

NAG Library Routine Document

F04BEF

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

F04BEF computes the solution to a real system of linear equations $AX = B$, where A is an n by n symmetric positive definite matrix, stored in packed format, and X and B are n by r matrices. An estimate of the condition number of A and an error bound for the computed solution are also returned.

2 Specification

```
SUBROUTINE F04BEF (UPLO, N, NRHS, AP, B, LDB, RCOND, ERBND, IFAIL)
  INTEGER          N, NRHS, LDB, IFAIL
  REAL (KIND=nag_wp) AP(*), B(LDB,*), RCOND, ERBND
  CHARACTER(1)     UPLO
```

3 Description

The Cholesky factorization is used to factor A as $A = U^T U$, if $UPLO = 'U'$, or $A = LL^T$, if $UPLO = 'L'$, where U is an upper triangular matrix and L is a lower triangular matrix. The factored form of A is then used to solve the system of equations $AX = B$.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia <http://www.netlib.org/lapack/lug>

Higham N J (2002) *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

5 Arguments

- 1: UPLO – CHARACTER(1) *Input*
On entry: if UPLO = 'U', the upper triangle of the matrix A is stored.
 If UPLO = 'L', the lower triangle of the matrix A is stored.
Constraint: UPLO = 'U' or 'L'.
- 2: N – INTEGER *Input*
On entry: the number of linear equations n , i.e., the order of the matrix A .
Constraint: $N \geq 0$.
- 3: NRHS – INTEGER *Input*
On entry: the number of right-hand sides r , i.e., the number of columns of the matrix B .
Constraint: NRHS ≥ 0 .

- 4: AP(*) – REAL (KIND=nag_wp) array Input/Output

Note: the dimension of the array AP must be at least $\max(1, N \times (N + 1)/2)$.

On entry: the n by n symmetric matrix A . The upper or lower triangular part of the symmetric matrix is packed column-wise in a linear array. The j th column of A is stored in the array AP as follows:

More precisely,

if UPLO = 'U', the upper triangle of A must be stored with element A_{ij} in $AP(i + j(j - 1)/2)$ for $i \leq j$;

if UPLO = 'L', the lower triangle of A must be stored with element A_{ij} in $AP(i + (2n - j)(j - 1)/2)$ for $i \geq j$.

On exit: if IFAIL = 0 or $N + 1$, the factor U or L from the Cholesky factorization $A = U^T U$ or $A = LL^T$, in the same storage format as A .

- 5: B(LDB, *) – REAL (KIND=nag_wp) array Input/Output

Note: the second dimension of the array B must be at least $\max(1, NRHS)$.

On entry: the n by r matrix of right-hand sides B .

On exit: if IFAIL = 0 or $N + 1$, the n by r solution matrix X .

- 6: LDB – INTEGER Input

On entry: the first dimension of the array B as declared in the (sub)program from which F04BEF is called.

Constraint: $LDB \geq \max(1, N)$.

- 7: RCOND – REAL (KIND=nag_wp) Output

On exit: if IFAIL = 0 or $N + 1$, an estimate of the reciprocal of the condition number of the matrix A , computed as $RCOND = 1 / (\|A\|_1 \|A^{-1}\|_1)$.

- 8: ERRBND – REAL (KIND=nag_wp) Output

On exit: if IFAIL = 0 or $N + 1$, an estimate of the forward error bound for a computed solution \hat{x} , such that $\|\hat{x} - x\|_1 / \|x\|_1 \leq ERRBND$, where \hat{x} is a column of the computed solution returned in the array B and x is the corresponding column of the exact solution X . If RCOND is less than **machine precision**, then ERRBND is returned as unity.

- 9: IFAIL – INTEGER Input/Output

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this argument, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (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 detected by the routine:

$IFAIL > 0$ and $IFAIL \leq N$

The principal minor of order $\langle value \rangle$ of the matrix A is not positive definite. The factorization has not been completed and the solution could not be computed.

$IFAIL = N + 1$

A solution has been computed, but $RCOND$ is less than *machine precision* so that the matrix A is numerically singular.

$IFAIL = -1$

On entry, $UPLO$ not one of 'U' or 'u' or 'L' or 'l': $UPLO = \langle value \rangle$.

$IFAIL = -2$

On entry, $N = \langle value \rangle$.
Constraint: $N \geq 0$.

$IFAIL = -3$

On entry, $NRHS = \langle value \rangle$.
Constraint: $NRHS \geq 0$.

$IFAIL = -6$

On entry, $LDB = \langle value \rangle$ and $N = \langle value \rangle$.
Constraint: $LDB \geq \max(1, N)$.

$IFAIL = -99$

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

$IFAIL = -399$

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

$IFAIL = -999$

Dynamic memory allocation failed.

The integer allocatable memory required is N , and the real allocatable memory required is $3 \times N$. Allocation failed before the solution could be computed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

The computed solution for a single right-hand side, \hat{x} , satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and ϵ is the *machine precision*. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A) \frac{\|E\|_1}{\|A\|_1},$$

where $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. F04BEF uses the approximation $\|E\|_1 = \epsilon \|A\|_1$ to estimate ERRBND. See Section 4.4 of Anderson *et al.* (1999) for further details.

8 Parallelism and Performance

F04BEF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F04BEF makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The packed storage scheme is illustrated by the following example when $n = 4$ and UPLO = 'U'. Two-dimensional storage of the symmetric matrix A :

$$\begin{array}{cccc} a_{11} & a_{12} & a_{13} & a_{14} \\ & a_{22} & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{array} \quad (a_{ij} = a_{ji})$$

Packed storage of the upper triangle of A :

$$AP = [a_{11}, a_{12}, a_{22}, a_{13}, a_{23}, a_{33}, a_{14}, a_{24}, a_{34}, a_{44}]$$

The total number of floating-point operations required to solve the equations $AX = B$ is proportional to $(\frac{1}{3}n^3 + n^2r)$. The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization.

In practice the condition number estimator is very reliable, but it can underestimate the true condition number; see Section 15.3 of Higham (2002) for further details.

The complex analogue of F04BEF is F04CEF.

10 Example

This example solves the equations

$$AX = B,$$

where A is the symmetric positive definite matrix

$$A = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.18 & 0.34 & 1.18 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 8.70 & 8.30 \\ -13.35 & 2.13 \\ 1.89 & 1.61 \\ -4.14 & 5.00 \end{pmatrix}.$$

An estimate of the condition number of A and an approximate error bound for the computed solutions are also printed.

10.1 Program Text

Program f04befe

```

!      F04BEF Example Program Text
!
!      Mark 26 Release. NAG Copyright 2016.
!
!      .. Use Statements ..
!      Use nag_library, Only: f04bef, nag_wp, x04caf
!      .. Implicit None Statement ..
!      Implicit None
!      .. Parameters ..
!      Integer, Parameter          :: nin = 5, nout = 6
!      Character (1), Parameter   :: uplo = 'U'
!      .. Local Scalars ..
!      Real (Kind=nag_wp)         :: errbnd, rcond
!      Integer                    :: i, ierr, ifail, j, ldb, n, nrhs
!      .. Local Arrays ..
!      Real (Kind=nag_wp), Allocatable :: ap(:), b(:, :)
!      .. Executable Statements ..
!      Write (nout,*) 'F04BEF Example Program Results'
!      Write (nout,*)
!      Flush (nout)
!      Skip heading in data file
!      Read (nin,*)
!      Read (nin,*) n, nrhs
!      ldb = n
!      Allocate (ap((n*(n+1))/2),b(ldb,nrhs))
!
!      Read the upper or lower triangular part of the matrix A from
!      data file
!
!      If (uplo=='U') Then
!        Read (nin,*)((ap(i+(j*(j-1))/2),j=i,n),i=1,n)
!      Else If (uplo=='L') Then
!        Read (nin,*)((ap(i+((2*n-j)*(j-1))/2),j=1,i),i=1,n)
!      End If
!
!      Read B from data file
!      Read (nin,*)(b(i,1:nrhs),i=1,n)
!
!      Solve the equations AX = B for X
!
!      ifail: behaviour on error exit
!      =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
!      ifail = 1
!      Call f04bef(uplo,n,nrhs,ap,b,ldb,rcond,errbnd,ifail)
!
!      If (ifail==0) Then
!        Print solution, estimate of condition number and approximate
!        error bound
!
!        ierr = 0
!        Call x04caf('General',' ',n,nrhs,b,ldb,'Solution', ierr)
!
!        Write (nout,*)
!        Write (nout,*) 'Estimate of condition number'
!        Write (nout,99999) 1.0E0_nag_wp/rcond
!        Write (nout,*)
!        Write (nout,*) 'Estimate of error bound for computed solutions'
!        Write (nout,99999) errbnd
!      Else If (ifail==n+1) Then
!        Matrix A is numerically singular. Print estimate of
!        reciprocal of condition number and solution
!        Write (nout,*)
!        Write (nout,*) 'Estimate of reciprocal of condition number'
!        Write (nout,99999) rcond
!        Write (nout,*)
!        Flush (nout)

```

```

      ierr = 0
      Call x04caf('General',' ',n,nrhs,b,ldb,'Solution',ierr)

      Else If (ifail>0 .And. ifail<=n) Then
!       The matrix A is not positive definite to working precision
        Write (nout,99998) 'The leading minor of order ', ifail,      &
          ' is not positive definite'
      Else
        Write (nout,99997) ifail
      End If

99999 Format (6X,1P,E9.1)
99998 Format (1X,A,I3,A)
99997 Format (1X,' ** F04BEF returned with IFAIL = ',I5)
      End Program f04befe

```

10.2 Program Data

F04BEF Example Program Data

```

      4          2          : n, nrhs

      4.16  -3.12   0.56  -0.10
           5.03  -0.83   1.18
                0.76   0.34
                1.18 : matrix A

      8.70   8.30
     -13.35  2.13
       1.89  1.61
      -4.14  5.00          : matrix B

```

10.3 Program Results

F04BEF Example Program Results

Solution

	1	2
1	1.0000	4.0000
2	-1.0000	3.0000
3	2.0000	2.0000
4	-3.0000	1.0000

Estimate of condition number
9.7E+01

Estimate of error bound for computed solutions
1.1E-14
