Lecture 20: Least Squares Problems

MAT2040 Linear Algebra

Theorem 19.23 (Orthogonal Decomposition Theorem)

If $\mathbf{x} \in \mathbb{R}^n$ *and* S *is a subspace of* $\mathbb{R}^n$*, then* $\mathbf{x}$ *can be* **uniquely** *expressed as* $\mathbf{x} = \hat{\mathbf{x}} + \mathbf{z}$*, where* $\hat{\mathbf{x}} \in S$ *and* $\mathbf{z} \in S^{\perp}$*.*

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The vector $\hat{\mathbf{x}}$ in the Orthogonal Decomposition Theorem is called the **orthogonal projection of x onto subspace** S.

Theorem 20.1 (Orthogonal Projection is Closest Point)

Let $\mathbf{b} \in \mathbb{R}^m$*,* S *be a subspace of* $\mathbb{R}^m$*, and* $\mathbf{p}$ *be the orthogonal projection of* $\mathbf{b}$ *onto* S*. Then* $\mathbf{p}$ *is the closest point in* S *to* $\mathbf{b}$*, i.e.,*

$$\|\mathbf{b} - \mathbf{p}\| < \|\mathbf{b} - \mathbf{s}\|$$

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$$\|\mathbf{b} - \mathbf{p}\| < \|\mathbf{b} - \mathbf{s}\|$$

for all $\mathbf{s} \in S$, $\mathbf{s} \neq \mathbf{p}$.

Note that "closest" here is with respect to Euclidean distance.

We have not yet seen how to **find** the orthogonal projection however (except for 1-dimensional subspaces).

We will now study how to finding the orthogonal projection in the context of "Least Squares Problems".

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Note that choosing the Euclidean norm as our measure was a choice.

Also note that
$\|A\hat{\mathbf{x}} - \mathbf{b}\| = \sqrt{(\vec{a}_1\mathbf{x} - b_1)^2 + (\vec{a}_2\mathbf{x} - b_2)^2 + \cdots + (\vec{a}_m\mathbf{x} - b_m)^2}$,
which explains the name "least squares".

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$A\mathbf{x} \in \operatorname{Col} A$! We are projecting on the column space of A.

To make sure $A\hat{\mathbf{x}}$ is the orthogonal projection of $\mathbf{b}$ onto $\operatorname{Col} A$, we want that $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to $\operatorname{Col} A$.

We want $\hat{\mathbf{x}}$ so that $\mathbf{b} - A\hat{\mathbf{x}} \in (\operatorname{Col} A)^{\perp}$.

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In other words, $\hat{x}$ is a solution to

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This system of equations is known as the **normal equations**.

Theorem 20.2

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

Example 20.3

Find the least squares solution to

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \\ -1 & 1 \end{bmatrix} \mathbf{x} = \begin{bmatrix} -3 \\ 0 \\ 6 \end{bmatrix}.$$

Theorem 20.4

Let A be an $m \times n$ matrix. The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for every $\mathbf{b} \in \mathbb{R}^m$ if and only if the columns of A are linearly independent.

Corollary 20.5

If the columns of A are linearly independent, then the orthogonal projection of $\mathbf{b}$ *on the subspace* $\operatorname{Col} A$ *is the vector*
$\mathbf{p} = A(A^T A)^{-1} A^T \mathbf{b}$.

The matrix $A(A^T A)^{-1} A^T$ is sometimes called the **projection matrix** (corresponding the projection on the subspace $\operatorname{Col} A$).