NAG Library Routine Document

F07QRF (ZSPTRF)

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

F07QRF (ZSPTRF) computes the Bunch–Kaufman factorization of a complex symmetric matrix, using packed storage.

2 Specification

```
SUBROUTINE F07QRF(UPLO, N, AP, IPIV, INFO)
INTEGER            N, IPIV(*), INFO
complex*16         AP(*)
CHARACTER*1        UPLO
```

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

3 Description

F07QRF (ZSPTRF) factorizes a complex symmetric matrix A, using the Bunch–Kaufman diagonal pivoting method and packed storage. A is factorized as either $A = PUDU^{\mathrm{T}}P^{\mathrm{T}}$ if UPLO = 'U' or $A = PLDL^{\mathrm{T}}P^{\mathrm{T}}$ 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.

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 $PUDU^{\mathrm{T}}P^{\mathrm{T}}$, where U is upper triangular.

UPLO = 'L'

The lower triangular part of A is stored and A is factorized as $PLDL^{\mathrm{T}}P^{\mathrm{T}}$, 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$(*)$ – ***complex*16*** array *Input/Output*

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

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 $\mathrm{AP}(i + j(j-1)/2)$ for $i \leq j$;

if UPLO = 'L', the lower triangle of A must be stored with element A_{ij} in $\mathrm{AP}(i + (2n-j)(j-1)/2)$ 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 $\max(1, \mathrm{N})$.

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

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

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

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

$$|E| \leq c(n)\epsilon P|U||D|\left|U^{\mathrm{T}}\right|P^{\mathrm{T}},$$

$c(n)$ 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 IPIV$(i) = i$, for $i = 1, 2, \ldots, n$, 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 real floating-point operations is approximately $\frac{4}{3}n^3$.

A call to F07QRF (ZSPTRF) may be followed by calls to the routines:

F07QSF (ZSPTRS) to solve $AX = B$;

F07QUF (ZSPCON) to estimate the condition number of A;

F07QWF (ZSPTRI) to compute the inverse of A.

The real analogue of this routine is F07PDF (DSPTRF).

9 Example

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

$$A = \begin{pmatrix} -0.39 - 0.71i & 5.14 - 0.64i & -7.86 - 2.96i & 3.80 + 0.92i \\ 5.14 - 0.64i & 8.86 + 1.81i & -3.52 + 0.58i & 5.32 - 1.59i \\ -7.86 - 2.96i & -3.52 + 0.58i & -2.83 - 0.03i & -1.54 - 2.86i \\ 3.80 + 0.92i & 5.32 - 1.59i & -1.54 - 2.86i & -0.56 + 0.12i \end{pmatrix},$$

using packed storage.

9.1 Program Text

```
*     F07QRF 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 ..
      COMPLEX *16      AP(NMAX*(NMAX+1)/2)
      INTEGER          IPIV(NMAX)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DDF, ZSPTRF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07QRF 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 ZSPTRF(UPLO,N,AP,IPIV,INFO)
*
         WRITE (NOUT,*)
*
*        Print details of factorization
*
         IFAIL = 0
         CALL X04DDF(UPLO,'Nonunit',N,AP,'Bracketed','F7.4',
     +               'Details of factorization','Integer',RLABS,
     +               'Integer',CLABS,80,0,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 ((1X,I12,3I18))
      END
```

9.2 Program Data

```
F07QRF Example Program Data
  4                                                       :Value of N
  'L'                                                     :Value of UPLO
 (-0.39,-0.71)
 ( 5.14,-0.64) ( 8.86, 1.81)
 (-7.86,-2.96) (-3.52, 0.58) (-2.83,-0.03)
 ( 3.80, 0.92) ( 5.32,-1.59) (-1.54,-2.86) (-0.56, 0.12)  :End of matrix A
```

9.3 Program Results

```
 F07QRF Example Program Results

 Details of factorization
                    1                 2                 3                 4
 1  (-0.3900,-0.7100)
 2  (-7.8600,-2.9600) (-2.8300,-0.0300)
 3  ( 0.5279,-0.3715) (-0.6078, 0.2811) ( 4.4079, 5.3991)
 4  ( 0.4426, 0.1936) (-0.4823, 0.0150) (-0.1071,-0.3157) (-2.0954,-2.2011)

 IPIV
           -3                -3                 3                 4
```