NAG Library Function Document

nag_zungqr (f08atc)

1 Purpose

nag_zungqr (f08atc) generates all or part of the complex unitary matrix Q from a QR factorization computed by nag_zgeqrf (f08asc), nag_zgeqpf (f08bsc) or nag_zgeqp3 (f08btc).

2 Specification

```
#include <nag.h>
#include <nagf08.h>
void nag_zungqr (Nag_OrderType order, Integer m, Integer n, Integer k,
     Complex a[], Integer pda, const Complex tau[], NagError *fail)
```

3 Description

nag_zungqr (f08atc) is intended to be used after a call to nag_zgeqrf (f08asc), nag_zgeqpf (f08bsc) or nag_zgeqp3 (f08btc), which perform a QR factorization of a complex matrix A. The unitary matrix Q is represented as a product of elementary reflectors.

This function may be used to generate Q explicitly as a square matrix, or to form only its leading columns.

Usually Q is determined from the QR factorization of an m by p matrix A with $m \geq p$. The whole of Q may be computed by:

```
nag_zungqr(order,m,m,p,a,pda,tau,&fail)
```

(note that the array **a** must have at least m columns) or its leading p columns by:

```
nag_zungqr(order,m,p,p,a,pda,tau,&fail)
```

The columns of Q returned by the last call form an orthonormal basis for the space spanned by the columns of A; thus nag_zgeqrf (f08asc) followed by nag_zungqr (f08atc) can be used to orthogonalize the columns of A.

The information returned by the QR factorization functions also yields the QR factorization of the leading k columns of A, where $k < p$. The unitary matrix arising from this factorization can be computed by:

```
nag_zungqr(order,m,m,k,a,pda,tau,&fail)
```

or its leading k columns by:

```
nag_zungqr(order,m,k,k,a,pda,tau,&fail)
```

4 References

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 2.3.1.3 in How to Use the NAG Library and its Documentation for a more detailed explanation of the use of this argument.

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

2: **m** – Integer *Input*

On entry: m, the order of the unitary matrix Q.

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

3: **n** – Integer *Input*

On entry: n, the number of columns of the matrix Q.

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

4: **k** – Integer *Input*

On entry: k, the number of elementary reflectors whose product defines the matrix Q.

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

5: **a**[dim] – Complex *Input/Output*

Note: the dimension, *dim*, of the array **a** must be at least

$\max(1, \mathbf{pda} \times \mathbf{n})$ when **order** = Nag_ColMajor;
$\max(1, \mathbf{m} \times \mathbf{pda})$ when **order** = Nag_RowMajor.

On entry: details of the vectors which define the elementary reflectors, as returned by nag_zgeqrf (f08asc), nag_zgeqpf (f08bsc) or nag_zgeqp3 (f08btc).

On exit: the m by n matrix Q.

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

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

6: **pda** – Integer *Input*

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

Constraints:

if **order** = Nag_ColMajor, $\mathbf{pda} \geq \max(1, \mathbf{m})$;
if **order** = Nag_RowMajor, $\mathbf{pda} \geq \max(1, \mathbf{n})$.

7: **tau**[dim] – const Complex *Input*

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

On entry: further details of the elementary reflectors, as returned by nag_zgeqrf (f08asc), nag_zgeqpf (f08bsc) or nag_zgeqp3 (f08btc).

8: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.
See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

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

NE_INT

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

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

NE_INT_2

On entry, **m** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **m** $\geq$ **n** ≥ 0.

On entry, **n** = ⟨*value*⟩ and **k** = ⟨*value*⟩.
Constraint: **n** $\geq$ **k** ≥ 0.

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

On entry, **pda** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **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 contact NAG for assistance.

An unexpected error has been triggered by this function. Please contact NAG.
See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.
See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

The computed matrix Q differs from an exactly unitary matrix by a matrix E such that

$$\|E\|_2 = O(\epsilon),$$

where ϵ is the ***machine precision***.

8 Parallelism and Performance

nag_zungqr (f08atc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_zungqr (f08atc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the x06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The total number of real floating-point operations is approximately $16mnk - 8(m+n)k^2 + \frac{16}{3}k^3$; when $n = k$, the number is approximately $\frac{8}{3}n^2(3m-n)$.

The real analogue of this function is nag_dorgqr (f08afc).

10 Example

This example forms the leading 4 columns of the unitary matrix Q from the QR factorization of the matrix A, where

$$A = \begin{pmatrix} 0.96-0.81i & -0.03+0.96i & -0.91+2.06i & -0.05+0.41i \\ -0.98+1.98i & -1.20+0.19i & -0.66+0.42i & -0.81+0.56i \\ 0.62-0.46i & 1.01+0.02i & 0.63-0.17i & -1.11+0.60i \\ -0.37+0.38i & 0.19-0.54i & -0.98-0.36i & 0.22-0.20i \\ 0.83+0.51i & 0.20+0.01i & -0.17-0.46i & 1.47+1.59i \\ 1.08-0.28i & 0.20-0.12i & -0.07+1.23i & 0.26+0.26i \end{pmatrix}.$$

The columns of Q form an orthonormal basis for the space spanned by the columns of A.

10.1 Program Text

```
/* nag_zungqr (f08atc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

int main(void)
{
  /* Scalars */
  Integer i, j, m, n, pda, tau_len;
  Integer exit_status = 0;
  NagError fail;
  Nag_OrderType order;
  /* Arrays */
  char *title = 0;
  Complex *a = 0, *tau = 0;
#ifdef NAG_LOAD_FP
  /* The following line is needed to force the Microsoft linker
     to load floating point support */
  float force_loading_of_ms_float_support = 0;
#endif /* NAG_LOAD_FP */

#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);

  printf("nag_zungqr (f08atc) Example Program Results\n\n");

  /* Skip heading in data file */
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &m, &n);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &m, &n);
#endif
#ifdef NAG_COLUMN_MAJOR
  pda = m;
#else
  pda = n;
#endif
  tau_len = MIN(m, n);

  /* Allocate memory */
  if (!(title = NAG_ALLOC(31, char)) ||
      !(a = NAG_ALLOC(m * n, Complex)) ||
      !(tau = NAG_ALLOC(tau_len, Complex)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* Read A from data file */
  for (i = 1; i <= m; ++i) {
    for (j = 1; j <= n; ++j)
#ifdef _WIN32
      scanf_s(" ( %lf , %lf )", &A(i, j).re, &A(i, j).im);
#else
      scanf(" ( %lf , %lf )", &A(i, j).re, &A(i, j).im);
#endif
  }
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

  /* Compute the QR factorization of A */
  /* nag_zgeqrf (f08asc).
   * QR factorization of complex general rectangular matrix
   */
  nag_zgeqrf(order, m, n, a, pda, tau, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_zgeqrf (f08asc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Form the leading N columns of Q explicitly */
  /* nag_zungqr (f08atc).
   * Form all or part of unitary Q from QR factorization
   * determined by nag_zgeqrf (f08asc) or nag_zgeqpf (f08bsc)
   */
  nag_zungqr(order, m, n, n, a, pda, tau, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_zungqr (f08atc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Print the leading N columns of Q only */
```

```
#ifdef _WIN32
  sprintf_s(title, 31, "The leading %2" NAG_IFMT " columns of Q\n", n);
#else
  sprintf(title, "The leading %2" NAG_IFMT " columns of Q\n", n);
#endif
  /* nag_gen_complx_mat_print_comp (x04dbc).
   * Print complex general matrix (comprehensive)
   */
  fflush(stdout);
  nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag, m,
                                n, a, pda, Nag_BracketForm, "%7.4f", title,
                                Nag_IntegerLabels, 0, Nag_IntegerLabels, 0,
                                80, 0, 0, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_complx_mat_print_comp (x04dbc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }
END:
  NAG_FREE(title);
  NAG_FREE(a);
  NAG_FREE(tau);

  return exit_status;
}
```

10.2 Program Data

```
nag_zungqr (f08atc) Example Program Data
  6  4                                                    :Values of M and N
 ( 0.96,-0.81) (-0.03, 0.96) (-0.91, 2.06) (-0.05, 0.41)
 (-0.98, 1.98) (-1.20, 0.19) (-0.66, 0.42) (-0.81, 0.56)
 ( 0.62,-0.46) ( 1.01, 0.02) ( 0.63,-0.17) (-1.11, 0.60)
 (-0.37, 0.38) ( 0.19,-0.54) (-0.98,-0.36) ( 0.22,-0.20)
 ( 0.83, 0.51) ( 0.20, 0.01) (-0.17,-0.46) ( 1.47, 1.59)
 ( 1.08,-0.28) ( 0.20,-0.12) (-0.07, 1.23) ( 0.26, 0.26)   :End of matrix A
```

10.3 Program Results

```
nag_zungqr (f08atc) Example Program Results

 The leading  4 columns of Q

                     1                   2                   3                   4
 1  (-0.3110, 0.2624)  (-0.3175, 0.4835)  ( 0.4966,-0.2997)  (-0.0072,-0.3718)
 2  ( 0.3175,-0.6414)  (-0.2062, 0.1577)  (-0.0793,-0.3094)  (-0.0282,-0.1491)
 3  (-0.2008, 0.1490)  ( 0.4892,-0.0900)  ( 0.0357,-0.0219)  ( 0.5625,-0.0710)
 4  ( 0.1199,-0.1231)  ( 0.2566,-0.3055)  ( 0.4489,-0.2141)  (-0.1651, 0.1800)
 5  (-0.2689,-0.1652)  ( 0.1697,-0.2491)  (-0.0496, 0.1158)  (-0.4885,-0.4540)
 6  (-0.3499, 0.0907)  (-0.0491,-0.3133)  (-0.1256,-0.5300)  ( 0.1039, 0.0450)
```