MTHSC 3110 Section 6.5 – Least Squares Solutions

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Definition

Suppose that A is an $m \times n$ matrix. A <u>least squares solution</u> of the matrix equation $A\vec{x} = \vec{b}$ is a vector $\hat{x} \in \mathbb{R}^n$ satisfying

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

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

Example

Find a least squares solution to $A\vec{x} = \vec{b}$ where

$$A = \begin{pmatrix} 1 & -6 \\ 1 & -2 \\ 1 & 1 \\ 1 & 7 \end{pmatrix}. \text{ and } \vec{b} = \begin{pmatrix} -1 \\ 2 \\ 1 \\ 6 \end{pmatrix}.$$

Solution

Note that the columns of A are orthogonal and thus give an orthogonal basis for $\mathrm{Col}(A)$.
We can compute

$$\begin{aligned}\hat{b} &= \mathrm{Proj}_{\mathrm{Col}(A)}(\vec{b}) = \frac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1}\vec{a}_1 + \frac{\vec{b}\cdot\vec{a}_2}{\vec{a}_2\cdot\vec{a}_2}\vec{a}_2 \\ &= \frac{8}{4}\vec{a}_1 + \frac{45}{90}\vec{a}_2 = 2\vec{a}_1 + \frac{1}{2}\vec{a}_2 = \begin{pmatrix} -1 \\ 1 \\ \frac{3}{2} \\ \frac{11}{2} \end{pmatrix}.\end{aligned}$$

Since $\hat{b} = \mathrm{Proj}_{\mathrm{Col}(A)}(\vec{b})$, it is the closest vector to $\vec{b}$ in $\mathrm{Col}(A)$.
Since $\hat{b} \in \mathrm{Col}(A)$ there is a solution to $A\hat{x} = \hat{b}$.
From our previous work, a solution is given by $\hat{x} = \begin{pmatrix} 2 \\ \frac{1}{2} \end{pmatrix}$.

Theorem

The set of least squares solutions to $A\vec{x} = \vec{b}$ is the nonempty set of solutions of

$$(A^T A)\vec{x} = A^T \vec{b}.$$

Proof.

Write $A = [\vec{a}_1, \dots, \vec{a}_n]$. Take $\hat{b} = \mathrm{Proj}_{\mathrm{Col}(A)}(\vec{b})$.
Then $\hat{b}$ is the closest vector to $\vec{b}$ for which $A\vec{x} = \hat{b}$ has a solution.
Since $\hat{b} \in \mathrm{Col}(A)$, there is $\hat{x} \in \mathbb{R}^n$ with $A\hat{x} = \hat{b}$.
Now, note that

$$\begin{aligned}
(\vec{b} - \hat{b}) \perp \mathrm{Col}(A) \quad &\Leftrightarrow \quad (\vec{b} - A\hat{x}) \perp \vec{a}_i \text{ for } 1 \le i \le n. \\
&\Leftrightarrow \quad \vec{a}_i^T(\vec{b} - A\hat{x}) = 0 \text{ for } 1 \le i \le n. \\
&\Leftrightarrow \quad \vec{0} = A^T(\vec{b} - A\hat{x}) = A^T\vec{b} - A^T A\hat{x}. \\
&\Leftrightarrow \quad A^T A\hat{x} = A^T\vec{b}.
\end{aligned}$$

$\square$

Theorem

The matrix $A^T A$ is invertible if and only if the columns of A are linearly independent. In this case, the equation $A\vec{x} = \vec{b}$ has a unique least squares solution, and it is given by

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

Theorem

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

$$\hat{x} = R^{-1} Q^T \vec{b}.$$