable Statements ..
      CALL X04AAF(0,NERR)
      WRITE (NERR,*)
      WRITE (NERR,*) 'This is a dummy error message'
      RETURN
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04AAF Example Program Results

This is a dummy error message
```

X04ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04ABF returns the value of the current advisory message unit number, or sets the current advisory message unit number to a new value.

2. Specification

```
SUBROUTINE X04ABF (IFLAG, NADV)
INTEGER          IFLAG, NADV
```

3. Description

This routine enables those library routines which output advisory messages, to determine the number of the output unit to which the advisory messages are to be sent; in this case X04ABF is called with IFLAG = 0. X04ABF may also be called with IFLAG = 1 to set the unit number to a specified value. Otherwise a default value (stated in the User's Note for your implementation) is returned.

Records written to this output unit by other library routines are at most 120 characters long (including a line-printer carriage control character), unless those library routines allow users to specify longer records.

Note that if the unit number is set < 0, no messages will be output.

4. References

None.

5. Parameters

1: IFLAG – INTEGER. *Input*

On entry: the action to be taken (see NADV).

Constraint: IFLAG = 0 or 1.

2: NADV – INTEGER. *Input/Output*

On entry:

if IFLAG = 0, NADV need not be set;
if IFLAG = 1, NADV must specify the new advisory message unit number.

On exit:

if IFLAG = 0, NADV is set to the current advisory message unit number;
if IFLAG = 1, NADV is unchanged.

Note that Fortran unit numbers must be positive or zero. If NADV is set < 0, output of advisory messages is totally suppressed.

6. Error Indicators and Warnings

None.

7. Accuracy

Not applicable.

8. Further Comments

The time taken by this routine is negligible.

9. Example

In this example X04ABF is called by the user's main program to make the advisory message from the routine DUMMY appear on the same unit as the rest of the output (unit 6). Normally a NAG Fortran Library routine with an IFAIL parameter (see Chapter P01) would take the place of DUMMY.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04ABF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. External Subroutines ..
      EXTERNAL         DUMMY, X04ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04ABF Example Program Results'
*
      CALL X04ABF(1,NOUT)
      CALL DUMMY
*
      STOP
      END
*
      SUBROUTINE DUMMY
*     .. Local Scalars ..
      INTEGER          NADV
*     .. External Subroutines ..
      EXTERNAL         X04ABF
*     .. Executable Statements ..
      CALL X04ABF(0,NADV)
      WRITE (NADV,*)
      WRITE (NADV,*) 'This is a dummy advisory message'
      RETURN
      END
```

9.2. Program Data

None.

9.3. Program Results

```
 X04ABF Example Program Results

 This is a dummy advisory message
```

X04ACF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

X04ACF opens a Fortran unit number for reading, writing or appending, and associates the unit with a named file.

2 Specification

```
SUBROUTINE X04ACF(IOUNIT, FILE, MODE, IFAIL)
INTEGER           IOUNIT, MODE, IFAIL
CHARACTER*(*)     FILE
```

3 Description

X04ACF is especially useful if the calling language is not Fortran. It opens a Fortran unit number for reading, writing or appending, and associates the unit with a filename specified by the parameter FILE.

Because it is not standard Fortran 77 to open a file for appending, this facility may not be available on all systems. See the Users' Note for your implementation for details.

4 References

None.

5 Parameters

1: IOUNIT — INTEGER *Input*

On entry: the Fortran unit number which identifies the file to be read from, written to or appended to. Note that this may be system dependent. Values in the range 7 to 1000 should however be safe on most systems.

2: FILE — CHARACTER*(*) *Input*

On entry: the name of the file to be opened.

Constraint: must contain a valid filename for the computer system being used.

3: MODE — INTEGER *Input*

On entry: specifies whether the file is to be opened for reading, writing or appending as follows.

If MODE = 0, the file is to be opened for reading.
If MODE = 1, the file is to be opened for writing.
If MODE = 2, the file is to be opened for appending.

Constraint: $0 \leq \text{MODE} \leq 2$.

4: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings specified by the routine:

IFAIL = 1

On entry, MODE is invalid.

IFAIL = 2

Failure to open the file for reading.

IFAIL = 3

Failure to open the file for writing.

IFAIL = 4

Failure to open the file for appending.

7 Accuracy

Not applicable.

8 Further Comments

None.

9 Example

This example program simply illustrates how to open a file for writing.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04ACF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          ICHAN
      PARAMETER        (ICHAN=4)
      CHARACTER*11     FNAME
      PARAMETER        (FNAME='success.res')
*     .. Local Scalars ..
      INTEGER          IFAIL
      LOGICAL          EX, OP
*     .. External Subroutines ..
      EXTERNAL         X04ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04ACF Example Program Results'
*
*     Test successful open for write
*
      IFAIL = 1
```

```
*
      CALL X04ACF(ICHAN,FNAME,1,IFAIL)
*
      INQUIRE (ICHAN,EXIST=EX,OPENED=OP)
      IF ((IFAIL.EQ.0) .AND. EX .AND. OP) THEN
         WRITE (NOUT,99998)
         WRITE (ICHAN,99998)
      ELSE
         WRITE (NOUT,99999) FNAME, ICHAN
      END IF
*
      STOP
*
99999 FORMAT (' ** FAILS to open "',A,'" and connect file to channel ',
     +       I2)
99998 FORMAT (' OK file successfully opened for writing')
      END
```

9.2 Program Data

None.

9.3 Program Results

```
X04ACF Example Program Results
OK file successfully opened for writing
```

X04ADF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

X04ADF closes a file associated with a given Fortran unit number.

2 Specification

```
SUBROUTINE X04ADF(IOUNIT, IFAIL)
INTEGER           IOUNIT, IFAIL
```

3 Description

X04ADF is especially useful if the calling language is not Fortran. It closes a file associated with a given Fortran unit number.

4 References

None.

5 Parameters

1: IOUNIT — INTEGER *Input*

On entry: the Fortran unit number which identifies the file to be closed.

2: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings specified by the routine:

IFAIL = 1

Failure to close the file.

7 Accuracy

Not applicable.

8 Further Comments

None.

9 Example

This example program simply illustrates how to close a file once it has been opened for writing followed by how to close a file once it has been opened for reading.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04ADF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          ICHAN
      PARAMETER        (ICHAN=4)
      CHARACTER*11     FNAME
      PARAMETER        (FNAME='success.res')
*     .. Local Scalars ..
      INTEGER          IFAIL
      LOGICAL          EX, OP
*     .. External Subroutines ..
      EXTERNAL         X04ACF, X04ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04ADF Example Program Results'
*
*     Test successful open and close for write
*
      IFAIL = 1
*
      CALL X04ACF(ICHAN,FNAME,1,IFAIL)
*
      INQUIRE (ICHAN,EXIST=EX,OPENED=OP)
      IF ((IFAIL.EQ.0) .AND. EX .AND. OP) THEN
         WRITE (NOUT,99998)
         WRITE (ICHAN,99998)
      ELSE
         WRITE (NOUT,99999) FNAME, ICHAN
      END IF
*
      IFAIL = 1
*
      CALL X04ADF(ICHAN,IFAIL)
*
      INQUIRE (ICHAN,OPENED=OP)
      IF ((IFAIL.EQ.0) .AND. ( .NOT. OP)) THEN
         WRITE (NOUT,99997)
      ELSE
         WRITE (NOUT,99996) FNAME, ICHAN
      END IF
*
*     Test successful open and close for read
*
      IFAIL = 1
*
      CALL X04ACF(ICHAN,FNAME,0,IFAIL)
*
```

```
      INQUIRE (ICHAN,EXIST=EX,OPENED=OP)
      IF ((IFAIL.EQ.0) .AND. EX .AND. OP) THEN
         WRITE (NOUT,99994)
      ELSE
         WRITE (NOUT,99995) FNAME, ICHAN
      END IF
*
      IFAIL = 1
*
      CALL X04ADF(ICHAN,IFAIL)
*
      INQUIRE (ICHAN,OPENED=OP)
      IF ((IFAIL.EQ.0) .AND. ( .NOT. OP)) THEN
         WRITE (NOUT,99997)
      ELSE
         WRITE (NOUT,99996) FNAME, ICHAN
      END IF
*
      STOP
*
99999 FORMAT (' ** FAILS to open "',A,'" and connect file to channel ',
     +       I2)
99998 FORMAT (' OK file successfully opened for writing')
99997 FORMAT (' OK file successfully closed')
99996 FORMAT (' ** FAILS to close "',A,'" on channel ',I2)
99995 FORMAT (' ** FAILS to open "',A,'" for reading on channel ',I2)
99994 FORMAT (' OK file successfully opened for reading')
      END
```

9.2 Program Data

None.

9.3 Program Results

```
X04ADF Example Program Results
OK file successfully opened for writing
OK file successfully closed
OK file successfully opened for reading
OK file successfully closed
```

X04BAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04BAF writes a single formatted record to an external file.

2. Specification

```
SUBROUTINE X04BAF (NOUT, REC)
INTEGER        NOUT
CHARACTER*(*) REC
```

3. Description

X04BAF is used by NAG Fortran Library routines to write formatted records to an external file. All formatted output to an external file from NAG Fortran Library routines is performed by calls to X04BAF.

4. References

None.

5. Parameters

1: NOUT – INTEGER. *Input*

On entry: the Fortran unit number which identifies the file to be written to. If NOUT < 0 (not a valid Fortran unit number), then no output occurs. Within the NAG Fortran Library NOUT is always determined by a call to X04AAF or X04ABF.

2: REC – CHARACTER*(*). *Input*

On entry: a character-string. This is written to the external file as a single record. Trailing blanks are not output, except that if REC is entirely blank, a single blank character is output. If the record is printed, the first character is treated as a carriage-control character.

6. Error Indicators and Warnings

System-dependent errors may occur if the unit specified by NOUT is not connected to an external file, or if REC exceeds the maximum record-length for that file.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

This example program simply illustrates how a formatted record is output from the NAG Fortran Library, by first writing it to the character-string REC, used as an internal file, and then passing the character-string to X04BAF.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*      X04BAF Example Program Text
*      Mark 14 Revised.  NAG Copyright 1989.
*      .. Parameters ..
       INTEGER          NOUT
       PARAMETER        (NOUT=6)
*      .. Local Scalars ..
       CHARACTER*40     REC
*      .. External Subroutines ..
       EXTERNAL         X04BAF
*      .. Executable Statements ..
       WRITE (NOUT,*) 'X04BAF Example Program Results'
       WRITE (NOUT,*)
       WRITE (REC,99999) 'This record was output by X04BAF'
*
       CALL X04BAF(NOUT,REC)
*
       STOP
*
99999 FORMAT (1X,A)
       END
```

9.2. Program Data

None.

9.3. Program Results

```
X04BAF Example Program Results

This record was output by X04BAF
```

X04BBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04BBF reads a single formatted record from an external file.

2. Specification

```
SUBROUTINE X04BBF (NIN, REC, IFAIL)
INTEGER        NIN, IFAIL
CHARACTER*(*) REC
```

3. Description

X04BBF is used by NAG Fortran Library routines to read formatted records from an external file. All formatted input from an external file by NAG Fortran Library routines is performed by calls to X04BBF.

4. References

None.

5. Parameters

1: NIN – INTEGER. *Input*

On entry: the Fortran unit number which identifies the file to be read from. If NIN < 0 (not a valid Fortran unit number), then no input occurs.

2: REC – CHARACTER*(*). *Output*

On exit: the first LEN(REC) characters of the record read from unit NIN, padded with trailing blanks if the record was shorter than LEN(REC).

3: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

An end-of-file was detected by the READ statement.

System-dependent errors may also occur if the unit specified by NIN is not connected to an external file, or if a read error occurs.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

This example program simply illustrates how a formatted record is read from the NAG Fortran Library, by first reading it into the character-string REC, used as an internal file, by X04BBF and then reading the internal file.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04BBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X
      INTEGER          I, IFAIL
      CHARACTER*40     REC
*     .. External Subroutines ..
      EXTERNAL         X04BBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04BBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
*
*     Read in values of I and X.
*
      CALL X04BBF(NIN,REC,IFAIL)
*
      READ (REC,99999) I, X
*
*     Write out I and X.
      WRITE (NOUT,99998) I, X
      STOP
*
99999 FORMAT (I3,F7.3)
99998 FORMAT (1X,I5,F11.3)
      END
```

9.2. Program Data

```
X04BBF Example Program Data
 20  2.996
```

9.3. Program Results

```
 X04BBF Example Program Results

    20      2.996
```

X04CAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04CAF is an easy-to-use routine to print a ***real*** matrix stored in a two-dimensional array.

2. Specification

```
SUBROUTINE X04CAF (MATRIX, DIAG, M, N, A, LDA, TITLE, IFAIL)
INTEGER          M, N, LDA, IFAIL
real             A(LDA,*)
CHARACTER*1      MATRIX, DIAG
CHARACTER*(*)    TITLE
```

3. Description

X04CAF prints a ***real*** matrix. It is an easy-to-use driver for X04CBF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length.

X04CAF will choose a format code such that numbers will be printed with either an F8.4, F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: MATRIX – CHARACTER*1. *Input*

On entry: indicates the part of the matrix to be printed, as follows:

MATRIX = 'G' or 'g' (General), the whole of the rectangular matrix.

MATRIX = 'L' or 'l' (Lower), the lower triangle of the matrix, or the lower trapezium if the matrix has more rows than columns.

MATRIX = 'U' or 'u' (Upper), the upper triangle of the matrix, or the upper trapezium if the matrix has more columns than rows.

Constraint: MATRIX must be one of 'G', 'g', 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: unless MATRIX = 'G' or 'g', DIAG must specify whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

If MATRIX = 'G' or 'g', then DIAG need not be set.

Constraint: If MATRIX ≠ 'G' or 'g', then DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: M – INTEGER. *Input*

4: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix, respectively, to be printed.

If either of M or N is less than 1, X04CAF will exit immediately after printing TITLE; no row or column labels are printed.

5: A(LDA,*) – ***real*** array. *Input*

The second dimension of A must be at least max(1,N).

On entry: the matrix to be printed. Only the elements that will be referred to, as specified by parameters MATRIX and DIAG, need be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04CAF is called.

Constraint: LDA ≥ M.

7: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, MATRIX ≠ 'G', 'g', 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, MATRIX = 'L', 'l', 'U' or 'u', but DIAG ≠ 'N', 'n', 'U', 'u', 'B' or 'b'.

IFAIL = 3

On entry, LDA < M.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04CAF is equivalent to a call to X04CBF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
```

9. Example

This example program calls X04CAF twice, first to print a 3 by 5 rectangular matrix, and then to print a 5 by 5 lower triangular matrix.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04CAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      real             A(LDA,NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04CAF Example Program Results'
      WRITE (NOUT,*)
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            A(I,J) = 10*I + J
   20    CONTINUE
   40 CONTINUE
*
      IFAIL = 0
*
*     Print 3 by 5 rectangular matrix
      CALL X04CAF('General',' ',3,5,A,LDA,'Example 1:',IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 5 by 5 lower triangular matrix
      CALL X04CAF('Lower','Non-unit',5,5,A,LDA,'Example 2:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04CAF Example Program Results

Example 1:
                1          2          3          4          5
1       11.0000    12.0000    13.0000    14.0000    15.0000
2       21.0000    22.0000    23.0000    24.0000    25.0000
3       31.0000    32.0000    33.0000    34.0000    35.0000

Example 2:
                1          2          3          4          5
1       11.0000
2       21.0000    22.0000
3       31.0000    32.0000    33.0000
4       41.0000    42.0000    43.0000    44.0000
5       51.0000    52.0000    53.0000    54.0000    55.0000
```

X04CBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04CBF prints a ***real*** matrix stored in a two-dimensional array.

2. Specification

```
SUBROUTINE X04CBF (MATRIX, DIAG, M, N, A, LDA, FORMAT, TITLE, LABROW,
                   RLABS, LABCOL, CLABS, NCOLS, INDENT, IFAIL)
INTEGER           M, N, LDA, NCOLS, INDENT, IFAIL
real              A(LDA,*)
CHARACTER*1       MATRIX, DIAG, LABROW, LABCOL
CHARACTER*(*)     FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04CBF prints a ***real*** matrix, or part of it, using a format specifier supplied by the user. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: MATRIX – CHARACTER*1. *Input*

On entry: indicates the part of the matrix to be printed, as follows:

MATRIX = 'G' or 'g' (General), the whole of the rectangular matrix.

MATRIX = 'L' or 'l' (Lower), the lower triangle of the matrix, or the lower trapezium if the matrix has more rows than columns.

MATRIX = 'U' or 'u' (Upper), the upper triangle of the matrix, or the upper trapezium if the matrix has more columns than rows.

Constraint: MATRIX must be one of 'G', 'g', 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: unless MATRIX = 'G' or 'g', DIAG must specify whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

If MATRIX = 'G' or 'g', then DIAG need not be set.

Constraint: If MATRIX $\neq$ 'G' or 'g', then DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: M – INTEGER. *Input*

4: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix, respectively, to be printed.

If either of M or N is less than 1, X04CBF will exit immediately after printing TITLE; no row or column labels are printed.

5: A(LDA,*) – ***real*** array. *Input*

The second dimension of A must be at least max(1,N).

On entry: the matrix to be printed. Only the elements that will be referred to, as specified by parameters MATRIX and DIAG, need be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04CBF is called.

Constraint: LDA ≥ M.

7: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(F11.4)', '1PE13.5', 'G14.5'.

In addition, there are two special codes which force X04CBF to choose its own format code:

FORMAT = ' ' means that X04CBF will choose a format code such that numbers will be printed with either an F8.4, an F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

FORMAT = '*' means that X04CBF will choose a format code such that numbers will be printed to as many significant digits as are necessary to distinguish between neighbouring machine numbers. Thus any two numbers that are stored with different internal representations should look different on output. Whether they do in fact look different will depend on the run-time library of the Fortran compiler in use.

Constraint: the character length of FORMAT must be ≤ 80.

8: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

9: LABROW – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04CBF prints no row labels.

If LABROW = 'I' or 'i', X04CBF prints integer row labels.

If LABROW = 'C' or 'c', X04CBF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C', or 'c'.

10: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length M and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

11: LABCOL – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04CBF prints no column labels.

If LABCOL = 'I' or 'i', X04CBF prints integer column labels.

If LABCOL = 'C' or 'c', X04CBF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C', 'c'.

12: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

13: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

14: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

15: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, MATRIX ≠ 'G', 'g', 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, MATRIX = 'L', 'l', 'U' or 'u', but DIAG ≠ 'N', 'n', 'U', 'u', 'B' or 'b'.

IFAIL = 3

On entry, LDA < M.

IFAIL = 4

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 5

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 6

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'I', 'i', 'C' or 'c'.

IFAIL = 7

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels), is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

X04CBF may be used to print a vector, either as a row or as a column. The following code fragment illustrates possible calls.

```
      real A(4)
      CHARACTER*1 RLABS(1), CLABS(1)
C     Print vector A as a column vector.
      LDA = 4
      IFAIL = 0
      CALL X04CBF('G', 'X', 1, 4, A, LDA, ' ', ' ', 'I', RLABS,
     *            'N', CLABS, 80, 0, IFAIL)
C     Print vector A as a row vector.
      LDA = 1
      IFAIL = 0
      CALL X04CBF('G', 'X', 4, 1, A, LDA, ' ', ' ', 'N', RLABS,
     *            'I', CLABS, 80, 0, IFAIL)
```

9. Example

This example program calls X04CBF twice, first to print a 3 by 5 rectangular matrix, and then to print a 5 by 5 upper triangular matrix, various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04CBF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INDENT, J, NCOLS
*     .. Local Arrays ..
      real             A(LDA,NMAX)
      CHARACTER*7      CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04CBF
*     .. Data statements ..
      DATA             CLABS/'Un', 'Deux', 'Trois', 'Quatre', 'Cinq'/
      DATA             RLABS/'Uno', 'Duo', 'Tre', 'Quattro', 'Cinque'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04CBF Example Program Results'
      WRITE (NOUT,*)
```

```
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            A(I,J) = 10*I + J
   20    CONTINUE
   40 CONTINUE
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
*
*     Print 3 by 5 rectangular matrix with default format and integer
*     row and column labels
      CALL X04CBF('General',' ',3,5,A,LDA,' ','Example 1:','Integer',
     +            RLABS,'Integer',CLABS,NCOLS,INDENT,IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 5 by 5 upper triangular matrix with user-supplied format
*     and row and column labels
      CALL X04CBF('Upper','Non-unit',5,5,A,LDA,'F8.2','Example 2:',
     +            'Character',RLABS,'Character',CLABS,NCOLS,INDENT,
     +            IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04CBF Example Program Results

Example 1:
             1          2          3          4          5
1     11.0000    12.0000    13.0000    14.0000    15.0000
2     21.0000    22.0000    23.0000    24.0000    25.0000
3     31.0000    32.0000    33.0000    34.0000    35.0000

Example 2:
              Un    Deux   Trois  Quatre    Cinq
    Uno    11.00   12.00   13.00   14.00   15.00
    Duo            22.00   23.00   24.00   25.00
    Tre                    33.00   34.00   35.00
Quattro                            44.00   45.00
 Cinque                                    55.00
```

X04CCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04CCF is an easy-to-use routine to print a ***real*** triangular matrix stored in a packed one-dimensional array.

2. Specification

```
SUBROUTINE X04CCF (UPLO, DIAG, N, A, TITLE, IFAIL)
INTEGER           N, IFAIL
real              A(*)
CHARACTER*1       UPLO, DIAG
CHARACTER*(*)     TITLE
```

3. Description

X04CCF prints a ***real*** triangular matrix stored in packed form. It is an easy-to-use driver for X04CDF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length. The matrix must be packed by column.

X04CCF will choose a format code such that numbers will be printed with either an F8.4, F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: UPLO – CHARACTER*1. *Input*

On entry: indicates the type of the matrix to be printed, as follows:

UPLO = 'L' or 'l' (Lower), the matrix is lower triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (2,1),..., (N,1), (2,2), (3,2),..., (N,2), etc.

UPLO = 'U' or 'u' (Upper), the matrix is upper triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (1,2), (2,2), (1,3), (2,3), (3,3), (1,4), etc.

Constraint: UPLO must be one of 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: indicates whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

Constraint: DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: N – INTEGER. *Input*

On entry: the order of the matrix to be printed.

If N is less than 1, X04CCF will exit immediately after printing TITLE; no row or column labels are printed.

4: A(*) – ***real*** array. *Input*

The dimension of A must be at least max(1,N*(N+1)/2).

On entry: the matrix to be printed. Note that A must have space for the diagonal elements of the matrix, even if these are not stored.

5: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, UPLO ≠ 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, DIAG ≠ 'N', 'n', 'U', 'u', 'B', or 'b'.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04CCF is equivalent to a call to X04CDF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
```

9. Example

This example program calls X04CCF twice, first to print a 4 by 4 lower triangular matrix, and then to print a 5 by 5 upper triangular matrix.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04CCF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LA
      PARAMETER        (NMAX=5,LA=(NMAX*(NMAX+1))/2)
*     .. Local Scalars ..
      INTEGER          I, IFAIL
*     .. Local Arrays ..
      real             A(LA)
*     .. External Subroutines ..
      EXTERNAL         X04CCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04CCF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 20 I = 1, LA
         A(I) = I
   20 CONTINUE
*
      IFAIL = 0
*
*     Print order 4 lower triangular matrix
      CALL X04CCF('Lower','Unit',4,A,'Example 1:',IFAIL)
*
      WRITE (NOUT,*)
*
*     Print order 5 upper triangular matrix
      CALL X04CCF('Upper','Non-unit',5,A,'Example 2:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04CCF Example Program Results

Example 1:
            1          2          3          4
1      1.0000
2      2.0000     1.0000
3      3.0000     6.0000     1.0000
4      4.0000     7.0000     9.0000     1.0000

Example 2:
            1          2          3          4          5
1      1.0000     2.0000     4.0000     7.0000    11.0000
2                 3.0000     5.0000     8.0000    12.0000
3                            6.0000     9.0000    13.0000
4                                      10.0000    14.0000
5                                                 15.0000
```

X04CDF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04CDF prints a ***real*** triangular matrix stored in a packed one-dimensional array.

2. Specification

```
SUBROUTINE X04CDF (UPLO, DIAG, N, A, FORMAT, TITLE, LABROW, RLABS,
1                  LABCOL, CLABS, NCOLS, INDENT, IFAIL)
INTEGER           N, NCOLS, INDENT, IFAIL
real              A(*)
CHARACTER*1       UPLO, DIAG, LABROW, LABCOL
CHARACTER*(*)     FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04CDF prints a ***real*** triangular matrix stored in packed form, using a format specifier supplied by the user. The matrix must be packed by column. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: UPLO – CHARACTER*1. *Input*

On entry: indicates the type of the matrix to be printed, as follows:

UPLO = 'L' or 'l' (Lower), the matrix is lower triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (2,1),..., (N,1), (2,2), (3,2),..., (N,2), etc.

UPLO = 'U' or 'u' (Upper), the matrix is upper triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (1,2), (2,2), (1,3), (2,3), (3,3), (1,4), etc.

Constraint: UPLO must be one of 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: indicates whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

Constraint: DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: N – INTEGER. *Input*

On entry: the order of the matrix to be printed.

If N is less than 1, X04CDF will exit immediately after printing TITLE; no row or column labels are printed.

4: A(*) – ***real*** array. *Input*

The dimension of A must be at least max(1,N*(N+1)/2).

On entry: the matrix to be printed. Note that A must have space for the diagonal elements of the matrix, even if these are not stored.

5: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(F11.4)', '1PE13.5', 'G14.5'.

In addition, there are two special codes which force X04CDF to choose its own format code:

FORMAT = ' ' means that X04CDF will choose a format code such that numbers will be printed with either an F8.4, an F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

FORMAT = '*' means that X04CDF will choose a format code such that numbers will be printed to as many significant digits as are necessary to distinguish between neighbouring machine numbers. Thus any two numbers that are stored with different internal representations should look different on output. Whether they do in fact look different will depend on the run-time library of the Fortran compiler in use.

Constraint: the character length of FORMAT must be ≤ 80.

6: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

7: LABROW – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04CDF prints no row labels.

If LABROW = 'I' or 'i', X04CDF prints integer row labels.

If LABROW = 'C' or 'c', X04CDF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

8: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length N and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

9: LABCOL – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04CDF prints no column labels.

If LABCOL = 'I' or 'i', X04CDF prints integer column labels.

If LABCOL = 'C' or 'c', X04CDF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

10: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

11: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

12: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

13: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, UPLO ≠ 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, DIAG ≠ 'N', 'n', 'U', 'u', 'B', or 'b'.

IFAIL = 3

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 4

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 5

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'T', 'i', 'C' or 'c'.

IFAIL = 6

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels) is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

This example program calls X04CDF twice, first to print a 4 by 4 lower triangular matrix, and then to print a 5 by 5 upper triangular matrix; various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04CDF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LA
      PARAMETER        (NMAX=5,LA=(NMAX*(NMAX+1))/2)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INDENT, NCOLS
*     .. Local Arrays ..
      real             A(LA)
      CHARACTER*7      CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04CDF
*     .. Data statements ..
      DATA             CLABS/'Un', 'Deux', 'Trois', 'Quatre', 'Cinq'/
      DATA             RLABS/'Uno', 'Duo', 'Tre', 'Quattro', 'Cinque'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04CDF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 20 I = 1, LA
         A(I) = I
   20 CONTINUE
*
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
*
*     Print order 4 lower triangular matrix with default format and
*     integer row and column labels
      CALL X04CDF('Lower','Non-unit',4,A,' ','Example 1:','Integer',
     +            RLABS,'Integer',CLABS,NCOLS,INDENT,IFAIL)
*
      WRITE (NOUT,*)
*
```

```
*     Print order 5 upper triangular matrix with user-supplied format
*     and row and column labels
      CALL X04CDF('Upper','Unit',5,A,'F8.2','Example 2:','Character',
     +            RLABS,'Character',CLABS,NCOLS,INDENT,IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04CDF Example Program Results

Example 1:
          1          2          3          4
1    1.0000
2    2.0000     5.0000
3    3.0000     6.0000     8.0000
4    4.0000     7.0000     9.0000    10.0000

Example 2:
            Un    Deux   Trois  Quatre    Cinq
   Uno    1.00    2.00    4.00    7.00   11.00
   Duo            1.00    5.00    8.00   12.00
   Tre                    1.00    9.00   13.00
Quattro                           1.00   14.00
 Cinque                                   1.00
```

X04CEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04CEF is an easy-to-use routine to print a ***real*** band matrix stored in a packed two-dimensional array.

2. Specification

```
SUBROUTINE X04CEF (M, N, KL, KU, A, LDA, TITLE, IFAIL)
INTEGER          M, N, KL, KU, LDA, IFAIL
real             A(LDA,*)
CHARACTER*(*)    TITLE
```

3. Description

X04CEF prints a ***real*** band matrix stored in a packed two-dimensional array. It is an easy-to-use driver for X04CFF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length.

X04CEF will choose a format code such that numbers will be printed with either an F8.4, F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: M – INTEGER. *Input*

2: N – INTEGER. *Input*

On entry: the number of rows and columns of the band matrix, respectively, to be printed.

If either of M or N is less than 1, X04CEF will exit immediately after printing TITLE; no row or column labels are printed.

3: KL – INTEGER. *Input*

On entry: the number of sub-diagonals of the band matrix A.

Constraint: KL $\geq$ 0.

4: KU – INTEGER. *Input*

On entry: the number of super-diagonals of the band matrix A.

Constraint: KU $\geq$ 0.

5: A(LDA,*) – ***real*** array. *Input*

Note: the second dimension of the array A must be at least max(1,min(M+KU,N)).

On entry: the band matrix to be printed. The leading (KL+KU+1) by min(M+KU,N) part of array A must contain the matrix, packed column by column, with the leading diagonal of the matrix in row (KU+1) of the array, the first super-diagonal starting at position 2 in row KU, the first sub-diagonal starting at position 1 in row (KU+2), and so on. Elements in the

array A that do not correspond to elements in the band matrix (such as the top left KU by KU triangle) are not referenced, and need not be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04CEF is called.

Constraint: LDA ≥ KL + KU + 1.

7: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, KL < 0.

IFAIL = 2

On entry, KU < 0.

IFAIL = 3

On entry, LDA < KL + KU + 1.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04CEF is equivalent to a call to X04CFF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
```

9. Example

This example program calls X04CEF to print a 5 by 5 band matrix with one sub-diagonal and one super-diagonal.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04CEF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      real             A(LDA,NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04CEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04CEF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            A(I,J) = 10*I + J
   20    CONTINUE
   40 CONTINUE
*
      IFAIL = 0
*
*     Print 5 by 5 band matrix with 1 sub-diagonal and 1 super-diagonal
      CALL X04CEF(5,5,1,1,A,LDA,'Band Matrix:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
 X04CEF Example Program Results

 Band Matrix:
                1           2           3           4           5
 1      21.0000     12.0000
 2      31.0000     22.0000     13.0000
 3                  32.0000     23.0000     14.0000
 4                              33.0000     24.0000     15.0000
 5                                          34.0000     25.0000
```

X04CFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04CFF prints a ***real*** band matrix stored in a packed two-dimensional array.

2. Specification

```
      SUBROUTINE X04CFF (M, N, KL, KU, A, LDA, FORMAT, TITLE, LABROW,
     1                   RLABS, LABCOL, CLABS, NCOLS, INDENT, IFAIL)
      INTEGER           M, N, KL, KU, LDA, NCOLS, INDENT, IFAIL
      real              A(LDA,*)
      CHARACTER*1       LABROW, LABCOL
      CHARACTER*(*)     FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04CFF prints a ***real*** band matrix stored in a packed two-dimensional array, using a format specifier supplied by the user. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: M – INTEGER. *Input*

2: N – INTEGER. *Input*

On entry: the number of rows and columns of the band matrix, respectively, to be printed.

If either of M or N is less than 1, X04CFF will exit immediately after printing TITLE; no row or column labels are printed.

3: KL – INTEGER. *Input*

On entry: the number of sub-diagonals of the band matrix A.

Constraint: KL $\geq$ 0.

4: KU – INTEGER. *Input*

On entry: the number of super-diagonals of the band matrix A.

Constraint: KU $\geq$ 0.

5: A(LDA,*) – ***real*** array. *Input*

The second dimension of A must be at least max(1,min(M+KU,N)).

On entry: the band matrix to be printed. The leading (KL+KU+1) by min(M+KU,N) part of array A must contain the matrix, packed column by column, with the leading diagonal of the matrix in row (KU+1) of the array, the first super-diagonal starting at position 2 in row KU, the first sub-diagonal starting at position 1 in row (KU+2), and so on. Elements in the array A that do not correspond to elements in the band matrix (such as the top left KU by KU triangle) are not referenced, and need not be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04CFF is called.

Constraint: LDA $\geq$ KL + KU + 1.

7: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(F11.4)', '1PE13.5', 'G14.5'.

In addition, there are two special codes which force X04CFF to choose its own format code:

FORMAT = ' ' means that X04CFF will choose a format code such that numbers will be printed with either an F8.4, an F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

FORMAT = '*' means that X04CFF will choose a format code such that numbers will be printed to as many significant digits as are necessary to distinguish between neighbouring machine numbers. Thus any two numbers that are stored with different internal representations should look different on output. Whether they do in fact look different will depend on the run-time library of the Fortran compiler in use.

Constraint: the character length of FORMAT must be ≤ 80.

8: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

9: LABROW – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04CFF prints no row labels.

If LABROW = 'I' or 'i', X04CFF prints integer row labels.

If LABROW = 'C' or 'c', X04CFF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

10: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length M and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

11: LABCOL – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04CFF prints no column labels.

If LABCOL = 'I' or 'i', X04CFF prints integer column labels.

If LABCOL = 'C' or 'c', X04CFF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

12: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

13: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

14: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

15: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, KL < 0.

IFAIL = 2

On entry, KU < 0.

IFAIL = 3

On entry, LDA < KL + KU + 1.

IFAIL = 4

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 5

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 6

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'I', 'i', 'C' or 'c'.

IFAIL = 7

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels) is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

This example program calls X04CFF twice, to print 5 by 5 matrices of different bandwidths; various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04CFF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INDENT, J, NCOLS
*     .. Local Arrays ..
      real             A(LDA,LDA)
      CHARACTER*7      CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04CFF
*     .. Data statements ..
      DATA             CLABS/'Un', 'Deux', 'Trois', 'Quatre', 'Cinq'/
      DATA             RLABS/'Uno', 'Duo', 'Tre', 'Quattro', 'Cinque'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04CFF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            A(I,J) = 10*I + J
   20    CONTINUE
   40 CONTINUE
*
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
*
*     Print 5 by 5 band matrix with 1 sub-diagonal, 1 super-diagonal,
*     default format and integer row and column labels
      CALL X04CFF(5,5,1,1,A,LDA,' ','Example 1:','Integer',RLABS,
     +            'Integer',CLABS,NCOLS,INDENT,IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 5 by 5 band matrix with 1 sub-diagonal, 2 super-diagonals,
*     user-supplied format and row and column labels
      CALL X04CFF(5,5,1,2,A,LDA,'F8.2','Example 2:','Character',RLABS,
     +            'Character',CLABS,NCOLS,INDENT,IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04CFF Example Program Results

Example 1:
             1          2          3          4          5
1     21.0000    12.0000
2     31.0000    22.0000    13.0000
3                32.0000    23.0000    14.0000
4                           33.0000    24.0000    15.0000
5                                      34.0000    25.0000

Example 2:
              Un     Deux    Trois  Quatre    Cinq
    Uno    31.00    22.00    13.00
    Duo    41.00    32.00    23.00   14.00
    Tre             42.00    33.00   24.00   15.00
Quattro              42.00    43.00   34.00   25.00
 Cinque                               44.00   35.00
```

X04DAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04DAF is an easy-to-use routine to print a ***complex*** matrix stored in a two-dimensional array.

2. Specification

```
SUBROUTINE X04DAF (MATRIX, DIAG, M, N, A, LDA, TITLE, IFAIL)
INTEGER          M, N, LDA, IFAIL
complex          A(LDA,*)
CHARACTER*1      MATRIX, DIAG
CHARACTER*(*)    TITLE
```

3. Description

X04DAF prints a ***complex*** matrix. It is an easy-to-use driver for X04DBF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length.

X04DAF will choose a format code such that numbers will be printed with either an F8.4, F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen. The chosen code is used to print each complex element of the matrix with the real part above the imaginary part.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: MATRIX – CHARACTER*1. *Input*

On entry: indicates the part of the matrix to be printed, as follows:

MATRIX = 'G' or 'g' (General), the whole of the rectangular matrix.

MATRIX = 'L' or 'l' (Lower), the lower triangle of the matrix, or the lower trapezium if the matrix has more rows than columns.

MATRIX = 'U' or 'u' (Upper), the upper triangle of the matrix, or the upper trapezium if the matrix has more columns than rows.

Constraint: MATRIX must be one of 'G', 'g', 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: unless MATRIX = 'G' or 'g', DIAG must specify whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

If MATRIX = 'G' or 'g', then DIAG need not be set.

Constraint: If MATRIX ≠ 'G' or 'g', then DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: M – INTEGER. *Input*

4: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix, respectively, to be printed.

If either of M or N is less than 1, X04DAF will exit immediately after printing TITLE; no row or column labels are printed.

5: A(LDA,*) – ***complex*** array. *Input*

The second dimension of A must be at least max(1,N).

On entry: the matrix to be printed. Only the elements that will be referred to, as specified by parameters MATRIX and DIAG, need be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04DAF is called.

Constraint: LDA ≥ M.

7: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, MATRIX ≠ 'G', 'g', 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, MATRIX = 'L', 'l', 'U' or 'u', but DIAG ≠ 'N', 'n', 'U', 'u', 'B' or 'b'.

IFAIL = 3

On entry, LDA < M.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04DAF is equivalent to a call to X04DBF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
USEFRM = 'A'
```

9. Example

This example program calls X04DAF twice, first to print a 4 by 3 rectangular matrix, and then to print a 4 by 4 lower triangular matrix.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04DAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=4,LDA=NMAX)
*     .. Local Scalars ..
      real             AA
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      complex          A(LDA,NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04DAF
*     .. Intrinsic Functions ..
      INTRINSIC        cmplx
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04DAF Example Program Results'
      WRITE (NOUT,*)
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            AA = 10*I + J
            A(I,J) = cmplx(AA,-AA)
   20    CONTINUE
   40 CONTINUE
*
      IFAIL = 0
*
*     Print 4 by 3 rectangular matrix
      CALL X04DAF('General',' ',4,3,A,LDA,'Example 1:',IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 4 by 4 lower triangular matrix
      CALL X04DAF('Lower','Non-unit',4,4,A,LDA,'Example 2:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04DAF Example Program Results

Example 1:
             1           2           3
1      11.0000     12.0000     13.0000
      -11.0000    -12.0000    -13.0000

2      21.0000     22.0000     23.0000
      -21.0000    -22.0000    -23.0000

3      31.0000     32.0000     33.0000
      -31.0000    -32.0000    -33.0000

4      41.0000     42.0000     43.0000
      -41.0000    -42.0000    -43.0000

Example 2:
             1           2           3           4
1      11.0000
      -11.0000

2      21.0000     22.0000
      -21.0000    -22.0000

3      31.0000     32.0000     33.0000
      -31.0000    -32.0000    -33.0000

4      41.0000     42.0000     43.0000     44.0000
      -41.0000    -42.0000    -43.0000    -44.0000
```

X04DBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04DBF prints a ***complex*** matrix stored in a two-dimensional array.

2. Specification

```
      SUBROUTINE X04DBF (MATRIX, DIAG, M, N, A, LDA, USEFRM, FORMAT,
     1                   TITLE, LABROW, RLABS, LABCOL, CLABS, NCOLS,
     2                   INDENT, IFAIL)
      INTEGER           M, N, LDA, NCOLS, INDENT, IFAIL
      complex           A(LDA,*)
      CHARACTER*1       MATRIX, DIAG, USEFRM, LABROW, LABCOL
      CHARACTER*(*)     FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04DBF prints a ***complex*** matrix, or part of it, using a format specifier supplied by the user. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: MATRIX – CHARACTER*1. *Input*

On entry: indicates the part of the matrix to be printed, as follows:

MATRIX = 'G' or 'g' (General), the whole of the rectangular matrix.

MATRIX = 'L' or 'l' (Lower), the lower triangle of the matrix, or the lower trapezium if the matrix has more rows than columns.

MATRIX = 'U' or 'u' (Upper), the upper triangle of the matrix, or the upper trapezium if the matrix has more rows than columns.

Constraint: MATRIX must be one of 'G', 'g', 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: unless MATRIX = 'G' or 'g', DIAG must specify whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

If MATRIX = 'G' or 'g', then DIAG need not be set.

Constraint: if MATRIX $\neq$ 'G' or 'g', then DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: M – INTEGER. *Input*

4: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix, respectively, to be printed.

If either of M or N is less than 1, X04DBF will exit immediately after printing TITLE; no row or column labels are printed.

5: A(LDA,*) – ***complex*** array. *Input*

The second dimension of A must be at least max(1,N).

On entry: the matrix to be printed. Only the elements that will be referred to, as specified by parameters MATRIX and DIAG, need be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04DBF is called.

Constraint: LDA ≥ M.

7: USEFRM – CHARACTER*1. *Input*

On entry: indicates how the value of FORMAT is to be used to print matrix elements.

USEFRM = 'A' or 'a' (Above), the format code in FORMAT is assumed to contain a single real edit-descriptor which is to be used to print the real and imaginary parts of each ***complex*** number one above the other. Each row of the matrix is separated by a blank line, and any row labels are attached only to the real parts. This option means that about twice as many columns can be fitted into NCOLS characters than if any other USEFRM option is used. A typical value of FORMAT for this USEFRM option might be FORMAT = 'E13.4', '*' or ' '.

USEFRM = 'B' or 'b' (Bracketed), the format code in FORMAT is assumed to contain a single edit-descriptor such as 'E13.4', '*' or ' ', which is used to print the real and imaginary parts of each ***complex*** number separated by a comma, and surrounded by brackets. Thus a matrix element printed with this USEFRM option might look like this: (12.345, −11.323)

USEFRM = 'D' or 'd' (Direct), the format code in FORMAT is used unaltered to print a ***complex*** number. This USEFRM option allows the user flexibility to specify exactly how the number is printed. With this option for USEFRM and a suitable value for FORMAT it is possible, for example, to print a ***complex*** number in the form (0.123 + 3.214*i*) or (0.123E−02,0.234E−01). See Section 9 for an example illustrating this option.

Constraint: USEFRM must be one of 'A', 'a', 'B', 'b', 'D' or 'd'.

8: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used in conjunction with parameter USEFRM, described above, to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(F11.4)', '1P,2E13.5'.

In addition, there are two special codes which force X04DBF to choose its own format code:

FORMAT = ' ' means that X04DBF will choose a format code such that numbers will be printed with either an F8.4, an F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of the real and imaginary parts of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the numbers to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

FORMAT = '*' means that X04DBF will choose a format code such that numbers will be printed to as many significant digits as are necessary to distinguish between neighbouring machine numbers. Thus any two numbers that are stored with different internal representations should look different on output. Whether they do in fact look different will depend on the run-time library of the Fortran compiler in use.

More complicated values of FORMAT, to print a ***complex*** number in a desired form, may be used. See the description of parameter USEFRM above for more details.

Constraint: the character length of FORMAT must be ≤ 80.

9: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

10: LABROW – CHARACTER*1. *Input*

On entry: the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04DBF prints no row labels.

If LABROW = 'I' or 'i', X04DBF prints integer row labels.

If LABROW = 'C' or 'c', X04DBF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

11: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length M and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

12: LABCOL – CHARACTER*1. *Input*

On entry: the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04DBF prints no column labels.

If LABCOL = 'I' or 'i', X04DBF prints integer column labels.

If LABCOL = 'C' or 'c', X04DBF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

13: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

14: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

15: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

16: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, MATRIX ≠ 'G', 'g', 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, MATRIX = 'L', 'l', 'U' or 'u', but DIAG ≠ 'N', 'n', 'U', 'u', 'B', or 'b'.

IFAIL = 3

On entry, LDA < M.

IFAIL = 4

On entry, USEFRM ≠ 'A', 'a', 'B', 'b', 'D' or 'd'.

IFAIL = 5

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 6

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 7

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'I', 'i', 'C' or 'c'.

IFAIL = 8

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels) is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

X04DBF may be used to print a vector, either as a row or as a column. The following code fragment illustrates possible calls.

```
      complex A(4)
      CHARACTER*1 RLABS(1), CLABS(1)
C     Print vector A as a column vector.
      LDA = 4
      IFAIL = 0
      CALL X04DBF('G', 'X', 1, 4, A, LDA, 'B', ' ', ' ', 'I', RLABS,
     *            'N', CLABS, 80, 0, IFAIL)
C     Print vector A as a row vector.
      LDA = 1
      IFAIL = 0
      CALL X04DBF('G', 'X', 4, 1, A, LDA, 'B', ' ', ' ', 'N', RLABS,
     *            'I', CLABS, 80, 0, IFAIL)
```

9. Example

This example program calls X04DBF twice, first to print a 3 by 4 rectangular matrix, and then to print a 4 by 4 upper triangular matrix; various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04DBF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=4,LDA=NMAX)
*     .. Local Scalars ..
      real             AA
      INTEGER          I, IFAIL, INDENT, J, NCOLS
*     .. Local Arrays ..
      complex          A(LDA,NMAX)
      CHARACTER*7      CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04DBF
*     .. Intrinsic Functions ..
      INTRINSIC        cmplx
*     .. Data statements ..
      DATA             CLABS/'Un', 'Deux', 'Trois', 'Quatre'/
      DATA             RLABS/'Uno', 'Duo', 'Tre', 'Quattro'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04DBF Example Program Results'
      WRITE (NOUT,*)
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            AA = 10*I + J
            A(I,J) = cmplx(AA,-AA)
   20    CONTINUE
   40 CONTINUE
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
*
*     Print 3 by 4 rectangular matrix with default format and integer
*     row and column labels, and bracketed complex elements
      CALL X04DBF('General',' ',3,4,A,LDA,'Bracketed',' ','Example 1:',
     +            'Integer',RLABS,'Integer',CLABS,NCOLS,INDENT,IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 4 by 4 upper triangular matrix with user-supplied format
*     and row and column labels, and complex elements with real part
*     above imaginary part
      CALL X04DBF('Upper','Non-unit',4,4,A,LDA,'Above','F8.2',
     +            'Example 2:','Character',RLABS,'Character',CLABS,
     +            NCOLS,INDENT,IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04DBF Example Program Results

Example 1:
                              1                              2
1  (    11.0000,   -11.0000) (    12.0000,   -12.0000)
2  (    21.0000,   -21.0000) (    22.0000,   -22.0000)
3  (    31.0000,   -31.0000) (    32.0000,   -32.0000)

                              3                              4
1  (    13.0000,   -13.0000) (    14.0000,   -14.0000)
2  (    23.0000,   -23.0000) (    24.0000,   -24.0000)
3  (    33.0000,   -33.0000) (    34.0000,   -34.0000)

Example 2:
            Un     Deux    Trois  Quatre
    Uno   11.00    12.00    13.00   14.00
         -11.00   -12.00   -13.00  -14.00

    Duo             22.00    23.00   24.00
                   -22.00   -23.00  -24.00

    Tre                      33.00   34.00
                            -33.00  -34.00

Quattro                              44.00
                                    -44.00
```

X04DCF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04DCF is an easy-to-use routine to print a ***complex*** triangular matrix stored in a packed one-dimensional array.

2. Specification

```
SUBROUTINE X04DCF (UPLO, DIAG, N, A, TITLE, IFAIL)
INTEGER           N, IFAIL
complex           A(*)
CHARACTER*1       UPLO, DIAG
CHARACTER*(*)     TITLE
```

3. Description

X04DCF prints a ***complex*** triangular matrix stored in packed form. It is an easy-to-use driver for X04DDF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length. The matrix must be packed by column.

X04DCF will choose a format code such that numbers will be printed with either an F8.4, F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen. The chosen code is used to print each complex element of the matrix with the real part above the imaginary part.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: UPLO – CHARACTER*1. *Input*

On entry: indicates the type of the matrix to be printed, as follows:

UPLO = 'L' or 'l' (Lower), the matrix is lower triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (2,1),..., (N,1), (2,2), (3,2),..., (N,2), etc.

UPLO = 'U' or 'u' (Upper), the matrix is upper triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (1,2), (2,2), (1,3), (2,3), (3,3), (1,4), etc.

Constraint: UPLO must be one of 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: indicates whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

Constraint: DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: N – INTEGER. *Input*

On entry: the order of the matrix to be printed.

If N is less than 1, X04DCF will exit immediately after printing TITLE; no row or column labels are printed.

4: A(*) – ***complex*** array. *Input*

The dimension of A must be at least max(1,N*(N+1)/2).

On entry: the matrix to be printed. Note that A must have space for the diagonal elements of the matrix, even if these are not stored.

5: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

6: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, UPLO ≠ 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, DIAG ≠ 'N', 'n', 'U', 'u', 'B' or 'b'.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04DCF is equivalent to a call to X04DDF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
USEFRM = 'A'
```

9. Example

This example program calls X04DCF twice, first to print a 3 by 3 lower triangular matrix, and then to print a 4 by 4 upper triangular matrix.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04DCF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LA
      PARAMETER        (NMAX=4,LA=(NMAX*(NMAX+1))/2)
*     .. Local Scalars ..
      real             AA
      INTEGER          I, IFAIL
*     .. Local Arrays ..
      complex          A(LA)
*     .. External Subroutines ..
      EXTERNAL         X04DCF
*     .. Intrinsic Functions ..
      INTRINSIC        cmplx
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04DCF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 20 I = 1, LA
         AA = I
         A(I) = cmplx(AA,-AA)
   20 CONTINUE
*
      IFAIL = 0
*
*     Print order 3 lower triangular matrix
      CALL X04DCF('Lower','Unit',3,A,'Example 1:',IFAIL)
*
      WRITE (NOUT,*)
*
*     Print order 4 upper triangular matrix
      CALL X04DCF('Upper','Non-unit',4,A,'Example 2:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
 X04DCF Example Program Results

 Example 1:
              1          2          3
 1       1.0000
         0.0000

 2       2.0000     1.0000
        -2.0000     0.0000

 3       3.0000     5.0000     1.0000
        -3.0000    -5.0000     0.0000
```

```
Example 2:
                1          2          3          4
1         1.0000     2.0000     4.0000     7.0000
         -1.0000    -2.0000    -4.0000    -7.0000

2                    3.0000     5.0000     8.0000
                    -3.0000    -5.0000    -8.0000

3                               6.0000     9.0000
                               -6.0000    -9.0000

4                                         10.0000
                                         -10.0000
```

X04DDF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04DDF prints a ***complex*** triangular matrix stored in a packed one-dimensional array.

2. Specification

```
SUBROUTINE X04DDF (UPLO, DIAG, N, A, USEFRM, FORMAT, TITLE, LABROW,
1                  RLABS, LABCOL, CLABS, NCOLS, INDENT, IFAIL)
INTEGER        N, NCOLS, INDENT, IFAIL
complex        A(*)
CHARACTER*1    UPLO, DIAG, USEFRM, LABROW, LABCOL
CHARACTER*(*)  FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04DDF prints a ***complex*** triangular matrix stored in packed form, using a format specifier supplied by the user. The matrix must be packed by column. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: UPLO – CHARACTER*1. *Input*

On entry: indicates the type of the matrix to be printed, as follows:

UPLO = 'L' or 'l' (Lower), the matrix is lower triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (2,1),..., (N,1), (2,2), (3,2),..., (N,2), etc.

UPLO = 'U' or 'u' (Upper), the matrix is upper triangular. In this case, the packed array A holds the matrix elements in the following order: (1,1), (1,2), (2,2), (1,3), (2,3), (3,3), (1,4), etc.

Constraint: UPLO must be one of 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: indicates whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

Constraint: DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix to be printed.

If N is less than 1, X04DDF will exit immediately after printing TITLE; no row or column labels are printed.

4: A(*) – ***complex*** array. *Input*

The dimension of A must be at least max(1,N*(N+1)/2).

On entry: the matrix to be printed. Note that A must have space for the diagonal elements of the matrix, even if these are not stored.

5: USEFRM – CHARACTER*1. *Input*

On entry: indicates how the value of FORMAT is to be used to print matrix elements.

USEFRM = 'A' or 'a' (Above), the format code in FORMAT is assumed to contain a single real edit-descriptor which is to be used to print the real and imaginary parts of each ***complex*** number one above the other. Each row of the matrix is separated by a blank line, and any row labels are attached only to the real parts. This option means that about twice as many columns can be fitted into NCOLS characters than if any other USEFRM option is used. A typical value of FORMAT for this USEFRM option might be FORMAT = 'E13.4', '*' or ' '.

USEFRM = 'B' or 'b' (Bracketed), the format code in FORMAT is assumed to contain a single edit-descriptor such as 'E13.4', '*' or ' ', which is used to print the real and imaginary parts of each ***complex*** number separated by a comma, and surrounded by brackets. Thus a matrix element printed with this USEFRM option might look like this: (12.345, -11.323)

USEFRM = 'D' or 'd' (Direct), the format code in FORMAT is used unaltered to print a ***complex*** number. This USEFRM option allows the user flexibility to specify exactly how the number is printed. With this option for USEFRM and a suitable value for FORMAT it is possible, for example, to print a ***complex*** number in the form (0.123 + 3.214i) or (0.123E-02,0.234E-01). See Section 9 for an example illustrating this option.

Constraint: USEFRM must be one of 'A', 'a', 'B', 'b', 'D' or 'd'.

6: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used in conjunction with parameter USEFRM, described above, to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(F11.4)', '1P,2E13.5'.

In addition, there are two special codes which force X04DDF to choose its own format code:

FORMAT = ' ' means that X04DDF will choose a format code such that numbers will be printed with either an F8.4, an F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of the real and imaginary parts of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the numbers to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

FORMAT = '*' means that X04DDF will choose a format code such that numbers will be printed to as many significant digits as are necessary to distinguish between neighbouring machine numbers. Thus any two numbers that are stored with different internal representations should look different on output. Whether they do in fact look different will depend on the run-time library of the Fortran compiler in use.

More complicated values of FORMAT, to print a ***complex*** number in a desired form, may be used. See the description of parameter USEFRM above for more details.

Constraint: the character length of FORMAT must be ≤ 80.

7: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

8: LABROW – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04DDF prints no row labels.

If LABROW = 'I' or 'i', X04DDF prints integer row labels.

If LABROW = 'C' or 'c', X04DDF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

9: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length N and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

10: LABCOL – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04DDF prints no column labels.

If LABCOL = 'I' or 'i', X04DDF prints integer column labels.

If LABCOL = 'C' or 'c', X04DDF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

11: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

12: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

13: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

14: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, UPLO ≠ 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, DIAG ≠ 'N', 'n', 'U', 'u', 'B', or 'b'.

IFAIL = 3

On entry, USEFRM ≠ 'A', 'a', 'B', 'b', 'D', or 'd'.

IFAIL = 4

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 5

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 6

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'I', 'i', 'C' or 'c'.

IFAIL = 7

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels) is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

This example program calls X04DDF twice, first to print a 4 by 4 lower triangular matrix, and then to print a 4 by 4 triangular matrix, various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04DDF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LA
      PARAMETER        (NMAX=4,LA=(NMAX*(NMAX+1))/2)
*     .. Local Scalars ..
      real             AA
      INTEGER          I, IFAIL, INDENT, NCOLS
      CHARACTER*19     FORMAT
```

```
*     .. Local Arrays ..
      complex           A(LA)
      CHARACTER*7       CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL          X04DDF
*     .. Intrinsic Functions ..
      INTRINSIC         cmplx
*     .. Data statements ..
      DATA              CLABS/'Un', 'Deux', 'Trois', 'Quatre'/
      DATA              RLABS/'Uno', 'Duo', 'Tre', 'Quattro'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04DDF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 20 I = 1, LA
         AA = I
         A(I) = cmplx(AA,-AA)
   20 CONTINUE
*
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
      FORMAT = ' '
*
*     Print order 4 lower triangular matrix with default format and
*     integer row and column labels, and bracketed complex elements
      CALL X04DDF('Lower','Non-unit',4,A,'Bracketed',FORMAT,
     +            'Example 1:','Integer',RLABS,'Integer',CLABS,NCOLS,
     +            INDENT,IFAIL)
*
      WRITE (NOUT,*)
      FORMAT = 'SS,F7.1,SP,F6.1,''i'''
*
*     Print order 4 upper triangular matrix with user-supplied format
*     and row and column labels, using the supplied format directly
      CALL X04DDF('Upper','Unit',4,A,'Direct',FORMAT,'Example 2:',
     +            'Character',RLABS,'Character',CLABS,NCOLS,INDENT,
     +            IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04DDF Example Program Results

Example 1:
                              1                          2
1  (     1.0000,    -1.0000)
2  (     2.0000,    -2.0000) (     5.0000,    -5.0000)
3  (     3.0000,    -3.0000) (     6.0000,    -6.0000)
4  (     4.0000,    -4.0000) (     7.0000,    -7.0000)

                              3                          4
1
2
3  (     8.0000,    -8.0000)
4  (     9.0000,    -9.0000) (    10.0000,   -10.0000)
```

Example 2:

	Un		Deux		Trois		Quatre	
Uno	1.0	+0.0i	2.0	-2.0i	4.0	-4.0i	7.0	-7.0i
Duo			1.0	+0.0i	5.0	-5.0i	8.0	-8.0i
Tre					1.0	+0.0i	9.0	-9.0i
Quattro							1.0	+0.0i

X04DEF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04DEF is an easy-to-use routine to print a ***complex*** band matrix stored in a packed two-dimensional array.

2. Specification

```
SUBROUTINE X04DEF (M, N, KL, KU, A, LDA, TITLE, IFAIL)
INTEGER          M, N, KL, KU, LDA, IFAIL
complex          A(LDA,*)
CHARACTER*(*)    TITLE
```

3. Description

X04DEF prints a ***complex*** band matrix stored in a packed two-dimensional array. It is an easy-to-use driver for X04DEF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length.

X04DEF will choose a format code such that numbers will be printed with either an F8.4, F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the matrix elements to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen. The chosen code is used to print each complex element of the matrix with the real part above the imaginary part.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: M – INTEGER. *Input*

2: N – INTEGER. *Input*

On entry: the number of rows and columns of the band matrix, respectively, to be printed.

If either of M or N is less than 1, X04DEF will exit immediately after printing TITLE; no row or column labels are printed.

3: KL – INTEGER. *Input*

On entry: the number of sub-diagonals of the band matrix A.

Constraint: KL $\geq$ 0.

4: KU – INTEGER. *Input*

On entry: the number of super-diagonals of the band matrix A.

Constraint: KU $\geq$ 0.

5: A(LDA,*) – ***complex*** array. *Input*

The second dimension of A must be at least max(1,min(M+KU,N)).

On entry: the band matrix to be printed. The leading (KL+KU+1) by min(M+KU,N) part of array A must contain the matrix, packed column by column, with the leading diagonal of the matrix in row (KU+1) of the array, the first super-diagonal starting at position 2 in row KU, the first sub-diagonal starting at position 1 in row (KU+2), and so on. Elements in the array A that do not correspond to elements in the band matrix (such as the top left KU by KU triangle) are not referenced, and need not be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04DEF is called.

Constraint: LDA ≥ KL + KU + 1.

7: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, KL < 0.

IFAIL = 2

On entry, KU < 0.

IFAIL = 3

On entry, LDA < KL + KU + 1.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04DEF is equivalent to a call to X04DFF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
USEFRM = 'A'
```

9. Example

This example program calls X04DEF to print a 5 by 5 band matrix with one sub-diagonal and one super-diagonal.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04DEF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      real             AA
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      complex          A(LDA,NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04DEF
*     .. Intrinsic Functions ..
      INTRINSIC        cmplx
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04DEF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            AA = 10*I + J
            A(I,J) = cmplx(AA,-AA)
   20    CONTINUE
   40 CONTINUE
*
      IFAIL = 0
*
*     Print 5 by 5 band matrix with 1 sub-diagonal and 1 super-diagonal
      CALL X04DEF(5,5,1,1,A,LDA,'Band Matrix:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04DEF Example Program Results

Band Matrix:
             1          2          3          4          5
1     21.0000    12.0000
     -21.0000   -12.0000

2     31.0000    22.0000    13.0000
     -31.0000   -22.0000   -13.0000

3                32.0000    23.0000    14.0000
                -32.0000   -23.0000   -14.0000

4                           33.0000    24.0000    15.0000
                           -33.0000   -24.0000   -15.0000

5                                      34.0000    25.0000
                                      -34.0000   -25.0000
```

X04DFF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04DFF prints a ***complex*** band matrix stored in a packed two-dimensional array.

2. Specification

```
      SUBROUTINE X04DFF (M, N, KL, KU, A, LDA, USEFRM, FORMAT, TITLE,
     1                   LABROW, RLABS, LABCOL, CLABS, NCOLS, INDENT,
     2                   IFAIL)
      INTEGER           M, N, KL, KU, LDA, NCOLS, INDENT, IFAIL
      complex           A(LDA,*)
      CHARACTER*1       USEFRM, LABROW, LABCOL
      CHARACTER*(*)     FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04DFF prints a ***complex*** band matrix stored in a packed two-dimensional array, using a format specifier supplied by the user. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: M – INTEGER. *Input*

2: N – INTEGER. *Input*

On entry: the number of rows and columns of the band matrix, respectively, to be printed.

If either of M or N is less than 1, X04DFF will exit immediately after printing TITLE; no row or column labels are printed.

3: KL – INTEGER. *Input*

On entry: the number of sub-diagonals of the band matrix A.

Constraint: KL $\geq$ 0.

4: KU – INTEGER. *Input*

On entry: the number of super-diagonals of the band matrix A.

Constraint: KU $\geq$ 0.

5: A(LDA,*) – ***complex*** array. *Input*

The second dimension of A must be at least max(1,min(M+KU,N)).

On entry: the band matrix to be printed. The leading (KL+KU+1) by min(M+KU,N) part of array A must contain the matrix, packed column by column, with the leading diagonal of the matrix in row (KU+1) of the array, the first super-diagonal starting at position 2 in row KU, the first sub-diagonal starting at position 1 in row (KU+2), and so on. Elements in the array A that do not correspond to elements in the band matrix (such as the top left KU by KU triangle) are not referenced, and need not be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04DFF is called.

Constraint: LDA $\geq$ KL + KU + 1.

7: USEFRM – CHARACTER*1. *Input*

On entry: indicates how the value of FORMAT is to be used to print matrix elements.

USEFRM = 'A' or 'a' (Above), the format code in FORMAT is assumed to contain a single real edit-descriptor which is to be used to print the real and imaginary parts of each ***complex*** number one above the other. Each row of the matrix is separated by a blank line, and any row labels are attached only to the real parts. This option means that about twice as many columns can be fitted into NCOLS characters than if any other USEFRM option is used. A typical value of FORMAT for this USEFRM option might be FORMAT = 'E13.4', '*' or ' '.

USEFRM = 'B' or 'b' (Bracketed), the format code in FORMAT is assumed to contain a single edit-descriptor such as 'E13.4', '*' or ' ', which is used to print the real and imaginary parts of each ***complex*** number separated by a comma, and surrounded by brackets. Thus a matrix element printed with this USEFRM option might look like this: (12.345, −11.323)

USEFRM = 'D' or 'd' (Direct), the format code in FORMAT is used unaltered to print a ***complex*** number. This USEFRM option allows the user flexibility to specify exactly how the number is printed. With this option for USEFRM and a suitable value for FORMAT it is possible, for example, to print a ***complex*** number in the form (0.123 + 3.214i) or (0.123E−02,0.234E−01). See Section 9 for an example illustrating this option.

Constraint: USEFRM must be one of 'A', 'a', 'B', 'b', 'D' or 'd'.

8: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used in conjunction with parameter USEFRM, described above, to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(F11.4)', '1P,2E13.5'.

In addition, there are two special codes which force X04DFF to choose its own format code:

FORMAT = ' ' means that X04DFF will choose a format code such that numbers will be printed with either an F8.4, an F11.4 or a 1PE13.4 format. The F8.4 code is chosen if the sizes of the real and imaginary parts of all the matrix elements to be printed lie between 0.001 and 1.0. The F11.4 code is chosen if the sizes of all the numbers to be printed lie between 0.001 and 9999.9999. Otherwise the 1PE13.4 code is chosen.

FORMAT = '*' means that X04DFF will choose a format code such that numbers will be printed to as many significant digits as are necessary to distinguish between neighbouring machine numbers. Thus any two numbers that are stored with different internal representations should look different on output. Whether they do in fact look different will depend on the run-time library of the Fortran compiler in use.

More complicated values of FORMAT, to print a ***complex*** number in a desired form, may be used. See the description of parameter USEFRM above for more details.

Constraint: the character length of FORMAT must be ≤ 80.

9: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

10: LABROW – CHARACTER*1. *Input*

On entry: the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04DFF prints no row labels.

If LABROW = 'I' or 'i', X04DFF prints integer row labels.

If LABROW = 'C' or 'c', X04DFF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

11: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length M and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

12: LABCOL – CHARACTER*1. *Input*

On entry: the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04DFF prints no column labels.

If LABCOL = 'I' or 'i', X04DFF prints integer column labels.

If LABCOL = 'C' or 'c', X04DFF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

13: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

14: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

15: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

16: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, KL < 0.

IFAIL = 2

On entry, KU < 0.

IFAIL = 3

On entry, LDA < KL + KU + 1.

IFAIL = 4

On entry, USEFRM ≠ 'A', 'a', 'B', 'b', 'D' or 'd'.

IFAIL = 5

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 6

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 7

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'I', 'i', 'C' or 'c'.

IFAIL = 8

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels) is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

None.

9. Example

This example program calls X04DFF twice, to print band matrices of different orders and bandwidths; various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04DFF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      real             AA
      INTEGER          I, IFAIL, INDENT, J, NCOLS
      CHARACTER*19     FORMAT
*     .. Local Arrays ..
      complex          A(LDA,LDA)
      CHARACTER*7      CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04DFF
```

```
*     .. Intrinsic Functions ..
      INTRINSIC        cmplx
*     .. Data statements ..
      DATA             CLABS/'Un', 'Deux', 'Trois', 'Quatre', 'Cinq'/
      DATA             RLABS/'Uno', 'Duo', 'Tre', 'Quattro', 'Cinque'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04DFF Example Program Results'
      WRITE (NOUT,*)
*
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            AA = 10*I + J
            A(I,J) = cmplx(AA,-AA)
   20    CONTINUE
   40 CONTINUE
*
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
      FORMAT = ' '
*
*     Print 5 by 5 band matrix with 1 sub-diagonal, 1 super-diagonal,
*     default format, bracketed complex numbers, and integer row and
*     column labels
      CALL X04DFF(5,5,1,1,A,LDA,'Bracketed',FORMAT,'Example 1:',
     +            'Integer',RLABS,'Integer',CLABS,NCOLS,INDENT,IFAIL)
*
      WRITE (NOUT,*)
      FORMAT = 'SS,F7.1,SP,F6.1,''i'''
*
*     Print 4 by 4 band matrix with 1 sub-diagonal, 2 super-diagonals,
*     user-supplied format and row and column labels
      CALL X04DFF(4,4,1,2,A,LDA,'Direct',FORMAT,'Example 2:',
     +            'Character',RLABS,'Character',CLABS,NCOLS,INDENT,
     +            IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04DFF Example Program Results

Example 1:
                              1                         2
1  (    21.0000,   -21.0000) (    12.0000,   -12.0000)
2  (    31.0000,   -31.0000) (    22.0000,   -22.0000)
3                            (    32.0000,   -32.0000)
4
5

                              3                         4
1
2  (    13.0000,   -13.0000)
3  (    23.0000,   -23.0000) (    14.0000,   -14.0000)
4  (    33.0000,   -33.0000) (    24.0000,   -24.0000)
5                            (    34.0000,   -34.0000)

                              5
1
2
3
4  (    15.0000,   -15.0000)
5  (    25.0000,   -25.0000)
```

Example 2:

	Un	Deux	Trois	Quatre
Uno	31.0 -31.0i	22.0 -22.0i	13.0 -13.0i	
Duo	41.0 -41.0i	32.0 -32.0i	23.0 -23.0i	14.0 -14.0i
Tre		42.0 -42.0i	33.0 -33.0i	24.0 -24.0i
Quattro			43.0 -43.0i	34.0 -34.0i

X04EAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04EAF is an easy-to-use routine to print an integer matrix stored in a two-dimensional array.

2. Specification

```
SUBROUTINE X04EAF (MATRIX, DIAG, M, N, A, LDA, TITLE, IFAIL)
INTEGER          M, N, A(LDA,*), LDA, IFAIL
CHARACTER*1      MATRIX, DIAG
CHARACTER*(*)    TITLE
```

3. Description

X04EAF prints an integer matrix. It is an easy-to-use driver for X04EBF. The routine uses default values for the format in which numbers are printed, for labelling the rows and columns, and for output record length.

X04EAF will choose a format code such that numbers will be printed with the smallest I edit descriptor that is large enough to hold all the numbers to be printed.

The matrix is printed with integer row and column labels, and with a maximum record length of 80.

The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: MATRIX – CHARACTER*1. *Input*

On entry: indicates the part of the matrix to be printed, as follows:

MATRIX = 'G' or 'G' (General), the whole of the rectangular matrix.

MATRIX = 'L' or 'l' (Lower), the lower triangle of the matrix, or the lower trapezium if the matrix has more rows than columns.

MATRIX = 'U' or 'u' (Upper), the upper triangle of the matrix, or the upper trapezium if the matrix has more columns than rows.

Constraint: MATRIX must be one of 'G', 'g', 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: unless MATRIX = 'G' or 'g', DIAG must specify whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

If MATRIX = 'G' or 'g', then DIAG need not be set.

Constraint: If MATRIX $\neq$ 'G' or 'g', then DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: M – INTEGER. *Input*

4: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix, respectively, to be printed.

If either of M or N is less than 1, X04EAF will exit immediately after printing TITLE; no row or column labels are printed.

5: A(LDA,*) – INTEGER array. *Input*

The second dimension of A must be at least max(1,N).

On entry: the matrix to be printed. Only the elements that will be referred to, as specified by parameters MATRIX and DIAG, need be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04EAF is called.

Constraint: LDA ≥ M.

7: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than 80 characters, the contents of TITLE will be wrapped onto more than one line, with the break after 80 characters.

Any trailing blank characters in TITLE are ignored.

8: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, MATRIX ≠ 'G', 'g', 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, MATRIX = 'L', 'l', 'U' or 'u', but DIAG ≠ 'N', 'n', 'U', 'u', 'B' or 'b'.

IFAIL = 3

On entry, LDA < M.

7. Accuracy

Not applicable.

8. Further Comments

A call to X04EAF is equivalent to a call to X04EBF with the following argument values:

```
NCOLS = 80
INDENT = 0
LABROW = 'I'
LABCOL = 'I'
FORMAT = ' '
```

9. Example

This example program calls X04EAF twice, first to print a 3 by 5 rectangular matrix, and then to print a 5 by 5 triangular matrix.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04EAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      INTEGER          A(LDA,NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04EAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04EAF Example Program Results'
      WRITE (NOUT,*)
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            A(I,J) = 10*I + J
   20    CONTINUE
   40 CONTINUE
*
      IFAIL = 0
*
*     Print 3 by 5 rectangular matrix
      CALL X04EAF('General',' ',3,5,A,LDA,'Example 1:',IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 5 by 5 lower triangular matrix
      CALL X04EAF('Lower','Non-unit',5,5,A,LDA,'Example 2:',IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04EAF Example Program Results

Example 1:
    1  2  3  4  5
1  11 12 13 14 15
2  21 22 23 24 25
3  31 32 33 34 35

Example 2:
    1  2  3  4  5
1  11
2  21 22
3  31 32 33
4  41 42 43 44
5  51 52 53 54 55
```

X04EBF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X04EBF prints an integer matrix stored in a two-dimensional array.

2. Specification

```
SUBROUTINE X04EBF (MATRIX, DIAG, M, N, A, LDA, FORMAT, TITLE, LABROW,
1                  RLABS, LABCOL, CLABS, NCOLS, INDENT, IFAIL)
INTEGER        M, N, A(LDA,*), LDA, NCOLS, INDENT, IFAIL
CHARACTER*1    MATRIX, DIAG, LABROW, LABCOL
CHARACTER*(*)  FORMAT, TITLE, RLABS(*), CLABS(*)
```

3. Description

X04EBF prints an integer matrix, or part of it, using a format specifier supplied by the user. The matrix is output to the unit defined by X04ABF.

4. References

None.

5. Parameters

1: MATRIX – CHARACTER*1. *Input*

On entry: indicates the part of the matrix to be printed, as follows:

MATRIX = 'G' or 'g' (General), the whole of the rectangular matrix.

MATRIX = 'L' or 'l' (Lower), the lower triangle of the matrix, or the lower trapezium if the matrix has more rows than columns.

MATRIX = 'U' or 'u' (Upper), the upper triangle of the matrix, or the upper trapezium if the matrix has more columns than rows.

Constraint: MATRIX must be one of 'G', 'g', 'L', 'l', 'U' or 'u'.

2: DIAG – CHARACTER*1. *Input*

On entry: unless MATRIX = 'G' or 'g', DIAG must specify whether the diagonal elements of the matrix are to be printed, as follows:

DIAG = 'B' or 'b' (Blank), the diagonal elements of the matrix are not referenced and not printed.

DIAG = 'U' or 'u' (Unit diagonal), the diagonal elements of the matrix are not referenced, but are assumed all to be unity, and are printed as such.

DIAG = 'N' or 'n' (Non-unit diagonal), the diagonal elements of the matrix are referenced and printed.

If MATRIX = 'G' or 'g', then DIAG need not be set.

Constraint: If MATRIX $\neq$ 'G' or 'g', then DIAG must be one of 'B', 'b', 'U', 'u', 'N' or 'n'.

3: M – INTEGER. *Input*

4: N – INTEGER. *Input*

On entry: the number of rows and columns of the matrix, respectively, to be printed.

If either of M or N is less than 1, X04EBF will exit immediately after printing TITLE; no row or column labels are printed.

5: A(LDA,*) – INTEGER array. *Input*

The second dimension of A must be at least max(1,N).

On entry: the matrix to be printed. Only the elements that will be referred to, as specified by parameters MATRIX and DIAG, need be set.

6: LDA – INTEGER. *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which X04EBF is called.

Constraint: LDA ≥ M.

7: FORMAT – CHARACTER*(*). *Input*

On entry: a valid Fortran format code. This may be any format code allowed on the system, whether it is standard Fortran or not. FORMAT is used to print elements of the matrix *A*. It may or may not be enclosed in brackets. Examples of valid values for FORMAT are '(I6)', 'I4,2X'.

In addition, there is a special code which forces X04EBF to choose its own format code:

FORMAT = ' ' means that X04EBF will choose a format code such that numbers will be printed using the smallest edit descriptor that is large enough to hold all the numbers to be printed.

Constraint: the character length of FORMAT must be ≤ 80.

8: TITLE – CHARACTER*(*). *Input*

On entry: a title to be printed above the matrix. If TITLE = ' ', no title (and no blank line) will be printed.

If TITLE contains more than NCOLS characters, the contents of TITLE will be wrapped onto more than one line, with the break after NCOLS characters.

Any trailing blank characters in TITLE are ignored.

9: LABROW – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the rows of the matrix, as follows:

If LABROW = 'N' or 'n', X04EBF prints no row labels.

If LABROW = 'I' or 'i', X04EBF prints integer row labels.

If LABROW = 'C' or 'c', X04EBF prints character labels, which must be supplied in array RLABS.

Constraint: LABROW must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

10: RLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABROW = 'C' or 'c', RLABS must be dimensioned at least of length M and must contain labels for the rows of the matrix, otherwise RLABS may be dimensioned of length 1.

Labels are right justified when output, in a field which is as wide as necessary to hold the longest row label. Note that this field width is subtracted from the number of usable columns, NCOLS.

11: LABCOL – CHARACTER*1. *Input*

On entry: indicates the type of labelling to be applied to the columns of the matrix, as follows:

If LABCOL = 'N' or 'n', X04EBF prints no column labels.

If LABCOL = 'I' or 'i', X04EBF prints integer column labels.

If LABCOL = 'C' or 'c', X04EBF prints character labels, which must be supplied in array CLABS.

Constraint: LABCOL must be one of 'N', 'n', 'I', 'i', 'C' or 'c'.

12: CLABS(*) – CHARACTER*(*) array. *Input*

On entry: if LABCOL = 'C' or 'c', CLABS must be dimensioned at least of length N and must contain labels for the columns of the matrix, otherwise CLABS may be dimensioned of length 1.

Labels are right-justified when output. Any label that is too long for the column width, which is determined by FORMAT, is truncated.

13: NCOLS – INTEGER. *Input*

On entry: the maximum output record length. If the number of columns of the matrix is too large to be accommodated in NCOLS characters, the matrix will be printed in parts, containing the largest possible number of matrix columns, and each part separated by a blank line.

NCOLS must be large enough to hold at least one column of the matrix using the format specifier in FORMAT. If a value less than 0 or greater than 132 is supplied for NCOLS, then the value 80 is used instead.

14: INDENT – INTEGER. *Input*

On entry: the number of columns by which the matrix (and any title and labels) should be indented. The effective value of NCOLS is reduced by INDENT columns. If a value less than 0 or greater than NCOLS is supplied for INDENT, the value 0 is used instead.

15: IFAIL – INTEGER. *Input/Output*

On entry: IFAIL must be set to 0, –1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6. Error Indicators and Warnings

Errors detected by the routine:

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

IFAIL = 1

On entry, MATRIX ≠ 'G', 'g', 'L', 'l', 'U' or 'u'.

IFAIL = 2

On entry, MATRIX = 'L', 'l', 'U' or 'u', but DIAG ≠ 'N', 'n', 'U', 'u', 'B' or 'b'.

IFAIL = 3

On entry, M > LDA.

IFAIL = 4

On entry, variable FORMAT is more than 80 characters long.

IFAIL = 5

The code supplied in FORMAT cannot be used to output a number. FORMAT probably has too wide a field width or contains an illegal edit descriptor.

IFAIL = 6

On entry, either LABROW or LABCOL ≠ 'N', 'n', 'I', 'i', 'C' or 'c'.

IFAIL = 7

The quantity NCOLS – INDENT – LABWID (where LABWID is the width needed for the row labels) is not large enough to hold at least one column of the matrix.

7. Accuracy

Not applicable.

8. Further Comments

X04EBF may be used to print a vector, either as a row or as a column. The following code fragment illustrates possible calls.

```
      INTEGER A(4)
      CHARACTER*1 RLABS(1), CLABS(1)
C     Print vector A as a column vector.
      LDA = 4
      IFAIL = 0
      CALL X04EBF('G', 'X', 1, 4, A, LDA, ' ', ' ', 'I', RLABS,
     *            'N', CLABS, 80, 0, IFAIL)
C     Print vector A as a row vector.
      LDA = 1
      IFAIL = 0
      CALL X04EBF('G', 'X', 4, 1, A, LDA, ' ', ' ', 'N', RLABS,
     *            'I', CLABS, 80, 0, IFAIL)
```

9. Example

This example program calls X04EBF twice, first to print a 3 by 5 rectangular matrix, and then to print a 5 by 5 upper triangular matrix; various options for labelling and formatting are illustrated.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X04EBF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NMAX, LDA
      PARAMETER        (NMAX=5,LDA=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INDENT, J, NCOLS
*     .. Local Arrays ..
      INTEGER          A(LDA,NMAX)
      CHARACTER*7      CLABS(NMAX), RLABS(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04EBF
*     .. Data statements ..
      DATA             CLABS/'Un', 'Deux', 'Trois', 'Quatre', 'Cinq'/
      DATA             RLABS/'Uno', 'Duo', 'Tre', 'Quattro', 'Cinque'/
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X04EBF Example Program Results'
      WRITE (NOUT,*)
*     Generate an array of data
      DO 40 J = 1, NMAX
         DO 20 I = 1, LDA
            A(I,J) = 10*I + J
   20    CONTINUE
   40 CONTINUE
      NCOLS = 80
      INDENT = 0
      IFAIL = 0
*
```

```
*     Print 3 by 5 rectangular matrix with default format and integer
*     row and column labels
      CALL X04EBF('General',' ',3,5,A,LDA,' ','Example 1:','Integer',
     +            RLABS,'Integer',CLABS,NCOLS,INDENT,IFAIL)
*
      WRITE (NOUT,*)
*
*     Print 5 by 5 upper triangular matrix with user-supplied format
*     and row and column labels
      CALL X04EBF('Upper','Non-unit',5,5,A,LDA,'I8','Example 2:',
     +            'Character',RLABS,'Character',CLABS,NCOLS,INDENT,
     +            IFAIL)
*
      STOP
      END
```

9.2. Program Data

None.

9.3. Program Results

```
X04EBF Example Program Results

Example 1:
     1  2  3  4  5
1   11 12 13 14 15
2   21 22 23 24 25
3   31 32 33 34 35

Example 2:
               Un    Deux   Trois  Quatre    Cinq
    Uno        11      12      13      14      15
    Duo              22      23      24      25
    Tre                      33      34      35
Quattro                              44      45
 Cinque                                      55
```

Chapter X05 – Date and Time Utilities

Note. Please refer to the Users' Note for your implementation to check that a routine is available.

Routine Name	Mark of Introduction	Purpose
X05AAF	14	Return date and time as an array of integers
X05ABF	14	Convert array of integers representing date and time to character string
X05ACF	14	Compare two character strings representing date and time
X05BAF	14	Return the CPU time

Chapter X05

Date and Time Utilities

Contents

1 Scope of the Chapter

This chapter provides routines to obtain the current real time, and the amount of processor time used.

2 Background to the Problems

2.1 Real Time

Routines are provided to obtain the current time in two different formats, and to compare two such times.

2.2 Processor Time

A routine is provided to return the current amount of processor time used. This allows the timing of a particular routine or section of code.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

X05AAF returns the current date/time in integer format.

X05ABF converts from integer to character string date/time.

X05ACF compares two date/time character strings.

X05BAF returns the amount of processor time used.

X05AAF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

X05AAF returns the current date and time.

2 Specification

```
SUBROUTINE X05AAF(ITIME)
INTEGER           ITIME(7)
```

3 Description

X05AAF returns the current date and time as a set of seven integers.

4 References

None.

5 Parameters

1: ITIME(7) — INTEGER array *Output*

On exit: the current date and time, as follows:

ITIME(1) contains the current year.

ITIME(2) contains the current month, in the range 1–12.

ITIME(3) contains the current day, in the range 1–31.

ITIME(4) contains the current hour, in the range 0–23.

ITIME(5) contains the current minute, in the range 0–59.

ITIME(6) contains the current second, in the range 0–59.

ITIME(7) contains the current millisecond, in the range 0–999.

6 Error Indicators and Warnings

None.

7 Accuracy

The accuracy of this routine depends on the accuracy of the host machine. In particular, on some machines it may not be possible to return a value for the current millisecond, for example. In this case, the value returned will be zero.

8 Further Comments

None.

9 Example

This program prints out the vector ITIME after a call to X05AAF.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X05AAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Arrays ..
      INTEGER          ITIME(7)
*     .. External Subroutines ..
      EXTERNAL         X05AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X05AAF Example Program Results'
*
      CALL X05AAF(ITIME)
*
      WRITE (NOUT,99999) '       Year : ', ITIME(1)
      WRITE (NOUT,99999) '      Month : ', ITIME(2)
      WRITE (NOUT,99999) '        Day : ', ITIME(3)
      WRITE (NOUT,99999) '       Hour : ', ITIME(4)
      WRITE (NOUT,99999) '     Minute : ', ITIME(5)
      WRITE (NOUT,99999) '     Second : ', ITIME(6)
      WRITE (NOUT,99999) 'Millisecond : ', ITIME(7)
      STOP
*
99999 FORMAT (1X,A,I4)
      END
```

9.2 Program Data

None.

9.3 Program Results

```
 X05AAF Example Program Results
        Year : 1997
       Month :    5
         Day :   21
        Hour :    9
      Minute :   36
      Second :   13
 Millisecond :  511
```

X05ABF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X05ABF converts from a seven-integer format time and date, as returned by X05AAF, into a character string, returned via the routine name.

2. Specification

```
CHARACTER*30 FUNCTION X05ABF(ITIME)
INTEGER      ITIME(7)
```

3. Description

X05ABF returns a character string of length 30 which contains the date and time as supplied in argument ITIME. On exit, the character string has the following format:

```
'DAY XXTH MTH YEAR HR:MN:SC.MIL',
```

where `DAY` is one of 'Sun', 'Mon', 'Tue', 'Wed', 'Thu', 'Fri', 'Sat',

`XX` is an integer denoting the day of the month,

`TH` is one of 'st', 'nd', 'rd', 'th',

`MTH` is one of 'Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul','Aug', 'Sep', 'Oct', 'Nov', 'Dec',

`YEAR` is the year as a four digit integer,

`HR` is the hour,

`MN` is the minute,

`SC` is the second,

`MIL` is the millisecond.

If on entry the date in ITIME is invalid, the string returned is ' `** Illegal date/time **` '

4. References

None.

5. Parameters

1: ITIME(7) – INTEGER array. *Input*

On entry: a date and time in the format returned by X05AAF, as follows:

ITIME(1) must contain the year as a positive integer.

ITIME(2) must contain the month, in the range 1-12.

ITIME(3) must contain the day, in the range 1 to p, where p = 28, 29, 30 or 31, depending on the month and year.

ITIME(4) must contain the hour, in the range 0-23.

ITIME(5) must contain the minute, in the range 0-59.

ITIME(6) must contain the second, in the range 0-59.

ITIME(7) must contain the millisecond, in the range 0-999.

6. Error Indicators and Warnings

None.

7. Accuracy

The day name included as part of the character string returned by this routine is calculated assuming that the date is part of the Gregorian calendar. This calendar has been in operation in Europe since October the 15th 1582, and in Great Britain since September the 14th 1752. Entry to this routine with a date earlier than these will therefore not return a day name that is historically accurate.

8. Further Comments

Two dates stored in character string format, as returned by this routine, may be compared by X05ACF.

9. Example

This program initialises a time in ITIME, and converts it to character format by a call to X05ABF.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X05ABF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      CHARACTER*30     CTIME
*     .. Local Arrays ..
      INTEGER          ITIME(7)
*     .. External Functions ..
      CHARACTER*30     X05ABF
      EXTERNAL         X05ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X05ABF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) ITIME
*
      CTIME = X05ABF(ITIME)
*
      WRITE (NOUT,99999) CTIME
      STOP
*
99999 FORMAT (1X,A)
      END
```

9.2. Program Data

```
X05ABF Example Program Data
1789 7 14 13 11 48 320
```

9.3. Program Results

```
 X05ABF Example Program Results
 Tue 14th Jul 1789 13:11:48.320
```

X05ACF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X05ACF compares two date/time character strings, each stored in the format returned by X05ABF.

2. Specification

```
INTEGER FUNCTION X05ACF (CTIME1, CTIME2)
CHARACTER*(*) CTIME1, CTIME2
```

3. Description

X05ACF compares two date/time character strings, and returns an integer that specifies which one is the earliest. The result is an integer returned through the routine name, with meaning as follows:

X05ACF = −1 : the first date/time string is earlier than the second.
X05ACF = 0 : the two date/time strings are equivalent.
X05ACF = 1 : the first date/time string is later than the second.

4. References

None.

5. Parameters

1: CTIME1 – CHARACTER*(*). *Input*
2: CTIME2 – CHARACTER*(*). *Input*

On entry: the date/time strings to be compared. These are expected be in the format returned by X05ABF, although X05ACF will still attempt to interpret the strings if they vary slightly from this format. See Section 8 for further details.

6. Error Indicators and Warnings

None.

7. Accuracy

Not applicable.

8. Further Comments

For flexibility, X05ACF will accept various formats for the two date/time strings CTIME1 and CTIME2.

The strings do not have to be the same length. It is permissible, for example, to enter with one or both of the strings truncated to a smaller length, in which case missing fields are treated as zero.

Each character string may be of any length, but everything after character 80 is ignored.

Each string may or may not include an alphabetic day name, such as 'Wednesday', at its start. These day names are ignored, and no check is made that the day name corresponds correctly to the rest of the date.

The month name may contain any number of characters provided it uniquely identifies the month, however all characters that are supplied are significant.

Each field in the character string must be separated by one or more spaces.

The case of all alphabetic characters is insignificant.

Any field in a date time string that is indecipherable according to the above rules will be converted to a zero value internally. Thus two strings that are completely indecipherable will compare equal.

According to these rules, all the following date/time strings are equivalent:

'Thursday 10th July 1958 12:43:17.320'
'THU 10th JULY 1958 12:43:17.320'
'10th Jul 1958 12:43:17.320'

9. Example

This program initialises two date/time strings, and compares them by a call to X05ACF.

9.1. Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X05ACF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          K
      CHARACTER*50     CTIME1, CTIME2
*     .. External Functions ..
      INTEGER          X05ACF
      EXTERNAL         X05ACF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X05ACF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) CTIME1, CTIME2
*
      K = X05ACF(CTIME1,CTIME2)
*
      IF (K.LT.0) THEN
         WRITE (NOUT,99999) CTIME1
         WRITE (NOUT,99999) 'is earlier than'
         WRITE (NOUT,99999) CTIME2
      ELSE IF (K.EQ.0) THEN
         WRITE (NOUT,99999) CTIME1
         WRITE (NOUT,99999) 'is equivalent to'
         WRITE (NOUT,99999) CTIME2
      ELSE
         WRITE (NOUT,99999) CTIME1
         WRITE (NOUT,99999) 'is later than'
         WRITE (NOUT,99999) CTIME2
      END IF
      STOP
*
99999 FORMAT (1X,A)
      END
```

9.2. Program Data

```
X05ACF Example Program Data
'Thu 27th April 1989 13:15:21.320'
'Wed 26th April 1989 11:23:14.130'
```

9.3. Program Results

```
X05ACF Example Program Results
Thu 27th April 1989 13:15:21.320
is later than
Wed 26th April 1989 11:23:14.130
```

X05BAF – NAG Fortran Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

X05BAF returns the amount of processor time used since an unspecified previous time, via the routine name.

2. Specification

```
real FUNCTION X05BAF ( )
```

3. Description

X05BAF returns the number of seconds of processor time used since some previous time. The previous time is system dependent, but may be, for example, the time the current job or the current program started running.

If the system clock of the host machine is inaccessible for any reason, X05BAF returns the value zero.

4. References

None.

5. Parameters

None.

6. Error Indicators and Warnings

None.

7. Accuracy

The accuracy of the value returned depends on the accuracy of the system clock on the host machine.

8. Further Comments

Since the value returned by X05BAF is the amount of processor time since some unspecified earlier time, no significance should be placed on the value other than as a marker to be compared with some later figure returned by X05BAF. The amount of processor time that has elapsed between two calls of X05BAF can be simply calculated as the earlier value subtracted from the later value.

9. Example

This program makes a call to X05BAF, performs some computations, makes another call to X05BAF, and gives the time used by the computations as the difference between the two returned values.

9.1. Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     X05BAF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      real             ONE
      PARAMETER        (ONE=1.0e0)
*     .. Local Scalars ..
      real             CPTIME, E, S1, S2, T
      INTEGER          N
*     .. External Functions ..
      real             X05BAF
      EXTERNAL         X05BAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'X05BAF Example Program Results'
*
      S1 = X05BAF()
*
      E = ONE
      T = ONE
      DO 20 N = 1, 10000
         T = T/N
         E = E + T
   20 CONTINUE
*
      S2 = X05BAF()
*
      CPTIME = S2 - S1
      WRITE (NOUT,99999) 'It took', CPTIME, ' seconds to compute e =', E
      STOP
*
99999 FORMAT (1X,A,1P,e10.2,A,e13.5)
      END
```

9.2. Program Data

None.

9.3. Program Results

```
 X05BAF Example Program Results
 It took  8.66E-01 seconds to compute e =  2.71828E+00
```