

NAG Library Routine Document

F07PBF (DSPSVX)

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

F07PBF (DSPSVX) uses the diagonal pivoting factorization

$$A = UDU^T \quad \text{or} \quad A = LDL^T$$

to compute 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. Error bounds on the solution and a condition estimate are also provided.

2 Specification

```
SUBROUTINE F07PBF (FACT, UPLO, N, NRHS, AP, AFP, IPIV, B, LDB, X, LDX,      &
                  RCOND, FERR, BERR, WORK, IWORK, INFO)
INTEGER          N, NRHS, IPIV(N), LDB, LDX, IWORK(N), INFO
REAL (KIND=nag_wp) AP(*), AFP(*), B(LDB,*), X(LDX,*), RCOND,      &
                  FERR(NRHS), BERR(NRHS), WORK(3*N)
CHARACTER(1)     FACT, UPLO
```

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

3 Description

F07PBF (DSPSVX) performs the following steps:

1. If FACT = 'N', the diagonal pivoting method is used to factor A as $A = UDU^T$ if UPLO = 'U' or $A = LDL^T$ if UPLO = 'L', where U (or L) is a product of permutation and unit upper (lower) triangular matrices and D is symmetric and block diagonal with 1 by 1 and 2 by 2 diagonal blocks.
2. If some $d_{ii} = 0$, so that D is exactly singular, then the routine returns with INFO = i . Otherwise, the factored form of A is used to estimate the condition number of the matrix A . If the reciprocal of the condition number is less than ***machine precision***, INFO = $N + 1$ is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.
3. The system of equations is solved for X using the factored form of A .
4. Iterative refinement is applied to improve the computed solution matrix and to calculate error bounds and backward error estimates for it.

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: FACT – CHARACTER(1) *Input*
On entry: specifies whether or not the factorized form of the matrix A has been supplied.
FACT = 'F'
AFP and IPIV contain the factorized form of the matrix A . AFP and IPIV will not be modified.
FACT = 'N'
The matrix A will be copied to AFP and factorized.
Constraint: FACT = 'F' or 'N'.
- 2: 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'.
- 3: N – INTEGER *Input*
On entry: n , the number of linear equations, i.e., the order of the matrix A .
Constraint: $N \geq 0$.
- 4: 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 .
- 5: AP(*) – REAL (KIND=nag_wp) array *Input*
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 $i \geq j$.
- 6: AFP(*) – REAL (KIND=nag_wp) array *Input/Output*
Note: the dimension of the array AFP must be at least $\max(1, N \times (N + 1)/2)$.
On entry: if FACT = 'F', AFP contains 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 F07PDF (DSPTRF), stored as a packed triangular matrix in the same storage format as A .
On exit: if FACT = 'N', AFP contains 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 F07PDF (DSPTRF), stored as a packed triangular matrix in the same storage format as A .
- 7: IPIV(N) – INTEGER array *Input/Output*
On entry: if FACT = 'F', IPIV contains details of the interchanges and the block structure of D , as determined by F07PDF (DSPTRF).

if $\text{IPIV}(i) = k > 0$, 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 $\text{UPLO} = 'U'$ and $\text{IPIV}(i-1) = \text{IPIV}(i) = -l < 0$, $\begin{pmatrix} d_{i-1,i-1} & \bar{d}_{i,i-1} \\ \bar{d}_{i,i-1} & d_{ii} \end{pmatrix}$ 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 $\text{UPLO} = 'L'$ and $\text{IPIV}(i) = \text{IPIV}(i+1) = -m < 0$, $\begin{pmatrix} d_{ii} & d_{i+1,i} \\ d_{i+1,i} & d_{i+1,i+1} \end{pmatrix}$ 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.

On exit: if $\text{FACT} = 'N'$, IPIV contains details of the interchanges and the block structure of D , as determined by F07PDF (DSPTRF), as described above.

8: $\text{B}(\text{LDB}, *)$ – REAL (KIND=nag_wp) array *Input*

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

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

9: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07PBF (DSPSVX) is called.

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

10: $\text{X}(\text{LDX}, *)$ – REAL (KIND=nag_wp) array *Output*

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

On exit: if $\text{INFO} = 0$ or $N+1$, the n by r solution matrix X .

11: LDX – INTEGER *Input*

On entry: the first dimension of the array X as declared in the (sub)program from which F07PBF (DSPSVX) is called.

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

12: RCOND – REAL (KIND=nag_wp) *Output*

On exit: the estimate of the reciprocal condition number of the matrix A . If $\text{RCOND} = 0.0$, the matrix may be exactly singular. This condition is indicated by $\text{INFO} > 0$ and $\text{INFO} \leq N$. Otherwise, if RCOND is less than the **machine precision**, the matrix is singular to working precision. This condition is indicated by $\text{INFO} = N+1$.

13: $\text{FERR}(\text{NRHS})$ – REAL (KIND=nag_wp) array *Output*

On exit: if $\text{INFO} = 0$ or $N+1$, an estimate of the forward error bound for each computed solution vector, such that $\|\hat{x}_j - x_j\|_\infty / \|x_j\|_\infty \leq \text{FERR}(j)$ where \hat{x}_j is the j th column of the computed solution returned in the array X and x_j is the corresponding column of the exact solution X . The estimate is as reliable as the estimate for RCOND , and is almost always a slight overestimate of the true error.

14: $\text{BERR}(\text{NRHS})$ – REAL (KIND=nag_wp) array *Output*

On exit: if $\text{INFO} = 0$ or $N+1$, an estimate of the component-wise relative backward error of each computed solution vector \hat{x}_j (i.e., the smallest relative change in any element of A or B that makes \hat{x}_j an exact solution).

15: $\text{WORK}(3 \times N)$ – REAL (KIND=nag_wp) array *Workspace*

- 16: IWORK(N) – INTEGER array Workspace
- 17: INFO – INTEGER Output
- On exit:* INFO = 0 unless the routine detects an error (see Section 6).

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 and INFO ≤ N

Element $\langle value \rangle$ of the diagonal is exactly zero. The factorization has been completed, but the factor D is exactly singular, so the solution and error bounds could not be computed. RCOND = 0.0 is returned.

INFO = N + 1

D is nonsingular, but RCOND is less than *machine precision*, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of RCOND would suggest.

7 Accuracy

For each right-hand side vector b , the computed solution \hat{x} is the exact solution of a perturbed system of equations $(A + E)\hat{x} = b$, where

$$\|E\|_1 = O(\epsilon)\|A\|_1,$$

where ϵ is the *machine precision*. See Chapter 11 of Higham (2002) for further details.

If \hat{x} is the true solution, then the computed solution x satisfies a forward error bound of the form

$$\frac{\|x - \hat{x}\|_\infty}{\|\hat{x}\|_\infty} \leq w_c \text{cond}(A, \hat{x}, b)$$

where $\text{cond}(A, \hat{x}, b) = \frac{\|A^{-1}(|A|\|\hat{x}\| + |b|)\|_\infty}{\|\hat{x}\|_\infty} \leq \text{cond}(A) = \|A^{-1}\|_\infty \|A\|_\infty \leq \kappa_\infty(A)$. If \hat{x} is the j th column of X , then w_c is returned in BERR(j) and a bound on $\|x - \hat{x}\|_\infty / \|\hat{x}\|_\infty$ is returned in FERR(j). See Section 4.4 of Anderson *et al.* (1999) for further details.

8 Parallelism and Performance

F07PBF (DSPSVX) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F07PBF (DSPSVX) 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 factorization of A requires approximately $\frac{1}{3}n^3$ floating-point operations.

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations. Each step of iterative refinement involves an additional $6n^2$ operations. At most five steps of iterative refinement are performed, but usually only one or two steps are required. Estimating the forward error involves solving a number of systems of equations of the form $Ax = b$; the number is usually 4 or 5 and never more than 11. Each solution involves approximately $2n^2$ operations.

The complex analogues of this routine are F07PPF (ZHPSVX) for Hermitian matrices, and F07QPF (ZSPSVX) for symmetric matrices.

10 Example

This example solves the equations

$$AX = B,$$

where A is the symmetric matrix

$$A = \begin{pmatrix} -1.81 & 2.06 & 0.63 & -1.15 \\ 2.06 & 1.15 & 1.87 & 4.20 \\ 0.63 & 1.87 & -0.21 & 3.87 \\ -1.15 & 4.20 & 3.87 & 2.07 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0.96 & 3.93 \\ 6.07 & 19.25 \\ 8.38 & 9.90 \\ 9.50 & 27.85 \end{pmatrix}.$$

Error estimates for the solutions, and an estimate of the reciprocal of the condition number of the matrix A are also output.

10.1 Program Text

```

Program f07pbfe

!      F07PBF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
      Use nag_library, Only: dspsvx, nag_wp, x04caf
!      .. Implicit None Statement ..
      Implicit None
!      .. Parameters ..
      Integer, Parameter          :: nin = 5, nout = 6
      Character (1), Parameter   :: uplo = 'U'
!      .. Local Scalars ..
      Real (Kind=nag_wp)         :: rcond
      Integer                    :: i, ifail, info, j, ldb, ldx, n, nrhs
!      .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable :: afp(:), ap(:), b(:, :), berr(:),      &
                                         ferr(:), work(:), x(:, :)
      Integer, Allocatable        :: ipiv(:), iwork(:)
!      .. Executable Statements ..
      Write (nout,*) 'F07PBF Example Program Results'
      Write (nout,*)
      Flush (nout)
!      Skip heading in data file
      Read (nin,*)
      Read (nin,*) n, nrhs
      ldb = n
      ldx = n
      Allocate (afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb,nrhs), berr(nrhs), ferr(  &
                                         nrhs), work(3*n), x(ldx,nrhs), ipiv(n), iwork(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(i,1:nrhs),i=1,n)

!      Solve the equations AX = B for X
!      The NAG name equivalent of dspsvx is f07pbf
!      Call dspsvx('Not factored',uplo,n,nrhs,ap,afp,ipiv,b,ldb,x,ldx,rcond,      &
         ferr,berr,work,iwork,info)

      If ((info==0) .Or. (info==n+1)) Then

!      Print solution, error bounds and condition number

!      ifail: behaviour on error exit
!      =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0
      Call x04caf('General',' ',n,nrhs,x,ldx,'Solution(s)',ifail)

      Write (nout,*)
      Write (nout,*) 'Backward errors (machine-dependent)'
      Write (nout,99999) berr(1:nrhs)
      Write (nout,*)
      Write (nout,*) 'Estimated forward error bounds (machine-dependent)'
      Write (nout,99999) ferr(1:nrhs)
      Write (nout,*)
      Write (nout,*) 'Estimate of reciprocal condition number'
      Write (nout,99999) rcond
      Write (nout,*)

      If (info==n+1) Then
        Write (nout,*)
        Write (nout,*) 'The matrix A is singular to working precision'
      End If
    Else
      Write (nout,99998) 'The diagonal block ', info, ' of D is zero'
    End If

99999 Format ((3X,1P,7E11.1))
99998 Format (1X,A,I3,A)
      End Program f07pbfe

```

10.2 Program Data

F07PBF Example Program Data

```

  4      2      :Values of N and NRHS
-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    3.93
6.07   19.25
8.38    9.90
9.50   27.85      :End of matrix B

```

10.3 Program Results

F07PBF Example Program Results

Solution(s)

	1	2
1	-5.0000	2.0000
2	-2.0000	3.0000
3	1.0000	4.0000
4	4.0000	1.0000

Backward errors (machine-dependent)
 1.4E-16 1.0E-16

Estimated forward error bounds (machine-dependent)

2.5E-14 3.2E-14

Estimate of reciprocal condition number
1.3E-02
