NAG C Library Function Document

nag_dgehrd (f08nec)

1 Purpose

nag_dgehrd (f08nec) reduces a real general matrix to Hessenberg form.

2 Specification

```
void nag_dgehrd (Nag_OrderType order, Integer n, Integer ilo, Integer ihi,
     double a[], Integer pda, double tau[], NagError *fail)
```

3 Description

nag_dgehrd (f08nec) reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation: $A = QHQ^T$.

The matrix Q is not formed explicitly, but is represented as a product of elementary reflectors (see the f08 Chapter Introduction for details). Functions are provided to work with Q in this representation (see Section 8).

The function can take advantage of a previous call to nag_dgebal (f08nhc), which may produce a matrix with the structure:

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ & A_{22} & A_{23} \\ & & A_{33} \end{pmatrix}$$

where A_{11} and A_{33} are upper triangular. If so, only the central diagonal block A_{22}, in rows and columns i_{lo} to i_{hi}, needs to be reduced to Hessenberg form (the blocks A_{12} and A_{23} will also be affected by the reduction). Therefore the values of i_{lo} and i_{hi} determined by nag_dgebal (f08nhc) can be supplied to the function directly. If nag_dgebal (f08nhc) has not previously been called however, then i_{lo} must be set to 1 and i_{hi} to 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: **n** – Integer *Input*

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

Constraint: **n** ≥ 0.

3: **ilo** – Integer *Input*
4: **ihi** – Integer *Input*

On entry: if A has been output by nag_dgebal (f08nhc), then **ilo** and **ihi** **must** contain the values returned by that function. Otherwise, **ilo** must be set to 1 and **ihi** to **n**.

Constraints:

if $\mathbf{n} > 0$, $1 \leq \mathbf{ilo} \leq \mathbf{ihi} \leq \mathbf{n}$;
if $\mathbf{n} = 0$, $\mathbf{ilo} = 1$ and $\mathbf{ihi} = 0$.

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

On entry: the n by n general matrix A.

On exit: A is overwritten by the upper Hessenberg matrix H and details of the orthogonal matrix Q.

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: **tau**$[dim]$ – double *Output*

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

On exit: further details of the orthogonal matrix Q.

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_INT_3

On entry, **n** = ⟨*value*⟩, **ilo** = ⟨*value*⟩, **ihi** = ⟨*value*⟩.
Constraint: if $\mathbf{n} > 0$, $1 \leq \mathbf{ilo} \leq \mathbf{ihi} \leq \mathbf{n}$;
if $\mathbf{n} = 0$, $\mathbf{ilo} = 1$ and $\mathbf{ihi} = 0$.

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 Hessenberg matrix H is exactly similar to a nearby matrix $A + E$, where

$$\|E\|_2 \leq c(n)\epsilon\|A\|_2,$$

$c(n)$ is a modestly increasing function of n, and ϵ is the ***machine precision***.

The elements of H themselves may be sensitive to small perturbations in A or to rounding errors in the computation, but this does not affect the stability of the eigenvalues, eigenvectors or Schur factorization.

8 Further Comments

The total number of floating-point operations is approximately $\frac{2}{3}q^2(2q + 3n)$, where $q = i_{hi} - i_{lo}$; if $i_{lo} = 1$ and $i_{hi} = n$, the number is approximately $\frac{10}{3}n^3$.

To form the orthogonal matrix Q this function may be followed by a call to nag_dorghr (f08nfc):

```
nag_dorghr (order,n,ilo,ihi,&a,pda,tau,&fail)
```

To apply Q to an m by n real matrix C this function may be followed by a call to nag_dormhr (f08ngc). For example,

```
nag_dormhr (order,Nag_LeftSide,Nag_NoTrans,m,n,ilo,ihi,&a,pda,
tau,&c,pdc,&fail)
```

forms the matrix product QC.

The complex analogue of this function is nag_zgehrd (f08nsc).

9 Example

To compute the upper Hessenberg form of the matrix A, where

$$A = \begin{pmatrix} 0.35 & 0.45 & -0.14 & -0.17 \\ 0.09 & 0.07 & -0.54 & 0.35 \\ -0.44 & -0.33 & -0.03 & 0.17 \\ 0.25 & -0.32 & -0.13 & 0.11 \end{pmatrix}.$$

9.1 Program Text

```
/* nag_dgehrd (f08nec) 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, tau_len;
  Integer  exit_status=0;
  NagError fail;
  Nag_OrderType order;
  /* Arrays */
```

```
  double *a=0, *tau=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("f08nec Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%*[^\n] ", &n);
#ifdef NAG_COLUMN_MAJOR
  pda = n;
#else
  pda = n;
#endif
  tau_len = n - 1;

  /* Allocate memory */
  if ( !(a = NAG_ALLOC(n * n, double)) ||
       !(tau = NAG_ALLOC(tau_len, double)) )
    {
      Vprintf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Read A from data file */
  for (i = 1; i <= n; ++i)
    {
      for (j = 1; j <= n; ++j)
        Vscanf("%lf", &A(i,j));
    }
  Vscanf("%*[^\n] ");

  /* Reduce A to upper Hessenberg form */
  f08nec(order, n, 1, n, a, pda, tau, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f08nec.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }

  /* Set the elements below the first sub-diagonal to zero */
  for (i = 1; i <= n - 2; ++i)
    {
      for (j = i + 2; j <= n; ++j)
        A(j, i) = 0.0;
    }

  /* Print upper Hessenberg form */
  x04cac(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, n,
         a, pda, "Upper Hessenberg form", 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 (tau) NAG_FREE(tau);
  return exit_status;
}
```

9.2 Program Data

```
f08nec Example Program Data
  4                              :Value of N
  0.35   0.45  -0.14  -0.17
  0.09   0.07  -0.54   0.35
 -0.44  -0.33  -0.03   0.17
  0.25  -0.32  -0.13   0.11   :End of matrix A
```

9.3 Program Results

```
f08nec Example Program Results

 Upper Hessenberg form
          1        2        3        4
 1   0.3500  -0.1160  -0.3886  -0.2942
 2  -0.5140   0.1225   0.1004   0.1126
 3   0.0000   0.6443  -0.1357  -0.0977
 4   0.0000   0.0000   0.4262   0.1632
```