NAG Library Routine Document

F07GVF (ZPPRFS)

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

F07GVF (ZPPRFS) returns error bounds for the solution of a complex Hermitian positive-definite system of linear equations with multiple right-hand sides, $AX = B$, using packed storage. It improves the solution by iterative refinement, in order to reduce the backward error as much as possible.

2 Specification

```
      SUBROUTINE F07GVF(UPLO, N, NRHS, AP, AFP, B, LDB, X, LDX, FERR, BERR,
     1                  WORK, RWORK, INFO)
      INTEGER           N, NRHS, LDB, LDX, INFO
      double precision  FERR(NRHS), BERR(NRHS), RWORK(N)
      complex*16        AP(*), AFP(*), B(LDB,*), X(LDX,*), WORK(2*N)
      CHARACTER*1       UPLO
```

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

3 Description

F07GVF (ZPPRFS) returns the backward errors and estimated bounds on the forward errors for the solution of a complex Hermitian positive-definite system of linear equations with multiple right-hand sides $AX = B$, using packed storage. The routine handles each right-hand side vector (stored as a column of the matrix B) independently, so we describe the function of F07GVF (ZPPRFS) in terms of a single right-hand side b and solution x.

Given a computed solution x, the routine computes the *component-wise backward error* β. This is the size of the smallest relative perturbation in each element of A and b such that x is the exact solution of a perturbed system

$$(A + \delta A)x = b + \delta b$$
$$\left|\delta a_{ij}\right| \leq \beta\left|a_{ij}\right| \quad \text{and} \quad \left|\delta b_i\right| \leq \beta\left|b_i\right|.$$

Then the routine estimates a bound for the *component-wise forward error* in the computed solution, defined by:

$$\max_i\left|x_i - \hat{x}_i\right| / \max_i\left|x_i\right|$$

where $\hat{x}$ is the true solution.

For details of the method, see the F07 Chapter Introduction.

4 References

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

5 Parameters

1: UPLO – CHARACTER*1 *Input*

On entry: indicates whether the upper or lower triangular part of A is stored and how A is to be factorized.

UPLO = 'U'
The upper triangular part of A is stored and A is factorized as $U^{\mathrm{H}}U$, where U is upper triangular.

UPLO = 'L'
The lower triangular part of A is stored and A is factorized as LL^{H}, where L is lower triangular.

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

2: N – INTEGER *Input*

On entry: n, the order of the matrix A.

Constraint: $\mathrm{N} \geq 0$.

3: NRHS – INTEGER *Input*

On entry: r, the number of right-hand sides.

Constraint: $\mathrm{NRHS} \geq 0$.

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

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 original Hermitian positive-definite matrix A as supplied to F07GRF (ZPPTRF).

5: AFP($*$) – ***complex*16*** array *Input*

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

On entry: the Cholesky factor of A stored in packed form, as returned by F07GRF (ZPPTRF).

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

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.

7: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07GVF (ZPPRFS) is called.

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

8: X(LDX,$*$) – ***complex*16*** array *Input/Output*

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

On entry: the n by r solution matrix X, as returned by F07GSF (ZPPTRS).

On exit: the improved solution matrix X.

9: LDX – INTEGER *Input*

On entry: the first dimension of the array X as declared in the (sub)program from which F07GVF (ZPPRFS) is called.

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

10: FERR(NRHS) – ***double precision*** array *Output*

On exit: $\mathrm{FERR}(j)$ contains an estimated error bound for the jth solution vector, that is, the jth column of X, for $j = 1, 2, \ldots, r$.

11: BERR(NRHS) – ***double precision*** array *Output*

On exit: $\mathrm{BERR}(j)$ contains the component-wise backward error bound β for the jth solution vector, that is, the jth column of X, for $j = 1, 2, \ldots, r$.

12: $\mathrm{WORK}(2 \times \mathrm{N})$ – ***complex*16*** array *Workspace*

13: RWORK(N) – ***double precision*** array *Workspace*

14: INFO – INTEGER *Output*

On exit: $\mathrm{INFO} = 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

$\mathrm{INFO} < 0$

If $\mathrm{INFO} = -i$, the ith parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

7 Accuracy

The bounds returned in FERR are not rigorous, because they are estimated, not computed exactly; but in practice they almost always overestimate the actual error.

8 Further Comments

For each right-hand side, computation of the backward error involves a minimum of $16n^2$ real floating-point operations. Each step of iterative refinement involves an additional $24n^2$ real 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 linear equations of the form $Ax = b$; the number is usually 5 and never more than 11. Each solution involves approximately $8n^2$ real operations.

The real analogue of this routine is F07GHF (DPPRFS).

9 Example

This example solves the system of equations $AX = B$ using iterative refinement and to compute the forward and backward error bounds, where

$$A = \begin{pmatrix} 3.23 + 0.00i & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 + 0.00i & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 + 0.00i & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 + 0.00i \end{pmatrix}$$

and

$$B = \begin{pmatrix} 3.93 - 6.14i & 1.48 + 6.58i \\ 6.17 + 9.42i & 4.65 - 4.75i \\ -7.17 - 21.83i & -4.91 + 2.29i \\ 1.99 - 14.38i & 7.64 - 10.79i \end{pmatrix}.$$

Here A is Hermitian positive-definite, stored in packed form, and must first be factorized by F07GRF (ZPPTRF).

9.1 Program Text

```
*     F07GVF Example Program Text
*     Mark 15 Release. NAG Copyright 1991.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, NRHMAX, LDB, LDX
      PARAMETER        (NMAX=8,NRHMAX=NMAX,LDB=NMAX,LDX=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N, NRHS
      CHARACTER        UPLO
*     .. Local Arrays ..
      COMPLEX *16      AFP(NMAX*(NMAX+1)/2), AP(NMAX*(NMAX+1)/2),
     +                 B(LDB,NRHMAX), WORK(2*NMAX), X(LDX,NMAX)
      DOUBLE PRECISION BERR(NRHMAX), FERR(NRHMAX), RWORK(NMAX)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         F06TFF, X04DBF, ZPPRFS, ZPPTRF, ZPPTRS
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07GVF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NRHS
      IF (N.LE.NMAX .AND. NRHS.LE.NRHMAX) THEN
*
*        Read A and B from data file, and copy A to AFP and B to X
*
         READ (NIN,*) UPLO
         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 (NIN,*) ((B(I,J),J=1,NRHS),I=1,N)
         DO 20 I = 1, N*(N+1)/2
            AFP(I) = AP(I)
   20    CONTINUE
         CALL F06TFF('General',N,NRHS,B,LDB,X,LDX)
*
*        Factorize A in the array AFP
*
         CALL ZPPTRF(UPLO,N,AFP,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.EQ.0) THEN
*
*           Compute solution in the array X
*
            CALL ZPPTRS(UPLO,N,NRHS,AFP,X,LDX,INFO)
*
*           Improve solution, and compute backward errors and
*           estimated bounds on the forward errors
*
            CALL ZPPRFS(UPLO,N,NRHS,AP,AFP,B,LDB,X,LDX,FERR,BERR,WORK,
     +                  RWORK,INFO)
*
*           Print solution
*
```

```
            IFAIL = 0
            CALL X04DBF('General',' ',N,NRHS,X,LDX,'Bracketed','F7.4',
     +                  'Solution(s)','Integer',RLABS,'Integer',CLABS,
     +                  80,0,IFAIL)
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Backward errors (machine-dependent)'
            WRITE (NOUT,99999) (BERR(J),J=1,NRHS)
            WRITE (NOUT,*)
     +        'Estimated forward error bounds (machine-dependent)'
            WRITE (NOUT,99999) (FERR(J),J=1,NRHS)
         ELSE
            WRITE (NOUT,*) 'A is not positive-definite'
         END IF
      END IF
*
99999 FORMAT ((5X,1P,4(E11.1,7X)))
      END
```

9.2 Program Data

```
F07GVF Example Program Data
  4  2                                                    :Values of N and NRHS
  'L'                                                     :Value of UPLO
 (3.23, 0.00)
 (1.51, 1.92) ( 3.58, 0.00)
 (1.90,-0.84) (-0.23,-1.11) ( 4.09, 0.00)
 (0.42,-2.50) (-1.18,-1.37) ( 2.33, 0.14) ( 4.29, 0.00)  :End of matrix A
 ( 3.93, -6.14) ( 1.48,  6.58)
 ( 6.17,  9.42) ( 4.65, -4.75)
 (-7.17,-21.83) (-4.91,  2.29)
 ( 1.99,-14.38) ( 7.64,-10.79)                            :End of matrix B
```

9.3 Program Results

```
 F07GVF Example Program Results

 Solution(s)
                    1                  2
 1  ( 1.0000,-1.0000) (-1.0000, 2.0000)
 2  ( 0.0000, 3.0000) ( 3.0000,-4.0000)
 3  (-4.0000,-5.0000) (-2.0000, 3.0000)
 4  ( 2.0000, 1.0000) ( 4.0000,-5.0000)

 Backward errors (machine-dependent)
        5.4E-17           7.4E-17
 Estimated forward error bounds (machine-dependent)
        5.9E-14           7.5E-14
```