NAG Library Routine Document

F08TPF (ZHPGVX)

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

F08TPF (ZHPGVX) computes selected eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

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

where A and B are Hermitian, stored in packed format, and B is also positive definite. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

2 Specification

```
SUBROUTINE F08TPF (ITYPE, JOBZ, RANGE, UPLO, N, AP, BP, VL, VU, IL, IU,        &
                   ABSTOL, M, W, Z, LDZ, WORK, RWORK, IWORK, JFAIL, INFO)

INTEGER               ITYPE, N, IL, IU, M, LDZ, IWORK(5*N), JFAIL(*), INFO
REAL (KIND=nag_wp)    VL, VU, ABSTOL, W(N), RWORK(7*N)
COMPLEX (KIND=nag_wp) AP(*), BP(*), Z(LDZ,*), WORK(2*N)
CHARACTER(1)          JOBZ, RANGE, UPLO
```

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

3 Description

F08TPF (ZHPGVX) first performs a Cholesky factorization of the matrix B as $B = U^{\mathrm{H}}U$, when UPLO = 'U' or $B = LL^{\mathrm{H}}$, when UPLO = 'L'. The generalized problem is then reduced to a standard symmetric eigenvalue problem

$$Cx = \lambda x,$$

which is solved for the desired eigenvalues and 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

$$Z^{\mathrm{H}}AZ = \Lambda \qquad \text{and} \qquad Z^{\mathrm{H}}BZ = I,$$

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

$$Z^{-1}AZ^{-\mathrm{H}} = \Lambda \qquad \text{and} \qquad Z^{\mathrm{H}}BZ = I,$$

and for $BAz = \lambda z$ we have

$$Z^{\mathrm{H}}AZ = \Lambda \qquad \text{and} \qquad Z^{\mathrm{H}}B^{-1}Z = I.$$

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 http://www.netlib.org/lapack/lug

Demmel J W and Kahan W (1990) Accurate singular values of bidiagonal matrices *SIAM J. Sci. Statist. Comput.* **11** 873–912

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.

ITYPE = 1
$Az = \lambda Bz$.

ITYPE = 2
$ABz = \lambda z$.

ITYPE = 3
$BAz = \lambda z$.

Constraint: ITYPE = 1, 2 or 3.

2: JOBZ – CHARACTER(1) *Input*

On entry: indicates whether eigenvectors are computed.

JOBZ = 'N'
Only eigenvalues are computed.

JOBZ = 'V'
Eigenvalues and eigenvectors are computed.

Constraint: JOBZ = 'N' or 'V'.

3: RANGE – CHARACTER(1) *Input*

On entry: if RANGE = 'A', all eigenvalues will be found.

If RANGE = 'V', all eigenvalues in the half-open interval $(\mathrm{VL}, \mathrm{VU}]$ will be found.

If RANGE = 'I', the ILth to IUth eigenvalues will be found.

Constraint: RANGE = 'A', 'V' or 'I'.

4: 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.

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

5: N – INTEGER *Input*

On entry: n, the order of the matrices A and B.

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

6: AP($*$) – COMPLEX (KIND=nag_wp) 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 upper or lower triangle of the n by n Hermitian 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 $i \geq j$.

On exit: the contents of AP are destroyed.

7: BP(*) – COMPLEX (KIND=nag_wp) array *Input/Output*

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

On entry: the upper or lower triangle of the n by n Hermitian matrix B, packed by columns.

More precisely,

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

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

On exit: the triangular factor U or L from the Cholesky factorization $B = U^{\mathrm{H}}U$ or $B = LL^{\mathrm{H}}$, in the same storage format as B.

8: VL – REAL (KIND=nag_wp) *Input*
9: VU – REAL (KIND=nag_wp) *Input*

On entry: if RANGE = 'V', the lower and upper bounds of the interval to be searched for eigenvalues.

If RANGE = 'A' or 'I', VL and VU are not referenced.

Constraint: if RANGE = 'V', VL < VU.

10: IL – INTEGER *Input*
11: IU – INTEGER *Input*

On entry: if RANGE = 'I', the indices (in ascending order) of the smallest and largest eigenvalues to be returned.

If RANGE = 'A' or 'V', IL and IU are not referenced.

Constraints:

if RANGE = 'I' and N = 0, IL = 1 and IU = 0;
if RANGE = 'I' and N > 0, $1 \leq \mathrm{IL} \leq \mathrm{IU} \leq \mathrm{N}$.

12: ABSTOL – REAL (KIND=nag_wp) *Input*

On entry: the absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a, b]$ of width less than or equal to

$$\mathrm{ABSTOL} + \epsilon \max(|a|, |b|),$$

where ϵ is the ***machine precision***. If ABSTOL is less than or equal to zero, then $\epsilon\|T\|_1$ will be used in its place, where T is the tridiagonal matrix obtained by reducing C to tridiagonal form. Eigenvalues will be computed most accurately when ABSTOL is set to twice the underflow threshold $2 \times$ X02AMF( ), not zero. If this routine returns with INFO = 1 to N, indicating that some eigenvectors did not converge, try setting ABSTOL to $2 \times$ X02AMF( ). See Demmel and Kahan (1990).

13: M – INTEGER *Output*

On exit: the total number of eigenvalues found. $0 \leq \mathrm{M} \leq \mathrm{N}$.

If RANGE = 'A', M = N.

If RANGE = 'I', M = IU − IL + 1.

14: W(N) – REAL (KIND=nag_wp) array *Output*

On exit: the first M elements contain the selected eigenvalues in ascending order.

15: Z(LDZ,∗) – COMPLEX (KIND=nag_wp) array *Output*

Note: the second dimension of the array Z must be at least max(1, M) if JOBZ = 'V', and at least 1 otherwise.

On exit: if JOBZ = 'V', then

if INFO = 0, the first M columns of Z contain the orthonormal eigenvectors of the matrix A corresponding to the selected eigenvalues, with the ith column of Z holding the eigenvector associated with W(i). The eigenvectors are normalized as follows:

if ITYPE = 1 or 2, $Z^{\mathrm{H}}BZ = I$;

if ITYPE = 3, $Z^{\mathrm{H}}B^{-1}Z = I$;

if an eigenvector fails to converge (INFO = 1 to N), then that column of Z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in JFAIL.

If JOBZ = 'N', Z is not referenced.

Note: you must ensure that at least max(1, M) columns are supplied in the array Z; if RANGE = 'V', the exact value of M is not known in advance and an upper bound of at least N must be used.

16: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08TPF (ZHPGVX) is called.

Constraints:

if JOBZ = 'V', LDZ ≥ max(1, N);
otherwise LDZ ≥ 1.

17: WORK(2 × N) – COMPLEX (KIND=nag_wp) array *Workspace*

18: RWORK(7 × N) – REAL (KIND=nag_wp) array *Workspace*

19: IWORK(5 × N) – INTEGER array *Workspace*

20: JFAIL(∗) – INTEGER array *Output*

Note: the dimension of the array JFAIL must be at least max(1, N).

On exit: if JOBZ = 'V', then

if INFO = 0, the first M elements of JFAIL are zero;

if INFO = 1 to N, JFAIL contains the indices of the eigenvectors that failed to converge.

If JOBZ = 'N', JFAIL is not referenced.

21: 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 $= -i$, argument i had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO $= 1$ to N

If INFO $= i$, F08GPF (ZHPEVX) failed to converge; i eigenvectors failed to converge. Their indices are stored in array JFAIL.

INFO $>$ N

F07GRF (ZPPTRF) returned an error code; i.e., if 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.

8 Further Comments

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

The real analogue of this routine is F08TBF (DSPGVX).

9 Example

This example finds the eigenvalues in the half-open interval $(-3, 3]$, and corresponding 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

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

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

9.1 Program Text

```
    Program f08tpfe

!     F08TPF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, x04daf, zhpgvx
```

```
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Real (Kind=nag_wp), Parameter    :: zero = 0.0E+0_nag_wp
      Integer, Parameter               :: nin = 5, nout = 6
      Character (1), Parameter         :: uplo = 'U'
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: abstol, vl, vu
      Integer                          :: i, ifail, il, info, iu, j, ldz, m, n
!     .. Local Arrays ..
      Complex (Kind=nag_wp), Allocatable :: ap(:), bp(:), work(:), z(:,:)
      Real (Kind=nag_wp), Allocatable  :: rwork(:), w(:)
      Integer, Allocatable             :: iwork(:), jfail(:)
!     .. Executable Statements ..
      Write (nout,*) 'F08TPF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n
      ldz = n
      m = n
      Allocate (ap((n*(n+1))/2),bp((n*(n+1))/2),work(2*n),z(ldz,m),rwork(7*n), &
        w(n),iwork(5*n),jfail(n))

!     Read the lower and upper bounds of the interval to be searched,
!     and read the upper or lower triangular parts of the matrices A
!     and B from data file

      Read (nin,*) vl, vu
      If (uplo=='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=='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

!     Set the absolute error tolerance for eigenvalues. With abstol
!     set to zero, the default value is used instead

      abstol = zero

!     Solve the generalized Hermitian eigenvalue problem
!     A*x = lambda*B*x (itype = 1)

!     The NAG name equivalent of zhpgvx is f08tpf
      Call zhpgvx(1,'Vectors','Values in range',uplo,n,ap,bp,vl,vu,il,iu, &
        abstol,m,w,z,ldz,work,rwork,iwork,jfail,info)

      If (info>=0 .And. info<=n) Then

!       Print solution

        Write (nout,99999) 'Number of eigenvalues found =', m
        Write (nout,*)
        Write (nout,*) 'Eigenvalues'
        Write (nout,99998) w(1:m)
        Flush (nout)

!       Normalize the eigenvectors
        Do i = 1, m
          z(1:n,i) = z(1:n,i)/z(1,i)
        End Do

!       ifail: behaviour on error exit
!              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
        Call x04daf('General',' ',n,m,z,ldz,'Selected eigenvectors',ifail)

        If (info>0) Then
          Write (nout,99999) 'INFO eigenvectors failed to converge, INFO =', &
```

```
            info
          Write (nout,*) 'Indices of eigenvectors that did not converge'
          Write (nout,99997) jfail(1:m)
        End If
      Else If (info>n .And. info<=2*n) Then
        i = info - n
        Write (nout,99996) 'The leading minor of order ', i, &
          ' of B is not positive definite'
      Else
        Write (nout,99999) 'Failure in ZHPGVX. INFO =', info
      End If

99999 Format (1X,A,I5)
99998 Format (3X,(8F8.4))
99997 Format (3X,(8I8))
99996 Format (1X,A,I4,A)
    End Program f08tpfe
```

9.2 Program Data

```
F08TPF Example Program Data

   4                                                          :Value of N

  -3.0          3.0                                           :Values of VL and VU

 (-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

```
 F08TPF Example Program Results

 Number of eigenvalues found =    2

 Eigenvalues
    -2.9936  0.5047
 Selected eigenvectors
             1          2
 1      1.0000     1.0000
       -0.0000    -0.0000

 2      0.1491     0.1882
        0.0777    -0.7410

 3     -1.2303    -0.2080
       -0.4192    -0.4733

 4      0.5811     0.4524
        1.0051     0.9265
```