

NAG Fortran Library Routine Document

F08TBF (DSPGVX)

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

F08TBF (DSPGVX) computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

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

where A and B are symmetric, stored in packed storage, 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 F08TBF (ITYPE, JOBZ, RANGE, UPLO, N, AP, BP, VL, VU, IL, IU,
1              ABSTOL, M, W, Z, LDZ, WORK, IWORK, JFAIL, INFO)
      INTEGER          ITYPE, N, IL, IU, M, LDZ, IWORK(*), JFAIL(*), INFO
      double precision  AP(*), BP(*), VL, VU, ABSTOL, W(*), Z(LDZ,*), WORK(*)
      CHARACTER*1      JOBZ, RANGE, UPLO

```

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

3 Description

F08TBF (DSPGVX) first performs a Cholesky factorization of the matrix B as $B = U^T U$, when $UPLO = 'U'$ or $B = LL^T$, 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 of C are then backtransformed to give the eigenvectors of the original problem.

For the problem $Az = \lambda Bz$ and $ABz = \lambda z$, the eigenvectors are normalized so that

$$z^T Bz = I.$$

For the problem $BAz = \lambda z$ we correspondingly have

$$z^T B^{-1} z = I.$$

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>

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:
 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: RANGE – CHARACTER*1 *Input*
On entry: if RANGE = 'A', all eigenvalues will be found.
 If RANGE = 'V', all eigenvalues in the half-open interval (VL, VU] will be found.
 If RANGE = 'I', the ILth to IUth eigenvalues will be found.
- 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.
- 5: N – INTEGER *Input*
On entry: n , the order of the matrix pencil (A, B) .
Constraint: $N \geq 0$.
- 6: AP(*) – **double precision** 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 symmetric 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.
- 7: BP(*) – **double precision** 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 symmetric 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 $B = U^T U$ or $B = LL^T$, in the same storage format as B .

- 8: VL – **double precision** Input
 9: VU – **double precision** Input
- On entry:* if RANGE = 'V', the lower and upper bounds of the interval to be searched for eigenvalues.
- Constraint:* VL < VU.
- If RANGE = 'A' or 'I', VL and VU are not referenced.
- 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 N = 0, IL = 1 and IU = 0;
 if N > 0, 1 ≤ IL ≤ IU ≤ N.
- 12: ABSTOL – **double precision** 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
- $$\text{ABSTOL} + \epsilon \max(|a|, |b|),$$
- 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 $2 \times \text{X02AMF}()$, not zero. If this routine returns with INFO > 0, indicating that some eigenvectors did not converge, try setting ABSTOL to $2 \times \text{X02AMF}()$. See Demmel and Kahan (1990).
- 13: M – INTEGER Output
- On exit:* the total number of eigenvalues found.
- If RANGE = 'A', M = N.
- If RANGE = 'I', M = IU – IL + 1.
- Constraint:* 0 ≤ M ≤ N.
- 14: W(*) – **double precision** array Output
- Note:** the dimension of the array W must be at least max(1, N).
- On exit:* the first M elements contain the selected eigenvalues in ascending order.
- 15: Z(LDZ,*) – **double precision** array Output
- Note:** the second dimension of the array Z must be at least max(1, M).
- 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 i th column of Z holding the eigenvector associated with W(i). The eigenvectors are normalized as follows:
- if ITYPE = 1 or 2, $Z^T B Z = I$;
 if ITYPE = 3, $Z^T B^{-1} Z = I$.
- If JOBZ = 'N', Z is not referenced.
- If an eigenvector fails to converge, then that column of Z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in JFAIL.

Note: the user 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 must be used.

16: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08TBF (DSPGVX) is called.

Constraints:

if $JOBZ = 'V'$, $LDZ \geq \max(1, N)$;
 $LDZ \geq 1$ otherwise.

17: WORK(*) – **double precision** array *Workspace*

Note: the dimension of the array WORK must be at least $\max(1, 8 \times N)$.

18: IWORK(*) – INTEGER array *Workspace*

Note: the dimension of the array IWORK must be at least $\max(1, 5 \times N)$.

19: 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 $INFO > 0$, JFAIL contains the indices of the eigenvectors that failed to converge.

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

20: 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 i th argument had an illegal value.

$INFO > 0$

F07GDF (DPPTRF) or F08GBF (DSPEVX) returned an error code:

$\leq N$ if $INFO = i$, F08GBF (DSPEVX) failed to converge; i eigenvectors failed to converge. Their indices are stored in array JFAIL;

$> N$ 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 complex analogue of this routine is F08TPF (ZHPGVX).

9 Example

To find the eigenvalues in the half-open interval $(-1.0, 1.0]$, and corresponding eigenvectors, of the generalized symmetric eigenproblem $Az = \lambda Bz$, where

$$A = \begin{pmatrix} 0.24 & 0.39 & 0.42 & -0.16 \\ 0.39 & -0.11 & 0.79 & 0.63 \\ 0.42 & 0.79 & -0.25 & 0.48 \\ -0.16 & 0.63 & 0.48 & -0.03 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.09 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.09 & 0.34 & 1.18 \end{pmatrix}.$$

The example program for F08TCF (DSPGVD) 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.

```
*      F08TBF Example Program Text
*      Mark 21.  NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX
      PARAMETER        (NMAX=10,MMAX=5)
      INTEGER          LDZ
      PARAMETER        (LDZ=NMAX)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
      DOUBLE PRECISION ZERO
      PARAMETER        (ZERO=0.0D+0)
*      .. Local Scalars ..
      DOUBLE PRECISION ABSTOL, VL, VU
      INTEGER          I, IFAIL, IL, INFO, IU, J, M, N
*      .. Local Arrays ..
      DOUBLE PRECISION AP((NMAX*(NMAX+1))/2), BP((NMAX*(NMAX+1))/2),
+      W(NMAX), WORK(8*NMAX), Z(LDZ,MMAX)
      INTEGER          INDEX(NMAX), IWORK(5*NMAX)
*      .. External Subroutines ..
      EXTERNAL         DSPGVX, X04CAF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08TBF Example Program Results'
      WRITE (NOUT,*)
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*          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.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
*

```

```

*      Set the absolute error tolerance for eigenvalues.  With ABSTOL
*      set to zero, the default value is used instead
*
      ABSTOL = ZERO
*
*      Solve the generalized symmetric eigenvalue problem
*      A*x = lambda*B*x (ITYPE = 1)
*
      CALL DSPGVX(1,'Vectors','Values in range',UPLO,N,AP,BP,VL,VU,
+               IL,IU,ABSTOL,M,W,Z,LDZ,WORK,IWORK,INDEX,INFO)
*
      IF (INFO.GE.0 .AND. INFO.LE.N .AND. M.LE.MMAX) THEN
*
*      Print solution
*
        WRITE (NOUT,99999) 'Number of eigenvalues found =', M
        WRITE (NOUT,*)
        WRITE (NOUT,*) 'Eigenvalues'
        WRITE (NOUT,99998) (W(J),J=1,M)
*
        IFAIL = 0
        CALL X04CAF('General',' ',N,M,Z,LDZ,'Selected eigenvectors',
+               IFAIL)
        IF (INFO.GT.0) THEN
+           WRITE (NOUT,99999)
+           'INFO eigenvectors failed to converge, INFO =', INFO
+           WRITE (NOUT,*)
+           'Indices of eigenvectors that did not converge'
+           WRITE (NOUT,99997) (INDEX(J),J=1,M)
        END IF
        ELSE IF (INFO.GT.N .AND. INFO.LE.2*N) THEN
          I = INFO - N
          WRITE (NOUT,99996) 'The leading minor of order ', I,
+          ' of B is not positive definite'
        ELSE IF (M.GT.MMAX) THEN
+           WRITE (NOUT,99995) 'M greater than MMAX, M =', M,
+           ', MMAX =', MMAX
        ELSE
          WRITE (NOUT,99999) 'Failure in DSPGVX. INFO =', INFO
        END IF
      ELSE
        WRITE (NOUT,*)
        WRITE (NOUT,*) 'NMAX too small'
      END IF
      STOP
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (3X,(8F8.4))
99997 FORMAT (3X,(8I8))
99996 FORMAT (1X,A,I4,A)
99995 FORMAT (1X,A,I5,A,I5)
      END

```

9.2 Program Data

F08TBF Example Program Data

```

4                               :Value of N

-1.0    1.0                     :Values of VL and VU

0.24    0.39    0.42   -0.16
      -0.11    0.79    0.63
              -0.25    0.48
                  -0.03   :End of matrix A

4.16   -3.12    0.56   -0.10
      5.03   -0.83    1.09
              0.76    0.34
                  1.18   :End of matrix B

```

9.3 Program Results

F08TBF Example Program Results

Number of eigenvalues found = 2

Eigenvalues

-0.4548 0.1001

Selected eigenvectors

1 2

1 0.3080 0.4469

2 0.5329 0.0371

3 -0.3496 -0.0505

4 -0.6211 -0.4743
