NAG Fortran Library Routine Document

F04BJF

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

F04BJF computes the solution to a real system of linear equations $AX = B$, where A is an n by n symmetric 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 F04BJF (UPLO, N, NRHS, AP, IPIV, B, LDB, RCOND, ERRBND,
     1                   IFAIL)
      INTEGER           N, NRHS, IPIV(*), LDB, IFAIL
      double precision  AP(*), B(LDB,*), RCOND, ERRBND
      CHARACTER*1       UPLO
```

3   Description

The diagonal pivoting method is used to factor A as $A = UDU^T$, if UPLO = 'U', or $A = LDL^T$, if UPLO = 'L', where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is symmetric and block diagonal with 1 by 1 and 2 by 2 diagonal blocks. 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 URL: http://www.netlib.org/lapack/lug

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

5   Parameters

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 $\geq$ 0.

4:     AP($*$) – **_double precision_** 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, packed columnwise in a linear array. The jth column of the matrix A is stored in the array AP as follows:

> if UPLO = 'U', $\text{AP}(i + (j - 1)j/2) = a_{ij}$ for $1 \leq i \leq j$
> if UPLO = 'L', $\text{AP}(i + (j - 1)(2n - j)/2) = a_{ij}$ for $j \leq i \leq n$

See Section 8 below for further details.

On exit: if IFAIL ≥ 0, the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^T$ or $A = LDL^T$ as computed by F07PDF (DSPTRF), stored as a packed triangular matrix in the same storage format as A.

5:     IPIV($*$) – INTEGER array   *Output*

Note: the dimension of the array IPIV must be at least $\max(1, N)$.

On exit: if IFAIL ≥ 0, details of the interchanges and the block structure of D, as determined by F07PDF (DSPTRF).

> If IPIV(k) > 0, then rows and columns k and IPIV(k) were interchanged, and d_{kk} is a 1 by 1 diagonal block;
> if UPLO = 'U' and IPIV(k) = IPIV($k - 1$) < 0, then rows and columns $k - 1$ and $-$IPIV(k) were interchanged and $d_{k-1:k,k-1:k}$ is a 2 by 2 diagonal block;
> if UPLO = 'L' and IPIV(k) = IPIV($k + 1$) < 0, then rows and columns $k + 1$ and $-$IPIV(k) were interchanged and $d_{k:k+1,k:k+1}$ is a 2 by 2 diagonal block.

6:     B(LDB,$*$) – **_double precision_** array   *Input/Output*

Note: the second dimension of the array B must be at least $\max(1, \text{NRHS})$. To solve the equations $Ax = b$, where b is a single right-hand side, B may be supplied as a one-dimensional array with length LDB $= \max(1, N)$.

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.

7:     LDB – INTEGER   *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F04BJF is called.

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

8:     RCOND – **_double precision_**   *Output*

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

9:     ERRBND – **_double precision_**   *Output*

On exit: if IFAIL $= 0$ or $N + 1$, an estimate of the forward error bound for a computed solution $\hat{x}$, such that $\|\hat{x} - x\|_1 / \|x\|_1 \leq \text{ERRBND}$, 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.

10:    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 (see Section 6).

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, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is 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 detected by the routine:

IFAIL < 0 and IFAIL $\neq -999$

If IFAIL $= -i$, the ith argument had an illegal value.

IFAIL $= -999$

Allocation of memory failed. The INTEGER allocatable memory required is N, and the **double precision** allocatable memory required is $2 \times$ N. Allocation failed before the solution could be computed.

IFAIL > 0 and IFAIL $\leq$ N

If IFAIL $= i$, d_{ii} is exactly zero. The factorization has been completed, but the block diagonal matrix D is exactly singular, so the solution could not be computed.

IFAIL $=$ N $+ 1$

RCOND is less than **machine precision**, so that the matrix A is numerically singular. A solution to the equations $AX = B$ has nevertheless been computed.

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. F04BJF uses the approximation $\|E\|_1 = \epsilon\|A\|_1$ to estimate ERRBND. See Section 4.4 of Anderson *et al.* (1999) for further details.

8   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:

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

Packed storage of the upper triangle of A:

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

The total number of floating-point operations required to solve the equations $AX = B$ is proportional to $\left(\frac{1}{3}n^3 + 2n^2 r\right)$. 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 analogues of F04BJF are F04CJF for complex Hermitian matrices, and F04DJF for complex symmetric matrices.

9 Example

To solve the equations

$$AX = B,$$

where A is the symmetric indefinite matrix

$$A = \begin{pmatrix} -1.81 & 2.06 & 0.63 & -1.15 \\ 2.06 & 1.15 & 1.87 & 4.20 \\ 0.63 & 1.87 & -0.21 & 3.87 \\ -1.15 & 4.20 & 3.87 & 2.07 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 0.96 & 3.93 \\ 6.07 & 19.25 \\ 8.38 & 9.90 \\ 9.50 & 27.85 \end{pmatrix}.$$

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

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.

```
*     F04BJF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, NRHSMX
      PARAMETER        (NMAX=8,NRHSMX=2)
      INTEGER          LDB
      PARAMETER        (LDB=NMAX)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*     .. Local Scalars ..
      DOUBLE PRECISION ERRBND, RCOND
      INTEGER          I, IERR, IFAIL, J, N, NRHS
*     .. Local Arrays ..
      DOUBLE PRECISION AP((NMAX*(NMAX+1))/2), B(LDB,NRHSMX)
      INTEGER          IPIV(NMAX)
*     .. External Subroutines ..
      EXTERNAL         F04BJF, X04CAF, X04CCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F04BJF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NRHS
```

```
      IF (N.LE.NMAX .AND. NRHS.LE.NRHSMX) THEN
*
*        Read the upper or lower triangular part of the matrix A from
*        data file
*
         IF (UPLO.EQ.'U') THEN
            READ (NIN,*) ((AP(I+(J*(J-1))/2),J=I,N),I=1,N)
         ELSE IF (UPLO.EQ.'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,J),J=1,NRHS),I=1,N)
*
*        Solve the equations AX = B for X
*
         IFAIL = -1
         CALL F04BJF(UPLO,N,NRHS,AP,IPIV,B,LDB,RCOND,ERRBND,IFAIL)
*
         IF (IFAIL.EQ.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) 1.0D0/RCOND
            WRITE (NOUT,*)
            WRITE (NOUT,*)
     +         'Estimate of error bound for computed solutions'
            WRITE (NOUT,99999) ERRBND
         ELSE IF (IFAIL.EQ.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,*)
            IERR = 0
            CALL X04CAF('General',' ',N,NRHS,B,LDB,'Solution',IERR)
*
         ELSE IF (IFAIL.GT.0 .AND. IFAIL.LE.N) THEN
*
*           The upper triangular matrix U is exactly singular.  Print
*           details of factorization
*
            WRITE (NOUT,*)
            IERR = 0
            CALL X04CCF(UPLO,'Non-unit diagonal',N,AP,
     +                  'Details of factorization',IERR)
*
*           Print pivot indices
*
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Pivot indices'
            WRITE (NOUT,99998) (IPIV(I),I=1,N)
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX and/or NRHSMX too small'
      END IF
      STOP
*
99999 FORMAT (6X,1P,E9.1)
99998 FORMAT ((3X,7I11))
```

```
     END
```

9.2   Program Data

```
F04BJF Example Program Data

  4      2                      :Values of N and NRHS

 -1.81   2.06   0.63  -1.15
         1.15   1.87   4.20
               -0.21   3.87
                       2.07 :End of matrix A

  0.96   3.93
  6.07  19.25
  8.38   9.90
  9.50  27.85                  :End of matrix B
```

9.3   Program Results

```
F04BJF Example Program Results

 Solution
            1         2
 1    -5.0000    2.0000
 2    -2.0000    3.0000
 3     1.0000    4.0000
 4     4.0000    1.0000

 Estimate of condition number
      7.6E+01

 Estimate of error bound for computed solutions
      8.4E-15
```