6.5 Least-Squares Problems

For an inconsistent system $A\mathbf{x} = \mathbf{b}$, where a solution does not exist, the best we can do is to find an $\mathbf{x}$ that makes $A\mathbf{x}$ as close as possible to $\mathbf{b}$. By the Best Approximation theorem, we have:

Definition. *If A is $m \times n$ and $\mathbf{b} \in \mathbb{R}^n$, a* least-squares *solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\hat{\mathbf{x}} \in \mathbb{R}^n$ such that*

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

for all $\mathbf{x} \in \mathbb{R}^n$.

The adjective "least-squares" arises from the fact that $\|\mathbf{b} - A\hat{\mathbf{x}}\|$ is the square root of a sum of squares. The most important aspect of the least-squares problem is that no matter what $\mathbf{x}$ we select, the vector $A\mathbf{x}$ will necessarily be in Col A. So we seek a vector $\mathbf{x}$ that makes $A\mathbf{x}$ the closest point in Col A to $\mathbf{b}$.

Given A and $\mathbf{b}$, we apply the Best Approximation theorem to the subspace Col A. Let

$$\hat{\mathbf{b}} = \text{proj}_{\text{Col }A}\mathbf{b}.$$

Because $\hat{\mathbf{b}}$ is in the column space of A, the equation $A\mathbf{x} = \hat{\mathbf{b}}$ is consistent, and there is an $\hat{\mathbf{x}} \in \mathbb{R}^n$ such that

$$A\hat{\mathbf{x}} = \hat{\mathbf{b}}. \tag{1}$$

Since $\hat{\mathbf{b}}$ is the closest point in Col A to $\mathbf{b}$, a vector $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $\hat{\mathbf{x}}$ satisfies (1). Such an $\hat{\mathbf{x}} \in \mathbb{R}^n$ is a list of weights that will build $\hat{\mathbf{b}}$ out of the columns of A.

Suppose $\hat{\mathbf{x}}$ satisfies (1). By the Orthogonal Decomposition theorem, the projection $\hat{\mathbf{b}}$ has the property that $\mathbf{b} - \hat{\mathbf{b}}$ is orthogonal to Col A, so $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to each column of A. If $\mathbf{a}_j$ is any column of A, then $\mathbf{a}_j \cdot (\mathbf{b} - A\hat{\mathbf{x}}) = 0$, and $\mathbf{a}_j^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0$. Since each $\mathbf{a}_j$ is a row of A^T,

$$A^T(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0}. \tag{2}$$

Thus

$$A^T\mathbf{b} - A^TA\hat{\mathbf{x}} = \mathbf{0}$$
$$\therefore A^TA\hat{\mathbf{x}} = A^T\mathbf{b}.$$

These calculations show that each least-squares solution of $A\mathbf{x} = \mathbf{b}$ satisfies the equation

$$A^TA\mathbf{x} = A^T\mathbf{b}. \tag{3}$$

The matrix equation (3) represents a system of equations called the *normal equations* for $A\mathbf{x} = \mathbf{b}$. A solution of (3) is often denoted by $\hat{\mathbf{x}}$.

Theorem 13. *The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.*

Theorem 14. *Let A be an $m \times n$ matrix. The following are equivalent:*

1. *The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each $\mathbf{b} \in \mathbb{R}^m$.*
2. *The columns of A are linearly independent.*
3. *The matrix A^TA is invertible.*

When these statements are true, the least-squares solution $\hat{\mathbf{x}}$ is given by

$$\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b} \tag{4}$$

The distance between $\mathbf{b}$ and $A\hat{\mathbf{x}}$ is called the least-squares error of this approximation.

Theorem 15. *Given an $m \times n$ matrix A with linearly independent columns, let $A = QR$ be a QR factorization of A. Then, for each $\mathbf{b} \in \mathbb{R}^m$, the equation $A\mathbf{x} = \mathbf{b}$ has a unique solution, given by*

$$\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}. \tag{5}$$

Example 1. *Find (a) the orthogonal projection of* $\mathbf{b} = \begin{bmatrix} 2 \\ 5 \\ 6 \\ 6 \end{bmatrix}$ *onto* Col A *and (b) a least-squares solution of* $A\mathbf{x} = \mathbf{b}$, *when* $A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & -1 \end{bmatrix}$.