Section 6.5 Least-Squares Problem

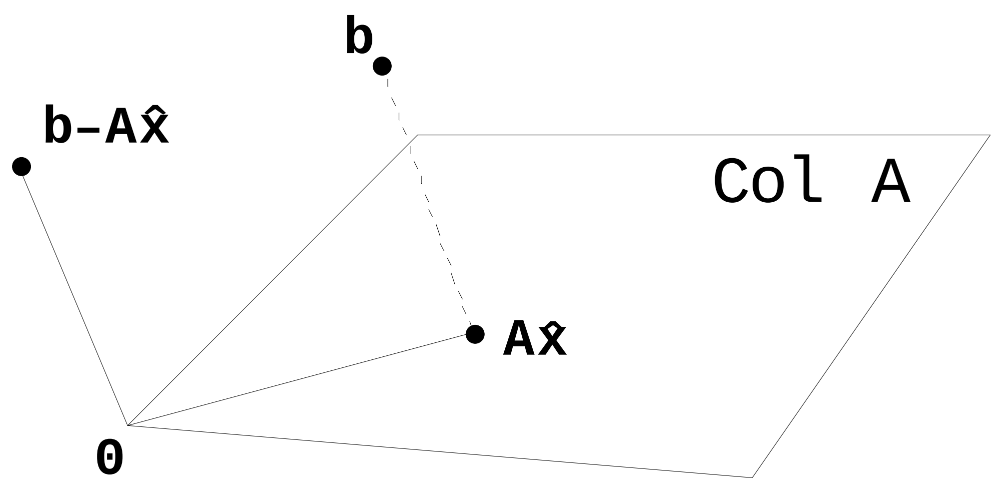
Problem: What do we do when $A\mathbf{x} = \mathbf{b}$ has no solution $\mathbf{x}$?

Answer: Find $\hat{\mathbf{x}}$ such that $A\hat{\mathbf{x}}$ is as "close" as possible to $\mathbf{b}$. (*Least Squares Problem*)

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

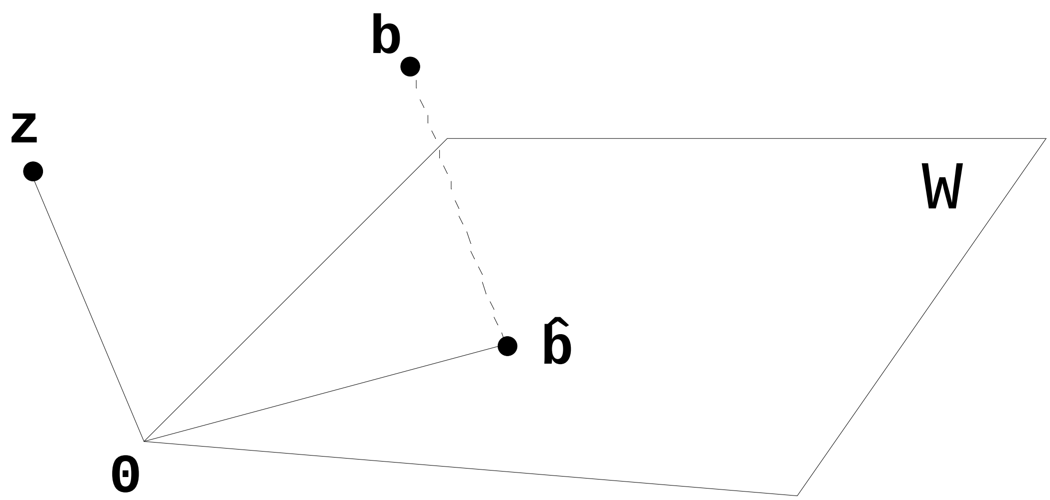
$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

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

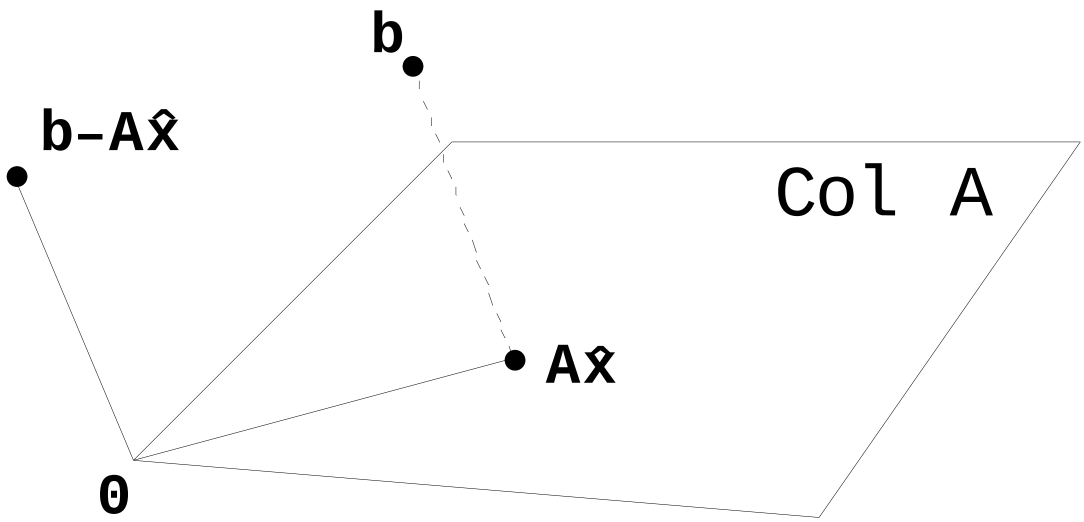


Let $W = \text{Col}\, A$ where A is $m \times n$ and $A = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n \end{bmatrix}$.

Suppose $\mathbf{b}$ is in $\mathbf{R}^m$ and $\hat{\mathbf{b}} = \text{proj}_W \mathbf{b}$.



$\hat{\mathbf{b}}$ is the point in $W = \text{Col}\, A$ closest to $\mathbf{b}$



Since $\widehat{\mathbf{b}}$ is in Col A, then $\hat{\mathbf{x}}$ is a vector in $\mathbf{R}^n$ such that $\widehat{\mathbf{b}} = A\hat{\mathbf{x}}$.

By the Orthogonal Projection Theorem, $\mathbf{z}$ is in $W^\perp$ where
$\mathbf{z} = \mathbf{b} - A\hat{\mathbf{x}}$.

Then $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to every column of A. Meaning that

$$\mathbf{a}_1^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \qquad \mathbf{a}_2^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \qquad \cdots \qquad \mathbf{a}_n^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0$$

$$\begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_n^T \end{bmatrix} (\mathbf{b} - A\hat{\mathbf{x}}) = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

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

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

$$\boxed{A^TA\hat{\mathbf{x}} = A^T\mathbf{b}}$$

(normal equations for $\hat{\mathbf{x}}$)

THEOREM 13

The set of least squares solutions of $A\mathbf{x} = \mathbf{b}$ is the set of all solutions of the normal equations $A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$.

EXAMPLE: Find a least squares solution to the inconsistent system $A\mathbf{x} = \mathbf{b}$ where

$$A = \begin{bmatrix} 2 & 0 \\ 0 & 1 \\ 2 & 2 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}.$$

Solution: Solve $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$ after first finding $A^T A$ and $A^T\mathbf{b}$.

$$A^T A = \begin{bmatrix} 2 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 1 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 8 & 2 \\ 4 & 3 \end{bmatrix}$$

$$A^T\mathbf{b} = \quad = \begin{bmatrix} 2 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 8 \\ 8 \end{bmatrix}$$

So solve the following:

$$\underbrace{\begin{bmatrix} 8 & 2 \\ 4 & 3 \end{bmatrix}}_{} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{} = \underbrace{\begin{bmatrix} 8 \\ 8 \end{bmatrix}}_{}$$

$$\begin{bmatrix} 8 & 2 & 8 \\ 4 & 3 & 8 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & 2 \end{bmatrix} \qquad \Rightarrow \qquad \hat{\mathbf{x}} = \begin{bmatrix} \frac{1}{2} \\ 2 \end{bmatrix}$$

When A^TA is invertible,

$$A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$$

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

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

So in the last example,

$$(A^TA)^{-1} = \begin{bmatrix} 8 & 2 \\ 4 & 3 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{3}{16} & -\frac{1}{8} \\ -\frac{1}{4} & \frac{1}{2} \end{bmatrix}$$

and

$$\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b} = \begin{bmatrix} \frac{3}{16} & -\frac{1}{8} \\ -\frac{1}{4} & \frac{1}{2} \end{bmatrix}\begin{bmatrix} 8 \\ 8 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ 2 \end{bmatrix}$$

THEOREM 14

The matrix A^TA is invertible if and only if the columns of A are linearly independent. In this case, the equation $A\mathbf{x} = \mathbf{b}$ has only one least-squares solution $\hat{\mathbf{x}}$, and it is given by

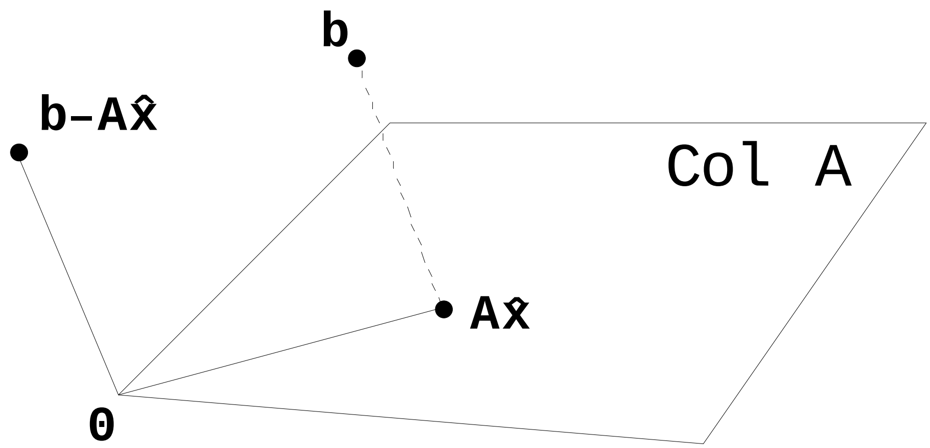
$$\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b}.$$

$$\textbf{least-squares error} = \|\mathbf{b} - A\hat{\mathbf{x}}\|$$

From the last example,

$$\mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \text{ and } A\hat{\mathbf{x}} = \begin{bmatrix} 2 & 0 \\ 0 & 1 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} \frac{1}{2} \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$$

$$\textbf{least-squares error} = \|\mathbf{b} - A\hat{\mathbf{x}}\| = \left\| \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix} \right\| = 2$$



For another way to compute $\hat{\mathbf{x}}$, see Theorem 15 (page 414) and Example 5, page 415.