NAG Library Routine Document

F08GAF (DSPEV)

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

F08GAF (DSPEV) computes all the eigenvalues and, optionally, all the eigenvectors of a real n by n symmetric matrix A in packed storage.

2 Specification

```
SUBROUTINE F08GAF (JOBZ, UPLO, N, AP, W, Z, LDZ, WORK, INFO)

INTEGER             N, LDZ, INFO
REAL (KIND=nag_wp) AP(*), W(N), Z(LDZ,*), WORK(3*N)
CHARACTER(1)        JOBZ, UPLO
```

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

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: indicates whether eigenvectors are computed.

JOBZ = 'N'
Only eigenvalues are computed.

JOBZ = 'V'
Eigenvalues and eigenvectors are computed.

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: AP($*$) – REAL (KIND=nag_wp) 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 n by n symmetric 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: AP is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.

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

On exit: the eigenvalues in ascending order.

6: Z(LDZ,$*$) – REAL (KIND=nag_wp) array *Output*

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

On exit: if JOBZ = 'V', Z contains the orthonormal eigenvectors of the matrix A, with the ith column of Z holding the eigenvector associated with W(i).

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

7: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08GAF (DSPEV) is called.

Constraints:

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

8: WORK($3 \times N$) – REAL (KIND=nag_wp) array *Workspace*

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 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 F08GNF (ZHPEV).

9 Example

This example finds all the eigenvalues 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.

9.1 Program Text

```
    Program f08gafe

!     F08GAF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: dspev, nag_wp, x02ajf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
      Character (1), Parameter         :: uplo = 'U'
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: eerrbd, eps
      Integer                          :: i, info, j, n
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: ap(:), w(:), work(:)
      Real (Kind=nag_wp)               :: dummy(1,1)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: abs, max
!     .. Executable Statements ..
      Write (nout,*) 'F08GAF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n

      Allocate (ap((n*(n+1))/2),w(n),work(3*n))

!     Read the upper or lower triangular part of the matrix A from
!     data file

      If (uplo=='U') Then
        Read (nin,*)((ap(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)
      End If

!     Solve the symmetric eigenvalue problem
```

```
!     The NAG name equivalent of dspev is f08gaf
      Call dspev('No vectors',uplo,n,ap,w,dummy,1,work,info)

      If (info==0) Then

!       Print solution

        Write (nout,*) 'Eigenvalues'
        Write (nout,99999) w(1:n)

!       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)))

!       Print the approximate error bound for the eigenvalues

        Write (nout,*)
        Write (nout,*) 'Error estimate for the eigenvalues'
        Write (nout,99998) eerrbd
      Else
        Write (nout,99997) 'Failure in DSPEV. INFO =', info
      End If

99999 Format (3X,(8F8.4))
99998 Format (4X,1P,6E11.1)
99997 Format (1X,A,I4)
    End Program f08gafe
```

9.2 Program Data

```
F08GAF 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

```
 F08GAF Example Program Results

 Eigenvalues
    -2.0531 -0.5146 -0.2943 12.8621

 Error estimate for the eigenvalues
        1.4E-15
```