Claim If Q has orthogonal columns, i.e. $Q^TQ = I$, then

(i) $\|Q\underline{x}\| = \|\underline{x}\|$ pf: $\|Q\underline{x}\|^2 = (Q\underline{x})^T(Q\underline{x}) = \underline{x}^TQ^TQ\underline{x} = \underline{x}^T\underline{x} = \|\underline{x}\|^2$

(ii) $(Q\underline{x})^TQ\underline{y} = \underline{x}^T\underline{y}$ pf: $(Q\underline{x})^T(Q\underline{y}) = \underline{x}^TQ^TQ\underline{y} = \underline{x}^T\underline{y}$

Projection using orthonormal bases

- Suppose the basis vectors are orthonormal.

  $Q = [\underline{q_1} \cdots \underline{q_n}] \Rightarrow Q^TQ = I$

  The least squares solution of $Q\underline{x} = \underline{b}$ is $Q^TQ\hat{\underline{x}} = Q^T\underline{b} \Rightarrow \hat{\underline{x}} = Q^T\underline{b}$

  The projection vector $\underline{p} = Q\hat{\underline{x}} = \underbrace{QQ^T}_{\text{projection matrix}}\underline{b} \Rightarrow \underline{p} = [\underline{q_1} \cdots \underline{q_n}]\begin{bmatrix} \underline{q_1}^T \\ \vdots \\ \underline{q_n}^T \end{bmatrix}\underline{b} = \underline{q_1}(\underline{q_1}^T\underline{b}) + \cdots + \underline{q_n}(\underline{q_n}^T\underline{b})$

- Projection $\underline{p} = \frac{\underline{a}^T\underline{b}}{\underline{a}^T\underline{a}}\underline{a} = \frac{\underline{a}^T\underline{b}}{\|\underline{a}\|^2}\underline{a} = \left(\frac{\underline{a}}{\|\underline{a}\|}\right)^T\underline{b}\,\frac{\underline{a}}{\|\underline{a}\|} = \underline{q}^T\underline{b}\,\underline{q} = \underline{q}(\underline{q}^T\underline{b})$

- When Q 為方陣, the subspace is the whole vector space $\mathbb{R}^n$ and $Q^T = Q^{-1}$

  $\hat{\underline{x}} = Q^T\underline{b} = Q^{-1}\underline{b}$ $\quad Q\underline{x} = \underline{b} \Rightarrow \underline{x} = Q^{-1}\underline{b}$

  which is the exact solution to $Q\underline{x} = \underline{b}$, and the projection of $\underline{b}$ is itself, i.e., $\underline{p} = \underline{b}$.

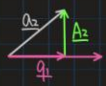
  Therefore, $\underline{b} = \underline{q_1}(\underline{q_1}^T\underline{b}) + \cdots + \underline{q_n}(\underline{q_n}^T\underline{b})$

The Gram-Schmidt (Orthogonalization) Process

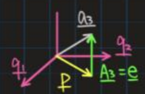
- Given n L.I. vectors $\underline{a_1} \cdots \underline{a_n}$, we want to find n orthonormal vectors $\underline{q_1} \cdots \underline{q_n}$ with the same span.

- 1. $\underline{A_1} = \underline{a_1}$. Then $\underline{q_1} = \frac{\underline{A_1}}{\|\underline{A_1}\|}$

  2. $\underline{A_2} = \underbrace{\underline{a_2} - (\underline{q_1}^T\underline{a_2})\underline{q_1}}_{\text{error } \underline{e}}$. Then $\underline{q_2} = \frac{\underline{A_2}}{\|\underline{A_2}\|}$

  3. $\underline{A_3} = \underbrace{\underline{a_3} - (\underline{q_1}^T\underline{a_3})\underline{q_1} - (\underline{q_2}^T\underline{a_3})\underline{q_2}}_{\text{error } \underline{e}}$. Then $\underline{q_3} = \frac{\underline{A_3}}{\|\underline{A_3}\|}$

- In general, $\underline{A_i} = \underline{a_i} - \sum_{j=1}^{i-1}(\underline{q_j}^T\underline{a_i})\underline{q_j}$ and $\underline{q_i} = \frac{\underline{A_i}}{\|\underline{A_i}\|}$ for $i = 1 \cdots n$

The Factorization $A = QR$

- Given L.I. vectors $\underline{a_1}, \underline{a_2}, \underline{a_3}$, we can use the Gram-Schmidt process to construct vectors q_1, q_2, q_3.

  $\underline{a_1}$ and $\underline{A_1}$, q_1 are in the same subspace.

  $\underline{a_1}, \underline{a_2}$ and $\underline{A_1}, \underline{A_2}$ and q_1, q_2 are in the same subspace.

  $\underline{a_1}, \underline{a_2}, \underline{a_3}$ and $\underline{A_1}, \underline{A_2}, \underline{A_3}$ and q_1, q_2, q_3 are in the same subspace.

  依此類推　Therefore, we can have

  $\underline{a_1} = (q_1^T \underline{a_1})\, q_1$

  $\underline{a_2} = (q_1^T \underline{a_2})\, q_1 + (q_2^T \underline{a_2})\, q_2$

  $\underline{a_3} = (q_1^T \underline{a_3})\, q_1 + (q_2^T \underline{a_3})\, q_2 + (q_3^T \underline{a_3})\, q_3$

- $$\underbrace{[\underline{a_1}\ \underline{a_2}\ \underline{a_3}]}_{A} = \underbrace{[q_1\ q_2\ q_3]}_{Q} \underbrace{\begin{bmatrix} q_1^T \underline{a_1} & q_1^T \underline{a_2} & q_1^T \underline{a_3} \\ 0 & q_2^T \underline{a_2} & q_2^T \underline{a_3} \\ 0 & 0 & q_3^T \underline{a_3} \end{bmatrix}}_{R} \Rightarrow A = QR$$

- In general, from independent vectors $\underline{a_1} \cdots \underline{a_n}$ the Gram-Schmidt process constructs $q_1 \cdots q_n$.

  $\underset{m\times n}{A} = \underset{m\times n}{Q}\ \underset{n\times n}{R} \Rightarrow [\underline{a_1} \cdots \underline{a_n}] = [q_1 \cdots q_n]\, R \Rightarrow Q^T A = Q^T Q R = IR = R$ (upper-triangular)

  Note: $\underline{A_1} = \|\underline{A_1}\|\, q_1 = \underline{a_1} \Rightarrow \underline{a_1} = \|\underline{A_1}\|\, q_1 \quad \therefore q_1^T \underline{a_1} = \|\underline{A_1}\|$

  $\underline{A_2} = \|\underline{A_2}\|\, q_2 = \underline{a_2} - (q_1^T \underline{a_2})\, q_1 \Rightarrow \underline{a_2} = (q_1^T \underline{a_2})\, q_1 + \|\underline{A_2}\|\, q_2 \quad \therefore q_2^T \underline{a_2} = \|\underline{A_2}\|$

  $\underline{A_3} = \|\underline{A_3}\|\, q_3 = \underline{a_3} - (q_1^T \underline{a_3})\, q_1 - (q_2^T \underline{a_3})\, q_2 \Rightarrow \underline{a_3} = (q_1^T \underline{a_3})\, q_1 + (q_2^T \underline{a_3})\, q_2 + \|\underline{A_3}\|\, q_3$

  $\therefore q_3^T \underline{a_3} = \|\underline{A_3}\|$

  Therefore, the diagonal elements of R are

  $q_1^T \underline{a_1} = \|\underline{A_1}\|$, $q_2^T \underline{a_2} = \|\underline{A_2}\|$, $q_3^T \underline{a_3} = \|\underline{A_3}\|$

  $\Rightarrow$ R is upper-triangular with positive diagonal

  $\Rightarrow$ R is invertible (n nonzero pivots)

- The least squares solution to $A\underline{x} = \underline{b}$ is $\hat{\underline{x}}$ satisfying

  $A^T A \hat{\underline{x}} = A^T \underline{b} \Rightarrow (QR)^T (QR) \hat{\underline{x}} = (QR)^T \underline{b} \Rightarrow R^T Q^T Q R \hat{\underline{x}} = R^T Q^T \underline{b} \Rightarrow R^T R \hat{\underline{x}} = R^T Q^T \underline{b}$

  $\Rightarrow (R^T)^{-1} R^T R \hat{\underline{x}} = (R^T)^{-1} R^T Q^T \underline{b} \Rightarrow R\hat{\underline{x}} = Q^T \underline{b}$, $\hat{\underline{x}} = R^{-1} Q^T \underline{b}$

  (can be solved by back substitution)