

## Gram–Schmidt Orthogonalization

Given independent vectors  $a_1, a_2, \dots, a_n$  the Gram–Schmidt orthogonalization algorithm constructs orthonormal vectors  $q_1, q_2, \dots, q_n$  as follows

$$\begin{array}{ll}
 \tilde{q}_1 = a_1 & q_1 = \tilde{q}_1 / \|\tilde{q}_1\| \\
 \tilde{q}_2 = a_2 - q_1(q_1 \cdot a_2) & q_2 = \tilde{q}_2 / \|\tilde{q}_2\| \\
 \tilde{q}_3 = a_3 - q_1(q_1 \cdot a_3) - q_2(q_2 \cdot a_3) & q_3 = \tilde{q}_3 / \|\tilde{q}_3\| \\
 \vdots & \vdots \\
 \tilde{q}_n = a_n - q_1(q_1 \cdot a_n) - q_2(q_2 \cdot a_n) - \cdots - q_{n-1}(q_{n-1} \cdot a_n) & q_n = \tilde{q}_n / \|\tilde{q}_n\|.
 \end{array}$$

Note that

$$\text{span}\{a_1, \dots, a_k\} = \text{span}\{q_1, \dots, q_k\} \quad \text{for every } k = 1, 2, \dots, n.$$

Let

$$A = \left[ \begin{array}{c|c|c|c} a_1 & a_2 & \cdots & a_n \end{array} \right] \quad \text{and} \quad Q = \left[ \begin{array}{c|c|c|c} q_1 & q_2 & \cdots & q_n \end{array} \right].$$

Since  $q_i \in \text{span}\{q_1, \dots, q_k\}^\perp = \text{span}\{a_1, \dots, a_k\}^\perp$  for every  $i > k$ , then

$$q_i \cdot a_j = 0 \quad \text{for every } i > j.$$

It follows that

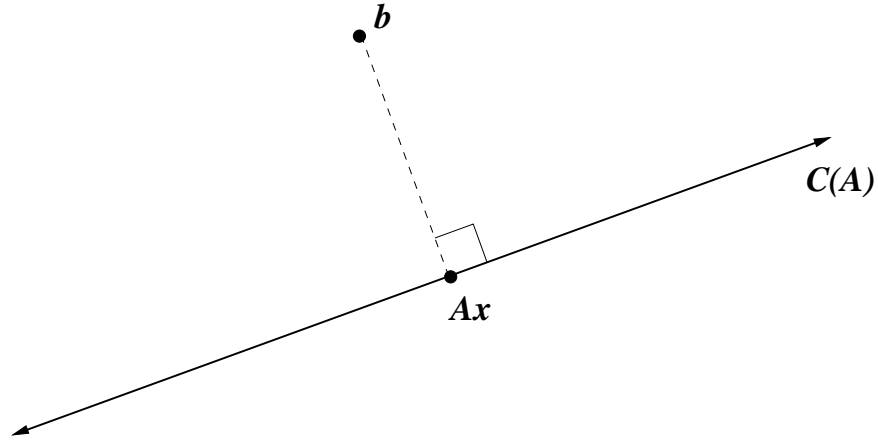
$$R = Q^T A = \left[ \begin{array}{c} \frac{q_1}{\|q_1\|} \\ \frac{q_2}{\|q_2\|} \\ \vdots \\ \frac{q_n}{\|q_n\|} \end{array} \right] \left[ \begin{array}{c|c|c|c} a_1 & a_2 & \cdots & a_n \end{array} \right] = \left[ \begin{array}{cccc} q_1 \cdot a_1 & q_1 \cdot a_2 & \cdots & q_1 \cdot a_n \\ 0 & q_2 \cdot a_2 & \cdots & q_2 \cdot a_n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & q_n \cdot a_n \end{array} \right]$$

is upper triangular. Moreover,

$$\begin{aligned}
 QR &= \left[ \begin{array}{c|c|c|c} q_1 & q_2 & \cdots & q_n \end{array} \right] \left[ \begin{array}{cccc} q_1 \cdot a_1 & q_1 \cdot a_2 & \cdots & q_1 \cdot a_n \\ 0 & q_2 \cdot a_2 & \cdots & q_2 \cdot a_n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & q_n \cdot a_n \end{array} \right] \\
 &= \left[ \begin{array}{c|c|c|c} q_1(q_1 \cdot a_1) & q_1(q_1 \cdot a_2) + q_2(q_2 \cdot a_2) & \cdots & q_1(q_1 \cdot a_n) + q_2(q_2 \cdot a_n) + \cdots + q_n(q_n \cdot a_n) \end{array} \right] \\
 &= \left[ \begin{array}{c|c|c|c} a_1 & a_2 & \cdots & a_n \end{array} \right] = A.
 \end{aligned}$$

## Least Squares Using $A = QR$

The least squares approximation is the point  $x$  such that  $\|Ax - b\|$  is minimized. This happens when  $Ax - b$  is orthogonal to  $\mathcal{C}(A)$ .



Since  $\mathcal{C}(A) = \mathcal{C}(Q)$ , then we are looking for  $x$  such that

$$q_i \cdot (Ax - b) = 0 \quad \text{for } i = 1, 2, \dots, n.$$

Therefore

$$\begin{aligned} Q^T(Ax - b) &= \mathbf{0} \\ Q^T Ax &= Q^T b \\ Q^T(QR)x &= Q^T b \\ (Q^T Q)Rx &= Q^T b \\ Rx &= Q^T b. \end{aligned}$$

Since  $R$  is upper triangular, this system may be easily solved by back substitution.