

NAG Library Routine Document

F08GCF (DSPEVD)

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.

Warning. The specification of the parameters LWORK and LIWORK changed at Mark 20 in the case where JOB = 'V' and N > 1: the minimum dimension of the array WORK has been reduced whereas the minimum dimension of the array IWORK has been increased.

1 Purpose

F08GCF (DSPEVD) computes all the eigenvalues and, optionally, all the eigenvectors of a real symmetric matrix held in packed storage. If the eigenvectors are requested, then it uses a divide-and-conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal–Walker–Kahan variant of the *QL* or *QR* algorithm.

2 Specification

```
SUBROUTINE F08GCF(JOB, UPLO, N, AP, W, Z, LDZ, WORK, LWORK, IWORK,
1                LIWORK, INFO)
    INTEGER          N, LDZ, LWORK, IWORK(max(1,LIWORK)), LIWORK, INFO
    double precision AP(*), W(*), Z(LDZ,*), WORK(max(1,LWORK))
    CHARACTER*1      JOB, UPLO
```

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

3 Description

F08GCF (DSPEVD) computes all the eigenvalues and, optionally, all the eigenvectors of a real symmetric matrix A (held in packed storage). In other words, it can compute the spectral factorization of A as

$$A = Z\Lambda Z^T,$$

where Λ is a diagonal matrix whose diagonal elements are the eigenvalues λ_i , and Z is the orthogonal matrix whose columns are the eigenvectors z_i . Thus

$$Az_i = \lambda_i z_i, \quad i = 1, 2, \dots, n.$$

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: JOB – CHARACTER*1 *Input*
On entry: indicates whether eigenvectors are computed.
 JOB = 'N'
 Only eigenvalues are computed.

JOB = 'V'

Eigenvalues and eigenvectors are computed.

Constraint: JOB = 'N' or 'V'.

2: UPLO – CHARACTER*1

Input

On entry: indicates whether the upper or lower triangular part of A is stored.

UPLO = 'U'

The upper triangular part of A is stored.

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(*) – **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 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(*) – **double precision** array

Output

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

On exit: the eigenvalues of the matrix A in ascending order.

6: Z(LDZ,*) – **double precision** array

Output

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

On exit: if JOB = 'V', Z is overwritten by the orthogonal matrix Z which contains the eigenvectors of A .

If JOB = '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 F08GCF (DSPEVD) is called.

Constraints:

if JOB = 'V', $LDZ \geq \max(1, N)$;

if JOB = 'N', $LDZ \geq 1$.

- 8: WORK(max(1,LWORK)) – **double precision** array *Workspace*
On exit: if INFO = 0, WORK(1) contains the required minimal size of LWORK.
- 9: LWORK – INTEGER *Input*
On entry: the dimension of the array WORK as declared in the (sub)program from which F08GCF (DSPEVD) is called.
 If LWORK = -1, a workspace query is assumed; the routine only calculates the minimum dimension of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.
Constraints:
 if $N \leq 1$, LWORK ≥ 1 or LWORK = -1;
 if JOB = 'N' and $N > 1$, LWORK $\geq 2 \times N$ or LWORK = -1;
 if JOB = 'V' and $N > 1$, LWORK $\geq N^2 + 6 \times N + 1$ or LWORK = -1.
- 10: IWORK(max(1,LIWORK)) – INTEGER array *Workspace*
On exit: if INFO = 0, IWORK(1) contains the required minimal size of LIWORK.
- 11: LIWORK – INTEGER *Input*
On entry: the dimension of the array IWORK as declared in the (sub)program from which F08GCF (DSPEVD) is called.
 If LIWORK = -1, a workspace query is assumed; the routine only calculates the minimum dimension of the IWORK array, returns this value as the first entry of the IWORK array, and no error message related to LIWORK is issued.
Constraints:
 if JOB = 'N' or $N \leq 1$, LIWORK ≥ 1 or LIWORK = -1;
 if JOB = 'V' and $N > 1$, LIWORK $\geq 5 \times N + 3$ or LIWORK = -1.
- 12: 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 and JOB = 'N', the algorithm failed to converge; i elements of an intermediate tridiagonal form did not converge to zero; if INFO = i and JOB = 'V', then the algorithm failed to compute an eigenvalue while working on the submatrix lying in rows and column $i/(N+1)$ through mod($i, N+1$).

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 complex analogue of this routine is F08GQF (ZHPEVD).

9 Example

This example computes all the eigenvalues and eigenvectors of the symmetric matrix A , where

$$A = \begin{pmatrix} 1.0 & 2.0 & 3.0 & 4.0 \\ 2.0 & 2.0 & 3.0 & 4.0 \\ 3.0 & 3.0 & 3.0 & 4.0 \\ 4.0 & 4.0 & 4.0 & 4.0 \end{pmatrix}.$$

9.1 Program Text

```
*      F08GCF Example Program Text
*      Mark 20 Revised. NAG Copyright 2001.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, LDZ
      PARAMETER        (NMAX=8,LDZ=NMAX)
      INTEGER          LWORK, LIWORK
      PARAMETER        (LWORK=NMAX*NMAX+6*NMAX+1,LIWORK=5*NMAX+3)
      INTEGER          MMAX
      PARAMETER        (MMAX=NMAX*(NMAX+1)/2)
*      .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N
      CHARACTER        JOB, UPLO
*      .. Local Arrays ..
      DOUBLE PRECISION AP(MMAX), W(NMAX), WORK(LWORK), Z(LDZ,NMAX)
      INTEGER          IWORK(LIWORK)
*      .. External Subroutines ..
      EXTERNAL         DSPEVD, X04CAF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08GCF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*          Read A from data file
*
*          READ (NIN,*) UPLO
*          IF (UPLO.EQ.'U') THEN
*              READ (NIN,*) ((AP(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)
*          END IF
*
*          READ (NIN,*) JOB
*
*          Calculate all the eigenvalues and eigenvectors of A
*
*          CALL DSPEVD(JOB,UPLO,N,AP,W,Z,LDZ,WORK,LWORK,IWORK,LIWORK,INFO)
*
*          WRITE (NOUT,*)
*          IF (INFO.GT.0) THEN
*              WRITE (NOUT,*) 'Failure to converge.'
*          ELSE
*
*              Print eigenvalues and eigenvectors
*
*              WRITE (NOUT,*) 'Eigenvalues'
*              WRITE (NOUT,99999) (W(I),I=1,N)
*              WRITE (NOUT,*)
*              IFAIL = 0
*
*              CALL X04CAF('General',' ',N,N,Z,LDZ,'Eigenvectors',IFAIL)
```

```

*
      END IF
END IF
*
99999 FORMAT (3X,(8F8.4))
      END

```

9.2 Program Data

```

F08GCF Example Program Data
  4                               :Value of N
  'L'                           :Value of UPLO
  1.0
  2.0  2.0
  3.0  3.0  3.0
  4.0  4.0  4.0  4.0           :End of matrix A
  'V'                           :Value of JOB

```

9.3 Program Results

F08GCF 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
