# QR and least square

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March 15, 2023

## 1 QR factorization

We study $A \in \mathbb{R}^{m\times n}$ matrix with linearly independent columns. QR algorithm is a key algorithm in numerical linear algebra. We want to study the column space of $A$.

Recall the Gram–Schmidt process for producing an orthogonal or an orthonormal basis for any nonzero subspace of $\mathbb{R}^n$. Given a basis $\{x_1, ..., x_p\}$ for a nonzero subspace $W$, define

$$\begin{aligned}
q_1 &= a_1/r_{11} \\
q_2 &= a_2/r_{22} - \frac{r_{12}}{r_{22}} q_1 \\
q_3 &= a_3/r_{33} - \frac{r_{13}}{r_{33}} q_1 - \frac{r_{23}}{r_{33}} q_2 \\
&\cdots \\
q_p &= a_p/r_{pp} - \frac{r_{1p}}{r_{pp}} a_1 - \frac{r_{2p}}{r_{pp}} q_2 - \frac{r_{(p-1)p}}{r_{pp}} q_{p-1},
\end{aligned}$$

where $r_{ij} = q_i^T a_j$ and $r_{jj} = \|a_j - \sum_{i=1}^j r_{ij} q_i\|$. Then $\{q_1, ..., q_p\}$ is an orthonormal basis for $W$, i.e., $span\{a_1, a_2, ..., a_p\} = span\{q_1, q_2, ..., q_p\}$.

**Theorem 1.1.** If $A$ is an $m \times n$ matrix with linearly independent columns, then $A$ can be factored as $A = QR$, where $Q$ is an $m \times n$ matrix whose columns form an orthonormal basis for Col $A$ and $R$ is an $n \times n$ upper triangular invertible matrix with positive entries on its diagonal.

*Proof.* Let $a_1, ..., a_n$ be columns of $A$. Perform Gram-Schmidt, we obtain $Q = [q_1, ..., q_n]$, which is an orthonormal set of vectors whose span is $col(A)$. For $a_k$, $a_k$ is in $span\{a_1, ..., a_k\} = span\{q_1, ..., q_k\}$. That is there exists $r_{1k}, ..., r_{kk}$ such that $a_k = r_{1k}q_1 + ... + r_{kk}q_k + 0q_{k+1}...0q_n$. Without loss of generality, we assume $r_{kk} > 0$, otherwise multiply $r_{kk}$ and $q_k$ by $-1$ simultaneously. Denote $Q = [q_1, q_2, ..., q_n]$, $R = [r_1, ..., r_n]$ where $r_k = [r_{1k}, ..., r_{kk}, 0, ..., 0]^t \in \mathbb{R}^n$, recall the matrix multiplication we have $A = QR$. We now claim that $R$ is upper triangular with a positive diagonal (easy to verify) and invertible. Recall $rank(QR) \leq min(rank(Q), rank(R))$. Since $rank(A) = n = rank(Q)$, this implies that $rank(R) = n$. $\square$

When $m > n$, we can append $m - n$ columns to $Q$ to make it a $m \times m$ unitary matrix $\tilde{Q}$. In this process, we will append $m - n$ $0$ rows to $R$ to obtain $\tilde{R}$. We call $A = \tilde{Q}\tilde{R}$ full QR of $A$.

## 2 Modified QR

The GS-QR algorithm is not numerically stable. For the moment, a stable algorithm is one that is not too sensitive to the effects of rounding off errors. The modified GS is the way to improve

**Algorithm 1:** Gram Schmidt

**Data:** $n \geq 0$

**for** $j = 1$ *to* $n$ **do**
- $v_j = a_j$
- **for** $i = 1$ *to* $j - 1$ **do**
  - $r_{ij} = q_i^t a_j$
  - $v_j = v_j - r_{ij} q_i$
- $r_{jj} = \|v_j\|_2$
- $q_j = v_j / r_{jj}$

the stability of the QR algorithm. GS can be expressed as an orthogonal projection:

$$q_1 = \frac{P_1 a_1}{\|P_1 a_1\|}, q_2 = \frac{P_2 a_2}{\|P_2 a_2\|}, ..., q_n = \frac{P_n a_n}{\|P_n a_n\|}, \tag{1}$$

where $P_j \in \mathbb{R}^{m \times m}$ denotes the orthogonal projector onto space spanned by $\{q_1, ...q_{j-1}\}$.

For each $j$, the GS algorithm computes a single orthogonal projection of rank $m - (j - 1)$, $v_j = P_j a_j$. Recall that: $P_{\perp q}$ denotes the rank $m - 1$ orthogonal projection onto the space orthogonal to $q$. By the definition of $P_j$, we can verify (without proof here):

$$P_j = P_{\perp q_{j-1}} ... P_{\perp q_2} P_{\perp q_1}, \tag{2}$$

and $P_{\perp q_1} = I$. As a result,

$$v_j = P_j a_j = P_{\perp q_{j-1}} ... P_{\perp q_2} P_{\perp q_1} a_j. \tag{3}$$

Specifically,

$$\begin{aligned}
v_j^1 &= a_j, \\
v_j^2 &= P_{\perp q_1} v_j^1 = v_j^1 - q_1 q_1^t v_j^1, \\
v_j^3 &= P_{\perp q_2} v_j^2 = v_j^2 - q_2 q_2^t v_j^2, \\
&... \quad ... \\
v_j &= P_{\perp q_{j-1}} v_j^{j-1} = v_j^{j-1} - q_{j-1} q_{j-1}^t v_j^{j-1}.
\end{aligned}$$

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We summarize the algorithm in 2.

**Algorithm 2:** Modified Gram Schmidt

1 **for** $i = 1$ *to* $n$ **do**

2    $v_i = a_i$

3 **for** $i = 1$ *to* $n$ **do**

inner product

3m

4    $r_{ii} = \|v_i\|$ → $2m-1 + 1$ → $\sqrt{\ }$

5    $q_i = v_i / r_{ii}$ → $m$

6    **for** $j = i + 1$ *to* $n$ **do**

7      $r_{ij} = q_i^t v_j$

8      $v_j = v_j - r_{ij} q_i$

The dominant steps are step 7 & 8 b/c we have to do 2 loops for 7 & 8.

step 7 : $m$ " x " + $m-1$ " + " = $2m-1 \sim 2m$

step 8 : $m$ " x " + $m$ " − " = $2m$

$q_i \in \mathbb{R}^m$

step 7 8 $\sum_{i=1}^{n} \sum_{j=i+1}^{n} (4m-1) = 2mn^2$

step 4 5 $\sum_{i=1}^{n} 3m = 3mn$

## 2.1 Operation counts

step 4 & 5 is of lower order, $\Rightarrow$ operation counts $\sim 2mn^2$

Each addition, subtraction, multiplication, division and square root counts as one flop. Operation count is the number of flops an algorithm requires.

**Theorem 2.1.** The Gram-Schmidt algorithm requires $\sim 2mn^2$ flops for a matrix $A$ of size $m \times n$.

**Remark 1.** The $\sim$ sign here is the asymptotic convergence, i.e.,

$$\lim_{m,n\to\infty} \frac{\text{the total number of flops}}{2mn^2} = 1. \tag{4}$$

In discussing the operation count, it is standard to discard lower-order terms, since they are usually of little significance unless $m$ and $n$ are small.

*Proof.* In each $i$ iteration, we have:

1. Line 7: $m$ multiplication and $m-1$ addition.
2. Line 8: $m$ multiplication and $m$ subtraction.

In total we have $\sum_{i=1}^{n}\sum_{j=1}^{n}(4m-1)i \sim 2mn^2$. $\square$

# 3 Housedolder triangularization

The target of the algorithm is to create a full $QR$ of $A$. The idea is to applies a sequence of unitary matrices $Q_k$ on the left of $A$ such that, $Q_n ... Q_2 Q_1 A = R$ is upper triangular. Denote $Q = Q_1^t Q_2^t ... Q_n^t$, $Q$ is also unitary. This implies that $A = QR$ is a full QR of $A$. We will discuss how to find $Q_i$.

## 3.1 Householder reflector

Each $Q_k$ is chosen to introduce zeros below the diagonal in the $k-$th column while preserving all the zeros previously introduced. In general $Q_k$ operates on rows $k, ..., m$. Each $Q_k$ has the following format:

$$Q_k = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix}, \tag{5}$$

where $I$ is the identity matrix of the size $(k-1)\times(k-1)$ and $F$ is unitray of size $(m-k+1)$. Multiplication by $F$ will introduce zeros into $k-$th column. $F$ is called a Householder reflector.

Suppose at the beginning of step $k$, the entries $k, ..., m$ of $k-$th column are given by the vector $x \in \mathbb{R}^{m-k+1}$. The Householder reflector $F$ should introduce some zeros to $x$ such that $Fx = [\|x\|, 0, ..., 0]^\intercal = \|x\| e_1$. The target now is to construct $F$ such that $F$ will map $x$ to $\|x\|e_1$.

Let us define $v = x - \|x\|e_1$ (please check the picture). By the orthogonal projection formula, we have,

$$Px = (I - \frac{vv^t}{\|v\|^2})x = x - \frac{vv^t}{\|v\|^2}x. \tag{6}$$

Householder

GS : orthogonalization process, it will gives us $Q$.

Hs : it will give us $R$.

Idea: Design & apply a sequence of unitary matrices $Q_1 \cdots Q_n \in \mathbb{R}^{m \times m}$

s.t. $Q_n Q_{n-1} \cdots Q_1 A = R$ is triangular.

$$A = \underbrace{Q_1^* \quad Q_{n-1}^* Q_n^*}_{Q} R$$

$$\underset{A}{\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}} \xrightarrow{Q_1} \underset{Q_1 A}{\begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix}} \xrightarrow{Q_2} \underset{Q_2 Q_1 A}{\begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \\ 0 & 0 & x \end{pmatrix}}$$

$$\xrightarrow{Q_3} \underset{Q_3 Q_2 Q_1 A}{\begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}$$

k th step

$$\underbrace{\begin{pmatrix} I_{(k-1)(k-1)} & 0 \\ 0 & F_{(m-k+1)(m-k+1)} \end{pmatrix}}_{Q_k} \underbrace{\begin{pmatrix} \begin{pmatrix} x & P & x \\ x & & x \end{pmatrix}_{(k-1)(k-1)} & \begin{pmatrix} x & R & x \\ x & & x \end{pmatrix}_{(k-1)\cdot(n-k+1)} \\ \begin{pmatrix} x & & x \\ x & & x \\ x & 0 & x \\ x & & x \end{pmatrix}_{(m-k+1)(k-1)} & \begin{pmatrix} x & & x \\ x & B & x \\ x & & x \\ x & & x \end{pmatrix}_{(m-k+1)(n-k+1)} \end{pmatrix}_{m\cdot n.}}_{Q_{k-1} Q_{k-2} \cdots Q_1 A}$$

$$= \begin{pmatrix} IP & R \\ 0 & FB \end{pmatrix} = \underbrace{\begin{pmatrix} P & R \\ 0 & FB \end{pmatrix}}_{Q_k Q_{k-1} \cdots Q_1 A}$$

Now, design an $\underbrace{F}_{\text{unitary}} \in \mathbb{R}^{(m-k+1)(m-k+1)}$ s.t. $FB = \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix}$

Householder reflector.

$$FB = \begin{pmatrix} x & \cdots \\ 0 & \\ 0 & \\ 0 & \\ 0 & \end{pmatrix} \quad \text{denote } x = \begin{pmatrix} x_1 \\ \vdots \\ x_{m-k+1} \end{pmatrix} \text{ as the 1st col}$$

of $B$.

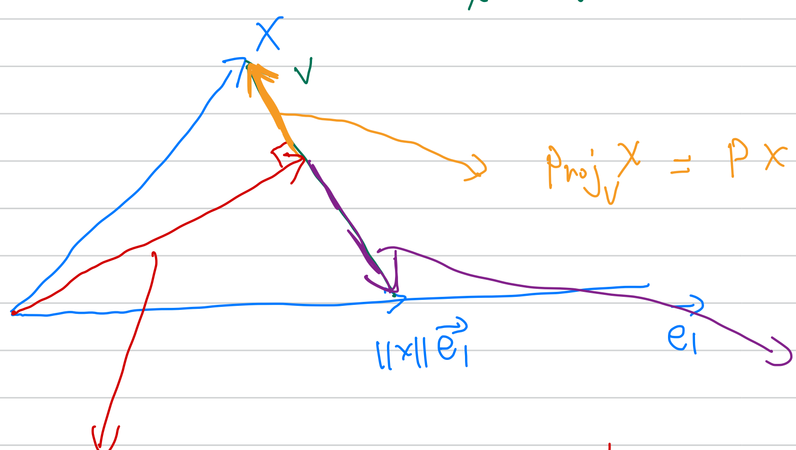
If

$$Fx = \underbrace{\|x\| \vec{e}_1}_{\text{try to make sure}}, \quad e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

then $F$ ✓

we have isosceles triangles.

$$x - v = \|x\| \vec{e}_1$$




$$\mathrm{Proj}_v x = Px$$

$$-\mathrm{Proj}_v x = \frac{vv^t}{\|v\|^2} x$$

$$(I - P)x = \Big(I - \underbrace{\frac{vv^t}{\|v\|^2}}_{\mathrm{Proj}_v x}\Big) x$$

Target $\|x\| \vec{e}_1$ = red + purple

$$= (I - P)x - Px$$

$$= \underbrace{\Big(I - \frac{2vv^t}{\|v\|^2}\Big)}_{F} x = Fx$$

( Household reflector )

This is the orthogonal projection of $x$ onto space which is orthogonal to $v$. Move twice as far in the same direction; we will have the target vector, i.e.,

$$Fx = x - 2\frac{vv^t}{\|v\|^2}x = (I - 2\frac{vv^t}{\|v\|^2})x. \tag{7}$$

We now derive the Household projector: $F = I - 2\frac{vv^t}{\|v\|^2}$.

**Theorem 3.1.** $F$ is unitary and Hermitian.