NAG Library Routine Document

F07PAF (DSPSV)

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

F07PAF (DSPSV) computes the solution to a real 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 F07PAF (UPLO, N, NRHS, AP, IPIV, B, LDB, INFO)

INTEGER            N, NRHS, IPIV(N), LDB, INFO
REAL (KIND=nag_wp) AP(*), B(LDB,*)
CHARACTER(1)       UPLO
```

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

3 Description

F07PAF (DSPSV) 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, 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 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$(*)$ – REAL (KIND=nag_wp) 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 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 $A = UDU^{\mathrm{T}}$ or $A = LDL^{\mathrm{T}}$ as computed by F07PDF (DSPTRF), 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 ith 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 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 mth row and column.

6: B(LDB,$*$) – REAL (KIND=nag_wp) array *Input/Output*

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

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 F07PAF (DSPSV) is called.

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

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.

F07PBF (DSPSVX) is a comprehensive LAPACK driver that returns forward and backward error bounds and an estimate of the condition number. Alternatively, F04BJF solves $AX = B$ and returns a forward error bound and condition estimate. F04BJF calls F07PAF (DSPSV) to solve the equations.

8 Further Comments

The total number of floating point operations is approximately $\frac{1}{3}n^3 + 2n^2r$, where r is the number of right-hand sides.

The complex analogues of F07PAF (DSPSV) are F07PNF (ZHPSV) for Hermitian matrices, and F07QNF (ZSPSV) for symmetric matrices.

9 Example

This example solves the equations

$$Ax = b,$$

where A is the symmetric matrix

$$A = \begin{pmatrix} -1.81 & 2.06 & 0.63 & -1.15 \\ 2.06 & 1.15 & 1.87 & 4.20 \\ 0.63 & 1.87 & -0.21 & 3.87 \\ -1.15 & 4.20 & 3.87 & 2.07 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 0.96 \\ 6.07 \\ 8.38 \\ 9.50 \end{pmatrix}.$$

Details of the factorization of A are also output.

9.1 Program Text

```
    Program f07pafe

!     F07PAF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: dspsv, nag_wp, x04ccf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
      Character (1), Parameter         :: uplo = 'U'
!     .. Local Scalars ..
      Integer                          :: i, ifail, info, j, n
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: ap(:), b(:)
      Integer, Allocatable             :: ipiv(:)
!     .. Executable Statements ..
      Write (nout,*) 'F07PAF 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 dspsv is f07paf
      Call dspsv(uplo,n,1,ap,ipiv,b,n,info)

      If (info==0) Then

!       Print solution

        Write (nout,*) 'Solution'
        Write (nout,99999) b(1:n)

!       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
        ifail = 0
        Call x04ccf(uplo,'Non-unit diagonal',n,ap, &
          'Details of the factorization',ifail)

!       Print pivot indices

        Write (nout,*)
        Write (nout,*) 'Pivot indices'
        Write (nout,99998) ipiv(1:n)

      Else
```

```
        Write (nout,99997) 'The diagonal block ', info, ' of D is zero'
      End If

99999 Format ((3X,7F11.4))
99998 Format (1X,7I11)
99997 Format (1X,A,I3,A)
    End Program f07pafe
```

9.2 Program Data

```
F07PAF Example Program Data
  4                          :Value of N
 -1.81   2.06   0.63  -1.15
         1.15   1.87   4.20
               -0.21   3.87
                       2.07 :End of matrix A
  0.96   6.07   8.38   9.50 :End of vector b
```

9.3 Program Results

```
 F07PAF Example Program Results

 Solution
       -5.0000    -2.0000     1.0000     4.0000

 Details of the factorization
             1          2          3          4
1       0.4074     0.3031    -0.5960     0.6537
2                 -2.5907     0.8115     0.2230
3                             1.1500     4.2000
4                                        2.0700

 Pivot indices
           1          2         -2         -2
```