MTHSC 3110 Section 6.5 – Least Squares Solutions

Kevin James

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DEFINITION

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

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

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

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EXAMPLE

Find a least squares solution to $A\vec{x} = \vec{b}$ where $A = \begin{pmatrix} 1 & -6 \\ 1 & -2 \\ 1 & 1 \\ 1 & 7 \end{pmatrix}$. and $\vec{b} = \begin{pmatrix} -1 \\ 2 \\ 1 \\ 6 \end{pmatrix}$.

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$$= \frac{8}{4} \vec{a}_1 + \frac{45}{90} \vec{a}_2 =$$

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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 $A = [\vec{a}_1, \ldots, \vec{a}_n]$.

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$$(ec{b}-\hat{b})\perp {\sf Col}({\it A}) \ \Leftrightarrow \ (ec{b}-{\it A}\hat{x})\perp ec{a_i} \ {\sf for} \ 1\leq i\leq n.$$

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$$(\vec{b} - \hat{b}) \perp \operatorname{Col}(A) \iff (\vec{b} - A\hat{x}) \perp \vec{a_i} \text{ for } 1 \leq i \leq n.$$

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

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

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

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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

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

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