NAG Library Routine Document

F07HDF (DPBTRF)

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

F07HDF (DPBTRF) computes the Cholesky factorization of a real symmetric positive-definite band matrix.

2 Specification

```
SUBROUTINE F07HDF(UPLO, N, KD, AB, LDAB, INFO)
INTEGER           N, KD, LDAB, INFO
double precision  AB(LDAB,*)
CHARACTER*1       UPLO
```

The routine may be called by its LAPACK name ***dpbtrf***.

3 Description

F07HDF (DPBTRF) forms the Cholesky factorization of a real symmetric positive-definite band matrix A either as $A = U^{\mathrm{T}}U$ if UPLO = 'U' or $A = LL^{\mathrm{T}}$ if UPLO = 'L', where U (or L) is an upper (or lower) triangular band matrix with the same number of superdiagonals (or subdiagonals) as A.

4 References

Demmel J W (1989) On floating-point errors in Cholesky *LAPACK Working Note No. 14* University of Tennessee, Knoxville

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1: UPLO – CHARACTER*1 *Input*

On entry: indicates whether the upper or lower triangular part of A is stored and how A is to be factorized.

UPLO = 'U'

The upper triangular part of A is stored and A is factorized as $U^{\mathrm{T}}U$, where U is upper triangular.

UPLO = 'L'

The lower triangular part of A is stored and A is factorized as LL^{T}, where L is lower triangular.

Constraint: UPLO = 'U' or 'L'.

2: N – INTEGER *Input*

On entry: n, the order of the matrix A.

Constraint: N $\geq$ 0.

3: KD – INTEGER *Input*

On entry: k_d, the number of superdiagonals or subdiagonals of the matrix A.

Constraint: KD ≥ 0.

4: AB(LDAB,$*$) – ***double precision*** array *Input/Output*

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

On entry: the n by n symmetric band matrix A.

The matrix is stored in rows 1 to $k_d + 1$, more precisely,

if UPLO = 'U', the elements of the upper triangle of A within the band must be stored with element A_{ij} in $\mathrm{AB}(k_d + 1 + i - j, j)$ for $\max(1, j - k_d) \leq i \leq j$;

if UPLO = 'L', the elements of the lower triangle of A within the band must be stored with element A_{ij} in $\mathrm{AB}(1 + i - j, j)$ for $j \leq i \leq \min(n, j + k_d)$.

On exit: the upper or lower triangle of A is overwritten by the Cholesky factor U or L as specified by UPLO, using the same storage format as described above.

5: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F07HDF (DPBTRF) is called.

Constraint: LDAB $\geq$ KD $+ 1$.

6: INFO – INTEGER *Output*

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

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

If INFO $= -i$, the ith parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO $= i$, the leading minor of order i is not positive-definite and the factorization could not be completed. Hence A itself is not positive-definite. This may indicate an error in forming the matrix A. There is no routine specifically designed to factorize a band matrix which is not positive-definite; the matrix must be treated either as a nonsymmetric band matrix, by calling F07BDF (DGBTRF) or as a full matrix, by calling F07MDF (DSYTRF).

7 Accuracy

If UPLO = 'U', the computed factor U is the exact factor of a perturbed matrix $A + E$, where

$$|E| \leq c(k+1)\epsilon \left|U^{\mathrm{T}}\right||U|,$$

$c(k+1)$ is a modest linear function of $k+1$, and ϵ is the ***machine precision***.

If UPLO = 'L', a similar statement holds for the computed factor L. It follows that $\left|e_{ij}\right| \leq c(k+1)\epsilon\sqrt{a_{ii}a_{jj}}$.

8 Further Comments

The total number of floating-point operations is approximately $n(k+1)^2$, assuming $n \gg k$.

A call to F07HDF (DPBTRF) may be followed by calls to the routines:

F07HEF (DPBTRS) to solve $AX = B$;

F07HGF (DPBCON) to estimate the condition number of A.

The complex analogue of this routine is F07HRF (ZPBTRF).

9 Example

This example computes the Cholesky factorization of the matrix A, where

$$A = \begin{pmatrix} 5.49 & 2.68 & 0.00 & 0.00 \\ 2.68 & 5.63 & -2.39 & 0.00 \\ 0.00 & -2.39 & 2.60 & -2.22 \\ 0.00 & 0.00 & -2.22 & 5.17 \end{pmatrix}.$$

9.1 Program Text

```
*     F07HDF Example Program Text
*     Mark 15 Release. NAG Copyright 1991.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, KMAX, LDAB
      PARAMETER        (NMAX=8,KMAX=8,LDAB=KMAX+1)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, KD, N
      CHARACTER        UPLO
*     .. Local Arrays ..
      DOUBLE PRECISION AB(LDAB,NMAX)
*     .. External Subroutines ..
      EXTERNAL         DPBTRF, X04CEF
*     .. Intrinsic Functions ..
      INTRINSIC        MAX, MIN
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07HDF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, KD
      IF (N.LE.NMAX .AND. KD.LE.KMAX) THEN
*
*        Read A from data file
*
         READ (NIN,*) UPLO
         IF (UPLO.EQ.'U') THEN
            DO 20 I = 1, N
               READ (NIN,*) (AB(KD+1+I-J,J),J=I,MIN(N,I+KD))
   20       CONTINUE
         ELSE IF (UPLO.EQ.'L') THEN
            DO 40 I = 1, N
               READ (NIN,*) (AB(1+I-J,J),J=MAX(1,I-KD),I)
   40       CONTINUE
         END IF
*
*        Factorize A
*
         CALL DPBTRF(UPLO,N,KD,AB,LDAB,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.EQ.0) THEN
*
*           Print factor
*
            IFAIL = 0
*
            IF (UPLO.EQ.'U') THEN
*
               CALL X04CEF(N,N,0,KD,AB,LDAB,'Factor',IFAIL)
```

```
*
            ELSE IF (UPLO.EQ.'L') THEN
*
               CALL X04CEF(N,N,KD,0,AB,LDAB,'Factor',IFAIL)
*
            END IF
*
         ELSE
            WRITE (NOUT,*) 'A is not positive-definite'
         END IF
      END IF
*
      END
```

9.2 Program Data

```
F07HDF Example Program Data
  4  1                         :Values of N and KD
  'L'                          :Value of UPLO
  5.49
  2.68   5.63
        -2.39   2.60
                -2.22   5.17   :End of matrix A
```

9.3 Program Results

```
 F07HDF Example Program Results

 Factor
              1          2          3          4
 1       2.3431
 2       1.1438     2.0789
 3                 -1.1497     1.1306
 4                            -1.9635     1.1465
```