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 (KIND=nag_wp) 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 $A = UDU^{\mathsf{T}}$ if UPLO = 'U' or $A = LDL^{\mathsf{T}}$ 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, Philadelphia http://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 Arguments

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: $N \ge 0$.

Mark 26 F07QNF.1

F07QNF NAG Library Manual

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 (KIND=nag_wp) 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,

column;

if UPLO = 'U', the upper triangle of A must be stored with element A_{ij} in AP(i+j(j-1)/2) for $i \le j$;

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

On exit: the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^{T}$ or $A = LDL^{T}$ 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. 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 kth 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 lth row and

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 mth row and column.

6: B(LDB,*) - COMPLEX (KIND=nag_wp) array Input/Output

Note: the second dimension of the array B must be at least max(1, NRHS).

Note: 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, 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 $\geq \max(1, N)$.

8: INFO – INTEGER Output

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

F07QNF.2 Mark 26

6 Error Indicators and Warnings

INFO < 0

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

INFO > 0

Element $\langle value \rangle$ of the diagonal 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

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \le \kappa(A) \frac{\|E\|_1}{\|A\|_1},$$

where $\kappa(A) = ||A^{-1}||_1 ||A||_1$, 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 Parallelism and Performance

F07QNF (ZSPSV) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 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). The complex Hermitian analogue of this routine is F07PNF (ZHPSV).

10 Example

This example solves the equations

$$Ax = b$$

where A is the complex symmetric matrix

Mark 26 F07QNF.3

F07QNF NAG Library Manual

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

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.

10.1 Program Text

```
Program f07qnfe
     F07QNF Example Program Text
!
!
     Mark 26 Release. NAG Copyright 2016.
     .. Use Statements ..
     Use nag_library, Only: nag_wp, x04ddf, zspsv
     .. Implicit None Statement ..
     Implicit None
!
     .. Parameters ..
     Integer, Parameter
                                       :: nin = 5, nout = 6
                                      :: uplo = 'U'
     Character (1), Parameter
!
     .. Local Scalars ..
     Integer
                                       :: i, ifail, info, j, n
     .. Local Arrays ..
     Complex (Kind=nag_wp), Allocatable :: ap(:), b(:)
     Integer, Allocatable :: ipiv(:)
     Character (1)
                                       :: clabs(1), rlabs(1)
!
     .. Executable Statements ..
     Write (nout,*) 'F07QNF Example Program Results'
     Write (nout,*)
!
     Skip heading in data file
     Read (nin,*)
     Read (nin,*) n
     Allocate (ap((n*(n+1))/2),b(n),ipiv(n))
!
     Read the upper or lower triangular part of the matrix A from
     data file
!
     If (uplo=='U') Then
       Read (nin,*)((ap(i+(j*(j-1))/2),j=i,n),i=1,n)
     Else If (uplo=='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(1:n)
     Solve the equations Ax = b for x
!
     The NAG name equivalent of zspsv is f07qnf
     Call zspsv(uplo,n,1,ap,ipiv,b,n,info)
     If (info==0) Then
       Print solution
!
       Write (nout,*) 'Solution'
       Write (nout, 99999) b(1:n)
```

F07QNF.4 Mark 26

```
Print details of factorization
        Write (nout,*)
        Flush (nout)
        ifail: behaviour on error exit
               =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        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(1:n)
        Write (nout,99997) 'The diagonal block ', info, ' of D is zero'
      End If
99999 Format ((3X,4(' (',F7.4,',',F7.4,')',:)))
99998 Format (1X,7I11)
99997 Format (1X,A,I3,A)
    End Program f07qnfe
10.2 Program Data
FO7QNF Example Program Data
                                                                    :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
10.3 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
                                       2
    (-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)
                                          (-2.8300,-0.0300) (-7.8600,-2.9600)
3
 4
                                                             (-0.3900, -0.7100)
Pivot indices
                       2
                                             -2
           1
                                 -2
```

Mark 26 F07QNF.5 (last)