

# NAG Library Function Document

## nag\_dtpqrt (f08bbc)

### 1 Purpose

nag\_dtpqrt (f08bbc) computes the  $QR$  factorization of a real  $(m+n)$  by  $n$  triangular-pentagonal matrix.

### 2 Specification

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

void nag_dtpqrt (Nag_OrderType order, Integer m, Integer n, Integer l,
                Integer nb, double a[], Integer pda, double b[], Integer pdb,
                double t[], Integer pdt, NagError *fail)
```

### 3 Description

nag\_dtpqrt (f08bbc) forms the  $QR$  factorization of a real  $(m+n)$  by  $n$  triangular-pentagonal matrix  $C$ ,

$$C = \begin{pmatrix} A \\ B \end{pmatrix}$$

where  $A$  is an upper triangular  $n$  by  $n$  matrix and  $B$  is an  $m$  by  $n$  pentagonal matrix consisting of an  $(m-l)$  by  $n$  rectangular matrix  $B_1$  on top of an  $l$  by  $n$  upper trapezoidal matrix  $B_2$ :

$$B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}.$$

The upper trapezoidal matrix  $B_2$  consists of the first  $l$  rows of an  $n$  by  $n$  upper triangular matrix, where  $0 \leq l \leq \min(m, n)$ . If  $l = 0$ ,  $B$  is  $m$  by  $n$  rectangular; if  $l = n$  and  $m = n$ ,  $B$  is upper triangular.

A recursive, explicitly blocked,  $QR$  factorization (see nag\_dgeqrt (f08abc)) is performed on the matrix  $C$ . The upper triangular matrix  $R$ , details of the orthogonal matrix  $Q$ , and further details (the block reflector factors) of  $Q$  are returned.

Typically the matrix  $A$  or  $B_2$  contains the matrix  $R$  from the  $QR$  factorization of a subproblem and nag\_dtpqrt (f08bbc) performs the  $QR$  update operation from the inclusion of matrix  $B_1$ .

For example, consider the  $QR$  factorization of an  $l$  by  $n$  matrix  $\hat{B}$  with  $l < n$ :  $\hat{B} = \hat{Q}\hat{R}$ ,  $\hat{R} = \begin{pmatrix} \hat{R}_1 & \hat{R}_2 \end{pmatrix}$ , where  $\hat{R}_1$  is  $l$  by  $l$  upper triangular and  $\hat{R}_2$  is  $(n-l)$  by  $n$  rectangular (this can be performed by nag\_dgeqrt (f08abc)). Given an initial least-squares problem  $\hat{B}\hat{X} = \hat{Y}$  where  $X$  and  $Y$  are  $l$  by  $n$  *nrhs* matrices, we have  $\hat{R}\hat{X} = \hat{Q}^T\hat{Y}$ .

Now, adding an additional  $m-l$  rows to the original system gives the augmented least squares problem

$$BX = Y$$

where  $B$  is an  $m$  by  $n$  matrix formed by adding  $m-l$  rows on top of  $\hat{R}$  and  $Y$  is an  $m$  by  $n$  *nrhs* matrix formed by adding  $m-l$  rows on top of  $\hat{Q}^T\hat{Y}$ .

nag\_dtpqrt (f08bbc) can then be used to perform the  $QR$  factorization of the pentagonal matrix  $B$ ; the  $n$  by  $n$  matrix  $A$  will be zero on input and contain  $R$  on output.

In the case where  $\hat{B}$  is  $r$  by  $n$ ,  $r \geq n$ ,  $\hat{R}$  is  $n$  by  $n$  upper triangular (forming  $A$ ) on top of  $r-n$  rows of zeros (forming first  $r-n$  rows of  $B$ ). Augmentation is then performed by adding rows to the bottom of  $B$  with  $l = 0$ .

## 4 References

Elmroth E and Gustavson F (2000) Applying Recursion to Serial and Parallel *QR* Factorization Leads to Better Performance *IBM Journal of Research and Development*. (Volume 44) 4 605–624

Golub G H and Van Loan C F (2012) *Matrix Computations* (4th 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 number of rows of the matrix *B*.

*Constraint:* **m** ≥ 0.

3: **n** – Integer *Input*

*On entry:* *n*, the number of columns of the matrix *B* and the order of the upper triangular matrix *A*.

*Constraint:* **n** ≥ 0.

4: **l** – Integer *Input*

*On entry:* *l*, the number of rows of the trapezoidal part of *B* (i.e., *B*<sub>2</sub>).

*Constraint:* 0 ≤ **l** ≤ min(**m**, **n**).

5: **nb** – Integer *Input*

*On entry:* the explicitly chosen block-size to be used in the algorithm for computing the *QR* factorization. See Section 9 for details.

*Constraints:*

**nb** ≥ 1;  
if **n** > 0, **nb** ≤ **n**.

6: **a**[*dim*] – double *Input/Output*

**Note:** the dimension, *dim*, of the array **a** must be at least max(1, **pda** × **n**).

The (*i*, *j*)th element of the matrix *A* is stored in

**a**[(*j* – 1) × **pda** + *i* – 1] when **order** = Nag\_ColMajor;  
**a**[(*i* – 1) × **pda** + *j* – 1] when **order** = Nag\_RowMajor.

*On entry:* the *n* by *n* upper triangular matrix *A*.

*On exit:* the upper triangle is overwritten by the corresponding elements of the *n* by *n* upper triangular matrix *R*.

- 7: **pda** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **a**.  
*Constraint:* **pda**  $\geq$   $\max(1, \mathbf{n})$ .
- 8: **b**[*dim*] – double *Input/Output*  
**Note:** the dimension, *dim*, of the array **b** must be at least  
 $\max(1, \mathbf{pdb} \times \mathbf{n})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{m} \times \mathbf{pdb})$  when **order** = Nag\_RowMajor.  
The (*i*, *j*)th element of the matrix *B* is stored in  
**b**[(*j* – 1)  $\times$  **pdb** + *i* – 1] when **order** = Nag\_ColMajor;  
**b**[(*i* – 1)  $\times$  **pdb** + *j* – 1] when **order** = Nag\_RowMajor.  
*On entry:* the *m* by *n* pentagonal matrix *B* composed of an (*m* – *l*) by *n* rectangular matrix *B*<sub>1</sub> above an *l* by *n* upper trapezoidal matrix *B*<sub>2</sub>.  
*On exit:* details of the orthogonal matrix *Q*.
- 9: **pdb** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **b**.  
*Constraints:*  
if **order** = Nag\_ColMajor, **pdb**  $\geq$   $\max(1, \mathbf{m})$ ;  
if **order** = Nag\_RowMajor, **pdb**  $\geq$   $\max(1, \mathbf{n})$ .
- 10: **t**[*dim*] – double *Output*  
**Note:** the dimension, *dim*, of the array **t** must be at least  
 $\max(1, \mathbf{pdt} \times \mathbf{n})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{nb} \times \mathbf{pdt})$  when **order** = Nag\_RowMajor.  
The (*i*, *j*)th element of the matrix *T* is stored in  
**t**[(*j* – 1)  $\times$  **pdt** + *i* – 1] when **order** = Nag\_ColMajor;  
**t**[(*i* – 1)  $\times$  **pdt** + *j* – 1] when **order** = Nag\_RowMajor.  
*On exit:* further details of the orthogonal matrix *Q*. The number of blocks is  $b = \lceil \frac{k}{\mathbf{nb}} \rceil$ , where  $k = \min(m, n)$  and each block is of order **nb** except for the last block, which is of order  $k - (b - 1) \times \mathbf{nb}$ . For each of the blocks, an upper triangular block reflector factor is computed: *T*<sub>1</sub>, *T*<sub>2</sub>, . . . , *T*<sub>*b*</sub>. These are stored in the **nb** by *n* matrix *T* as  $\mathbf{T} = [\mathbf{T}_1 | \mathbf{T}_2 | \dots | \mathbf{T}_b]$ .
- 11: **pdt** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **t**.  
*Constraints:*  
if **order** = Nag\_ColMajor, **pdt**  $\geq$  **nb**;  
if **order** = Nag\_RowMajor, **pdt**  $\geq$  **n**.
- 12: **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  $\langle value \rangle$  had an illegal value.

### NE\_INT

On entry,  $\mathbf{m} = \langle value \rangle$ .

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

On entry,  $\mathbf{n} = \langle value \rangle$ .

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

### NE\_INT\_2

On entry,  $\mathbf{nb} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $\mathbf{nb} \geq 1$  and

if  $\mathbf{n} > 0$ ,  $\mathbf{nb} \leq \mathbf{n}$ .

On entry,  $\mathbf{pda} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

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

On entry,  $\mathbf{pdb} = \langle value \rangle$  and  $\mathbf{m} = \langle value \rangle$ .

Constraint:  $\mathbf{pdb} \geq \max(1, \mathbf{m})$ .

On entry,  $\mathbf{pdb} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

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

On entry,  $\mathbf{pdt} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $\mathbf{pdt} \geq \mathbf{n}$ .

On entry,  $\mathbf{pdt} = \langle value \rangle$  and  $\mathbf{nb} = \langle value \rangle$ .

Constraint:  $\mathbf{pdt} \geq \mathbf{nb}$ .

### NE\_INT\_3

On entry,  $\mathbf{l} = \langle value \rangle$ ,  $\mathbf{m} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $0 \leq \mathbf{l} \leq \min(\mathbf{m}, \mathbf{n})$ .

### 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 factorization is the exact factorization of a nearby matrix  $(A + E)$ , where

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

and  $\epsilon$  is the *machine precision*.

## 8 Parallelism and Performance

nag\_dtpqrt (f08bbc) 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 floating-point operations is approximately  $\frac{2}{3}n^2(3m - n)$  if  $m \geq n$  or  $\frac{2}{3}m^2(3n - m)$  if  $m < n$ .

The block size, **nb**, used by nag\_dtpqrt (f08bbc) is supplied explicitly through the interface. For moderate and large sizes of matrix, the block size can have a marked effect on the efficiency of the algorithm with the optimal value being dependent on problem size and platform. A value of **nb** = 64  $\ll$  min( $m, n$ ) is likely to achieve good efficiency and it is unlikely that an optimal value would exceed 340.

To apply  $Q$  to an arbitrary real rectangular matrix  $C$ , nag\_dtpqrt (f08bbc) may be followed by a call to nag\_dtpmqrt (f08bcc). For example,

```
nag_dtpmqrt(Nag_ColMajor, Nag_LeftSide, Nag_Trans, m, p, n, l, nb, b, p, db,
            t, pdt, c, pdc, &c(n+1, 1), ldc, &fail)
```

forms  $C = Q^T C$ , where  $C$  is  $(m + n)$  by  $p$ .

To form the orthogonal matrix  $Q$  explicitly set  $p = m + n$ , initialize  $C$  to the identity matrix and make a call to nag\_dtpmqrt (f08bcc) as above.

## 10 Example

This example finds the basic solutions for the linear least squares problems

$$\text{minimize } \|Ax_i - b_i\|_2, \quad i = 1, 2$$

where  $b_1$  and  $b_2$  are the columns of the matrix  $B$ ,

$$A = \begin{pmatrix} -0.57 & -1.28 & -0.39 & 0.25 \\ -1.93 & 1.08 & -0.31 & -2.14 \\ 2.30 & 0.24 & 0.40 & -0.35 \\ -1.93 & 0.64 & -0.66 & 0.08 \\ 0.15 & 0.30 & 0.15 & -2.13 \\ -0.02 & 1.03 & -1.43 & 0.50 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} -2.67 & 0.41 \\ -0.55 & -3.10 \\ 3.34 & -4.01 \\ -0.77 & 2.76 \\ 0.48 & -6.17 \\ 4.10 & 0.21 \end{pmatrix}.$$

A  $QR$  factorization is performed on the first 4 rows of  $A$  using nag\_dgeqrt (f08abc) after which the first 4 rows of  $B$  are updated by applying  $Q^T$  using nag\_dgemqrt (f08acc). The remaining row is added by performing a  $QR$  update using nag\_dtpqrt (f08bbc);  $B$  is updated by applying the new  $Q^T$  using nag\_dtpmqrt (f08bcc); the solution is finally obtained by triangular solve using  $R$  from the updated  $QR$ .

### 10.1 Program Text

```
/* nag_dtpqrt (f08bbc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

```

#include <nagf07.h>
#include <nagf08.h>
#include <nagf16.h>
#include <nagx04.h>

int main(void)
{
    /* Scalars */
    double rnorm;
    Integer exit_status = 0;
    Integer pda, pdb, pdt;
    Integer i, j, m, n, nb, nrhs;
    /* Arrays */
    double *a = 0, *b = 0, *c = 0, *t = 0;
    /* Nag Types */
    Nag_OrderType order;
    NagError fail;

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

    INIT_FAIL(fail);

    printf("nag_dtpqrt (f08bbc) Example Program Results\n\n");
    fflush(stdout);

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[\n]", &m, &n, &nrhs);
#else
    scanf("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[\n]", &m, &n, &nrhs);
#endif
    nb = MIN(m, n);
    if (!(a = NAG_ALLOC(m * n, double)) ||
        !(b = NAG_ALLOC(m * nrhs, double)) ||
        !(c = NAG_ALLOC(m * nrhs, double)) ||
        !(t = NAG_ALLOC(nb * MIN(m, n), double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
#ifdef NAG_COLUMN_MAJOR
    pda = m;
    pdb = m;
    pdt = nb;
#else
    pda = n;
    pdb = nrhs;
    pdt = MIN(m, n);
#endif

    /* Read A and B from data file */
    for (i = 1; i <= m; ++i)
        for (j = 1; j <= n; ++j)
#ifdef _WIN32
            scanf_s("%lf", &A(i, j));

```

```

#else
    scanf("%lf", &A(i, j));
#endif
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif

    for (i = 1; i <= m; ++i)
        for (j = 1; j <= nrhs; ++j)
#ifdef _WIN32
            scanf_s("%lf", &B(i, j));
#else
            scanf("%lf", &B(i, j));
#endif
#ifdef _WIN32
            scanf_s("%*[\n]");
#else
            scanf("%*[\n]");
#endif

    for (i = 1; i <= m; ++i)
        for (j = 1; j <= nrhs; ++j)
            C(i, j) = B(i, j);

/* nag_dgeqrt (f08abc).
 * Compute the QR factorization of first n rows of A by recursive algorithm.
 */
nag_dgeqrt(order, n, n, nb, a, pda, t, pdt, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dgeqrt (f08abc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_dgemqrt (f08acc).
 * Compute  $C = (C1) = (Q^T) * B$ , storing the result in C
 *
 * (C2)
 * by applying  $Q^T$  from left.
 */
nag_dgemqrt(order, Nag_LeftSide, Nag_Trans, n, nrhs, n, nb, a, pda, t, pdt,
            c, pdb, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dgemqrt (f08acc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

for (i = 1; i <= n; ++i)
    for (j = 1; j <= nrhs; ++j)
        B(i, j) = C(i, j);

/* nag_dtrtrs (f07tec).
 * Compute least squares solutions for first n rows
 * by back-substitution in  $R * X = C1$ .
 */
nag_dtrtrs(order, Nag_Upper, Nag_NoTrans, Nag_NonUnitDiag, n, nrhs, a, pda,
            c, pdb, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dtrtrs (f07tec).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_gen_real_mat_print (x04cac).
 * Print least squares solutions using first n rows.
 */
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs,
                        c, pdb, "Solution(s) for n rows", 0, &fail);
if (fail.code != NE_NOERROR) {

```

```

    printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_dtpqrt (f08bbc).
 * Now add the remaining rows and perform QR update.
 */
nag_dtpqrt(order, m - n, n, 0, nb, a, pda, &A(n + 1, 1), pda, t, pdt,
           &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dtpqrt (f08bbc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_dtpmqrt (f08bcc).
 * Apply orthogonal transformations to C.
 */
nag_dtpmqrt(order, Nag_LeftSide, Nag_Trans, m - n, nrhs, n, 0, nb,
            &A(n + 1, 1), pda, t, pdt, b, pdb, &B(5, 1), pdb, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dtpmqrt (f08bcc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_dtrtrs (f07tec).
 * Compute least squares solutions for first n rows
 * by back-substitution in R*X = C1.
 */
nag_dtrtrs(order, Nag_Upper, Nag_NoTrans, Nag_NonUnitDiag, n, nrhs, a, pda,
           b, pdb, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dtrtrs (f07tec).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_gen_real_mat_print (x04cac).
 * Print least squares solutions.
 */
printf("\n");
fflush(stdout);
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs,
                      b, pdb, "Least squares solution(s) for all rows", 0,
                      &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

printf("\n Square root(s) of the residual sum(s) of squares\n");
for (j = 1; j <= nrhs; j++) {
    /* nag_dge_norm (f16rac).
     * Compute and print estimate of the square root of the residual
     * sum of squares.
     */
    nag_dge_norm(order, Nag_FrobeniusNorm, m - n, 1, &B(n + 1, j), pdb,
                &rnorm, &fail);
    if (fail.code != NE_NOERROR) {
        printf("\nError from nag_dge_norm (f16rac).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    printf("  %11.2e ", rnorm);
}
printf("\n");

```

END:



```

NAG_FREE(a);
NAG_FREE(b);
NAG_FREE(c);
NAG_FREE(t);

return exit_status;
}

```

## 10.2 Program Data

nag\_dtpqrt (f08bbc) Example Program Data

```

6      4      2      : m, n and nrhs
-0.57 -1.28 -0.39  0.25
-1.93  1.08 -0.31 -2.14
 2.30  0.24  0.40 -0.35
-1.93  0.64 -0.66  0.08
 0.15  0.30  0.15 -2.13
-0.02  1.03 -1.43  0.50 : matrix A

-2.67  0.41
-0.55 -3.10
 3.34 -4.01
-0.77  2.76
 0.48 -6.17
 4.10  0.21      : matrix B

```

## 10.3 Program Results

nag\_dtpqrt (f08bbc) Example Program Results

Solution(s) for n rows

	1	2
1	1.5179	-1.5850
2	1.8629	0.5531
3	-1.4608	1.3485
4	0.0398	2.9619

Least squares solution(s) for all rows

	1	2
1	1.5339	-1.5753
2	1.8707	0.5559
3	-1.5241	1.3119
4	0.0392	2.9585

Square root(s) of the residual sum(s) of squares

2.22e-02	1.38e-02
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