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REVIEW

Linear equality-constrained least-square problems by generalized QR factorization

El problema de los mínimos cuadrados con restricciones de igualdad mediante la factorización QR generalizada

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Abstract
The generalized QR factorization, also known as GQR factorization, is a method that simultaneously transforms two matrices A and B in a triangular form. In this paper, we show the application of GQR factorization in solving linear equality-constrained least square problems; in addition, we explain how to use GQR factorization for solving quaternion least-square problems through the matrix representation of quaternions.
Keywords . GQR factorization, linear equality-constrained least square problems, quaternions.

Resumen
La factorización QR generalizada, también conocida como factorización GQR, permite descomponer dos matrices A y B simultáneamente a una forma triangular. En este artículo, se muestra como aplicar la factorización GQR para resolver problemas de mínimos cuadrados con restricciones de igualdad; además, se emplea esta factorización para resolver problemas de mínimos cuadrados sobre cuaterniones.
Palabras clave. Factorización QR generalizada, problema de los mínimos cuadrados con restricciones de igualdad, cuaterniones.

1. Introduction. The QR factorization is a decomposition of A into a product of an orthogonal matrix Q and an upper triangular matrix R, i.e. $A = QR$. The generalized QR factorization, known as GQR factorization, was introduced in [3] and has been widely studied as a method that simultaneously transform two matrices $A_{m\times n}$ and $B_{m\times p}$ in a triangular form.

QR factorization approaches has been successfully used to solve linear least-square problems (LS) and linear equality-constrained least square problems (LSE), cf. [2]. The GQR factorization allows us to solve LSE problems more efficiently, in terms of computation, providing information on the conditioning of these generalized problems just as QR factorization [1]. Least square methods can be used to solve quaternion linear equations $AX \sim B$ [5].

Recently, quaternion least-squares problems (QLS) and linear equality-constrained quaternion least-square problem (QLSE) and its applications have been studied [9]. In this paper, we use GQR factorization to solve LSE problems; in addition, we show that QLS and QLSE problems can also be solved by GQR factorization through the matrix representation of quaternions.

2. The generalized QR factorization. The generalized QR factorization simultaneously transform two matrices A and B to triangular form. Following [1], we present the generalized QR and RQ factorizations as follows.

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Proposition 2.1. *Let $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{m\times p}$, then*

1. ***GQR factorization:*** *If $m \geq n$, there are orthogonal matrices Q and V such that $Q^TA = R$ and $Q^TBV = S$, where R and S are upper trapezoidal.*
2. ***GRQ factorization:*** *If $m < n$, there are orthogonal matrices $Q_{m\times m}$ and $U_{n\times n}$ such that $Q^TAU = R$ and $Q^TB = S$.*

Proof: Here we prove 1.; 2. can be similarly proved. If $m \geq n$, by QR factorization, there exist Q orthogonal and R upper trapezoidal matrices such that $A = QR$, therefore

$$R = Q^TA = \begin{bmatrix} R_1 \\ 0_{m-n,n} \end{bmatrix} \text{ where } R_1 \text{ has } n \text{ rows and columns.}$$

By RQ factorization, there are S and W such that $Q^TB = SW$, where S is upper triangular and W is orthogonal, so $[Q^TB]W^T = S$. Let $V = W^T$, then $[Q^TB]V = S$.

- If $m \leq p$, $[Q^TB]V = S = [S_1 \; 0_{m,p-m}]$ with $S_1 \in \mathbb{R}^{m\times m}$.
- If $m > p$, $[Q^TB]V = S = \begin{bmatrix} S_1 \\ S_2 \end{bmatrix}$. Where S_1 has $m - p$ rows and S_2 has p rows.

In the above proof, for the case $m \leq p$, S can be expressed in the form $S = [0_{m,p-m} \; S_2]$ with $S_2 \in \mathbb{R}^{m\times m}$, cf. [1]. The GQR and GRQ factorization can be defined with pivoting, in this paper we use these decompositions without pivoting.

Example 2.1. *Let A and B be matrices given by*

$$A = \begin{bmatrix} 1 & 2 & 3 \\ -3 & 2 & 1 \\ 2 & 0 & -1 \\ 3 & -1 & 2 \end{bmatrix}, \; B = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ -3 & 2 & -2 & 1 & 2 \\ 2 & 3 & 4 & -2 & -1 \\ 1 & 3 & -2 & 2 & 1 \end{bmatrix}.$$

A GQR factorization for A and B, presented in [1], is given by the following matrices

$$Q = \begin{bmatrix} -0.2085 & -0.8792 & 0.1562 & -0.3989 \\ 0.6255 & -0.4147 & 0.1465 & 0.6444 \\ -0.4170 & -0.2322 & -0.7665 & 0.4296 \\ -0.6255 & 0.0332 & 0.6054 & 0.4910 \end{bmatrix}, \; R = \begin{bmatrix} -4.7958 & 1.4596 & -0.8341 \\ 0 & -2.6210 & -2.7537 \\ 0 & 0 & 2.5926 \\ 0 & 0 & 0 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.3375 & -0.0791 & -0.2690 & -0.6363 & 0.6345 \\ -0.8926 & -0.2044 & 0.1635 & -0.2770 & 0.2407 \\ -0.0534 & -0.5118 & -0.5793 & -0.2833 & -0.5651 \\ -0.1584 & -0.1280 & -0.6087 & 0.6280 & 0.4401 \\ -0.2478 & 0.8208 & -0.4413 & -0.2091 & -0.1626 \end{bmatrix}$$

$$S = \begin{bmatrix} 0 & -3.431 & 2.8692 & -1.8585 & 0.1388 \\ 0 & 0 & 7.0240 & 2.1937 & 0.1571 \\ 0 & 0 & 0 & -5.9566 & 1.0776 \\ 0 & 0 & 0 & 0 & 3.9630 \end{bmatrix}.$$

Another GQR factorization is given by Q and R as above, and V and S given by

$$V = \begin{bmatrix} -0.8926 & -0.2044 & 0.1635 & -0.2771 & 0.2407 \\ -0.0534 & -0.5118 & -0.5793 & -0.2833 & -0.5651 \\ -0.1584 & -0.1280 & -0.6087 & 0.6280 & 0.4401 \\ -0.2478 & 0.8208 & -0.4413 & -0.2091 & -0.1626 \\ 0.3375 & -0.0791 & -0.2689 & -0.6363 & 0.6345 \end{bmatrix}$$

$$S = \begin{bmatrix} 3.4311 & 2.8692 & 1.8585 & 0.1388 & 0 \\ 0 & 7.0240 & -2.1937 & 0.1571 & 0 \\ 0 & 0 & 5.9566 & 1.0776 & 0 \\ 0 & 0 & 0 & 3.9630 & 0 \end{bmatrix}.$$

3. Linear equality-constrained least-squares problems. Linear equality-constrained least-squares problems, also known as LSE problems, consist in find a vector $x \in \mathbb{R}^n$ satisfying

$$\min_x \|Ax - b\|, \quad \text{subject to } Bx = d, \tag{3.1}$$

where $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{p\times n}$, $b \in \mathbb{R}^m$ and $d \in \mathbb{R}^p$. It is assumed that $m \geq n$, the most frequently case. LSE problem is abbreviated in the following form

$$\min_{Bx=d} \|Ax - b\|. \tag{3.2}$$

LSE problems can be solved by means of QR factorization cf. [10], here we use a more efficient method based on the decompositions presented in Proposition 2.1.

By GRQ factorization there are Q and U orthogonal matrices such that $A^T = QRU$ and $B^T = QS$, with $S \in \mathbb{R}^{p\times n}$ and $R \in \mathbb{R}^{n\times m}$ upper triangular matrices, then

$$\min_{Bx=d} \|Ax - b\| = \min_{Bx=d} \|[QRU]^T x - b\|.$$

By taking $y = Q^T x$, the problem is rewritten as

$$\min_{[QS]^T[Qy]=d} \|[U^T R^T Q^T]x - b\|.$$

Since U is an unitary matrix we have

$$\min_{[S^T Q^T][Qy]=d} \|U(U^T R^T Q^T x - b)\| = \min_{S^T y=d} \|R^T Q^T x - Ub\| = \min_{S^T y=d} \|R^T y - Ub\|.$$

Since $m \geq n$, $S = \begin{bmatrix} S_1 \\ 0 \end{bmatrix}$, and $S^T y = [S_1^T \; 0] \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$, then $S_1^T y_1 = d$. Assuming that $C = Ub$ and $R = \begin{bmatrix} R_{11} & R_{12} & 0 \\ 0 & R_{22} & 0 \end{bmatrix}$, we obtain

$$\min_{S^T y=d} \|R^T y - Ub\| = \min_{S^T y=d} \left\| \begin{bmatrix} R_{11}^T & 0 \\ R_{12}^T & R_{22}^T \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} - \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} \right\|$$

In terms of y_1 and y_2 we have

$$\min_{y_2} \|R_{12}^T y_1 + R_{22}^T y_2 - c_2\| = \min_{y_2} \|R_{22}^T y_2 - (c_2 - R_{12}^T y_1)\|.$$

Solving the problem $S_1^T y_1 = d$ we get y_1. On the other hand, we obtain that $y_2 = [R_{22}^T]^{-1}(c_2 - R_{12}^T y_1)$, therefore we get y. Hence $x = Qy = Q_1 y_1 + Q_2 y_2$ is the solution. R can also be considered in the form $R = \begin{bmatrix} 0 & R_{11} & R_{12} \\ 0 & 0 & R_{22} \end{bmatrix}$ but it does not affect the solution of the problem.

We generate a program for solving linear equality-constrained least-squares problems through GQR factorization, with A, B, b and d as parameters. Here we present a comparison, in terms of the residuals, among several methods for solving LSE problems; simulations were performed with $n = 100$ random problems with $m = 50$ rows.

Thus, we verify that the GQR factorization is a stable method for solving LSE problems.

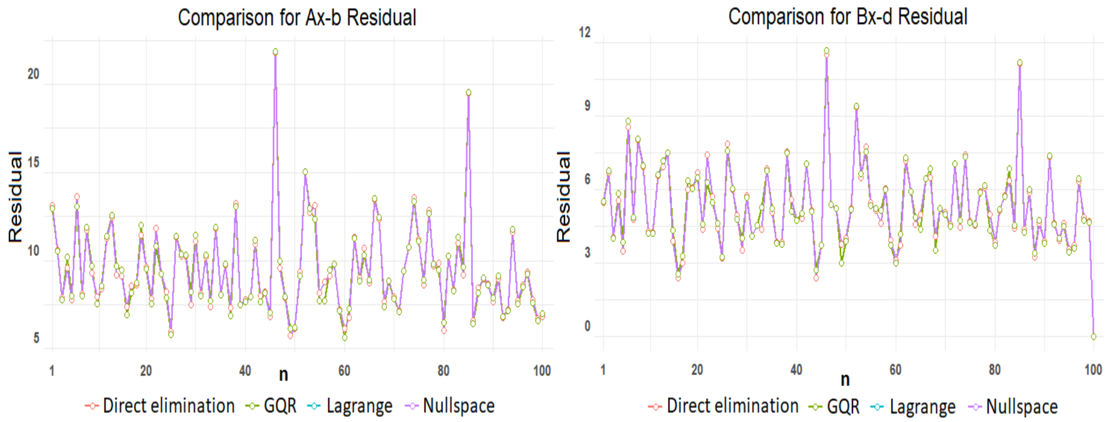

Figure 3.1: Residuals values were obtained by solving random problems through R via direct elimination, GQR factorization, Lagrange method, and nullspace method.

Example 3.1. *Solve the LSE problem*

$$\min_{x_1+x_2=1} \left\| \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} 7 \\ 1 \\ 3 \end{bmatrix} \right\|.$$

Let $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$, $b = \begin{bmatrix} 7 \\ 1 \\ 3 \end{bmatrix}$, $B = \begin{bmatrix} 1 & 1 \end{bmatrix}$, $d = [1]$, by GQR factorization we get

$$Q = \begin{bmatrix} -0.7071 & -0.7071 \\ -0.7071 & 0.7071 \end{bmatrix}, R = \begin{bmatrix} 4 & 8.5732 & 0 \\ 0 & -1.2247 & 0 \end{bmatrix}$$

$$U = \begin{bmatrix} 0.7071 & 0 & -0.7071 \\ -0.5773 & -0.5773 & -0.5773 \\ 0.04082 & -0.8165 & 0.4082 \end{bmatrix}, S = \begin{bmatrix} -1.4142 \\ 0 \end{bmatrix}.$$

Thus, the solution is $x_1 = 0.33333$ and $x_2 = 0.66667$.

Example 3.1 was presented in [12], and it was solved by several methods.

4. Quaternion least squares problems. The study of quaternion least-squares problems, also known as QLS problems, and the different ways to solve them have gained continued interest [7]. Here we present a method for solving quaternion least-squares problems through GQR factorization.

For the quaternion $q = a + bi + cj + dk$, there is a matrix representation [11], given by

$$\begin{bmatrix} a & -b & d & -c \\ b & a & -c & -d \\ -d & c & a & -b \\ c & d & b & a \end{bmatrix}.$$

For instance, $q = -1 + j$ is represented as the matrix $\begin{bmatrix} -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix}$.

Example 4.1. *Solve the problem*

$$\min_x \left\| \begin{bmatrix} -1+j & -k \\ i & 1+j \end{bmatrix} x - \begin{bmatrix} -1 \\ i \end{bmatrix} \right\|.$$

In [8] a technique of quaternion least squares problem was presented, and this problem was solved by this technique. Here we will use the GQR factorization to solve the equivalent problem $\min_x \|Ax - b\|$. It is easy to check that

$$A = \begin{bmatrix} -1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}, \; b = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Since we do not have any constraints, we use $B = A$ and $d = b$. Therefore we have the solution of the least squares problem

$$X = \begin{bmatrix} \frac{2}{3} & 0 & 0 & -\frac{1}{3} \\ 0 & \frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{2}{3} & 0 \\ \frac{1}{3} & 0 & 0 & \frac{2}{3} \\ 0 & -\frac{1}{3} & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} \\ 0 & 0 & \frac{1}{3} & 0 \end{bmatrix}.$$

Thus, the solution of the QLS problem is $\begin{bmatrix} \frac{2}{3} + \frac{1}{3}j \\ \frac{1}{3}i \end{bmatrix}$.

Following the Examples 3.1 and 4.1, we solve the following equality-constrained quaternion least-square problem, known as QLSE problem [6], through GQR factorization.

Example 4.2. *Solve the problem*

$$\min \left\| \begin{bmatrix} 3j & -3i \end{bmatrix} x - 2j \right\| \quad \textit{subject to} \quad \begin{bmatrix} -1+j & -k \\ i & 1+j \end{bmatrix} x = \begin{bmatrix} -1 \\ i \end{bmatrix}$$

Let B and d be the matrices $\begin{bmatrix} -1+j & -k \\ i & 1+j \end{bmatrix}$ and $\begin{bmatrix} -1 \\ i \end{bmatrix}$, respectively, thus we have

$$B = \begin{bmatrix} -1 & -0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}, \; d = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

On the other hand, $\begin{bmatrix} 3j & -3i \end{bmatrix}$ and $2j$ are represented by the following matrices

$$A = \begin{bmatrix} 0 & 0 & 0 & -3 & 0 & 3 & 0 & 0 \\ 0 & 0 & -3 & 0 & -3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 3 \\ 3 & 0 & 0 & 0 & 0 & 0 & -3 & 0 \end{bmatrix}, \; b = \begin{bmatrix} 0 & 0 & 0 & -2 \\ 0 & 0 & -2 & 0 \\ 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 \end{bmatrix}.$$

By GQR factorization we obtain $Q_{8\times8}$, $R_{8\times4}$, $S_{8\times8}$ and $V_{8\times8}$, some blocks of these matrices can be rewritten by quaternions. Thus, the solution of the QLSE problem is $\begin{bmatrix} \frac{2}{3} + \frac{1}{3}j \\ \frac{1}{3}i \end{bmatrix}$.

As an interesting fact, A^T and B can be written by quaternionic matrices in the form

$$A^T = \begin{bmatrix} 0.7071j & 0.2357i + 0.6667k \\ -0.7071i & 0.6667 - 0.2357j \end{bmatrix} \begin{bmatrix} -4.2426 \\ 0 \end{bmatrix},$$

$$B = \begin{bmatrix} -0.5774 + 0.5774j & 0.5774k \\ 0.5774i & -0.5774 - 0.5774j \end{bmatrix} \begin{bmatrix} 1.7321 & 0 \\ 0 & -1.7321 \end{bmatrix}.$$

Conclusions. The GQR factorization is an efficient method for solving linear equality-constrained least square problems, it can be extended to solve quaternion least square problems through matrix representation of quaternions.

It is necessary to establish the theoretical conditions to guarantee that in a QLSE problem, when we consider the problem through decompositions of the matrix representation of the quaternions, the solution is a quaternionic matrix.

In order to obtain an efficient method for solving QLS and QLSE problems, based on matrix factorization, structure-preserving quaternion QR algorithm could be considered [4].

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