NAG C Library Function Document

nag_zheevd (f08fqc)

1 Purpose

nag_zheevd (f08fqc) computes all the eigenvalues and, optionally, all the eigenvectors of a complex Hermitian 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

```
#include <nag.h>
#include <nagf08.h>

void nag_zheevd (Nag_OrderType order, Nag_JobType job, Nag_UploType uplo,
     Integer n, Complex a[], Integer pda, double w[], NagError *fail)
```

3 Description

nag_zheevd (f08fqc) computes all the eigenvalues and, optionally, all the eigenvectors of a complex Hermitian matrix A. In other words, it can compute the spectral factorization of A as

$$A = Z\Lambda Z^{\mathrm{H}},$$

where Λ is a real diagonal matrix whose diagonal elements are the eigenvalues λ_i, and Z is the (complex) unitary matrix whose columns are the eigenvectors z_i. Thus

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

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 URL: 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 Arguments

1: **order** – Nag_OrderType *Input*

On entry: the **order** argument 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 argument.

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

2: **job** – Nag_JobType *Input*

On entry: indicates whether eigenvectors are computed.

job = **Nag_DoNothing**

Only eigenvalues are computed.

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.

uplo = **Nag_Upper**

The upper triangular part of A is stored.

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] – Complex *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 $\mathbf{a}[(j-1) \times \mathbf{pda} + i - 1]$.

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 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 unitary matrix Z which contains the eigenvectors of A.

6: **pda** – Integer *Input*

On entry: the stride separating row or column elements (depending on the value of **order**) of the matrix A 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 * *Input/Output*

The NAG error argument (see Section 2.6 of the Essential Introduction).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

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

NE_CONVERGENCE

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

NE_INT

On entry, $\mathbf{n} = \langle value \rangle$.
Constraint: $\mathbf{n} \geq 0$.

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

NE_INT_2

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

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

$$\|E\|_2 = \mathrm{O}(\epsilon)\|A\|_2,$$

and ϵ is the ***machine precision***. See Section 4.7 of Anderson *et al.* (1999) for further details.

8 Further Comments

The real analogue of this function is nag_dsyevd (f08fcc).

9 Example

To compute all the eigenvalues and eigenvectors of the Hermitian matrix A, where

$$A = \begin{pmatrix} 1.0 + 0.0i & 2.0 - 1.0i & 3.0 - 1.0i & 4.0 - 1.0i \\ 2.0 + 1.0i & 2.0 + 0.0i & 3.0 - 2.0i & 4.0 - 2.0i \\ 3.0 + 1.0i & 3.0 + 2.0i & 3.0 + 0.0i & 4.0 - 3.0i \\ 4.0 + 1.0i & 4.0 + 2.0i & 4.0 + 3.0i & 4.0 + 0.0i \end{pmatrix}.$$

The example program for nag_zheevd (f08fqc) illustrates the computation of error bounds for the eigenvalues and eigenvectors.

9.1 Program Text

```
/* nag_zheevd (f08fqc) 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  *w=0;
  Complex *a=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("nag_zheevd (f08fqc) 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, Complex)) ||
       !(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 , %lf )", &A(i,j).re, &A(i,j).im);
        }
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf(" ( %lf , %lf )", &A(i,j).re, &A(i,j).im);
        }
      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 */
  /* nag_zheevd (f08fqc).
   * All eigenvalues and optionally all eigenvectors of
   * complex Hermitian matrix (divide-and-conquer)
   */
  nag_zheevd(order, job, uplo, n, a, pda, w, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from nag_zheevd (f08fqc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print eigenvalues and eigenvectors */
  Vprintf("Eigenvalues\n");
  for (i = 0; i < n; ++i)
    Vprintf("   %5ld     %8.4f\n",i+1,w[i]);
  Vprintf("\n");
  /* nag_gen_complx_mat_print_comp (x04dbc).
   * Print complex general matrix (comprehensive)
   */
  nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n,
                                n, a, pda, Nag_AboveForm, "%7.4f",
                                "Eigenvectors", Nag_IntegerLabels,
                                0, Nag_IntegerLabels, 0, 80, 0, 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from nag_gen_complx_mat_print_comp (x04dbc).\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

```
nag_zheevd (f08fqc) Example Program Data
  4                                                     :Value of N
  'L'                                                   :Value of UPLO
  (1.0, 0.0)
  (2.0, 1.0)  (2.0, 0.0)
  (3.0, 1.0)  (3.0, 2.0)  (3.0, 0.0)
  (4.0, 1.0)  (4.0, 2.0)  (4.0, 3.0)  (4.0, 0.0)     :End of matrix A
  'V'                                                   :Value of JOB
```

9.3 Program Results

```
nag_zheevd (f08fqc) Example Program Results

Eigenvalues
       1      -4.2443
       2      -0.6886
       3       1.1412
       4      13.7916

 Eigenvectors

         1       2       3       4
 1  0.4836  0.6470 -0.4456 -0.3859
    0.0000  0.0000  0.0000 -0.0000
```

```
 2  0.2912 -0.4984 -0.0230 -0.4441
   -0.3618 -0.1130 -0.5702  0.0156

 3 -0.3163  0.2949  0.5331 -0.5173
   -0.3696  0.3165  0.1317 -0.0844

 4 -0.4447 -0.2241 -0.3510 -0.5277
    0.3406 -0.2878  0.2261 -0.3168
```