# NAG Toolbox

# nag\_lapack\_dtpqrt (f08bb)

#### 1 Purpose

nag\_lapack\_dtpqrt (f08bb) computes the QR factorization of a real (m+n) by n triangular-pentagonal matrix.

# 2 Syntax

```
[a, b, t, info] = nag_lapack_dtpqrt(l, nb, a, b, 'm', m, 'n', n)
[a, b, t, info] = f08bb(l, nb, a, b, 'm', m, 'n', n)
```

#### **3** Description

nag\_lapack\_dtpqrt (f08bb) 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  $0 \le l \le \min(m, n)$ . 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\_lapack\_dgeqrt (f08ab)) 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\_lapack\_dtpqrt (f08bb) 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\_lapack\_dgeqrt (f08ab)). Given an initial least-squares problem  $\hat{B}\hat{X} = \hat{Y}$  where X and Y are l by 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 nrhs matrix formed by adding m - l rows on top of  $\hat{Q}^T \hat{Y}$ .

nag\_lapack\_dtpqrt (f08bb) 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  $n, r \ge n$ ,  $\hat{R}$  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 Parameters

### 5.1 Compulsory Input Parameters

1: **I** – INTEGER

l, the number of rows of the trapezoidal part of B (i.e.,  $B_2$ ).

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

### 2: **nb** – INTEGER

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

Constraints:

 $\begin{array}{l} \mathbf{nb} \geq 1; \\ \text{if } \mathbf{n} > 0, \ \mathbf{nb} \leq \mathbf{n}. \end{array}$ 

3:  $\mathbf{a}(lda,:) - \text{REAL} (\text{KIND=nag_wp}) \text{ array}$ 

The first dimension of the array **a** must be at least  $max(1, \mathbf{n})$ .

The second dimension of the array **a** must be at least  $max(1, \mathbf{n})$ .

The n by n upper triangular matrix A.

4:  $\mathbf{b}(ldb,:) - \text{REAL} (\text{KIND=nag_wp}) \text{ array}$ 

The first dimension of the array **b** must be at least  $max(1, \mathbf{m})$ .

The second dimension of the array **b** must be at least  $max(1, \mathbf{n})$ .

The m by n pentagonal matrix B composed of an (m-l) by n rectangular matrix  $B_1$  above an l by n upper trapezoidal matrix  $B_2$ .

### 5.2 Optional Input Parameters

1: **m** – INTEGER

Default: the first dimension of the array b.

m, the number of rows of the matrix B.

*Constraint*:  $\mathbf{m} \ge 0$ .

### 2: **n** – INTEGER

*Default*: the first dimension of the array **a** and the second dimension of the arrays **a**, **b**. (An error is raised if these dimensions are not equal.)

n, the number of columns of the matrix B and the order of the upper triangular matrix A.

*Constraint*:  $\mathbf{n} \ge 0$ .

### 5.3 Output Parameters

- a(lda,:) REAL (KIND=nag\_wp) array
  The first dimension of the array a will be max(1, n).
  The second dimension of the array a will be max(1, n).
  The upper triangle stores the corresponding elements of the n by n upper triangular matrix R.
- 2:  $\mathbf{b}(ldb,:) \text{REAL} (\text{KIND=nag_wp}) \text{ array}$

The first dimension of the array **b** will be  $max(1, \mathbf{m})$ . The second dimension of the array **b** will be  $max(1, \mathbf{n})$ . Details of the orthogonal matrix Q.

3:  $t(ldt,:) - REAL (KIND=nag_wp) array$ 

The first dimension of the array t will be nb.

The second dimension of the array  $\mathbf{t}$  will be  $\mathbf{n}$ .

Further details of the orthogonal matrix Q. The number of blocks is  $b = \lfloor \frac{k}{nb} \rfloor$ , 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:  $T_1, T_2, \ldots, T_b$ . These are stored in the **nb** by n matrix T as  $T = [T_1|T_2|\ldots|T_b]$ .

```
4: info – INTEGER
```

info = 0 unless the function detects an error (see Section 6).

### 6 Error Indicators and Warnings

info < 0

If info = -i, argument *i* had an illegal value. An explanatory message is output, and execution of the program is terminated.

### 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 Further Comments

The total number of floating-point operations is approximately  $\frac{2}{3}n^2(3m-n)$  if  $m \ge n$  or  $\frac{2}{3}m^2(3n-m)$  if m < n.

The block size, **nb**, used by nag\_lapack\_dtpqrt (f08bb) 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  $\mathbf{nb} = 64 \ll \min(m, n)$  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\_lapack\_dtpqrt (f08bb) may be followed by a call to nag\_lapack\_dtpmqrt (f08bc). For example,

```
[t, c, info] = f08bc('Left','Transpose', nb, a(:,1:min(m,n)), t, c);
```

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\_lapack\_dtpmqrt (f08bc) as above.

### 9 Example

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

m

inimize 
$$||Ax_i - b_i||_2$$
,  $i = 1, 2$ 

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\_lapack\_dgeqrt (f08ab) after which the first 4 rows of B are updated by applying  $Q^T$  using nag\_lapack\_dgemqrt (f08ac). The remaining row is added by performing a QR update using nag\_lapack\_dtpqrt (f08bb); B is updated by applying the new  $Q^T$  using nag\_lapack\_dtpmqrt (f08bc); the solution is finally obtained by triangular solve using R from the updated QR.

#### 9.1 Program Text

function f08bb\_example

```
fprintf('f08bb example results\n\n');
```

```
% Minimize ||Ax - b|| using recursive QR for m-by-n A and m-by-p B
m = nag_int(6);
n = nag_{int}(4);
p = nag_int(2);
a = [-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];
      -1.93,
      -0.02,
b = [-2.67, 0.41;
      -0.55, -3.10;
       3.34, -4.01;
      -0.77, 2.76;
0.48, -6.17;
       4.10, 0.21];
nb = n;
% Compute the QR Factorisation of first n rows of A
[QRn, Tn, info] = f08ab( ...
  nb,a(1:n,:));
% Compute C = (C1) = (Q^T)*B
[c1, info] = f08ac(...
      'Left', 'Transpose', QRn, Tn, b(1:n,:));
% Compute least-squares solutions by backsubstitution in R*X = C1
[x, info] = f07te( ...
     'Upper', 'No Transpose', 'Non-Unit', QRn, c1);
% Print first n-row solutions
disp('Solution for n rows');
disp(x(1:n,:));
% Add the remaining rows and perform QR update
nb2 = m-n;
```

```
l = nag_int(0);
[R, Q, T, info] = f08bb( ...
  l, nb2, QRn, a(n+1:m,:));
% Apply orthogonal transformations to C
[c1,c2,info] = f08bc( ...
 'Left','Transpose', l, Q, T, c1, b(n+1:m,:));
% Compute least-squares solutions for first n rows: R*X = C1
[x, info] = f07te( ...
    'Upper', 'No transpose', 'Non-Unit', R, c1);
% Print least-squares solutions for all m rows
disp('Least squares solution');
disp(x(1:n,:));
% Compute and print estimates of the square roots of the residual
% sums of squares
for j=1:p
 rnorm(j) = norm(c2(:,j));
end
fprintf('Square roots of the residual sums of squaresn');
fprintf('%12.2e', rnorm);
fprintf('\n');
```

#### 9.2 Program Results

f08bb example results

Solution for n rows 1.5179 -1.5850 1.8629 0.5531 -1.4608 1.3485 0.0398 2.9619 Least squares solution 1.5339 -1.5753 0.5559 1.8707 -1.5241 1.3119 0.0392 2.9585 Square roots of the residual sums of squares 1.38e-02 2.22e-02