NAG C Library Function Document

nag_dspevd (f08gcc)

1 Purpose

nag_dspevd (f08gcc) 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

```
void nag_dspevd (Nag_OrderType order, Nag_JobType job, Nag_UploType uplo,
     Integer n, double ap[], double w[], double z[], Integer pdz, NagError *fail)
```

3 Description

nag_dspevd (f08gcc) 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

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1: **order** – Nag_OrderType *Input*

On entry: the **order** parameter specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = **Nag_RowMajor**. See Section 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this parameter.

Constraint: **order** = **Nag_RowMajor** or **Nag_ColMajor**.

2: **job** – Nag_JobType *Input*

On entry: indicates whether eigenvectors are computed as follows:

if **job** = **Nag_DoNothing**, only eigenvalues are computed;

if **job** = **Nag_EigVecs**, eigenvalues and eigenvectors are computed.

Constraint: **job** = **Nag_DoNothing** or **Nag_EigVecs**.

3: **uplo** – Nag_UploType *Input*

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

if **uplo** = **Nag_Upper**, the upper triangular part of A is stored;

if **uplo** = **Nag_Lower**, the lower triangular part of A is stored.

Constraint: **uplo** = **Nag_Upper** or **Nag_Lower**.

4: **n** – Integer *Input*

On entry: n, the order of the matrix A.

Constraint: $\mathbf{n} \geq 0$.

5: **ap**[dim] – double *Input/Output*

Note: the dimension, dim, of the array **ap** must be at least $\max(1, \mathbf{n} \times (\mathbf{n} + 1)/2)$.

On entry: the symmetric matrix A, packed by rows or columns. The storage of elements a_{ij} depends on the **order** and **uplo** parameters as follows:

if **order** = **Nag_ColMajor** and **uplo** = **Nag_Upper**,
a_{ij} is stored in **ap**$[(j-1) \times j/2 + i - 1]$, for $i \leq j$;

if **order** = **Nag_ColMajor** and **uplo** = **Nag_Lower**,
a_{ij} is stored in **ap**$[(2n-j) \times (j-1)/2 + i - 1]$, for $i \geq j$;

if **order** = **Nag_RowMajor** and **uplo** = **Nag_Upper**,
a_{ij} is stored in **ap**$[(2n-i) \times (i-1)/2 + j - 1]$, for $i \leq j$;

if **order** = **Nag_RowMajor** and **uplo** = **Nag_Lower**,
a_{ij} is stored in **ap**$[(i-1) \times i/2 + j - 1]$, 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.

6: **w**[dim] – double *Output*

Note: the dimension, dim, of the array **w** must be at least $\max(1, \mathbf{n})$.

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

7: **z**[dim] – double *Output*

Note: the dimension, dim, of the array **z** must be at least
$\max(1, \mathbf{pdz} \times \mathbf{n})$ when **job** = **Nag_EigVecs**;
1 when **job** = **Nag_DoNothing**.

If **order** = **Nag_ColMajor**, the (i, j)th element of the matrix Z is stored in **z**$[(j-1) \times \mathbf{pdz} + i - 1]$ and if **order** = **Nag_RowMajor**, the (i, j)th element of the matrix Z is stored in **z**$[(i-1) \times \mathbf{pdz} + j - 1]$.

On exit: if **job** = **Nag_EigVecs**, **z** is overwritten by the orthogonal matrix Z which contains the eigenvectors of A.

If **job** = **Nag_DoNothing**, **z** is not referenced.

8: **pdz** – Integer *Input*

On entry: the stride separating matrix row or column elements (depending on the value of **order**) in the array **z**.

Constraints:

if **job** = **Nag_EigVecs**, $\mathbf{pdz} \geq \max(1, \mathbf{n})$;
if **job** = **Nag_DoNothing**, $\mathbf{pdz} \geq 1$.

9: **fail** – NagError * *Output*

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** ≥ 0.

On entry, **pdz** = ⟨*value*⟩.
Constraint: **pdz** > 0.

NE_ENUM_INT_2

On entry, **job** = ⟨*value*⟩, **n** = ⟨*value*⟩, **pdz** = ⟨*value*⟩.
Constraint: if **job** = **Nag_EigVecs**, **pdz** $\geq \max(1, \mathbf{n})$;
if **job** = **Nag_DoNothing**, **pdz** ≥ 1.

NE_CONVERGENCE

The algorithm failed to converge, ⟨*value*⟩ elements of an intermediate tridiagonal form did not converge to zero.

NE_ALLOC_FAIL

Memory allocation failed.

NE_BAD_PARAM

On entry, parameter ⟨*value*⟩ had an illegal value.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

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***.

8 Further Comments

The complex analogue of this function is nag_zhpevd (f08gqc).

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

```
/* nag_dspevd (f08gcc) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */
```

```
#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf08.h>
#include <nagx04.h>

int main(void)
{
  /* Scalars */
  Integer  i, j, n, ap_len, pdz, w_len;
  Integer  exit_status=0;
  NagError fail;
  Nag_JobType    job;
  Nag_UploType   uplo;
  Nag_OrderType  order;
  /* Arrays */
  char   uplo_char[2], job_char[2];
  double *ap=0, *w=0, *z=0;

#ifdef NAG_COLUMN_MAJOR
#define A_UPPER(I,J) ap[J*(J-1)/2 + I - 1]
#define A_LOWER(I,J) ap[(2*n-J)*(J-1)/2 + I - 1]
  order = Nag_ColMajor;
#else
#define A_LOWER(I,J) ap[I*(I-1)/2 + J - 1]
#define A_UPPER(I,J) ap[(2*n-I)*(I-1)/2 + J - 1]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);
  Vprintf("f08gcc Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%*[^\n] ", &n);
  ap_len = n*(n+1)/2;
  w_len = n;
  pdz =n;

  /* Allocate memory */
  if ( !(ap = NAG_ALLOC(ap_len, double)) ||
       !(z = NAG_ALLOC(n * n, double)) ||
       !(w = NAG_ALLOC(w_len, double)) )
    {
      Vprintf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }
  /* Read whether Upper or Lower part of A is stored */
  Vscanf(" ' %1s '%*[^\n] ", uplo_char);
  if (*(unsigned char *)uplo_char == 'L')
    uplo = Nag_Lower;
  else if (*(unsigned char *)uplo_char == 'U')
    uplo = Nag_Upper;
  else
    {
      Vprintf("Unrecognised character for Nag_UploType type\n");
      exit_status = -1;
      goto END;
    }
  /* Read A from data file */
  if (uplo == Nag_Upper)
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = i; j <= n; ++j)
            Vscanf("%lf", &A_UPPER(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  else
```

```
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf("%lf", &A_LOWER(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  /* Read type of job to be performed */
  Vscanf(" ' %1s '%*[^\n] ", job_char);
  if (*(unsigned char *)job_char == 'V')
    job = Nag_EigVecs;
  else
    job = Nag_DoNothing;
  /* Calculate all the eigenvalues and eigenvectors of A */
  f08gcc(order, job, uplo, n, ap, w, z, pdz, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f08gcc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print eigenvalues and eigenvectors */
  Vprintf("Eigenvalues \n");
  for (i = 0; i < n; ++i)
    Vprintf(" %8.4lf",w[i]);
  Vprintf("\n");
  x04cac(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, n,
         z, pdz, "Eigenvectors", 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from x04cac.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
 END:
  if (ap) NAG_FREE(ap);
  if (w) NAG_FREE(w);
  if (z) NAG_FREE(z);
  return exit_status;
}
```

9.2 Program Data

```
f08gcc 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

```
f08gcc 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
```