

# NAG Library Routine Document

## F08FAF (DSYEV)

**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

F08FAF (DSYEV) computes all the eigenvalues and, optionally, all the eigenvectors of a real  $n$  by  $n$  symmetric matrix  $A$ .

### 2 Specification

```
SUBROUTINE F08FAF(JOBZ, UPLO, N, A, LDA, W, WORK, LWORK, INFO)
INTEGER          N, LDA, LWORK, INFO
double precision A(LDA,*), W(*), WORK(max(1,LWORK))
CHARACTER*1      JOBZ, UPLO
```

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

### 3 Description

The symmetric matrix  $A$  is first reduced to tridiagonal form, using orthogonal similarity transformations, and then the  $QR$  algorithm is applied to the tridiagonal matrix to compute the eigenvalues and (optionally) the eigenvectors.

### 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>

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: UPLO – CHARACTER\*1 *Input*  
*On entry:* if UPLO = 'U', the upper triangular part of  $A$  is stored.  
 If UPLO = 'L', the lower triangular part of  $A$  is stored.  
*Constraint:* UPLO = 'U' or 'L'.
- 3: N – INTEGER *Input*  
*On entry:*  $n$ , the order of the matrix  $A$ .  
*Constraint:*  $N \geq 0$ .

- 4: 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 upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced.

If UPLO = 'L', the lower triangular part of A must be stored and the elements of the array above the diagonal are not referenced.

*On exit:* if JOBZ = 'V', then if INFO = 0, A contains the orthonormal eigenvectors of the matrix  $A$ .

If JOBZ = 'N', then on exit the lower triangle (if UPLO = 'L') or the upper triangle (if UPLO = 'U') of A, including the diagonal, is destroyed.

- 5: LDA – INTEGER *Input*

*On entry:* the first dimension of the array A as declared in the (sub)program from which F08FAF (DSYEV) is called.

*Constraint:*  $LDA \geq \max(1, N)$ .

- 6: 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.

- 7: WORK( $\max(1, LWORK)$ ) – **double precision** array *Workspace*

*On exit:* if INFO = 0, WORK(1) contains the minimum value of LWORK required for optimal performance.

- 8: LWORK – INTEGER *Input*

*On entry:* the dimension of the array WORK as declared in the (sub)program from which F08FAF (DSYEV) is called.

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.

*Suggested value:* for optimal performance,  $LWORK \geq (nb + 2) \times N$ , where  $nb$  is the optimal **block size** for F08FEF (DSYTRD).

*Constraint:*  $LWORK \geq \max(1, 3 \times N - 1)$ .

- 9: 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 > 0

If INFO =  $i$ , the algorithm failed to converge;  $i$  off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

## 7 Accuracy

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

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

and  $\epsilon$  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 F08FNF (ZHEEV).

## 9 Example

This example finds all the eigenvalues and eigenvectors of the symmetric matrix

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

together with approximate error bounds for the computed eigenvalues and eigenvectors.

### 9.1 Program Text

```
*      F08FAF Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NB, NMAX
      PARAMETER        (NB=64,NMAX=10)
      INTEGER          LDA, LWORK
      PARAMETER        (LDA=NMAX,LWORK=(NB+2)*NMAX)
*      .. Local Scalars ..
      DOUBLE PRECISION EERRBD, EPS
      INTEGER          I, IFAIL, INFO, J, LWKOPT, N
*      .. Local Arrays ..
      DOUBLE PRECISION A(LDA,NMAX), RCONDZ(NMAX), W(NMAX), WORK(LWORK),
+      ZERRBD(NMAX)
*      .. External Functions ..
      DOUBLE PRECISION X02AJF
      EXTERNAL          X02AJF
*      .. External Subroutines ..
      EXTERNAL          DDISNA, DSYEV, X04CAF
*      .. Intrinsic Functions ..
      INTRINSIC          ABS, INT, MAX
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08FAF Example Program Results'
      WRITE (NOUT,*)
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*          Read the upper triangular part of the matrix A from data file
*
*          READ (NIN,*) ((A(I,J),J=I,N),I=1,N)
*
*          Solve the symmetric eigenvalue problem
*
*          CALL DSYEV('Vectors','Upper',N,A,LDA,W,WORK,LWORK,INFO)
      LWKOPT = INT(WORK(1))
*
*          IF (INFO.EQ.0) THEN
```

```

*
*      Print solution
*
*      WRITE (NOUT,*) 'Eigenvalues'
*      WRITE (NOUT,99999) (W(J),J=1,N)
*
*      IFAIL = 0
*      CALL X04CAF('General',' ',N,N,A,LDA,'Eigenvectors',IFAIL)
*
*      Get the machine precision, EPS and compute the approximate
*      error bound for the computed eigenvalues. Note that for
*      the 2-norm, max( abs(W(i)) ) = norm(A), and since the
*      eigenvalues are returned in ascending order
*      max( abs(W(i)) ) = max( abs(W(1)), abs(W(n)) )
*
*      EPS = X02AJF()
*      EERRBD = EPS*MAX(ABS(W(1)),ABS(W(N)))
*
*      Call DDISNA (F08FLF) to estimate reciprocal condition
*      numbers for the eigenvectors
*
*      CALL DDISNA('Eigenvectors',N,N,W,RCONDZ,INFO)
*
*      Compute the error estimates for the eigenvectors
*
*      DO 20 I = 1, N
*          ZERRBD(I) = EERRBD/RCONDZ(I)
20      CONTINUE
*
*      Print the approximate error bounds for the eigenvalues
*      and vectors
*
*      WRITE (NOUT,*)
*      WRITE (NOUT,*) 'Error estimate for the eigenvalues'
*      WRITE (NOUT,99998) EERRBD
*      WRITE (NOUT,*)
*      WRITE (NOUT,*) 'Error estimates for the eigenvectors'
*      WRITE (NOUT,99998) (ZERRBD(I),I=1,N)
*      ELSE
*          WRITE (NOUT,99997) 'Failure in DSYEV. INFO =', INFO
*      END IF
*
*      Print workspace information
*
*      IF (LWORK.LT.LWKOPT) THEN
*          WRITE (NOUT,*)
*          WRITE (NOUT,99996) 'Optimum workspace required = ', LWKOPT,
+          'Workspace provided          = ', LWORK
*      END IF
*      ELSE
*          WRITE (NOUT,*) 'NMAX too small'
*      END IF
*
99999 FORMAT (3X,(8F8.4))
99998 FORMAT (4X,1P,6E11.1)
99997 FORMAT (1X,A,I4)
99996 FORMAT (1X,A,I5,/1X,A,I5)
END

```

## 9.2 Program Data

F08FAF Example Program Data

```

4                      :Value of N

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

F08FAF Example Program Results

Eigenvalues

-2.0531 -0.5146 -0.2943 12.8621

Eigenvectors

|   | 1       | 2       | 3       | 4      |
|---|---------|---------|---------|--------|
| 1 | 0.7003  | -0.5144 | -0.2767 | 0.4103 |
| 2 | 0.3592  | 0.4851  | 0.6634  | 0.4422 |
| 3 | -0.1569 | 0.5420  | -0.6504 | 0.5085 |
| 4 | -0.5965 | -0.4543 | 0.2457  | 0.6144 |

Error estimate for the eigenvalues

1.4E-15

Error estimates for the eigenvectors

|         |         |         |         |
|---------|---------|---------|---------|
| 9.3E-16 | 6.5E-15 | 6.5E-15 | 1.1E-16 |
|---------|---------|---------|---------|

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