

NAG Fortran Library Routine Document

F08UBF (DSBGVX)

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

F08UBF (DSBGVX) computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite banded eigenproblem, of the form

$$Ax = \lambda Bx,$$

where A and B are symmetric and banded, and B is also positive-definite. Eigenvalues and eigenvectors can be selected by specifying either all eigenvalues, a range of values or a range of indices for the desired eigenvalues.

2 Specification

```

SUBROUTINE F08UBF (JOBZ, RANGE, UPLO, N, KA, KB, AB, LDAB, BB, LDBB, Q,
1                LDQ, VL, VU, IL, IU, ABSTOL, M, W, Z, LDZ, WORK,
2                IWORK, JFAIL, INFO)

    INTEGER          N, KA, KB, LDAB, LDBB, LDQ, IL, IU, M, LDZ, IWORK(*),
1                JFAIL(*), INFO
    double precision AB(LDAB,*), BB(LDBB,*), Q(LDQ,*), VL, VU, ABSTOL,
1                W(*), Z(LDZ,*), WORK(*)
    CHARACTER*1      JOBZ, RANGE, UPLO

```

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

3 Description

The generalized symmetric-definite band problem

$$Az = \lambda Bz$$

is first reduced to a standard band symmetric problem

$$Cx = \lambda x,$$

where C is a symmetric band matrix, using Wilkinson's modification to Crawford's algorithm (see Crawford (1973) and Wilkinson (1977)). The symmetric eigenvalue problem is then solved for the required eigenvalues and eigenvectors, and the eigenvectors are then backtransformed to the eigenvectors of the original problem.

The eigenvectors are normalized so that

$$z^T A z = \lambda \quad \text{and} \quad z^T B z = 1.$$

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>

Crawford C R (1973) Reduction of a band-symmetric generalized eigenvalue problem *Comm. ACM* **16** 41–44

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

Wilkinson J H (1977) Some recent advances in numerical linear algebra *The State of the Art in Numerical Analysis* (ed D A H Jacobs) Academic Press

5 Parameters

- 1: JOBZ – CHARACTER*1 *Input*
On entry: if JOBZ = 'N', compute eigenvalues only.
 If JOBZ = 'V', compute eigenvalues and eigenvectors.
Constraint: JOBZ = 'N' or 'V'.

- 2: 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.

- 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: KA – INTEGER *Input*
On entry: *ka*, the number of super-diagonals of the matrix *A* if UPLO = 'U', or the number of sub-diagonals if UPLO = 'L'.
Constraint: $KA \geq 0$.

- 6: KB – INTEGER *Input*
On entry: *kb*, the number of super-diagonals of the matrix *B* if UPLO = 'U', or the number of sub-diagonals if UPLO = 'L'.
Constraint: $KB \geq 0$.

- 7: AB(LDAB,*) – **double precision** array *Input/Output*
Note: the second dimension of the array AB must be at least $\max(1, N)$.
On entry: the upper or lower triangle of the symmetric band matrix *A*, stored in the first *ka* + 1 rows of the array. The *j*th column of *A* is stored in the *j*th column of the array AB as follows:
 if UPLO = 'U', $AB(ka + 1 + i - j, j) = a_{ij}$ for $\max(1, j - ka) \leq i \leq j$;
 if UPLO = 'L', $AB(1 + i - j, j) = a_{ij}$ for $j \leq i \leq \min(n, j + ka)$.
On exit: the contents of AB are destroyed.

- 8: LDAB – INTEGER *Input*
On entry: the first dimension of the array AB as declared in the (sub)program from which F08UBF (DSBGVX) is called.
Constraint: $LDAB \geq KA + 1$.

- 9: BB(LDBB,*) – **double precision** array *Input/Output*
Note: the second dimension of the array BB must be at least $\max(1, N)$.
On entry: the upper or lower triangle of the symmetric band matrix B , stored in the first $kb + 1$ rows of the array. The j th column of B is stored in the j th column of the array BB as follows:
if UPLO = 'U', $BB(kb + 1 + i - j, j) = b_{ij}$ for $\max(1, j - kb) \leq i \leq j$;
if UPLO = 'L', $BB(1 + i - j, j) = b_{ij}$ for $j \leq i \leq \min(n, j + kb)$.
On exit: the factor S from the split Cholesky factorization $B = S^T S$, as returned by F08UFF (DPBSTF).
- 10: LDBB – INTEGER *Input*
On entry: the first dimension of the array BB as declared in the (sub)program from which F08UBF (DSBGVX) is called.
Constraint: $LDBB \geq KB + 1$.
- 11: Q(LDQ,*) – **double precision** array *Output*
Note: the second dimension of the array Q must be at least $\max(1, N)$.
On exit: if JOBZ = 'V', the n by n matrix used in the reduction of $Az = \lambda Bz$ to standard form, i.e., $Cx = \lambda x$, and subsequently C to tridiagonal form.
If JOBZ = 'N', Q is not referenced.
- 12: LDQ – INTEGER *Input*
On entry: the first dimension of the array Q as declared in the (sub)program from which F08UBF (DSBGVX) is called.
Constraints:
if JOBZ = 'N', $LDQ \geq 1$;
if JOBZ = 'V', $LDQ \geq \max(1, N)$.
- 13: VL – **double precision** *Input*
14: 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 'T', VL and VU are not referenced.
- 15: IL – INTEGER *Input*
16: IU – INTEGER *Input*
On entry: if RANGE = 'T', 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 $N > 0$, $1 \leq IL \leq IU \leq N$.
- 17: 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

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

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 > 0, indicating that some eigenvectors did not converge, try setting ABSTOL to $2 \times X02AMF()$. See Demmel and Kahan (1990).

- 18: M – INTEGER *Output*
On exit: the total number of eigenvalues found.
 If RANGE = 'A', M = N.
 If RANGE = 'I', M = IU – IL + 1.
Constraint: $0 \leq M \leq N$.
- 19: 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.
- 20: Z(LDZ,*) – *double precision* array *Output*
Note: the second dimension of the array Z must be at least max(1, N).
On exit: if JOBZ = 'V', then if INFO = 0, Z contains the matrix Z of eigenvectors, with the i th column of Z holding the eigenvector associated with $W(i)$. The eigenvectors are normalized so that $Z^T B Z = I$.
 If JOBZ = 'N', Z is not referenced.
- 21: LDZ – INTEGER *Input*
On entry: the first dimension of the array Z as declared in the (sub)program from which F08UBF (DSBGVX) is called.
Constraints:
 if JOBZ = 'V', LDZ $\geq$ max(1, N);
 LDZ $\geq$ 1 otherwise.
- 22: WORK(*) – *double precision* array *Workspace*
Note: the dimension of the array WORK must be at least max(1, 7 $\times$ N).
- 23: IWORK(*) – INTEGER array *Workspace*
Note: the dimension of the array IWORK must be at least max(1, 5 $\times$ N).
- 24: JFAIL(*) – INTEGER array *Output*
Note: the dimension of the array JFAIL must be at least max(1, M).
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 eigenvalues that failed to converge.
 If JOBZ = 'N', JFAIL is not referenced.
- 25: 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 and INFO ≤ N

if INFO = i , then i eigenvectors failed to converge. Their indices are stored in JFAIL. Please see ABSTOL.

INFO > N

F08UFF (DPBSTF) 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 if JOBZ = 'V' and RANGE = 'A', and assuming that $n \gg k_a$, is approximately proportional to $n^2 k_a$ if JOBZ = 'N'. Otherwise the number of floating point operations depends upon the number of eigenvectors computed.

The complex analogue of this routine is F08UPF (ZHBGVX).

9 Example

To find the eigenvalues in the half-open interval $(0.0, 1.0]$, and corresponding eigenvectors, of the generalized band symmetric eigenproblem $Ax = \lambda Bx$, where

$$A = \begin{pmatrix} 0.24 & 0.39 & 0.42 & 0 \\ 0.39 & -0.11 & 0.79 & 0.63 \\ 0.42 & 0.79 & -0.25 & 0.48 \\ 0 & 0.63 & 0.48 & -0.03 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 2.07 & 0.95 & 0 & 0 \\ 0.95 & 1.69 & -0.29 & 0 \\ 0 & -0.29 & 0.65 & -0.33 \\ 0 & 0 & -0.33 & 1.17 \end{pmatrix}.$$

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.

```
*      F08UBF Example Program Text
*      Mark 21.  NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5, NOUT=6)
      INTEGER          KAMAX, KBMAX, NMAX, MMAX
      PARAMETER        (KAMAX=5, KBMAX=5, NMAX=20, MMAX=10)
```

```

INTEGER          LDAB, LDBB, LDQ, LDZ
PARAMETER        (LDAB=KAMAX+1,LDBB=KBMAX+1,LDQ=NMAX,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, KA, KB, M, N
*
.. Local Arrays ..
DOUBLE PRECISION AB(LDAB,NMAX), BB(LDBB,NMAX), Q(LDQ,NMAX),
+                W(NMAX), WORK(7*NMAX), Z(LDZ,MMAX)
INTEGER          INDEX(NMAX), IWORK(5*NMAX)
*
.. External Subroutines ..
EXTERNAL         DSBGVX, X04CAF
*
.. Intrinsic Functions ..
INTRINSIC        MAX, MIN
*
.. Executable Statements ..
WRITE (NOUT,*) 'F08UBF Example Program Results'
WRITE (NOUT,*)
*
Skip heading in data file
READ (NIN,*)
READ (NIN,*) N, KA, KB
IF (N.LE.NMAX .AND. KA.LE.KAMAX .AND. KB.LE.KBMAX) 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,*) ((AB(KA+1+I-J,J),J=I,MIN(N,I+KA)),I=1,N)
  READ (NIN,*) ((BB(KB+1+I-J,J),J=I,MIN(N,I+KB)),I=1,N)
ELSE IF (UPLO.EQ.'L') THEN
  READ (NIN,*) ((AB(1+I-J,J),J=MAX(1,I-KA),I),I=1,N)
  READ (NIN,*) ((BB(1+I-J,J),J=MAX(1,I-KB),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
*
CALL DSBGVX('Vectors','Values in range',UPLO,N,KA,KB,AB,LDAB,
+          BB,LDBB,Q,LDQ,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 DSBGVX. 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

F08UBF Example Program Data

```

4      2      1      :Values of N, KA and KB

0.0    1.0      :Values of VL and VU

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

2.07   0.95
      1.69  -0.29
           0.65  -0.33
           1.17 :End of matrix B

```

9.3 Program Results

F08UBF Example Program Results

Number of eigenvalues found = 1

Eigenvalues

0.0992

Selected eigenvectors

```

1
1  0.6729
2 -0.1009
3  0.0155
4 -0.3806

```
