

NAG Fortran Library Routine Document

F08FBF (DSYEVX)

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

F08FBF (DSYEVX) computes selected eigenvalues and, optionally, eigenvectors of a real n by n symmetric matrix A . 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 F08FBF (JOBZ, RANGE, UPLO, N, A, LDA, VL, VU, IL, IU, ABSTOL,
1                M, W, Z, LDZ, WORK, LWORK, IWORK, JFAIL, INFO)
    INTEGER       N, LDA, IL, IU, M, LDZ, LWORK, IWORK(*), JFAIL(*),
1                INFO
    double precision A(LDA,*), VL, VU, ABSTOL, W(*), Z(LDZ,*), WORK(*)
    CHARACTER*1   JOBZ, RANGE, UPLO

```

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

3 Description

The symmetric matrix A is first reduced to tridiagonal form, using orthogonal similarity transformations. The required eigenvalues and eigenvectors are then computed from the tridiagonal matrix; the method used depends upon whether all, or selected, eigenvalues and eigenvectors are required.

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: 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 triangle of A is stored.
 If UPLO = 'L', the lower triangle of A is stored.
- 4: N – INTEGER *Input*
On entry: n , the order of the matrix A .
Constraint: $N \geq 0$.
- 5: A(LDA,*) – **double precision** array *Input/Output*
Note: the second dimension of the array A must be at least $\max(1, N)$.
On entry: the n by n symmetric matrix A .
 If UPLO = 'U', the leading n by n upper triangular part of A contains the upper triangular part of the matrix A .
 If UPLO = 'L', the leading n by n lower triangular part of A contains the lower triangular part of the matrix A .
On exit: the lower triangle (if UPLO = 'L') or the upper triangle (if UPLO = 'U') of A , including the diagonal, is destroyed.
- 6: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F08FBF (DSYEVX) is called.
Constraint: $LDA \geq \max(1, N)$.
- 7: VL – **double precision** *Input*
 8: 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.
- 9: IL – INTEGER *Input*
 10: 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 $N > 0$, $1 \leq IL \leq IU \leq N$.
- 11: 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 A 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).
- 12: M – INTEGER *Output*
On exit: the total number of eigenvalues found.
 If RANGE = 'A', $M = N$.
 If RANGE = 'I', $M = IU - IL + 1$.
Constraint: $0 \leq M \leq N$.
- 13: 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.
- 14: 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 $W(i)$.
 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.
 If JOBZ = 'N', Z is not referenced.
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.
- 15: LDZ – INTEGER *Input*
On entry: the first dimension of the array Z as declared in the (sub)program from which F08FBF (DSYEVX) is called.
Constraints:
 if JOBZ = 'V', $LDZ \geq \max(1, N)$;
 $LDZ \geq 1$ otherwise.
- 16: WORK(*) – *double precision* array *Workspace*
Note: the dimension of the array WORK must be at least $\max(1, LWORK)$.
On exit: if INFO = 0, WORK(1) returns the optimal LWORK.
- 17: LWORK – INTEGER *Input*
On entry: the dimension of the array WORK as declared in the (sub)program from which F08FBF (DSYEVX) is called.
 For optimal efficiency, $LWORK \geq (nb + 3) \times N$, where nb is the largest optimal block size for F08FEF (DSYTRD) and F08FGF (DORMTR).
 If LWORK = -1, a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.
Constraint: $LWORK \geq \max(1, 8 \times N)$.
- 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

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

7 Accuracy

The computed eigenvalues and eigenvectors are exact for a nearby matrix $(A + E)$, where

$$\|E\|_2 = O(\epsilon)\|A\|_2,$$

and ϵ is the *machine precision*. See Section 4.7 of Anderson *et al.* (1999) for further details.

8 Further Comments

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

The complex analogue of this routine is F08FPF (ZHHEEVX).

9 Example

To find the eigenvalues in the half-open interval $(-1, 1]$, and the corresponding eigenvectors, of the symmetric matrix

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 2 & 3 & 4 \\ 3 & 3 & 3 & 4 \\ 4 & 4 & 4 & 4 \end{pmatrix}.$$

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.

```
*      F08FBB Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
INTEGER          NIN, NOUT
PARAMETER       (NIN=5, NOUT=6)
INTEGER          NB, NMAX, MMAX
PARAMETER       (NB=64, NMAX=10, MMAX=5)
INTEGER          LDA, LDZ, LWORK
PARAMETER       (LDA=NMAX, LDZ=NMAX, LWORK=(NB+3)*NMAX)
DOUBLE PRECISION ZERO
```

```

PARAMETER          (ZERO=0.0D+0)
*
* .. Local Scalars ..
DOUBLE PRECISION  ABSTOL, VL, VU
INTEGER           I, IFAIL, IL, INFO, IU, J, LWKOPT, M, N
*
* .. Local Arrays ..
DOUBLE PRECISION  A(LDA,NMAX), W(NMAX), WORK(LWORK), Z(LDZ,MMAX)
INTEGER           INDEX(NMAX), IWORK(5*NMAX)
*
* .. External Subroutines ..
EXTERNAL          DSYEVX, X04CAF
*
* .. Executable Statements ..
WRITE (NOUT,*) 'F08FBF 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 triangular part of the matrix A from data
*   file
*
*   READ (NIN,*) VL, VU
*   READ (NIN,*) ((A(I,J),J=I,N),I=1,N)
*
*   Set the absolute error tolerance for eigenvalues.  With ABSTOL
*   set to zero, the default value is used instead
*
*   ABSTOL = ZERO
*
*   Solve the symmetric eigenvalue problem
*
*   CALL DSYEVX('Vectors','Values in range','Upper',N,A,LDA,VL,VU,
+           IL,IU,ABSTOL,M,W,Z,LDZ,WORK,LWORK,IWORK,INDEX,INFO)
*   LWKOPT = WORK(1)
*
*   IF (INFO.GE.0 .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 (M.GT.MMAX) THEN
*           WRITE (NOUT,99996) 'M greater than MMAX, M =', M,
+           ', MMAX =', MMAX
*       ELSE
*           WRITE (NOUT,99999) 'Failure in DSYEVX. INFO =', INFO
*       END IF
*
*   Print workspace information
*
*   IF (LWORK.LT.LWKOPT) THEN
*       WRITE (NOUT,*)
*       WRITE (NOUT,99995) 'Optimum workspace required = ', LWKOPT,
+       'Workspace provided      = ', LWORK
*   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,I5,A,I5)
99995 FORMAT (1X,A,I5,/1X,A,I5)
      END

```

9.2 Program Data

```

F08FBF Example Program Data
  4                               :Value of N
-1.0  1.0                        :Values of VL and VU
  1.0  2.0  3.0  4.0
      2.0  3.0  4.0
          3.0  4.0
              4.0 :End of matrix A

```

9.3 Program Results

F08FBF Example Program Results

Number of eigenvalues found = 2

```

Eigenvalues
  -0.5146 -0.2943
Selected eigenvectors
      1      2
1  -0.5144  0.2767
2   0.4851 -0.6634
3   0.5420  0.6504
4  -0.4543 -0.2457

```
