NAG C Library Function Document

nag_dsyevd (f08fcc)

1 Purpose

nag_dsyevd (f08fcc) computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric matrix. 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_dsyevd (Nag_OrderType order, Nag_JobType job, Nag_UploType uplo,
     Integer n, double a[], Integer pda, double w[], NagError *fail)
```

3 Description

nag_dsyevd (f08fcc) computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric matrix A. 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

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

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: **a**[dim] – double *Input/Output*

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

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

On entry: the n by n symmetric matrix A. If **uplo** = **Nag_Upper**, the upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced; if **uplo** = **Nag_Lower**, the lower triangular part of A must be stored and the elements of the array above the diagonal are not referenced.

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

6: **pda** – Integer *Input*

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

Constraint: $\mathbf{pda} \geq \max(1, \mathbf{n})$.

7: **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.

8: **fail** – NagError * *Output*

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: $\mathbf{n} \geq 0$.

On entry, **pda** = ⟨*value*⟩.
Constraint: $\mathbf{pda} > 0$.

NE_INT_2

On entry, **pda** = ⟨*value*⟩, **n** = ⟨*value*⟩.
Constraint: $\mathbf{pda} \geq \max(1, \mathbf{n})$.

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_zheevd (f08fqc).

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_dsyevd (f08fcc) 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, pda, 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 *a=0, *w=0;

#ifdef NAG_COLUMN_MAJOR
#define A(I,J) a[(J-1)*pda + I - 1]
  order = Nag_ColMajor;
#else
#define A(I,J) a[(I-1)*pda + J - 1]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);
  Vprintf("f08fcc Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
```

```
  Vscanf("%ld%*[^\n] ", &n);
  pda = n;
  w_len = n;

  /* Allocate memory */
  if ( !(a = 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(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf("%lf", &A(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 */
  f08fcc(order, job, uplo, n, a, pda, w, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f08fcc.\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, a, pda,
         "Eigenvectors", 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from x04cac.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
 END:
```

```
  if (a) NAG_FREE(a);
  if (w) NAG_FREE(w);
  return exit_status;
}
```

9.2 Program Data

```
F08FCC 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

```
f08fcc 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
```