

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

```
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

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

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

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

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: $n \geq 0$.
- 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 **a**[($j - 1$) \times **pda** + $i - 1$] and if **order** = **Nag_RowMajor**, the (i, j) th element of the matrix A is stored in **a**[($i - 1$) \times **pda** + $j - 1$].
On entry: the n by n Hermitian 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 * *Output*
 The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

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

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

NE_INT_2

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

NE_CONVERGENCE

The algorithm failed to converge, $\langle value \rangle$ elements of an intermediate tridiagonal form did not converge to zero.

NE_ALLOC_FAIL

Memory allocation failed.

NE_BAD_PARAM

On entry, parameter $\langle value \rangle$ 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 real analogue of this function is nag_dsyevd (f08fcc).

9 Example

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

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

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("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(" ( %1f , %1f )", &A(i,j).re, &A(i,j).im);
    }
    Vscanf("%*[\n] ");
}
else
{
    for (i = 1; i <= n; ++i)
    {
        for (j = 1; j <= i; ++j)
            Vscanf(" ( %1f , %1f )", &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 */
f08fqc(order, job, uplo, n, a, pda, w, &fail);
if (fail.code != NE_NOERROR)
{
    Vprintf("Error from 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");
x04dbc(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 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

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

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

```
