NAG Library Routine Document

F04BGF

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

F04BGF computes the solution to a real system of linear equations $AX = B$, where A is an n by n symmetric positive-definite tridiagonal 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 F04BGF(N, NRHS, D, E, B, LDB, RCOND, ERRBND, IFAIL)
INTEGER             N, NRHS, LDB, IFAIL
double precision    D(*), E(*), B(LDB,*), RCOND, ERRBND
```

3 Description

A is factorized as $A = LDL^{\mathrm{T}}$, where L is a unit lower bidiagonal matrix and D is diagonal, and the factored form of A is then used to solve the system of equations.

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, Philadelphiahttp://www.netlib.org/lapack/lug

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

5 Parameters

1: N – INTEGER *Input*

On entry: the number of linear equations n, i.e., the order of the matrix A.

Constraint: $\mathrm{N} \geq 0$.

2: NRHS – INTEGER *Input*

On entry: the number of right-hand sides r, i.e., the number of columns of the matrix B.

Constraint: $\mathrm{NRHS} \geq 0$.

3: D($*$) – ***double precision*** array *Input/Output*

Note: the dimension of the array D must be at least $\max(1, \mathrm{N})$.

On entry: must contain the n diagonal elements of the tridiagonal matrix A.

On exit: if $\mathrm{IFAIL} = 0$ or $\mathrm{N} + 1$, D is overwritten by the n diagonal elements of the diagonal matrix D from the LDL^{T} factorization of A.

4: E($*$) – ***double precision*** array *Input/Output*

Note: the dimension of the array E must be at least $\max(1, \mathrm{N} - 1)$.

On entry: must contain the $(n - 1)$ subdiagonal elements of the tridiagonal matrix A.

On exit: if IFAIL $= 0$ or $\mathrm{N}+1$, E is overwritten by the $(n-1)$ subdiagonal elements of the unit lower bidiagonal matrix L from the LDL^{T} factorization of A. (E can also be regarded as the superdiagonal of the unit upper bidiagonal factor U from the $U^{\mathrm{T}}DU$ factorization of A.)

5: B(LDB,$*$) – ***double precision*** array *Input/Output*

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

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

On exit: if IFAIL $= 0$ or $\mathrm{N}+1$, 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 F04BGF is called.

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

7: RCOND – ***double precision*** *Output*

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

8: ERRBND – ***double precision*** *Output*

On exit: if IFAIL $= 0$ or $\mathrm{N}+1$, 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 parameter you should refer to Section 3.3 in the Essential Introduction 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, if you are 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 ***double precision*** allocatable memory required is N. In this case the factorization and the solution X have been computed, but RCOND and ERRBND have not been computed.

IFAIL > 0 and IFAIL $\leq$ 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 $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. F04BGF 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 nr. The condition number estimation requires $O(n)$ floating-point operations.

See Section 15.3 of Higham (2002) for further details on computing the condition number of tridiagonal matrices.

The complex analogue of F04BGF is F04CGF.

9 Example

This example solves the equations

$$AX = B,$$

where A is the symmetric positive-definite tridiagonal matrix

$$A = \begin{pmatrix} 4.0 & -2.0 & 0 & 0 & 0 \\ -2.0 & 10.0 & -6.0 & 0 & 0 \\ 0 & -6.0 & 29.0 & 15.0 & 0 \\ 0 & 0 & 15.0 & 25.0 & 8.0 \\ 0 & 0 & 0 & 8.0 & 5.0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 6.0 & 10.0 \\ 9.0 & 4.0 \\ 2.0 & 9.0 \\ 14.0 & 65.0 \\ 7.0 & 23.0 \end{pmatrix}.$$

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

9.1 Program Text

```
*     F04BGF 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)
*     .. Local Scalars ..
      DOUBLE PRECISION ERRBND, RCOND
      INTEGER          I, IERR, IFAIL, J, N, NRHS
*     .. Local Arrays ..
      DOUBLE PRECISION B(LDB,NRHSMX), D(NMAX), E(NMAX-1)
*     .. External Subroutines ..
      EXTERNAL         F04BGF, X04CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F04BGF 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 A from data file
*
         READ (NIN,*) (D(I),I=1,N)
         READ (NIN,*) (E(I),I=1,N-1)
*
*        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 F04BGF(N,NRHS,D,E,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
            WRITE (NOUT,99998) 'The leading minor of order ', IFAIL,
     +        ' is not positive definite'
         ELSE
            WRITE (NOUT,99997) IFAIL
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX and/or NRHSMX too small'
      END IF
```

```
*
99999 FORMAT (6X,1P,E9.1)
99998 FORMAT (1X,A,I3,A)
99997 FORMAT (1X,' ** F04BGF returned with IFAIL = ',I5)
      END
```

9.2 Program Data

```
F04BGF Example Program Data

  5     2                     :Values of N and NRHS

  4.0  10.0  29.0  25.0   5.0 :End of diagonal D
 -2.0  -6.0  15.0   8.0       :End of sub-diagonal E

  6.0  10.0
  9.0   4.0
  2.0   9.0
 14.0  65.0
  7.0  23.0                   :End of matrix B
```

9.3 Program Results

```
 F04BGF Example Program Results

 Solution
             1          2
 1      2.5000     2.0000
 2      2.0000    -1.0000
 3      1.0000    -3.0000
 4     -1.0000     6.0000
 5      3.0000    -5.0000

 Estimate of condition number
        1.1E+02

 Estimate of error bound for computed solutions
        1.2E-14
```