

NAG Library Routine Document

F07FCF (DSPOSV)

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

F07FCF (DSPOSV) uses the Cholesky factorization

$$A = U^T U \quad \text{or} \quad A = LL^T$$

to compute the solution to a real system of linear equations

$$AX = B,$$

where A is an n by n symmetric positive definite matrix and X and B are n by r matrices.

2 Specification

```
SUBROUTINE F07FCF (UPLO, N, NRHS, A, LDA, B, LDB, X, LDX, WORK, SWORK,      &
                  ITER, INFO)
INTEGER                N, NRHS, LDA, LDB, LDX, ITER, INFO
REAL (KIND=nag_wp)    A(LDA,*), B(LDB,*), X(LDX,*), WORK(N,NRHS)
REAL (KIND=nag_rp)    SWORK(N*(N+NRHS))
CHARACTER(1)          UPLO
```

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

3 Description

F07FCF (DSPOSV) first attempts to factorize the matrix in reduced precision and use this factorization within an iterative refinement procedure to produce a solution with full precision normwise backward error quality (see below). If the approach fails the method switches to a full precision factorization and solve.

The iterative refinement can be more efficient than the corresponding direct full precision algorithm. Since the strategy implemented by F07FCF (DSPOSV) must perform iterative refinement on each right-hand side, any efficiency gains will reduce as the number of right-hand sides increases. Conversely, as the matrix size increases the cost of these iterative refinements become less significant relative to the cost of factorization. Thus, any efficiency gains will be greatest for a very small number of right-hand sides and for large matrix sizes. The cut-off values for the number of right-hand sides and matrix size, for which the iterative refinement strategy performs better, depends on the relative performance of the reduced and full precision factorization and back-substitution. F07FCF (DSPOSV) always attempts the iterative refinement strategy first; you are advised to compare the performance of F07FCF (DSPOSV) with that of its full precision counterpart F07FAF (DPOSV) to determine whether this strategy is worthwhile for your particular problem dimensions.

The iterative refinement process is stopped if $ITER > 30$ where $ITER$ is the number of iterations carried out thus far. The process is also stopped if for all right-hand sides we have

$$\|resid\| < \sqrt{N}\|x\|\|A\|\epsilon,$$

where $\|resid\|$ is the ∞ -norm of the residual, $\|x\|$ is the ∞ -norm of the solution, $\|A\|$ is the ∞ -norm of the matrix A and ϵ is the ***machine precision*** returned by X02AJF.

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: specifies whether the upper or lower triangular part of A is stored.
UPLO = 'U'
The upper triangular part of A is stored.
UPLO = 'L'
The lower triangular part 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: A(LDA,*) – REAL (KIND=nag_wp) array *Input/Output*
Note: the second dimension of the array A must be at least $\max(1, N)$.
On entry: the n by n symmetric positive definite matrix A .
If UPLO = 'U', the upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced.
If UPLO = 'L', the lower triangular part of A must be stored and the elements of the array above the diagonal are not referenced.
On exit: if iterative refinement has been successfully used (INFO = 0 and ITER ≥ 0 , see description below), then A is unchanged. If full precision factorization has been used (INFO = 0 and ITER < 0, see description below), then the array A contains the factor U or L from the Cholesky factorization $A = U^T U$ or $A = L L^T$.
- 5: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F07FCF (DSPOSV) is called.
Constraint: LDA $\geq \max(1, N)$.
- 6: B(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 right-hand side matrix B .

- 7: LDB – INTEGER *Input*
On entry: the first dimension of the array B as declared in the (sub)program from which F07FCF (DSPOSV) is called.
Constraint: $LDB \geq \max(1, N)$.
- 8: X(LDX,*) – REAL (KIND=nag_wp) array *Output*
Note: the second dimension of the array X must be at least $\max(1, NRHS)$.
On exit: if $INFO = 0$, the n by r solution matrix X .
- 9: LDX – INTEGER *Input*
On entry: the first dimension of the array X as declared in the (sub)program from which F07FCF (DSPOSV) is called.
Constraint: $LDX \geq \max(1, N)$.
- 10: WORK(N, NRHS) – REAL (KIND=nag_wp) array *Workspace*
- 11: SWORK($N \times (N + NRHS)$) – REAL (KIND=nag_rp) array *Workspace*
Note: this array is utilized in the reduced precision computation, consequently its type nag_rp reflects this usage.
- 12: ITER – INTEGER *Output*
On exit: information on the progress of the iterative refinement process.
 $ITER < 0$
Iterative refinement has failed for one of the reasons given below, full precision factorization has been performed instead.
 - 1 The routine fell back to full precision for implementation- or machine-specific reasons.
 - 2 Narrowing the precision induced an overflow, the routine fell back to full precision.
 - 3 An intermediate reduced precision factorization failed.
 - 31 The maximum permitted number of iterations was exceeded. $ITER > 0$
Iterative refinement has been successfully used. ITER returns the number of iterations.
- 13: 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 $INFO \leq N$

The leading minor of order $\langle value \rangle$ of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.

7 Accuracy

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

if UPLO = 'U', $|E| \leq c(n)\epsilon|U^T||U|$;

if UPLO = 'L', $|E| \leq c(n)\epsilon|L||L^T|$,

$c(n)$ is a modest linear function of n , and ϵ is the *machine precision*. See Section 10.1 of Higham (2002) for further details.

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 $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. See Section 4.4 of Anderson *et al.* (1999) for further details.

8 Parallelism and Performance

F07FCF (DSPOSV) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F07FCF (DSPOSV) 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 complex analogue of this routine is F07FQF (ZCPOSV).

10 Example

This example solves the equations

$$AX = B,$$

where A is the symmetric positive definite matrix

$$A = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.18 & 0.34 & 1.18 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 8.70 \\ -13.35 \\ 1.89 \\ -4.14 \end{pmatrix}.$$

10.1 Program Text

```

Program f07fcfe

!      F07FCF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
      Use nag_library, Only: dsposv, nag_rp, nag_wp
!      .. Implicit None Statement ..
      Implicit None
!      .. Parameters ..

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Integer, Parameter :: nin = 5, nout = 6
! .. Local Scalars ..
Integer :: i, info, iter, lda, ldb, ldx, n, r
! .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: a(:,:), b(:,:), work(:,:), x(:,:)
Real (Kind=nag_rp), Allocatable :: swork(:)
! .. Executable Statements ..
Write (nout,*) 'F07FCF Example Program Results'
Write (nout,*)
! Skip heading in data file
Read (nin,*)
Read (nin,*) n, r
lda = n
ldb = n
ldx = n
Allocate (a(lda,n),b(n,r),work(n,r),x(ldx,r),swork(n*(n+r)))

! Read the upper triangular part of A from data file

Read (nin,*)(a(i,i:n),i=1,n)

! Read B from data file

Read (nin,*)(b(i,1:r),i=1,n)

! Solve the equations Ax = b for x
! The NAG name equivalent of dsposv is f07fcf
Call dsposv('U',n,r,a,lda,b,ldb,x,ldx,work,swork,iter,info)

If (info==0) Then

! Print solution

Write (nout,*) 'Solution'
Write (nout,99999)(x(i,1:r),i=1,n)
Else
Write (nout,99998) 'The leading minor of order ', info,
' is not positive definite'
End If

99999 Format ((3X,7F11.4))
99998 Format ((1X,A,I3,A))
End Program f07fcfe

```

10.2 Program Data

F07FCF Example Program Data

4	1			:Value of N, R
4.16	-3.12	0.56	-0.10	
	5.03	-0.83	1.18	
		0.76	0.34	
			1.18	:End of matrix A
8.70	-13.35	1.89	-4.14	:End of vector b

10.3 Program Results

F07FCF Example Program Results

Solution

1.0000	-1.0000	2.0000	-3.0000
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