

NAG Library Routine Document

F07PDF (DSPTRF)

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

F07PDF (DSPTRF) computes the Bunch–Kaufman factorization of a real symmetric indefinite matrix, using packed storage.

2 Specification

```
SUBROUTINE F07PDF(UPLO, N, AP, IPIV, INFO)
```

```
INTEGER          N, IPIV(*), INFO
```

```
double precision AP(*)
```

```
CHARACTER*1      UPLO
```

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

3 Description

F07PDF (DSPTRF) factorizes a real symmetric matrix A , using the Bunch–Kaufman diagonal pivoting method and packed storage. A is factorized as either $A = PUDU^T P^T$ if $UPLO = 'U'$ or $A = PLDL^T P^T$ if $UPLO = 'L'$, where P is a permutation matrix, U (or L) is a unit upper (or lower) triangular matrix and D is a symmetric block diagonal matrix with 1 by 1 and 2 by 2 diagonal blocks; U (or L) has 2 by 2 unit diagonal blocks corresponding to the 2 by 2 blocks of D . Row and column interchanges are performed to ensure numerical stability while preserving symmetry.

This method is suitable for symmetric matrices which are not known to be positive-definite. If A is in fact positive-definite, no interchanges are performed and no 2 by 2 blocks occur in D .

4 References

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 $PUDU^T P^T$, where U is upper triangular.

UPLO = 'L'

The lower triangular part of A is stored and A is factorized as $PLDL^T P^T$, 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: 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 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: A is overwritten by details of the block diagonal matrix D and the multipliers used to obtain the factor U or L as specified by UPLO.

4: IPIV(*) – INTEGER array Output

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

On exit: details of the interchanges and the block structure of D . More precisely,

if $IPIV(i) = k > 0$, d_{ii} is a 1 by 1 pivot block and the i th row and column of A were interchanged with the k th row and column;

if UPLO = 'U' and $IPIV(i - 1) = IPIV(i) = -l < 0$, $\begin{pmatrix} d_{i-1,i-1} & \bar{d}_{i,i-1} \\ \bar{d}_{i,i-1} & d_{ii} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i - 1)$ th row and column of A were interchanged with the l th row and column;

if UPLO = 'L' and $IPIV(i) = IPIV(i + 1) = -m < 0$, $\begin{pmatrix} d_{ii} & d_{i+1,i} \\ d_{i+1,i} & d_{i+1,i+1} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i + 1)$ th row and column of A were interchanged with the m th row and column.

5: 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 i th parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO = i , $d(i, i)$ is exactly zero. The factorization has been completed, but the block diagonal matrix D is exactly singular, and division by zero will occur if it is used to solve a system of equations.

7 Accuracy

If UPLO = 'U', the computed factors U and D are the exact factors of a perturbed matrix $A + E$, where

$$|E| \leq c(n)\epsilon P|U||D||U^T|P^T,$$

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

If UPLO = 'L', a similar statement holds for the computed factors L and D .

8 Further Comments

The elements of D overwrite the corresponding elements of A ; if D has 2 by 2 blocks, only the upper or lower triangle is stored, as specified by UPLO.

The unit diagonal elements of U or L and the 2 by 2 unit diagonal blocks are not stored. The remaining elements of U or L overwrite elements in the corresponding columns of A , but additional row interchanges must be applied to recover U or L explicitly (this is seldom necessary). If $\text{IPIV}(i) = i$, for $i = 1, 2, \dots, n$ (as is the case when A is positive-definite), then U or L are stored explicitly in packed form (except for their unit diagonal elements which are equal to 1).

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

A call to F07PDF (DSPTRF) may be followed by calls to the routines:

F07PEF (DSPTRS) to solve $AX = B$;

F07PGF (DSPCON) to estimate the condition number of A ;

F07PJF (DSPTRI) to compute the inverse of A .

The complex analogues of this routine are F07PRF (ZHPTRF) for Hermitian matrices and F07QRF (ZSPTRF) for symmetric matrices.

9 Example

This example computes the Bunch–Kaufman factorization of the matrix A , where

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

using packed storage.

9.1 Program Text

```
*      F07PDF 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 ..
      DOUBLE PRECISION AP(NMAX*(NMAX+1)/2)
      INTEGER          IPIV(NMAX)
*      .. External Subroutines ..
      EXTERNAL         DSPTRF, X04CCF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F07PDF 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
      END IF
*
```

```

*      Factorize A
*
*      CALL DSPTRF(UPLO,N,AP,IPIV,INFO)
*
*      WRITE (NOUT,*)
*
*      Print details of factorization
*
*      IFAIL = 0
*
*      CALL X04CCF(UPLO,'Nonunit',N,AP,'Details of factorization',
+                IFAIL)
*
*      Print pivot indices
*
*      WRITE (NOUT,*)
*      WRITE (NOUT,*) 'IPIV'
*      WRITE (NOUT,99999) (IPIV(I),I=1,N)
*
*      IF (INFO.NE.0) WRITE (NOUT,*) 'The factor D is singular'
*
*      END IF
*
99999 FORMAT ((3X,7I11))
      END

```

9.2 Program Data

F07PDF Example Program Data

```

4                                :Value of N
'L'                             :Value of UPLO
2.07
3.87 -0.21
4.20  1.87  1.15
-1.15  0.63  2.06 -1.81 :End of matrix A

```

9.3 Program Results

F07PDF Example Program Results

Details of factorization

	1	2	3	4
1	2.0700			
2	4.2000	1.1500		
3	0.2230	0.8115	-2.5907	
4	0.6537	-0.5960	0.3031	0.4074

IPIV				
	-3	-3	3	4
