Review: $n \times n$ matrix $Q = [v_1 \; v_2 \; \cdots \; v_n]$ is ORTHOGONAL if $Q^T Q = I_n \Leftrightarrow v_i \bullet v_j = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$

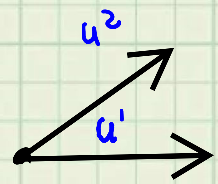
$\Leftrightarrow v_i \perp v_j \;\; i \neq j \;\; \& \;\; \|v_i\| = 1 \Leftrightarrow$ columns of Q are $\underbrace{\text{ORTHO}}_{\text{"}\perp\text{"}}\underbrace{\text{NORMAL}}_{\|\cdot\|=1}$

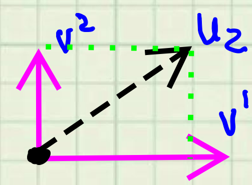
$$\left(v_i \bullet v_j = (v_i)^T v_j \right)$$

- **Gram-Schmidt Process** Takes $\{u_1, u_2, \ldots, u_m\}$ linearly independent $\longrightarrow$ $\{v_1, v_2, \ldots, v_m\}$ orthogonal

$v_1 = u_1$

$$v_2 = u_2 - \frac{u_2 \bullet v_1}{v_1 \bullet v_1} v_1$$





$$v_3 = u_3 - \frac{u_3 \bullet v_1}{v_1 \bullet v_1} v_1 - \frac{u_3 \bullet v_2}{v_2 \bullet v_2} v_2$$

$$v_4 = u_4 - \frac{u_4 \bullet v_1}{v_1 \bullet v_1} v_1 - \frac{u_4 \bullet v_2}{v_2 \bullet v_2} v_2 - \frac{u_4 \bullet v_3}{v_3 \bullet v_3} v_3$$

etc.

Consequence: Triangular Structure!

$u_1 \in \text{span}\{v_1\}$	$v_1 \in \text{span}\{u_1\}$
$u_2 \in \text{span}\{v_1, v_2\}$	$v_2 \in \text{span}\{u_1, u_2\}$
$u_3 \in \text{span}\{v_1, v_2, v_3\}$	$v_3 \in \text{span}\{u_1, u_2, u_3\}$
$\vdots$	$\vdots$

$u_k \in \text{span}\{v_1, v_2, \ldots, v_k\}$ | $v_k \in \text{span}\{u_1, u_2, \ldots, u_k\}$

• **Normalization:** Can integrate with G.S. or do after $v_i \to \frac{v_i}{\|v_i\|}$

Orthonormal and Orthognal Matrices

An $n \times m$ rectangular matrix Q is **orthonormal**:

- if $n > m$ (tall matrices), its columns are orthonormal vectors, which is equivalent to $Q^\top \cdot Q = I_m$; and
- if $n < m$ (wide matrices), its rows are orthonormal vectors, which is equivalent to $Q \cdot Q^\top = I_n$.

A square $n \times n$ matrix is **orthogonal** if $Q^\top \cdot Q = I_n$ and $Q \cdot Q^\top = I_n$, and hence, $Q^{-1} = Q^\top$.

Remarks:

- For a **square matrix**, $n = m$, $(Q^\top \cdot Q = I_n) \iff (Q \cdot Q^\top = I_n) \iff (Q^{-1} = Q^\top)$.
- For a tall matrix, $n > m$, $(Q^\top \cdot Q = I_m) \not\Longrightarrow (Q \cdot Q^\top = I_n)$.
- For a wide matrix, $m > n$, $(Q \cdot Q^\top = I_n) \not\Longrightarrow (Q^\top \cdot Q = I_m)$.

} Be careful!

Today QR Factorization

Suppose $A = n \times m$ with linearly independent columns. Then there exist an $n \times m$ matrix Q with orthonormal columns and an $m \times m$ matrix R that is upper triangular and invertible such that

$$\underset{n\times m}{A} = \underset{n\times m}{Q} \cdot R_{m \times m}$$

- $Q^T Q = I_m$
- $\det(R) \neq 0$

Moreover Q and R are constructed as follows

$$A = [u_1 \ u_2 \ \cdots \ u_m] \longrightarrow \{u_1, u_2, \ldots, u_m\}$$

lin. indep. in $\mathbb{R}^n$

$$\{u_1, u_2, \ldots, u_m\} \xrightarrow{G.S} \{v_1, v_2, \ldots, v_m\}$$ orthogonal

$$Q := \left[\frac{v_1}{\|v_1\|} \ \frac{v_2}{\|v_2\|} \ \cdots \ \frac{v_m}{\|v_m\|}\right]$$

columns of Q are orthonormal

Because $A = QR$ and $Q^T Q = I_m$

then it must be true that

$$Q^T \cdot A = \underbrace{Q^T Q}_{I_m} \cdot R = R$$

$$\boxed{R = Q^T \cdot A}$$

Book: Details how to extract the coefficients of R from G.S.

Book: $\det(R) \neq 0$.

$\square$

Why is $Q^T Q$ when $A = n \times m$?

$Q = \left[\frac{v_1}{\|v_1\|} \cdots \frac{v_m}{\|v_m\|} \right]$ orthonormal

$$Q^T Q = \begin{bmatrix} v_1^T / \|v_1\| \\ v_2^T / \|v_2\| \\ \vdots \\ v_m^T / \|v_m\| \end{bmatrix}_{m \times n} \cdot \left[\frac{v_1}{\|v_1\|} \ \frac{v_2}{\|v_2\|} \cdots \frac{v_m}{\|v_m\|} \right]_{n \times m}$$

$i\text{-}j$ entry $\left(\frac{v_i^T}{\|v_i\|} \right) \left(\frac{v_j}{\|v_j\|} \right) = \begin{cases} 0 & i \neq j \\ \frac{v_i^T v_i}{\|v_i\|^2} = 1 \end{cases}$

Example

Example 9.20 *Compute the QR Factorization of* $A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 3 & 1 \end{bmatrix}$.

Solution: We extract the columns of A and obtain

$$\{u_1, u_2, u_3\} = \left\{ \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \right\}$$

From Example 9.19, we have that

$$\left\{ \tilde{v}_1 = \frac{v_1}{\|v_1\|} = \frac{\sqrt{2}}{2} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \tilde{v}_2 = \frac{v_2}{\|v_2\|} = \frac{\sqrt{38}}{38} \begin{bmatrix} -1 \\ 1 \\ 6 \end{bmatrix}, \tilde{v}_3 = \frac{v_3}{\|v_3\|} = \frac{\sqrt{19}}{19} \begin{bmatrix} -3 \\ 3 \\ -1 \end{bmatrix} \right\}$$

and therefore,

$$Q \approx \begin{bmatrix} 0.707107 & -0.162221 & -0.688247 \\ 0.707107 & 0.162221 & 0.688247 \\ 0.000000 & 0.973329 & -0.229416 \end{bmatrix}$$

and

$$R = Q^\top A \approx \begin{bmatrix} 1.41421 & 2.12132 & 0.707107 \\ 0.00000 & 3.08221 & 1.13555 \\ 0.00000 & 0.00000 & 0.458831 \end{bmatrix}.$$

As a numerical check, we also compute how close $Q^\top$ is to being a matrix inverse of Q,

$$Q^\top \cdot Q - I = \begin{bmatrix} -2.22045e-16 & 9.71445e-17 & 1.11022e-16 \\ 9.71445e-17 & 0.00000e-17 & -2.49800e-16 \\ 1.11022e-16 & -2.49800e-16 & 0.00000e-17 \end{bmatrix}.$$

In addition, we check that $\det(Q) = -1.0$. ■

Fact Rotation matrices are orthogonal matrices!

$$\begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

How to Solve $Ax=b$ using QR Factorization

$A = n\times m$ suppose columns of A are linearly indep. and that $b\in\mathbb{R}^n$ that is a linear combination of the columns of A. We Factor A as $Q\cdot R$. Then

$$(Ax=b) \Leftrightarrow (Q\cdot Rx=b)$$
$$\Leftrightarrow (Rx=Q^Tb)$$

Standard "pipeline" for solving $Ax=b$!

- Factor $A=QR$
- multiply $Q^T\cdot b$
- Solve $Rx=Q^Tb$ via back substitution.

{Used by all the pros!}

See book for an example

Matlab for sure, Julia likely

$Ax = b$ $\quad$ $x = \mathrm{inv}(A) * b$ $\quad$ not good

$x = A\backslash b$ $\quad$ back slash

our pipeline

Least Squares (Regression) via QR

$Ax = b$ $\qquad b \notin \mathrm{range}(A)$

$\notin \mathrm{col\,span}(A)$

Assume columns of A are linearly indep.

$$x^* = \underset{x \in \mathbb{R}^m}{\arg\min} \|Ax - b\|^2 \qquad A = n \times m$$

$$x^* = (A^TA)^{-1}A^Tb \longleftrightarrow \boxed{(A^TA)x^* = A^Tb}$$

$A = QR$

$$A^T A = (R^T \cdot Q^T) \cdot (Q \cdot R) = R^T R$$

$$Q^T \cdot Q = I$$

$$A^T A x^* = A^T b = \cancel{R^T} Q^T \cdot b$$

$$\| \quad \cancel{R^T} R x^*$$

R invertible, $\mathrm{rank}(A^T) = \mathrm{rank}(A)$

$\therefore R^T$ invertible

$$\boxed{R x^* = Q^T \cdot b}$$

Least Squares

Hint: $Ax = b \Longrightarrow A^T A x = A^T b$

$\overset{?}{\Longleftarrow}$

What to do when $Ax = b$ has an infinite number of solutions?