NAG Library Routine Document

F07QNF (ZSPSV)

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

F07QNF (ZSPSV) computes the solution to a complex system of linear equations

$$AX = B,$$

where A is an n by n symmetric matrix stored in packed format and X and B are n by r matrices.

2 Specification

```
SUBROUTINE F07QNF(UPLO, N, NRHS, AP, IPIV, B, LDB, INFO)
INTEGER           N, NRHS, IPIV(N), LDB, INFO
complex*16        AP(*), B(LDB,*)
CHARACTER*1       UPLO
```

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

3 Description

F07QNF (ZSPSV) uses the diagonal pivoting method to factor A as $A = UDU^{\mathrm{T}}$ if UPLO = 'U' or $A = LDL^{\mathrm{T}}$ if UPLO = 'L', where U (or L) is a product of permutation and unit upper (lower) triangular matrices, D is symmetric and block diagonal with 1 by 1 and 2 by 2 diagonal blocks. The factored form of A is then used to solve the system of equations $AX = B$.

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

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

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

5 Parameters

1: UPLO – CHARACTER*1 *Input*

On entry: if UPLO = 'U', the upper triangle of A is stored.

If UPLO = 'L', the lower triangle of A is stored.

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

2: N – INTEGER *Input*

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

Constraint: N $\geq$ 0.

3: NRHS – INTEGER *Input*

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

Constraint: NRHS ≥ 0.

4: AP$(*)$ – ***complex*16*** array *Input/Output*

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

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: the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^{\text{T}}$ or $A = LDL^{\text{T}}$ as computed by F07QRF (ZSPTRF), stored as a packed triangular matrix in the same storage format as A.

5: IPIV(N) – INTEGER array *Output*

On exit: details of the interchanges and the block structure of D, as determined by F07QRF (ZSPTRF).

IPIV$(k) > 0$
Rows and columns k and IPIV(k) were interchanged, and $D(k,k)$ is a 1 by 1 diagonal block.

UPLO = 'U' and IPIV(k) = IPIV$(k-1) < 0$
Rows and columns $k-1$ and $-$IPIV(k) were interchanged and $D(k-1:k, k-1:k)$ is a 2 by 2 diagonal block.

UPLO = 'L' and IPIV(k) = IPIV$(k+1) < 0$
Rows and columns $k+1$ and $-$IPIV(k) were interchanged and $D(k:k+1, k:k+1)$ is a 2 by 2 diagonal block.

6: B(LDB,$*$) – ***complex*16*** array *Input/Output*

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

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 = $\max(1, \text{N})$

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

On exit: if INFO = 0, the n by r solution matrix X.

7: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07QNF (ZSPSV) is called.

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

8: 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 argument had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO $= i$, d_{ii} is exactly zero. The factorization has been completed, but the block diagonal matrix D is exactly singular, so the solution could not be 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 $\kappa(A) = \left\|A^{-1}\right\|_1\|A\|_1$, the condition number of A with respect to the solution of the linear equations. See Section 4.4 of Anderson *et al.* (1999) and Chapter 11 of Higham (2002) for further details.

F07QPF (ZSPSVX) is a comprehensive LAPACK driver that returns forward and backward error bounds and an estimate of the condition number. Alternatively, F04DJF solves $Ax = b$ and returns a forward error bound and condition estimate. F04DJF calls F07QNF (ZSPSV) to solve the equations.

8 Further Comments

The total number of floating-point operations is approximately $\frac{4}{3}n^3 + 8n^2r$, where r is the number of right-hand sides.

The real analogue of this routine is F07PAF (DSPSV).

9 Example

This example solves the equations

$$Ax = b,$$

where A is the complex symmetric matrix

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

and

$$b = \begin{pmatrix} -6.43 + 19.24i \\ -0.49 - 1.47i \\ -48.18 + 66.00i \\ -55.64 + 41.22i \end{pmatrix}.$$

Details of the factorization of A are also output.

9.1 Program Text

```
*     F07QNF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=8)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N
*     .. Local Arrays ..
      COMPLEX *16      AP((NMAX*(NMAX+1))/2), B(NMAX)
      INTEGER          IPIV(NMAX)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DDF, ZSPSV
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07QNF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read the upper or lower triangular part of the matrix A from
*        data file
*
         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
*
*        Read b from data file
*
         READ (NIN,*) (B(I),I=1,N)
*
*        Solve the equations Ax = b for x
*
         CALL ZSPSV(UPLO,N,1,AP,IPIV,B,N,INFO)
*
         IF (INFO.EQ.0) THEN
*
*           Print solution
*
            WRITE (NOUT,*) 'Solution'
            WRITE (NOUT,99999) (B(I),I=1,N)
*
*           Print details of factorization
*
            WRITE (NOUT,*)
            IFAIL = 0
            CALL X04DDF(UPLO,'Non-unit diagonal',N,AP,'Bracketed',
     +                  'F7.4','Details of factorization','Integer',
     +                  RLABS,'Integer',CLABS,80,0,IFAIL)
*
*           Print pivot indices
*
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Pivot indices'
            WRITE (NOUT,99998) (IPIV(I),I=1,N)
*
         ELSE
            WRITE (NOUT,99997) 'The diagonal block ', INFO,
     +        ' of D is zero'
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX too small'
```

```
      END IF
*
99999 FORMAT ((3X,4(' (',F7.4,',',F7.4,')',:)))
99998 FORMAT (1X,7I11)
99997 FORMAT (1X,A,I3,A)
      END
```

9.2 Program Data

```
F07QNF Example Program Data
    4                                                          :Value of N
 ( -0.56,  0.12) ( -1.54, -2.86) (  5.32, -1.59) (  3.80,  0.92)
                 ( -2.83 ,-0.03) ( -3.52,  0.58) ( -7.86, -2.96)
                                 (  8.86,  1.81) (  5.14, -0.64)
                                                 ( -0.39 ,-0.71) :End matrix A
 ( -6.43, 19.24) ( -0.49, -1.47) (-48.18, 66.00) (-55.64, 41.22) :End vector b
```

9.3 Program Results

```
 F07QNF Example Program Results

 Solution
    (-4.0000, 3.0000) ( 3.0000,-2.0000) (-2.0000, 5.0000) ( 1.0000,-1.0000)

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

 Pivot indices
           1          2         -2         -2
```