# QR Factorization

Recall: $A = LU$ factorization was used to encode (via matrices) Gaussian elimination. In §4.1 we introduced the least squares method to solve insoluble, "overdetermined" (i.e. $m > n$) systems. However, one drawback of this form of Least Squares is that $\text{cond}(A^T A)$ could be large, yielding an unstable system.

## Gram-Schmidt Orthogonalization & Least Squares

Review of the G-S Process. Given an input of a set of ($n$ LID) $m$-dimensional vectors, G-S outputs $n$ mutually orthogonal unit vectors that span the same subspace as the original set of vectors:

Let: $A_1, \dots, A_n$ be LID vectors in $\mathbb{R}^m$ (so $n \leq m$, why?).

The G-S method begins by dividing $A_1$ by $\|A_1\|_2$. Define:

$$\boxed{y_1 = A_1, \quad q_1 = \frac{y_1}{\|y_1\|_2}}$$

To find the second unit vector, subtract away the projection of $A_2$ in the direction of $q_1$ & normalize.

$$\boxed{y_2 = A_2 - q_1(q_1^T A_2) \quad \& \quad q_2 = \frac{y_2}{\|y_2\|_2}}$$

Notice that $g_1$ & $g_2$ are pairwise orthogonal, since:

$$g_1^T \cdot y_2 = g_1^T\left(A_2 - g_1\left(g_1^T A_2\right)\right)$$
$$= g_1^T A_2 - \underbrace{\left(g_1^T g_1\right)}\left(g_1^T A_2\right)$$
$$= g_1^T A_2 - 1\cdot\left(g_1^T A_2\right) = \underline{\underline{0}}.$$

Thus, $g_1 \perp g_2$

In general then, the $j^{th}$ step of the G-S method yields:

$$y_j = A_j - g_1\left(g_1^T A_j\right) - g_2\left(g_2^T A_j\right) - \cdots - g_{j-1}\left(g_{j-1}^T A_j\right)$$
& $$g_j = \frac{y_j}{\|y_j\|_2}.$$

Note that $g_j$ is orthogonal to each of $g_i$ for $i = 1, \dots, j-1$, since:

(*)(= 0 by induction for $i<j$).

$$g_i^T y_j = g_i^T A_j - \underbrace{g_i^T g_1}_{(*)} g_1^T A_j - \cdots - g_i^T g_{j-1} g_{j-1}^T A_j$$
$$= g_i^T A_j - 0 - \cdots - 0 - g_i^T g_i g_i^T A_j = g_i^T A_j - g_i^T A_j = \underline{\underline{0}}.$$

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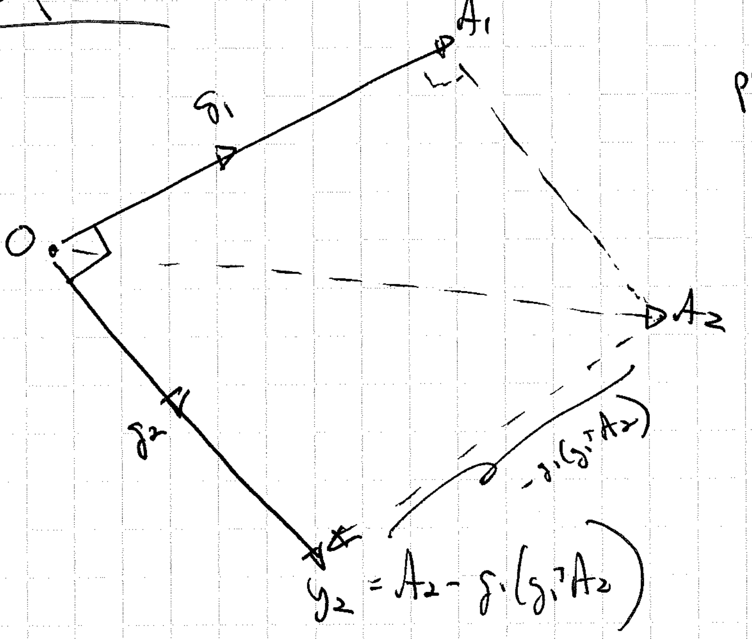
The Geometry of G-S: We subtract from $A_j$ the projections of $A_j$ onto the previously determined orthogonal vectors: $g_i$ $(i = 1, \dots, j-1)$. What remains is orthogonal to the $g_i$ (& make into a unit vector). Since orthogonal vectors form a LID set (why?), these vectors span the same subspace of $\mathbb{R}^m$ as the original set.

Picture of G-S process:




$$\text{proj}_{q_1}(A_2) = \left(\frac{q_1 \cdot A_2}{q_1 \cdot q_1}\right) q_1 = (q_1^T A_2)\, q_1$$

The result of GS orthogonalization can be put into Matrix form by introducing new notation for the dot products in the above calculation.

$\boxed{\text{Define: } r_{jj} = \|y_j\|_2}$ & $\boxed{r_{ij} = q_i^T A_j}$. Then:

$$A_1 = r_{11} q_1 \qquad \left(\text{since } \frac{A_1}{\|y_1\|} = q_1\right)$$

$$A_2 = r_{12} q_1 + r_{22} q_2 \qquad \left(\text{since } q_2 = \frac{A_2}{\|y_2\|} - \frac{(q_1^T A_2) q_1}{\|y_2\|}\right)$$

In general, $A_j = r_{1j} q_1 + \cdots + r_{j-1,j} q_{j-1} + r_{jj} q_j \longrightarrow$

Thus, ← Remember: we assume $A_1, \dots, A_n$ are LID!

$$\begin{bmatrix} | & | & & | \\ A_1 & A_2 & \cdots & A_n \\ | & | & & | \end{bmatrix} = \underbrace{\begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix}}_{\text{"}Q\text{"}} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & 0 & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}}_{\text{"}R\text{"}}$$

$(A = QR)$ → This is called the Reduced QR Factorization.

**Ex.** Find the reduced QR factorization to:

$$A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}. \quad \text{Set } y_1 = A_1 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}. \quad r_{11} = \|y_1\| = \boxed{3}$$

$$(*) \quad q_1 = \frac{y_1}{\|y_1\|} = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

$$y_2 = A_2 - q_1 q_1^T A_2 = \begin{bmatrix} -4 \\ 3 \\ 2 \end{bmatrix} - \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix} \begin{bmatrix} 1/3 & 2/3 & 2/3 \end{bmatrix} \begin{bmatrix} -4 \\ 3 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} -4 \\ 3 \\ 2 \end{bmatrix} - \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix} \cdot 2 = \begin{bmatrix} -\frac{14}{3} \\ \frac{5}{3} \\ \frac{2}{3} \end{bmatrix}$$

$$(*) \quad q_2 = \frac{y_2}{\|y_2\|} = \frac{1}{5} y_2 = \begin{bmatrix} -\frac{14}{15} \\ \frac{1}{3} \\ \frac{2}{15} \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix} = \begin{bmatrix} 1/3 & -14/15 \\ 2/3 & 1/3 \\ 2/3 & 2/15 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & 5 \end{bmatrix} = \underline{QR}.$$

<u>"Classical"</u> G-M orthogonalization:

Let $A_j$, $j=1,\dots,N$ be LID vectors

```
for j=1,...,n
    y = A_j
    for i=1,...,j-1
        r_ij = q_i^T A_j
        y = y - r_ij q_i
    end
    r_jj = ||y||,  q_j = y / r_jj
end
```

When the method is successful, it is customary to fill out the matrix with orthogonal unit vectors to achieve a "full" QR factorization. This can be done by adding $(m-n)$ extra vectors to the set $\{A_j\}$ so that the $m$ vectors span $\mathbb{R}^m$. This gives the full QR factorization:

$$\underbrace{\begin{bmatrix} | & | & & | \\ A_1 & A_2 & \cdots & A_n \\ | & | & & | \end{bmatrix}}_{(A:\ m\times n)} = \underbrace{\begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_m \\ | & | & & | \end{bmatrix}}_{(Q:\ m\times m)} \cdot \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ \emptyset & & \ddots & \vdots \\ & & & r_{nn} \\ \hline \emptyset & & & \emptyset \end{bmatrix}}_{(R:\ m\times n)}$$

added $(m-n)$ vectors

Note

$\boxed{\text{Def}}$ A square matrix $Q$ is $\boxed{\text{orthogonal}}$ if $Q^T = Q^{-1}$.

Note that a square matrix is orthogonal iff its columns are pairwise orthogonal unit vectors ($Q$ from the full QR is one such matrix).

The key property of an orthogonal matrix is that it is length-preserving!

$\boxed{\text{Lemma}}$ If $Q$ is an orthogonal $m\times m$ matrix, then

$$\|Q\vec{x}\|_2 = \|\vec{x}\|_2 \quad \forall \vec{x} \in \mathbb{R}^m.$$

Pf: $\|Q\vec{x}\|_2^2 = (Q\vec{x})^T \cdot (Q\vec{x}) = x^T Q^T Q \vec{x} = x^T (Q^T Q)\vec{x} =$

$x^T I x = \vec{x}\cdot\vec{x} = \|\vec{x}\|_2^2.$

Note: The product of orthogonal matrices is orthogonal (HW #10).

•) The QR factorization of an $m \times m$ matrix by the G-S method requires $\boxed{O(m^3)}$ multiplications & divisions (3 times more than LU) plus approximately the same number of additions.

(Note: Performing matrix calculations w/ orthogonal matrices is in generally much more efficient than for non-orthogonal vectors; furthermore orthogonal matrices are easily inverted, & they do not suffer from error magnification).

Ex. Find the full QR factorization: $A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$

Recall: $q_1 = \begin{bmatrix} \frac{1}{3} \\ \frac{2}{3} \\ \frac{2}{3} \end{bmatrix}$, $q_2 = \begin{bmatrix} -\frac{4}{15} \\ \frac{1}{5} \\ \frac{2}{15} \end{bmatrix}$. Adding a third vector, $A_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$

gives: $y_3 = A_3 - q_1 q_1^T A_3 - q_2 q_2^T A_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} \frac{1}{3} \\ \frac{2}{3} \\ \frac{2}{3} \end{bmatrix} \frac{1}{3} - \begin{bmatrix} -\frac{14}{15} \\ \frac{1}{3} \\ -\frac{2}{15} \end{bmatrix} \left(-\frac{14}{15}\right)$

$= \frac{2}{225} \begin{bmatrix} 2 \\ 10 \\ -11 \end{bmatrix} \to q_3 = \frac{y_3}{\|y_3\|} = \begin{bmatrix} \frac{2}{15} \\ \frac{10}{15} \\ -\frac{11}{15} \end{bmatrix}$.

Full QR:

$$A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix} = \begin{bmatrix} 1/3 & -14/15 & 2/15 \\ 2/3 & 1/3 & 2/3 \\ 2/3 & 2/15 & -11/15 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & 5 \\ 0 & 0 \end{bmatrix} = QR$$

Note that the choice of $A_3$ was arbitrary; any third column vector LID of the first two can be used.

(3) Major Applications of QR:

(1) QR to solve a system of n equations: $A\vec{x}=\vec{b}$

$A = QR \to A\vec{x}=\vec{b} \to QR\vec{x}=\vec{b} \to \boxed{R\vec{x}=Q^T\vec{b}}$;

Now solve the simple system w/ triangular back-sub.

This approach is roughly three times more expensive than LU.

(2) Apply QR to least squares. $A_{m\times n}$, $m \geq n \to$ let $\vec{d}=Q^T\vec{b}$

minimize $\|A\vec{x}-\vec{b}\|_2 \to \|QR\vec{x}-\vec{b}\|_2 = \underbrace{\cancel{Q}}_{\text{constant wrt } x}\|Rx - Q^T\vec{b}\|$ & minimize this

$$\text{error} = \begin{bmatrix} e_1 \\ \vdots \\ e_n \\ \hline e_{n+1} \\ \vdots \\ e_m \end{bmatrix} = \underbrace{\begin{bmatrix} \overbrace{\begin{matrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & \varnothing & \ddots & \vdots \\ & & & r_{nn} \end{matrix}}^{\hat{R}} \\ \hline \varnothing \end{bmatrix}}_{R} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{\vec{x}} - \underbrace{\begin{bmatrix} d_1 \\ \vdots \\ d_n \\ \hline d_{n+1} \\ \vdots \\ d_m \end{bmatrix}}_{Q^T\vec{b}} \to \vec{d}$$

(*) Observe that $\langle e_{n+1}, \dots, e_m\rangle = \langle -d_{n+1}, \dots, -d_m\rangle$ & so we can minimize the error with a choice of $\vec{x}$ for $\langle e_1, \dots, e_n\rangle$ that minimizes the upper part of the system!

The least squares error is consequently:

$$\|\vec{e}\|_2^2 = d_{n+1}^2 + \dots + d_m^2 \to \text{This error is irreducible.}$$

## Least Squares By QR Factorization

Given the $m \times n$ inconsistent system: $A\vec{x} = \vec{b}$

Find the full QR factorization: $A = QR$ and set:

$\hat{R}$ = upper $n \times n$ submatrix of $R$

$\hat{d}$ = upper $n$ entries of $d = Q^T\vec{b}$.

(*) Solve: $\hat{R}\bar{x} = \hat{d}$ for the least-squares solution: $\bar{x}$.

**Ex.** Use the full QR factorization to solve the least squares problem:

$$\begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -3 \\ 15 \\ 9 \end{bmatrix} \rightarrow R\vec{x} = Q^T\vec{b}:$$

$$\underbrace{\begin{bmatrix} 3 & 2 \\ 0 & 5 \\ \hdashline 0 & 0 \end{bmatrix}}_{\hat{R}}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \underbrace{\frac{1}{15}\begin{bmatrix} 5 & 10 & 10 \\ -14 & 5 & 2 \\ 2 & 10 & -11 \end{bmatrix}}_{Q^T} \cdot \underbrace{\begin{bmatrix} -3 \\ 15 \\ 9 \end{bmatrix}}_{\vec{b}} = \underbrace{\begin{bmatrix} 15 \\ 9 \\ \hdashline 3 \end{bmatrix}}_{d}$$

$\hat{d}$ = $\begin{bmatrix} 15 \\ 9 \end{bmatrix}$, 3 (error)

$$\rightarrow \hat{R}\bar{x} = \hat{d} \rightarrow \begin{bmatrix} 3 & 2 \\ 0 & 5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 15 \\ 9 \end{bmatrix} \Bigg\} \boxed{\begin{matrix} \bar{x}_1 = 3.8 \\ \bar{x}_2 = 1.8 \end{matrix}}$$

Recall: In chapter 2 we avoided solving ill-conditioned problems. While the normal equations of a problem may often be ill-conditioned, the QR approach solves the least squares w/o constructing $A^TA$.

# Modified G-S Orthogonalization

Let $A_j$, $j=1,\dots,n$ be LID vectors.

for $j = 1,2,\dots,n$
 $y = A_j$
 for $i = 1,2,\dots,j-1$
  $r_{ij} = q_i^+ y$ Note: immediate replacement
  $y = y - r_{ij} q_i$
 end
 $r_{jj} = \|y\|_2$
 $q_j = y / r_{jj}$
end

**Ex.** (Modified) G-S $A = \begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$ Let $\delta = 10^{-10}$.

(I) Classical G-S:

$y_1 = A_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}$, $q_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}$ ($\delta^2 = 10^{-20}$ < machine precision)

$\dots q_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \dots q_3 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ Note $q_2 \cdot q_3 \neq 0$!

(II) Now use Modified G-S. ($q_1, q_2$ are the same as before)

$$y_3' = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \delta \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} q_1^+ A_3 = \begin{bmatrix} 0 \\ -\delta \\ 0 \\ \delta \end{bmatrix} \to y_3 = y_3' - \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} q_2^+ y_3' = \begin{bmatrix} 0 \\ -\delta/2 \\ -\delta/2 \\ \delta \end{bmatrix}$$

$$\to q_3 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \end{bmatrix}$$