NAG Library Routine Document

F07GWF (ZPPTRI)

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

F07GWF (ZPPTRI) computes the inverse of a complex Hermitian positive-definite matrix A, where A has been factorized by F07GRF (ZPPTRF), using packed storage.

2 Specification

```
SUBROUTINE F07GWF(UPLO, N, AP, INFO)
INTEGER            N, INFO
complex*16         AP(*)
CHARACTER*1        UPLO
```

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

3 Description

F07GWF (ZPPTRI) is used to compute the inverse of a complex Hermitian positive-definite matrix A, the routine must be preceded by a call to F07GRF (ZPPTRF), which computes the Cholesky factorization of A, using packed storage.

If UPLO = 'U', $A = U^{\mathrm{H}}U$ and A^{-1} is computed by first inverting U and then forming $\left(U^{-1}\right)U^{-\mathrm{H}}$.

If UPLO = 'L', $A = LL^{\mathrm{H}}$ and A^{-1} is computed by first inverting L and then forming $L^{-\mathrm{H}}\left(L^{-1}\right)$.

4 References

Du Croz J J and Higham N J (1992) Stability of methods for matrix inversion *IMA J. Numer. Anal.* **12** 1–19

5 Parameters

1: UPLO – CHARACTER*1 *Input*

On entry: indicates how A has been factorized.

UPLO = 'U'
$A = U^{\mathrm{H}}U$, where U is upper triangular.

UPLO = 'L'
$A = LL^{\mathrm{H}}$, 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: AP$(*)$ – ***complex*16*** 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 Cholesky factor of A stored in packed form, as returned by F07GRF (ZPPTRF).

On exit: the factorization is overwritten by the n by n matrix A^{-1}.

More precisely,

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

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

4: 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 parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO $= i$, the ith diagonal element of the Cholesky factor is zero; the Cholesky factor is singular and the inverse of A cannot be computed.

7 Accuracy

The computed inverse X satisfies

$$\|XA - I\|_2 \leq c(n)\epsilon\kappa_2(A) \qquad \text{and} \qquad \|AX - I\|_2 \leq c(n)\epsilon\kappa_2(A),$$

where $c(n)$ is a modest function of n, ϵ is the ***machine precision*** and $\kappa_2(A)$ is the condition number of A defined by

$$\kappa_2(A) = \|A\|_2\|A^{-1}\|_2.$$

8 Further Comments

The total number of real floating-point operations is approximately $\frac{8}{3}n^3$.

The real analogue of this routine is F07GJF (DPPTRI).

9 Example

This example computes the inverse of the matrix A, where

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

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

9.1 Program Text

```
*     F07GWF Example Program Text
*     Mark 15 Release. NAG Copyright 1991.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=8)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N
      CHARACTER        UPLO
*     .. Local Arrays ..
      COMPLEX *16      AP(NMAX*(NMAX+1)/2)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DDF, ZPPTRF, ZPPTRI
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07GWF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read A from data file
*
         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
*
*        Factorize A
*
         CALL ZPPTRF(UPLO,N,AP,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.EQ.0) THEN
*
*           Compute inverse of A
*
            CALL ZPPTRI(UPLO,N,AP,INFO)
*
*           Print inverse
*
            IFAIL = 0
            CALL X04DDF(UPLO,'Nonunit',N,AP,'Bracketed','F7.4',
     +                  'Inverse','Integer',RLABS,'Integer',CLABS,80,0,
     +                  IFAIL)
         ELSE
            WRITE (NOUT,*) 'A is not positive-definite'
         END IF
      END IF
*
      END
```

9.2 Program Data

```
F07GWF Example Program Data
  4                                                        :Value of N
  '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
```

9.3 Program Results

```
 F07GWF Example Program Results

 Inverse
                     1                   2                   3                   4
 1  ( 5.4691, 0.0000)
 2  (-1.2624,-1.5491) ( 1.1024, 0.0000)
 3  (-2.9746,-0.9616) ( 0.8989,-0.5672) ( 2.1589, 0.0000)
 4  ( 1.1962, 2.9772) (-0.9826,-0.2566) (-1.3756,-1.4550) ( 2.2934, 0.0000)
```