F07GDF (SPPTRF/DPPTRF) – NAG Fortran Library Routine Document

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

F07GDF (SPPTRF/DPPTRF) computes the Cholesky factorization of a real symmetric positive-definite matrix, using packed storage.

2 Specification

SUBROUTINE F07GDF(UPLO, N, AP, INFO)ENTRYspptrf(UPLO, N, AP, INFO)INTEGERN, INFOrealAP(*)CHARACTER*1UPLO

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

This routine forms the Cholesky factorization of a real symmetric positive-definite matrix A either 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 lower triangular, using packed storage.

4 References

- [1] Demmel J W (1989) On floating-point errors in Cholesky LAPACK Working Note No. 14 University of Tennessee, Knoxville
- [2] Golub G H and van Loan C F (1996) Matrix Computations Johns Hopkins University Press (3rd Edition), Baltimore

5 Parameters

On entry: indicates whether the upper or lower triangular part of A is stored and how A is factorized, as follows:

if UPLO = 'U', then the upper triangular part of A is stored and A is factorized as $U^T U$, where U is upper triangular;

if UPLO = 'L', then 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

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

Constraint: $N \ge 0$.

Input

Input

^{1:} UPLO — CHARACTER*1

Input/Output

Output

3: AP(*) - real array

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

On entry: the n by n symmetric positive-definite matrix A, packed by columns. 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: the upper or lower triangle of A is overwritten by the Cholesky factor U or L as specified by UPLO, using the same packed storage format as described above.

4: INFO — INTEGER

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

6 Error Indicators and Warnings

```
INFO < 0
```

If INFO = -i, the *i*th 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. To factorize a symmetric matrix which is not positive-definite, call F07PDF (SSPTRF/DSPTRF) instead.

7 Accuracy

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

$$|E| \le c(n)\epsilon |U^T||U|,$$

c(n) is a modest linear function of n, and ϵ is the **machine precision**. If UPLO = 'L', a similar statement holds for the computed factor L. It follows that $|e_{ij}| \leq c(n)\epsilon \sqrt{a_{ii}a_{jj}}$.

8 Further Comments

The total number of floating-point operations is approximately $\frac{1}{3}n^3$.

A call to this routine may be followed by calls to the routines:

F07GEF (SPPTRS/DPPTRS) to solve AX = B;

F07GGF (SPPCON/DPPCON) to estimate the condition number of A;

F07GJF (SPPTRI/DPPTRI) to compute the inverse of A.

The complex analogue of this routine is F07GRF (CPPTRF/ZPPTRF).

9 Example

To compute the Cholesky factorization of the matrix A, where

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

using packed storage.

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.

```
F07GDF Example Program Text
*
     Mark 15 Release. NAG Copyright 1991.
*
*
      .. Parameters ..
      INTEGER
                       NIN, NOUT
     PARAMETER
                       (NIN=5,NOUT=6)
      INTEGER
                       NMAX
     PARAMETER
                       (NMAX=8)
      .. Local Scalars ..
      INTEGER
                      I, IFAIL, INFO, J, N
     CHARACTER
                       UPLO
      .. Local Arrays ..
     real
                       AP(NMAX*(NMAX+1)/2)
      .. External Subroutines ..
                       spptrf, X04CCF
     EXTERNAL
      .. Executable Statements ..
     WRITE (NOUT,*) 'F07GDF Example Program Results'
     Skip heading in data file
×
     READ (NIN,*)
     READ (NIN,*) N
      IF (N.LE.NMAX) THEN
         Read A from data file
*
         READ (NIN,*) UPLO
         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
*
         Factorize A
*
         CALL spptrf(UPLO, N, AP, INFO)
*
         WRITE (NOUT,*)
         IF (INFO.EQ.O) THEN
            Print factor
            IFAIL = 0
*
            CALL X04CCF(UPLO, 'Nonunit', N, AP, 'Factor', IFAIL)
*
         ELSE
            WRITE (NOUT, *) 'A is not positive-definite'
         END IF
     END IF
     STOP
*
     END
```

9.2 Program Data

 F07GDF Example Program Data

 4
 :Value of N

 'L'
 :Value of UPLO

 4.16
 -3.12
 5.03

 0.56
 -0.83
 0.76

 -0.10
 1.18
 0.34
 1.18

9.3 Program Results

F07GDF Example Program Results

Factor

1 40001				
	1	2	3	4
1	2.0396			
2	-1.5297	1.6401		
3	0.2746	-0.2500	0.7887	
4	-0.0490	0.6737	0.6617	0.5347