NAG Fortran Library Routine Document

F04BDF

1   Purpose

F04BDF computes the solution to a real system of linear equations $AX = B$, where A is an n by n symmetric positive-definite matrix 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 F04BDF (UPLO, N, NRHS, A, LDA, B, LDB, RCOND, ERRBND, IFAIL)

INTEGER          N, NRHS, LDA, LDB, IFAIL
double precision A(LDA,*), B(LDB,*), RCOND, ERRBND
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 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:    A(LDA,∗) – *double precision* array   *Input/Output*

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

On entry: the n by n symmetric matrix A.

If UPLO = 'U', the leading N by N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced;
if UPLO = 'L', the leading N by N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

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

5:      LDA – INTEGER   *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F04BDF is called.

Constraint: $\text{LDA} \geq \max(1, \text{N})$.

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 $\text{LDB} = \max(1, \text{N})$.

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 F04BDF is called.

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

8:      RCOND – ***double precision***   *Output*

On exit: if IFAIL = 0 or N + 1, 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 ≠ −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 $3 \times$ N. Allocation failed before the solution could be computed.

IFAIL > 0 and IFAIL ≤ N

>   If IFAIL = i, the leading minor of order i of A is not positive-definite. The factorization could not be completed, and the solution has not been 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 $\kappa(A) = \left\|A^{-1}\right\|_1\|A\|_1$, the condition number of A with respect to the solution of the linear equations. F04BDF 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 total number of floating-point operations required to solve the equations $AX = B$ is proportional to $\left(\frac{1}{3}n^3 + n^2r\right)$. 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 analogue of F04BDF is F04CDF.

9   Example

To solve the equations

$$AX = B,$$

where A is the symmetric positive-definite matrix

$$A = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.18 & 0.34 & 1.18 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 8.70 & 8.30 \\ -13.35 & 2.13 \\ 1.89 & 1.61 \\ -4.14 & 5.00 \end{pmatrix}.$$

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

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.

```
*       F04BDF 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           LDA, LDB
        PARAMETER         (LDA=NMAX,LDB=NMAX)
*       .. Local Scalars ..
        DOUBLE PRECISION ERRBND, RCOND
        INTEGER           I, IERR, IFAIL, J, N, NRHS
*       .. Local Arrays ..
        DOUBLE PRECISION A(LDA,NMAX), B(LDB,NRHSMX)
*       .. External Subroutines ..
        EXTERNAL          F04BDF, X04CAF
*       .. Executable Statements ..
        WRITE (NOUT,*) 'F04BDF 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 triangular part of A from data file
*
           READ (NIN,*) ((A(I,J),J=I,N),I=1,N)
*
*          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 F04BDF('Upper',N,NRHS,A,LDA,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 matrix A is not positive definite to working precision
*
              WRITE (NOUT,99998) 'The leading minor of order ', IFAIL,
     +          ' is not positive definite'
           END IF
         ELSE
           WRITE (NOUT,*) 'NMAX and/or NRHSMX too small'
         END IF
         STOP
*
99999 FORMAT (6X,1P,E9.1)
99998 FORMAT (1X,A,I3,A)
      END
```

9.2 Program Data

```
F04BDF Example Program Data

   4       2                      :Values of N and NRHS

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

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

9.3 Program Results

```
F04BDF 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
```