

# NAG Fortran Library Routine Document

## F08GCF (SSPEVD/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 (SSPEVD/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)
ENTRY          sspevd (JOB, UPLO, N, AP, W, Z, LDZ, WORK, LWORK, IWORK,
1                LIWORK, INFO)
INTEGER        N, LDZ, LWORK, IWORK(*), LIWORK, INFO
real          AP(*), W(*), Z(LDZ,*), WORK(*)
CHARACTER*1    JOB, UPLO

```

The ENTRY statement enables the routine to be called by its LAPACK name.

### 3 Description

This routine 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  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , 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

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 as follows:

if JOB = 'N', only eigenvalues are computed;

if 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 as follows:  
 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* array *Input/Output*  
**Note:** the dimension of the array AP must be at least  $\max(1, N * (N + 1) / 2)$ .  
*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:*  $A$  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(\*) – *real* 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,\*) – *real* 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 (SSPEVD/DSPEVD) is called.  
*Constraints:*  
 $LDZ \geq \max(1, N)$  if JOB = 'V',  
 $LDZ \geq 1$  if JOB = 'N'.
- 8: WORK(\*) – *real* array *Workspace*  
**Note:** the dimension of the array WORK must be at least  $\max(1, LWORK)$ .  
*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 (SSPEVD/DSPEVD) is called, unless LWORK = -1, in which case a workspace query is assumed and the routine only calculates the minimum dimension of WORK.

*Constraints:*

- if  $N \leq 1$ , LWORK  $\geq 1$  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(\*) – INTEGER array

*Workspace*

**Note:** the dimension of the array IWORK must be at least  $\max(1, \text{LIWORK})$ .

*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 (SSPEVD/DSPEVD) is called, unless LIWORK = -1, in which case a workspace query is assumed and the routine only calculates the minimum dimension of IWORK.

*Constraints:*

- if JOB = 'N' or  $N \leq 1$ , LIWORK  $\geq 1$  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 = - $i$ , the  $i$ th parameter 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;  $i$  indicates the number of elements of an intermediate tridiagonal form which 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*.

## 8 Further Comments

The complex analogue of this routine is F08GQF (CHPEVD/ZHPEVD).

## 9 Example

To compute 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

**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.

```
*      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 ..
      real            AP(MMAX), W(NMAX), WORK(LWORK), Z(LDZ,NMAX)
      INTEGER          IWORK(LIWORK)
*      .. External Subroutines ..
      EXTERNAL         sspevd, 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 sspevd(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
      STOP
*
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

```

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