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ON QR FACTORIZATION UPDATINGS

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Resumen y motivación

Recientemente, se han propuesto varios métodos para modificar los factores Q y R de una matrix una vez que se ha eliminado (o añadido) una fila ó una columna. Normalmente, la descripción de estos métodos se efectua en el contexto de una determinada aplicación; quizá sea ésta la causa de su escasa difusión.

La aplicación de la factorización QR se puede concretar, básicamente, en las tres siguientes posibilidades: resolución de un sistema sobredeterminado de ecuaciones lineales, obtención del vector que ajusta por mínimos cuadrados una linea a una serie de observaciones, y estimación de los coeficientes multiplicadores de Lagrange en programación no lineal con restricciones. Aunque esta última aplicación es la motivación de este trabajo y predecesores (ver referencias), los métodos descritos pueden aplicarse de forma análoga en las dos situaciones anteriores.

Sea A una matrix $n \times t$ (donde $n \geqslant t$) de rango t tal que $\underline{\underline{Q}}'A = (R'^t\, 0^t)^t$ es su factorization QR donde $\underline{\underline{Q}}'$ y $\underline{\underline{Q}}'^t$ son matrices no simétricas ortonormales $n \times n$, R' es una matrix triangular superior no singular $t \times t$ de rango t, y 0 es la matrix nula $(n-t) \times t$. Sea $\underline{\underline{Q}}'^t = (Q'\, Q_2')$ donde Q' y Q_2' son, por tanto, matrices ortonormales. De donde, $A = Q'R'$. Sean $\underline{\underline{Q}}$ y $\underline{\underline{Q}}^t$ matrices ortogonales $n \times n$ tal que $\underline{\underline{Q}}^t = (Q\, Q_2)$,

(*) Recibido, Enero, 1982

$Q = Q'D$ y $R = D^{-1}R'$, donde D es una matrix diagonal $t \times t$ que recoge la norma euclidea de las columnas de Q.

Aunque teóricamente $A = Q'R'$ y $A = QR$, las expresiones anteriores no son necesariamente correctas desde un punto de vista computacional debido a los errores de redondeo y cancelación que existen en las operaciones intermedias para obtener los factores. En trabajos anteriores demostramos que la utilización de Q y R es mas estable que Q' y R'.

Ocurre frecuentemente que una vez obtenidos los factores Q y R (ó Q' y R'), se modifica la matrix A tal que se elimina ó añade una de sus filas o columnas (ver las aplicaciones apuntadas más arriba); en este caso, no es preciso calcular los nuevos factores de la matrix A totalmente desde el principio, aunque computacionalmente sería lo más correcto. Ahorros considerables de tiempo de cálculo se pueden obtener si se elimina ó añade una columna ó fila en los factores Q y R (ó Q' y R') y, posteriormente, se efectua la correspondiente transformación a base de aplicar matrices Givens.

En este trabajo describimos métodos, computacionalmente estables, para actualizar los factores Q y R de la matrix A una vez que se ha eliminado una fila o una columna en dicha matrix.

Abstract

In recent years several algorithms have appeared in the literature for modifying the factors of a matrix following a rank-1 change. These methods have always been given in the context of specific applications and this has probably inhibited their use over a wider field. In this report a method is given for obtaining the QR factors of a matrix and its updatings after a row or a column has been deleted.

1. INTRODUCTION

Let A be a $n \times t$ (where $n \geqslant t$) full column rank matrix being $\underline{Q}'A = (R'^t 0^t)^t$ its QR factorization, such that $\underline{Q}'$ and $\underline{Q}'^t$ are $n \times n$ nonsymmetric orthonormal matrices and R' is a $t \times t$ nonsingular full rank triangular matrix. Let $\underline{Q}'^t$ be partitioned such that $\underline{Q}'^t = (Q' Q_2')$ where Q' and Q_2' are $n \times t$ and $n \times (n - t)$ matrices, respectively.

Note that $\underline{Q}'^t\underline{Q}' = I$ and, then, $Q'^tQ' = \mathrm{I}$, $Q_2'^tQ_2' = I$ and $Q'^tQ_2' = 0$. Note also that $\underline{Q}'\underline{Q}'^t = I = Q'Q'^t + Q_2'Q_2'^t$ and $A = Q'R'$. Elsewhere [3] we survey the applicability of the QR-factorization and, specially, the expresion $A = Q'R'$ in linear least square fitting and nonlinear programming.

Let $\underline{Q}$ and $\underline{Q}^t$ be $n \times n$ nonsymmetric orthogonal matrices; let $\underline{Q}^t$ be partitioned such that $\underline{Q}^t = (Q\,Q_2)$ where $Q = Q'D$, being D a $t \times t$ diagonal matrix such that d_i takes the euclidean norm of the i-th column vector of matrix Q.

Note that theoretically $A = Q'R' = QR$ where $R = D^{-1}R'$; but it is not computationally guaranteed that it is correct. Elsewhere [2] we describe a version of the modified Gram-Schmidt QR-factorization that obtains factors Q and R with the maximun accuracy that is possible in today computers. See in [12, 7, 10, 9, 5, 1, 4 and 11] different versions for obtaining factors Q' and R'. Our results show that factorizing A with Q and R is far more stable that using Q' and R'; the reason is that rounding errors are reduced if some computational calculations are substituted by their values derived from theoretical properties.

Very frequently it happens that once obtained factors Q and R (or Q' and R'), matrix A is modified by adding or deleting a row or a column. Let $\bar{A}$ be the new matrix and $\bar{Q}$ and $\bar{R}$ the new factors. Considerable savings can be made if $\bar{Q}$ and $\bar{R}$ are not completely calculated anew, but Q and R are updated after being selected the row or column to be added or deleted. The general idea consists in adding or deleting a row or column to matrices Q and R such that $\bar{A} = \bar{Q}\bar{R}$ and, by applying Givens matrices, modifiy $\bar{Q}$ and $\bar{R}$ such that they become QR-factors. Elsewhere [3] we describe the procedures for updating Q and R when adding a column or a row; see in [5, 1] procedures for updating factors $\underline{Q}'$, Q' and R'. In this paper we describe computationally stable procedures for updating Q and R when a column or a row is deleted from matrix A.

Notation. Small letters denote column vectors (and, sometimes, scalars), subindexed capital letters denote row vectors, and capital letters denote matrices.

Through the paper we will extensively use Givens matrices [6, 8]. Recall that a Givens matrix, say P_j^i is the identity matrix where its (i, i)-th, (i, j)-th, (j, i)-th and (j, j)-th elements are substituted by c, s, s and

-c, respectively, such that $c^2 + s^2 = 1$. Note that P_j^i and $P_j^{i^t}$ are orthonormal matrices. One of the most useful applications of Givens matrices is the possibility of anninhilating a single element, say j of a vector based on other element, say i such that if we set

$$\varrho^2 = v_i^2 + v_j^2, \quad c = -+v_i/\varrho, \quad s = -+v_j/\varrho$$

then $\bar{v} = P_j^i v$ is such that $\bar{v}_i = -+\varrho$, $\bar{v}_j = 0$ and $\bar{v}_k = v_k$ for $k \neq i, j$

An efficient computation $P_j^i z$ (where z is any vector distint of v) is as follows.

(1) Compute $y = s/(1 + c)$.

(2) $\bar{z}_i = cz_i + sz_j$; $\bar{z}_j = y(z_i + \bar{z}_i) - z_j$; $\bar{z}_k = z_k$ for $k \neq i, j$.

2. DELETING A COLUMN VECTOR FROM MATRIX A

Let delete column vector a from matrix $A = QR$ whose dimensions are as above; then,

$$\begin{aligned} A &\equiv (A_1 \, \mathrm{a} \, A_2) = Q(R_1 \, \mathrm{r} \, R_2) \\ \bar{A} &\equiv (A_1 A_2) = Q(R_1 R_2) = Q\hat{R} \end{aligned} \tag{2.1}$$

where $\hat{R}$ is a $t \times (t-1)$ upper Hessenberg matrix (whose diagonal is not necessarily the identity in its last part R_2) with identity subdiagonal from row $p+1$ to t, such that column vector r is the p-th column of matrix R. Note that if $p = t$ then R_2 vanishes and $\hat{R} = R_1$ is already upper triangular with identity diagonal. For transforming $\hat{R}$ in an upper triangular form, it could be written

$$\bar{A} = QP^tP\hat{R} \tag{2.2}$$

where P is the product of Givens matrices such that

$$P = P_t^{t-1}, \ldots, P_{p+2}^{p+1} P_{p+1}^{p} \tag{2.3}$$

Note that Q is non-normalized (and, then, QP^t is not orthogonal). But since $A = Q'R'$ where $Q' = QD^{-1}$ and $R' = DR$ and $Q'P^t$ is orthonormal, it results

$$\bar{A} = QD^{-1}P^tP\hat{R}' \tag{2.4}$$

where

$$\hat{R}' = (R_1' R_2') \tag{2.5}$$

such that R_1' takes the first $p - 1$ columns of DR, and R_2' takes the last $t - p$ columns of DR. After applying P to $\hat{R}'$ we have matrix

$$\begin{pmatrix} \bar{R}' \\ 0 \end{pmatrix} = P\hat{R}' \tag{2.6}$$

where $\bar{R}'$ is a $(t - 1) \times (t - 1)$ upper triangular matrix whose diagonal is not necessarily the identity, and 0 is the zero $(t - 1)$-row vector.

Assuming that $\bar{d}_i = \bar{r}'_{ii}$, it results

$$\bar{R}' = \bar{D}\bar{R} \tag{2.7}$$

where $\bar{R}$ is a $(t - 1) \times (t - 1)$ upper triangular matrix with identity diagonal. Then, denoting

$$(\bar{Q}' \, \bar{q}') \equiv QD^{-1}P^t \tag{2.8}$$

it results

$$\bar{A} = QD^{-1}P^t\bar{D}\begin{pmatrix} \bar{R} \\ 0 \end{pmatrix} = (\bar{Q}' \, \bar{q}')\bar{D}\begin{pmatrix} \bar{R} \\ 0 \end{pmatrix}$$

where $(\bar{Q}' \, \bar{q}')$ is a $n \times t$ orthonormal matrix and, then $\bar{Q}'$ is a $n \times (t - 1)$ orthonormal matrix.

By using (2.7) and (2.8), it results

$$\bar{A} = (\bar{Q}' \, \bar{q}')\begin{pmatrix} \bar{R}' \\ 0 \end{pmatrix} = \bar{Q}'\bar{R}'$$

Note that $\|\bar{q}_i\|_2 \equiv \bar{d}_i$ is already available; then, it results

$$\bar{A} = \bar{Q}'\bar{R}' = \bar{Q}\bar{D}^{-1}\bar{D}\bar{R} = \bar{Q}\bar{R}$$

where $\bar{Q}$ is a $n \times (t - 1)$ orthogonal matrix and $\bar{R}$ is a $(t - 1) \times (t - 1)$ upper triangular matrix with identity diagonal. Note that $|| \cdot ||_2$ is the norm that has been used. Although comparing this procedure with the direct calculation of Q and R [2] where $|| \cdot ||_2^2$ is used, it is not so stable, the time savings are considerable; however, matrix $\bar{A}$ must be directly factorized after a given number of updatings.

The computational procedure is as follows.

QRDEC (*QR updating when the p-th column vector is deleted from* *matrix A*).

Step 0. If $p = t$ then reset $\bar{R} = R_1$ (2.1), delete column vector q_t from Q, reset $\bar{Q} = Q$, and end the procedure.

Note. In the description of the procedure we will refer to several matrices (Q', $\bar{Q}'$, $\bar{Q}$ and, so $\hat{R}'$, $\bar{R}'$, $\bar{R}$); but for the sake of storage saving we will only work with matrices Q and R;.

Step 1. Obtain matrix Q' such that reset $q_i = q_i/d_i$ for $i = p, \ldots, t$.

Step 2. Obtain matrix $\hat{R}'$ such that reset $r_i = r_{i+1}$ for $i = p, \ldots, t-1$, $r_{pj} = r_{pj}d_p$ for $j = p, \ldots, t-1$, $r_{t,t-1} = d_t$, $r_{ij} = r_{ij}d_i$ for $j = i-1, \ldots, t-1$ and $i = p+1, \ldots, t-1$.

Step 3. Obtain matrices $\bar{R}'$ and $\bar{Q}'$; that is, obtain row vector $\bar{R}'_k$ and column vector $\bar{q}'_k$ for $k = 1, \ldots, t-1$. Note that since $\bar{q}'_k = q'_k$ and $\bar{R}'_k = R'_k$ for $k = 1, \ldots, p-1$ then step 3 is restricted to $k = p, \ldots, t-1$.

Obtain $P^k_{k+1}r_k$ where r_k is the k-th column of $\bar{R}'$; that is, obtain r_{hk} for $h = k, k+1$:

$$\begin{aligned} a &= (r^2_{kk} + r^2_{k+1,k})^{1/2} \\ c &= r_{kk}/a; \quad s = r_{k+1,k}/a \\ r_{kk} &= a; \quad r_{k+1,k} = 0 \\ y &= s/(1+c) \end{aligned}$$

Obtain $P^k_{k+1}r_i$ for $i = k+1, \ldots, t-1$; trhat is, obtain r_{hi} for $h = k, k+1$:

$$\begin{aligned} a &= cr_{ki} + sr_{k+1,i} \\ r_{k+1,i} &= y(r_{ki} + a) - r_{k+1,i} \\ r_{ki} &= a \end{aligned}$$

Obtain $Q'P^k_{k+1}$; that is, obtain $q_{hk}P^k_{k+1}$ and $q_{h,k+1}P^k_{k+1}$ for h $= 1, \ldots, n$:

$$\begin{aligned} a &= cq_{hk} + sq_{h,k+1} \\ q_{h,k+1} &= y(q_{hk} + a) - q_{h,k+1}. \text{ It is not required for } k = t-1 \\ q_{hk} &= a \end{aligned}$$

Step 4. Obtain matrices $\bar{R}$ and $\bar{Q}$; that is, obtain row vector $\bar{R}_i$ and column vector $\bar{q}_i$ for $i = p, \ldots, t-1$, such that reset

$$r_{ij} = r_{ij}/r_{ii} \text{ for } j = i+1, \ldots, t-1$$
$$q_{hi} = q_{hi}r_{ii} \text{ for } h = 1, \ldots, n$$
$$d_i^2 = r_{ii}^2; \quad r_{ii} = 1$$

such that $d_i = (d_i^2)^{1/2}$.

3. DELETING A ROW VECTOR FROM MATRIX A

Assume matrix $A = QR$ has the same dimensions as above being $n > t$ and row vector A_n is to be deleted from A. Without loss of generality we may assume that the vector is in the bottom of matrix A; if it is not then we may permute the rows in A and Q so that

$$\begin{pmatrix} \bar{A} \\ A_n \end{pmatrix} = \begin{pmatrix} \tilde{Q} & 0 \\ Q_n & 1 \end{pmatrix} \begin{pmatrix} R \\ 0 \end{pmatrix} \equiv (Q \quad e_n) \begin{pmatrix} R \\ 0 \end{pmatrix} \tag{3.1}$$

where $\tilde{Q}$ is a $(n-1) \times t$ matrix obtained by deleting row vector Q_n from the $n \times t$ orthogonal matrix Q; then $\tilde{Q}$ is not orthogonal, nor it is matrix $(Q \times e_n)$ since

$$\begin{pmatrix} \tilde{Q}^t & Q_n^t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{Q} & 0 \\ Q_n & 1 \end{pmatrix} = \begin{pmatrix} D^2 & Q_n^t \\ Q_n & 1 \end{pmatrix}$$

and $Q_n \neq 0$ by definition of the QR factorization.

Let as usual $Q' = QD^{-1}$ be the corresponding orthornomal matrix, being $R' = DR$

The aim is to transform matrix $\tilde{Q}'$ in orthonormal so that the new matrix $\bar{Q}'$ is such that

$$\begin{pmatrix} \bar{A} \\ A_n \end{pmatrix} = \begin{pmatrix} \bar{Q}' & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{R}' \\ A_n \end{pmatrix} \tag{3.2}$$

where $\bar{Q}'$ and $\bar{R}'$ are the factors of $\bar{A}$, being $\bar{Q}'$ orthornormal and $\bar{R}'$ upper triangular.

For obtaining (3.2) we must transform matrix

$$\begin{pmatrix} \tilde{Q}' & 0 \\ Q_n' & 1 \end{pmatrix} \tag{3.3}$$

in orthornormal without modifying the upper triangular structure of matrix R'; that is, we must obtain the scalars σ and ϱ, the $(n-1)$-column vector $\tilde{q}$ and the t-column vector r, such that the QR factorization of matrix (3.3) can be written

$$\begin{pmatrix} \tilde{Q}' & 0 \\ Q_n' & 1 \end{pmatrix} = \begin{pmatrix} \tilde{Q}' & \tilde{q} \\ Q_n' & \sigma \end{pmatrix} \begin{pmatrix} \mathrm{I} & r \\ & \varrho \end{pmatrix} \tag{3.4}$$

since in that case

$$\begin{pmatrix} \bar{A} \\ A_n \end{pmatrix} = \begin{pmatrix} \tilde{Q}' & \tilde{q} \\ Q_n' & \sigma \end{pmatrix} \begin{pmatrix} I & r \\ & \varrho \end{pmatrix} \begin{pmatrix} R' \\ 0 \end{pmatrix} = \begin{pmatrix} \tilde{Q}' & \tilde{q} \\ Q_n' & \sigma \end{pmatrix} \begin{pmatrix} R' \\ 0 \end{pmatrix} \tag{3.5}$$

Since matrix

$$\begin{pmatrix} \tilde{Q}' & \tilde{q} \\ Q_n' & \sigma \end{pmatrix} \tag{3.6}$$

is orthonormal, if it is postmultiplied by P^t, where P is an appropiate sweep of Givens matrices (see below) then the new matrix is also orthonormal. If matrix P is such that

$$(Q_n' \quad \sigma)P^t = (0 \quad -+1) \tag{3.7a}$$

then

$$(\tilde{Q}' \quad \tilde{q})P^t \equiv (\bar{Q}' \quad \bar{q}') = (\bar{Q}' \quad \bar{0}) \tag{3.7b}$$

since matrix

$$\begin{pmatrix} \bar{Q}' & \bar{q}' \\ 0 & -+1 \end{pmatrix}$$

is also orthonormal.

Note that $\bar{q}' = 0$ since $1 = ||(\bar{q}'^t \quad -+1)||_2^2$. Let $(\bar{q}_i'^t \quad 0)$ be the i-th row of matrix $(\bar{Q}'^t \quad 0)$; then, we also have that $1 = ||(\bar{q}_i'^t \quad 0)||_2^2 = ||\bar{q}_i'||_2^2$.

From (3.5) it finally results (see below)

$$\begin{pmatrix} \bar{A} \\ A_n \end{pmatrix} = \begin{pmatrix} \tilde{Q}' & \tilde{q} \\ Q_n' & \sigma \end{pmatrix} P^t P \begin{pmatrix} R' \\ 0 \end{pmatrix} = \begin{pmatrix} \bar{Q}' & 0 \\ 0 & -+1 \end{pmatrix} \begin{pmatrix} \bar{R}' \\ C \end{pmatrix} = \begin{pmatrix} \bar{Q}'\bar{R}' \\ C' \end{pmatrix}$$

where C is a t-row vector (note that $A_n = C'$), such that

$$\bar{A} = \bar{Q}'\bar{R}' = \bar{Q}\bar{D}^{-1}\bar{D}\bar{R} = \bar{Q}\bar{R}$$

where $\bar{D}$ is a $t \times t$ diagonal matrix such that $\bar{d}_i = r'_{ii}$, $\bar{Q}$ is a $(n-1) \times t$ orthogonal matrix, and $\bar{R}$ is a $t \times t$ upper triangular matrix with identity diagonal.

For obtaining σ, ϱ, $\tilde{q}$ and r we may proceed as follows.

The QR factorization of matrix (3.3) means that

$$\begin{pmatrix} Q'^t & \\ \tilde{q}^t & \sigma \end{pmatrix} \begin{pmatrix} Q' & \tilde{q} \\ & \sigma \end{pmatrix} = \begin{pmatrix} I & Q'^t\begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix} \\ (\tilde{q}^t \quad \sigma)Q' & ||\tilde{q}||_2^2 + \sigma^2 \end{pmatrix} = I$$

where

$$Q' \equiv \begin{pmatrix} \tilde{Q}' \\ Q'_n \end{pmatrix}$$

and, then

$$Q'^t\begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix} = 0 \tag{3.8}$$

such that from (3.4) we have

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = Q'r + \begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix}\varrho \tag{3.9}$$

Premultiplying it by Q'^t, it results

$$Q'^t\begin{pmatrix} 0 \\ 1 \end{pmatrix} = Q'^tQ'r + Q'^t\begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix}\varrho$$

and, then

$$Q'^t_n = r + Q'^t\begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix}\varrho = r \tag{3.9}$$

since expression (3.8) must hold. If $\varrho \neq 0$ then matrix (3.3) is QR-factorized provided that $||\tilde{q}||_2^2 + \sigma^2 = 1$ (i.e., it is a unit length vector); otherwise, any vector $\tilde{q}$ with unit length (since $\sigma = \varrho$ as we may see below) that satisfies the orthogonality property $\tilde{Q}'^t\tilde{q} = 0$ may produce the QR factorization of matrix (3.3); see (3.8). See below that should $\varrho \neq 0$ it may be made positive.

Note that if theoretically $\tilde{q}\varrho = 0$ then matrix (3.3) is not a full column rank matrix since from (3.9) it results that the $(n+1)$-th column of matrix (3.3) is a linear combination of its n first columns (matrix

Q'). In this case, matrix (3.3) has not a QR factorization; the corresponding factorization is termed complete QR factorization.

If ϱ as given by expression (3.13) is 'small' the procedure may become ill-conditioned when calculating $\tilde{q}$ and the orthogonality property (3.8) of matrix (3.3) may be lost. The calculated value (3.13a) of ϱ may be small due to rounding errors in the calculation of Q'_n

$$Q'_n = \sum_{i=1}^{t} q_{ni}/d_i$$

since in $d_i \equiv ||q_i||_2$ square root operations are used. However, by using expression (3.13b) where square roots operations are avoided, the risk of losing orthogonality is strongly reduced.

Expression (3.9) can also be written

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \tilde{Q}'r + \tilde{q}\varrho \\ Q'_n r + \sigma\varrho \end{pmatrix} = \begin{pmatrix} \tilde{Q}'\tilde{Q}'^t_n \\ Q'_n Q'^t_n \end{pmatrix} + \begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix}\varrho$$

from where

$$\begin{pmatrix} 0 - \tilde{Q}'Q'^t_n \\ 1 - Q'_n Q'^t_n \end{pmatrix} = \begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix}\varrho \tag{3.11}$$

Since matrix (3.6) is orthonormal, it results that

$$||\tilde{q}||_2^2 + \sigma^2 = 1$$

and then

$$\begin{aligned} \left|\left|\begin{pmatrix} \tilde{q} \\ \sigma \end{pmatrix}\varrho\right|\right|_2^2 &= \varrho^2(||\tilde{q}||_2^2 + \sigma^2) = \varrho^2 \\ &\equiv ||\tilde{Q}'Q'^t_n||_2^2 + (1 - Q'_n Q'^t_n)^2 \\ &= Q'_n\tilde{Q}'^t\tilde{Q}'Q'^t_n + (1 - Q'_n Q'^t_n)^2 \end{aligned} \tag{3.12}$$

Since $Q' \equiv \begin{pmatrix} \tilde{Q}' \\ Q'_n \end{pmatrix}$ is orthonormal and, then

$$I = Q'^t Q' \equiv (\tilde{Q}'^t Q'^t_n)\begin{pmatrix} \tilde{Q}' \\ Q'_n \end{pmatrix} = \tilde{Q}'^t\tilde{Q}' + Q'^t_n Q'_n$$

it results that (3.12) can be written

$$\varrho^2 = Q'_n(I - Q'^t_n Q'_n)Q'^t_n + (1 - Q'_n Q'^t_n)^2$$

$$= 1 - Q'_n Q'^t_n \qquad (3.13a)$$

$$= 1 - \sum_{i=1}^{t} q^2_{ni}/d^2_i \qquad (3.13b)$$

By using the last part of matrix (3.11) and (3.13*a*), it results that $\varrho^2 = \sigma\varrho$. Then, if $\varrho \neq 0$ we have $\varrho = \sigma$; if $\varrho = 0$ it results that $Q'_n Q'^t_n = 1$ and, since $Q'_n Q'^t_n + \sigma^2 \leqslant 1$ (see below), it finally results that $\sigma = 0$. We may see that in any case $\varrho = \sigma$.

As a result we have

$$r = Q'^t_n \qquad (3.10)$$

$$\varrho = \sigma$$

$$\varrho^2 = 1 - Q'_n Q'^t_n \quad \text{but using expression} \qquad (3.13b)$$

$$\tilde{q}_h = -\left(\sum_{i=1}^{t} q_{hi} q_{ni}/d^2_i\right)/\varrho \quad \text{for} \quad h = 1, \ldots, n \qquad (3.14)$$

by using (3.11) and avoiding square root operations.

Note that $Q'_n Q'^t_n + \sigma^2 \leqslant 1$; in effect, let $\underline{Q}'$ be the $n \times n$ orthonormal matrix, such that

$$\underline{Q}'\begin{pmatrix} \tilde{Q}' & 0 \\ Q'_n & 1 \end{pmatrix} = \begin{pmatrix} \underline{R}' \\ 0 \end{pmatrix}$$

where

$$\underline{R}' \equiv \begin{pmatrix} I & r \\ & \varrho \end{pmatrix}$$

Note that matrix (3.3) is a $n \times (t + 1)$ full column rank matrix. Matrix $\underline{Q}''$ can be written $\underline{Q}'^t_2 = (\underline{Q}'_1 \quad \underline{Q}'_2)$ where Q'_1 is matrix (3.6). Then.

$$I = \underline{Q}''\underline{Q}' = (\underline{Q}'_1 \quad \underline{Q}'_2)\begin{pmatrix} \underline{Q}'^t_1 \\ \underline{Q}'^t_2 \end{pmatrix} = \underline{Q}'_1\underline{Q}'^t_1 + \underline{Q}'_2\underline{Q}'^t_2$$

Let $\underline{Q}'_n$ denote the n-th row of matrix $\underline{Q}''$; then

$$1 = \underline{Q}'_n\underline{Q}'^t_n = \underline{Q}'_{1n}\underline{Q}'^t_{1n} + \underline{Q}'_{2n}\underline{Q}'^t_{2n}$$

Note that $0 < \underline{Q}'_{1n}\underline{Q}'^{t}_{1n} \leqslant 1$ and, then, equivalently

$$(Q'_n \quad \sigma)\begin{pmatrix} Q'^{t}_n \\ \sigma \end{pmatrix} \leqslant 1$$

Matrix P in transformation (3.7a) can be expressed such that

$$P\begin{pmatrix} Q'^{t}_n \\ \varrho \end{pmatrix} = P_1^{t+1}P_2^{t+1}\cdots P_t^{t+1}\begin{pmatrix} Q'^{t}_n \\ \varrho \end{pmatrix} = \gamma e_{t+1} \qquad (3.15)$$

Note that $\gamma = -+1$ since

$$\left|\left|P\begin{pmatrix} Q'^{t}_n \\ \varrho \end{pmatrix}\right|\right|_2^2 = (Q'_n \quad \varrho)P^tP\begin{pmatrix} Q'^{t}_n \\ \varrho \end{pmatrix} = Q'_nQ'^{t}_n + \varrho^2$$

and from (3.13), and by using (3.15), it results

$$1 = ||\gamma e_{t+1}||_2^2 = \gamma^2$$

Note that the application of P^tP to matrix (3.5) can be expressed

$$\begin{pmatrix} \tilde{Q}' & \tilde{q} \\ Q'_n & \varrho \end{pmatrix} P_t^{t+1}\cdots P_2^{t+1}P_1^{t+1}P_1^{t+1}P_2^{t+1}\cdots P_t^{t+1}\begin{pmatrix} R' \\ 0 \end{pmatrix}$$

The computational procedure is as follows.

QRDER (*QR updating when the last row vector is deleted from matrix A*)

Assume that A is a full column rank $n \times t$ matrix where $n > t$.

Step 1. Obtain scalar ϱ (3.13b) such that

$$\varrho^2 = 1 - \sum_{i=1}^{t} q_{ni}^2/d_i^2; \quad \varrho = (\varrho^2)^{1/2}$$

Step 2. Obtain the $(n-1)$-column vector $\tilde{q}$ (3.14) such that

$$q_h = -\left(\sum_{i=1}^{t} q_{hi}q_{ni}/d_i^2\right)/\varrho \quad \text{for} \quad h = 1, \ldots, n-1$$

Step 3. Obtain matrices $R' = DR$ and $Q' = QD$, such that R and Q are reset to the normalized values.

Note that the t-column vector r (3.10) is not required by the procedure.

Step 4 Obtain matrices $\bar{Q}'$ and $\bar{R}'$; that is, obtain column vector $\bar{q}'_k$

and row vector $\bar{R}'_k$ for $k = t, \ldots, 1$ by using matrix P in (3.15). For that purpose, the operations to be perfomed are as follows. Obtain updating of ϱ by reducing to zero the k-th element of Q'_n, such that the operation $(Q'_n \quad \varrho)P_k^{t+1}$ (3.7a) is performed:

$$\varrho^2 = q_{nk}^2 + \varrho^2; \quad a = (\varrho^2)^{1/2}; \quad \text{if } \varrho > 0 \text{ then } a = -a.$$
$$c = \varrho/a; \quad s = q_{nk}/a. \text{ Note that } -1 < c < 0$$
$$\varrho = a; \quad q_{nk} = 0$$
$$y = s/(1 + c)$$

Obtain $(\bar{Q}' \quad \bar{q}')P_k^{t+1}$ (3.7b); that is, obtain $\bar{q}'_k$ and $\bar{q}'$. Note that it consists in resetting q_{hk} and q_h for $h = 1, \ldots, n - 1$:

$$a = cq_h + sq_{hk}$$
$$q_{hk} = y(q_h + a) - q_{hk}$$
$$q_h = a$$

Obtain $P_k^{t+1}R'$; that is, obtain $P_k^{t+1}R'_i$ for $i = k, \ldots, t$:

Obtain r_{kk} and c_k, where c_k is the k-th element of row vector C:

$$c_k = sr_{kk}$$
$$r_{kk} = -cr_{kk} > 0$$

Obtain r_{ki} and c_i for $i = k + 1, \ldots, t$:

$$a = -cr_{ki} + sc_i$$
$$c_i = sr_{ki} + cc_i$$
$$r_{ki} = a$$

Step 5. Obtain matrices $\bar{R}$, $\bar{Q}$ and $\bar{D}$ as in procedure ORDEC such that $i = 1, \ldots, t$, $j = i + 1, \ldots, t$ and $h = 1, \ldots, n - 1$.

For avoiding computational rounding errors and noting that $\bar{d}_k^2 = \bar{r}'^2_{kk}$ for $k = 1, \ldots, t$, the above calculation of r_{kk} is substituted by the following:

$$c_k = sd_k \quad \text{and} \quad \bar{d}_k^2 = c^2 d_k^2 > 0$$

such that vectors $\bar{q}_k$ and $\bar{R}_k$ for $k = 1, \ldots, t$ are calculated in step 5 as follows. Reset:

$$\bar{r}_{ki} = \bar{r}_{ki}/\bar{d}_k \quad \text{for} \quad i = k+1, \ldots, t \quad \text{and} \quad \bar{r}_{kk} = 1$$
$$\bar{q}_{hk} = \bar{q}_{hk}\bar{d}_k$$

where $\bar{d}_k = (\bar{d}_k^2)^{1/2}$.

8. CONCLUSIONES

In this report we have presented a set of methods that can be used to update the QR factorization of a $n \times t$ matrix after the most frequently used matrix modifications. These methods keep updated two matrices and one vector whose storage needs are $n \times t$, $t \times (t-1)/2$ and t, respectively. The computational time in each updating is very small; special care has been taken in computational stability.

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