

NAG Fortran Library Routine Document

F08TNF (ZHPGV)

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

F08TNF (ZHPGV) computes all the eigenvalues and, optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

$$Az = \lambda Bz, \quad ABz = \lambda z \quad \text{or} \quad BAz = \lambda z,$$

where A and B are Hermitian, stored in packed format, and B is also positive-definite.

2 Specification

```

SUBROUTINE F08TNF (ITYPE, JOBZ, UPLO, N, AP, BP, W, Z, LDZ, WORK, RWORK,
1                  INFO)
    INTEGER          ITYPE, N, LDZ, INFO
    double precision W(*), RWORK(*)
    complex*16       AP(*), BP(*), Z(LDZ,*), WORK(*)
    CHARACTER*1      JOBZ, UPLO

```

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

3 Description

F08TNF (ZHPGV) first performs a Cholesky factorization of the matrix B as $B = U^H U$, when UPLO = 'U' or $B = LL^H$, when UPLO = 'L'. The generalized problem is then reduced to a standard symmetric eigenvalue problem

$$Cx = \lambda x,$$

which is solved for the eigenvalues and, optionally, the eigenvectors; the eigenvectors are then backtransformed to give the eigenvectors of the original problem.

For the problem $Az = \lambda Bz$, the eigenvectors are normalized so that the matrix of eigenvectors, z , satisfies

$$Z^H A Z = \Lambda \quad \text{and} \quad Z^H B Z = I,$$

where Λ is the diagonal matrix whose diagonal elements are the eigenvalues. For the problem $ABz = \lambda z$ we correspondingly have

$$Z^{-1} A Z^{-H} = \Lambda \quad \text{and} \quad Z^H B Z = I,$$

and for $BAz = \lambda z$ we have

$$Z^H A Z = \Lambda \quad \text{and} \quad Z^H B^{-1} Z = I.$$

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 URL: <http://www.netlib.org/lapack/lug>

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

5 Parameters

- 1: ITYPE – INTEGER *Input*
On entry: specifies the problem type to be solved:
 if ITYPE = 1, $Az = \lambda Bz$;
 if ITYPE = 2, $ABz = \lambda z$;
 if ITYPE = 3, $BAz = \lambda z$.
- 2: JOBZ – CHARACTER*1 *Input*
On entry: if JOBZ = 'N', compute eigenvalues only.
 If JOBZ = 'V', compute eigenvalues and eigenvectors.
Constraint: JOBZ = 'N' or 'V'.
- 3: UPLO – CHARACTER*1 *Input*
On entry: if UPLO = 'U', the upper triangles of A and B are stored.
 If UPLO = 'L', the lower triangles of A and B are stored.
- 4: N – INTEGER *Input*
On entry: n , the order of the matrices A and B .
Constraint: $N \geq 0$.
- 5: AP(*) – **complex*16** array *Input/Output*
Note: the dimension of the array AP must be at least $\max(1, N \times (N + 1)/2)$.
On entry: the upper or lower triangle of the Hermitian matrix A , packed columnwise in a linear array. The j th column of A is stored in the array AP as follows:
 if UPLO = 'U', $AP(i + (j - 1) \times j/2) = a_{ij}$ for $1 \leq i \leq j$;
 if UPLO = 'L', $AP(i + (j - 1) \times (2 \times n - j)/2) = a_{ij}$ for $j \leq i \leq n$.
On exit: the contents of AP are destroyed.
- 6: BP(*) – **complex*16** array *Input/Output*
Note: the dimension of the array BP must be at least $\max(1, N \times (N + 1)/2)$.
On entry: the upper or lower triangle of the Hermitian matrix B , packed columnwise in a linear array. The j th column of B is stored in the array BP as follows:
 if UPLO = 'U', $BP(i + (j - 1) \times j/2) = b_{ij}$ for $1 \leq i \leq j$;
 if UPLO = 'L', $BP(i + (j - 1) \times (2 \times n - j)/2) = b_{ij}$ for $j \leq i \leq n$.
On exit: the triangular factor U or L from the Cholesky factorization $B = U^H U$ or $B = LL^H$, in the same storage format as B .
- 7: W(*) – **double precision** array *Output*
Note: the dimension of the array W must be at least $\max(1, N)$.
On exit: if INFO = 0, the eigenvalues in ascending order.

- 8: $Z(\text{LDZ},*)$ – **complex*16** array *Output*
Note: the second dimension of the array Z must be at least $\max(1, N)$.
On exit: if $\text{JOBZ} = 'V'$, then if $\text{INFO} = 0$, Z contains the matrix Z of eigenvectors. The eigenvectors are normalized as follows:
 if $\text{ITYPE} = 1$ or 2 , $Z^H B Z = I$;
 if $\text{ITYPE} = 3$, $Z^H B^{-1} Z = I$.
 If $\text{JOBZ} = 'N'$, Z is not referenced.
- 9: LDZ – INTEGER *Input*
On entry: the first dimension of the array Z as declared in the (sub)program from which F08TNF (ZHPGV) is called.
Constraints:
 if $\text{JOBZ} = 'V'$, $\text{LDZ} \geq \max(1, N)$;
 $\text{LDZ} \geq 1$ otherwise.
- 10: $\text{WORK}(*)$ – **complex*16** array *Workspace*
Note: the dimension of the array WORK must be at least $\max(1, 2 \times N - 1)$.
- 11: $\text{RWORK}(*)$ – **double precision** array *Workspace*
Note: the dimension of the array RWORK must be at least $\max(1, 3 \times N - 2)$.
- 12: INFO – INTEGER *Output*
On exit: $\text{INFO} = 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

$\text{INFO} < 0$

If $\text{INFO} = -i$, the i th argument had an illegal value.

$\text{INFO} > 0$

F07GRF (ZPPTRF) or F08GNF (ZHPEV) returned an error code:

$\leq N$ if $\text{INFO} = i$, F08GNF (ZHPEV) failed to converge; i off-diagonal elements of an intermediate tridiagonal form did not converge to zero;

$> N$ if $\text{INFO} = N + i$, for $1 \leq i \leq N$, then the leading minor of order i of B is not positive-definite. The factorization of B could not be completed and no eigenvalues or eigenvectors were computed.

7 Accuracy

If B is ill-conditioned with respect to inversion, then the error bounds for the computed eigenvalues and vectors may be large, although when the diagonal elements of B differ widely in magnitude the eigenvalues and eigenvectors may be less sensitive than the condition of B would suggest. See Section 4.10 of Anderson *et al.* (1999) for details of the error bounds.

The example program below illustrates the computation of approximate error bounds.

8 Further Comments

The total number of floating point operations is proportional to n^3 .

The real analogue of this routine is F08TAF (DSPGV).

9 Example

To find all the eigenvalues and eigenvectors of the generalized Hermitian eigenproblem $Az = \lambda Bz$, where

$$A = \begin{pmatrix} -7.36 & 0.77 - 0.43i & -0.64 - 0.92i & 3.01 - 6.97i \\ 0.77 + 0.43i & 3.49 & 2.19 + 4.45i & 1.90 + 3.73i \\ -0.64 + 0.92i & 2.19 - 4.45i & 0.12 & 2.88 - 3.17i \\ 3.01 + 6.97i & 1.90 - 3.73i & 2.88 + 3.17i & -2.54 \end{pmatrix}$$

and

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

together with an estimate of the condition number of B , and approximate error bounds for the computed eigenvalues and eigenvectors.

The example program for F08TQF (ZHPGVD) illustrates solving a generalized symmetric eigenproblem of the form $ABz = \lambda z$.

9.1 Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*      F08TNF Example Program Text
*      Mark 21.  NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=10)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*      .. Local Scalars ..
      DOUBLE PRECISION ANORM, BNORM, EPS, RCOND, RCONDB, T1, T2
      INTEGER          I, INFO, J, N
*      .. Local Arrays ..
      COMPLEX *16      AP((NMAX*(NMAX+1))/2), BP((NMAX*(NMAX+1))/2),
+      DUMMY(1,1), WORK(2*NMAX)
      DOUBLE PRECISION EERBND(NMAX), RWORK(3*(NMAX-2)), W(NMAX)
*      .. External Functions ..
      DOUBLE PRECISION F06UDF, X02AJF
      EXTERNAL         F06UDF, X02AJF
*      .. External Subroutines ..
      EXTERNAL         ZHPGV, ZTPCON
*      .. Intrinsic Functions ..
      INTRINSIC        ABS
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08TNF Example Program Results'
      WRITE (NOUT,*)
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN

*
*          Read the upper or lower triangular parts of the matrices A and
*          B from data file
*

```

```

      IF (UPLO.EQ.'U') THEN
        READ (NIN,*) ((AP(I+(J*(J-1))/2),J=I,N),I=1,N)
        READ (NIN,*) ((BP(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)
        READ (NIN,*) ((BP(I+((2*N-J)*(J-1))/2),J=1,I),I=1,N)
      END IF

*
*   Compute the one-norms of the symmetric matrices A and B
*
      ANORM = F06UDF('One norm',UPLO,N,AP,RWORK)
      BNORM = F06UDF('One norm',UPLO,N,BP,RWORK)

*
*   Solve the generalized symmetric eigenvalue problem
*   A*x = lambda*B*x (ITYPE = 1)
*
      CALL ZHPGV(1,'No vectors',UPLO,N,AP,BP,W,DUMMY,1,WORK,RWORK,
+           INFO)

*
      IF (INFO.EQ.0) THEN

*
*       Print solution
*
        WRITE (NOUT,*) 'Eigenvalues'
        WRITE (NOUT,99999) (W(J),J=1,N)

*
*       Call ZTPCON (F07UUF) to estimate the reciprocal condition
*       number of the Cholesky factor of B. Note that:
*       cond(B) = 1/RCOND**2
*
        CALL ZTPCON('One norm',UPLO,'Non-unit',N,BP,RCOND,WORK,
+           RWORK,INFO)

*
*       Print the reciprocal condition number of B
*
        RCONDB = RCOND**2
        WRITE (NOUT,*)
        WRITE (NOUT,*)
+       'Estimate of reciprocal condition number for B'
        WRITE (NOUT,99998) RCONDB

*
*       Get the machine precision, EPS, and if RCONDB is not less
*       than EPS**2, compute error estimates for the eigenvalues
*
        EPS = X02AJF()
        IF (RCOND.GE.EPS) THEN
          T1 = EPS/RCONDB
          T2 = ANORM/BNORM
          DO 20 I = 1, N
            EERBND(I) = T1*(T2+ABS(W(I)))
20          CONTINUE

*
*       Print the approximate error bounds for the eigenvalues
*
          WRITE (NOUT,*)
          WRITE (NOUT,*) 'Error estimates for the eigenvalues'
          WRITE (NOUT,99998) (EERBND(I),I=1,N)
        ELSE
          WRITE (NOUT,*)
          WRITE (NOUT,*) 'B is very ill-conditioned, error ',
+           'estimates have not been computed'
        END IF
      ELSE IF (INFO.GT.N .AND. INFO.LE.2*N) THEN
        I = INFO - N
        WRITE (NOUT,99997) 'The leading minor of order ', I,
+       ' of B is not positive definite'
      ELSE
        WRITE (NOUT,99996) 'Failure in ZHPGV. INFO =', INFO
      END IF
    ELSE
      WRITE (NOUT,*) 'NMAX too small'
    
```

```

      END IF
      STOP
*
99999 FORMAT (3X,(6F11.4))
99998 FORMAT (4X,1P,6E11.1)
99997 FORMAT (1X,A,I4,A)
99996 FORMAT (1X,A,I4)
      END

```

9.2 Program Data

F08TNF Example Program Data

```

      4                                     :Value of N

(-7.36, 0.00) ( 0.77, -0.43) (-0.64, -0.92) ( 3.01, -6.97)
              ( 3.49, 0.00) ( 2.19, 4.45) ( 1.90, 3.73)
              ( 0.12, 0.00) ( 2.88, -3.17)
              (-2.54, 0.00) :End of matrix A

( 3.23, 0.00) ( 1.51, -1.92) ( 1.90, 0.84) ( 0.42, 2.50)
              ( 3.58, 0.00) (-0.23, 1.11) (-1.18, 1.37)
              ( 4.09, 0.00) ( 2.33, -0.14)
              ( 4.29, 0.00) :End of matrix B

```

9.3 Program Results

F08TNF Example Program Results

```

Eigenvalues
-5.9990    -2.9936    0.5047    3.9990

Estimate of reciprocal condition number for B
2.5E-03

Error estimates for the eigenvalues
3.4E-13    2.0E-13    9.6E-14    2.5E-13

```
