Least Squares Solutions and Orthogonal Projection

Linear Algebra
MATH 2076

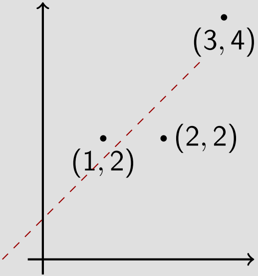
Two Examples

Suppose we want to solve $A\vec{x} = \vec{b}$ where A is an 8×3 matrix.

This corresponds to an SLE with 8 equations but only 3 unknowns. Such a system is highly overdetermined, and almost surely will be inconsistent. In fact, $\vec{b}$ is a vector in $\mathbb{R}^8$, however, $\dim \mathcal{CS}(A) \leq 3$.

But, what if we (our boss) really wants a "solution"?

Suppose we want to find the "best fit" line for the data points $(1, 2), (2, 2), (3, 4)$? We see—look at the pix—that no line goes through all 3 points. How should we proceed?



Recall that $A\vec{x} = \vec{b}$ has a solution iff $\vec{b}$ lies in $\mathcal{CS}(A)$.

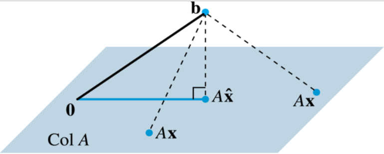
"Solving" an Inconsistent System of Linear Equations

We need to solve $A\vec{x} = \vec{b}$, but $\vec{b}$ is **not** in $\mathcal{CS}(A)$. How should we proceed?

We search for $\vec{x}$ so that $A\vec{x}$ is "as close to $\vec{b}$" as possible. That is, we find a vector $\hat{\mathbf{x}}$ with the property that for any $\vec{x}$,

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

Such a vector $\hat{\mathbf{x}}$ is called a *least squares solution* to $A\vec{x} = \vec{b}$.



The vector $\mathbf{b}$ is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other $\mathbf{x}$.

Least Squares Solution to a System of Linear Equations

A vector $\hat{\mathbf{x}}$ is a *least squares solution* to $A\vec{x} = \vec{b}$ provided for any $\vec{x}$,

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

Here, when A is $m \times n$, $\vec{x}$ is any vector in $\mathbb{R}^n$.
Thus we must solve the **minimization** problem:

$$\text{Find} \quad \min_{\vec{x} \text{ in } \mathbb{R}^n} \|A\vec{x} - \vec{b}\|^2 = \sum_{j=1}^{m} \big((A\vec{x})_j - b_j\big)^2$$

How should we proceed?
Calculus works! You see this approach in a statistics course.

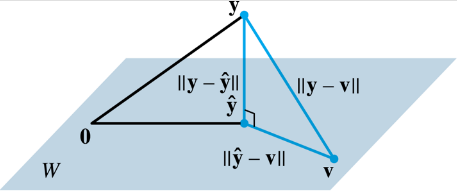
It's more elegant, and easier too, to use Geometry and Linear Algebra.

Best Approximation Theorem for Orthogonal Projection

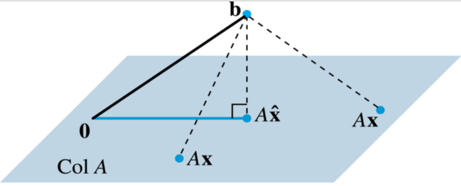
Recall that the orthogonal projection of a vector $\vec{y}$ onto a vector subspace $\mathbb{W}$ **gives us** the vector $\hat{\mathbf{y}}$ in $\mathbb{W}$ that is nearest to $\vec{y}$. Let's apply this with $\vec{y} = \vec{b}$ and $\mathbb{W} = \mathcal{CS}(A)$. We see that the vector in $\mathcal{CS}(A)$ that is nearest/closest to $\vec{b}$ is

$$\hat{\mathbf{b}} = \text{Proj}_{\mathcal{CS}(A)}(\vec{b}).$$

Since $\hat{\mathbf{b}}$ lies in $\mathcal{CS}(A)$, we can solve $A\vec{x} = \hat{\mathbf{b}}$, and any solution to this is a least squares solution to $A\vec{x} = \vec{b}$, right?



The orthogonal projection of **y** onto W is the closest point in W to **y**.



The vector **b** is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other **x**.

Least Squares Solution to a System of Linear Equations

A vector $\hat{\mathbf{x}}$ is a *least squares solution* to $A\vec{x} = \vec{b}$ provided for any $\vec{x}$,

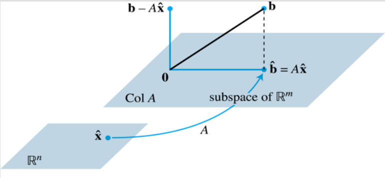
$$\|A\hat{\mathbf{x}} - \vec{b}\| \leq \|A\vec{x} - \vec{b}\| .$$

Here, when A is $m \times n$, $\vec{x}$ is any vector in $\mathbb{R}^n$.

The vector $\hat{\mathbf{b}} = \text{Proj}_{\mathcal{CS}(A)}(\vec{b})$ lies in $\mathcal{CS}(A)$ and is nearest/closest to $\vec{b}$, so any solution $\hat{\mathbf{x}}$ to

$$A\vec{x} = \hat{\mathbf{b}}$$

is a least squares solution.



The least-squares solution $\hat{\mathbf{x}}$ is in $\mathbb{R}^n$.

To find a least squares solution to $A\vec{x} = \vec{b}$:

- Calculate the orthogonal projection $\hat{\mathbf{b}} = \text{Proj}_{\mathcal{CS}(A)}(\vec{b})$. Work!
- Solve $A\vec{x} = \hat{\mathbf{b}}$. Not difficult, right?

Using Geometry to Get a Least Squares Solution

We want to find a solution $\hat{\mathbf{x}}$ to $A\vec{x} = \hat{\mathbf{b}} = \text{Proj}_{\mathcal{CS}(A)}(\vec{b})$.

Recall that $\vec{b} = \hat{\mathbf{b}} + \vec{z}$ where $\vec{z}$ is orthogonal to $\mathcal{CS}(A)$. Thus, $\vec{z}$ lies in the orthogonal complement $\left(\mathcal{CS}(A)\right)^{\perp} = \mathcal{NS}(A^T)$. So,

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

That is,

$$A\hat{\mathbf{x}} = \hat{\mathbf{b}} \iff A^T A\hat{\mathbf{x}} = A^T\vec{b}.$$

Any solution $\hat{\mathbf{x}}$ to $\boxed{A^T A\vec{x} = A^T\vec{b}}$ is a least squares solution to $A\vec{x} = \vec{b}$.

Least Squares Example

We find a least squares solution to $\begin{bmatrix} 1 & 4 \\ -3 & 3 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -16 \\ 28 \\ 6 \end{bmatrix}$.

We compute

$$\begin{bmatrix} 1 & -3 & 5 \\ 4 & 3 & 1 \end{bmatrix} \begin{bmatrix} 1 & 4 \\ -3 & 3 \\ 5 & 1 \end{bmatrix} = \begin{bmatrix} 35 & 0 \\ 0 & 26 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & -3 & 5 \\ 4 & 3 & 1 \end{bmatrix} \begin{bmatrix} -16 \\ 28 \\ 6 \end{bmatrix} = \begin{bmatrix} -70 \\ 26 \end{bmatrix}.$$

So, we must solve

$$\begin{bmatrix} 35 & 0 \\ 0 & 26 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -70 \\ 26 \end{bmatrix}$$

which has the unique solution

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -2 \\ 1 \end{bmatrix}.$$

When will we get a unique least squares solution?

Least Squares Example—"Line Fitting"

Let's find the "best fit" line $y = b + mx$ for the points $(1,2),(2,2),(3,4)$. Here b, m are the unknowns (aka, the variables) and we wish to solve the SLE

$$\begin{cases} b + 1m = 2 \\ b + 2m = 2 \\ b + 3m = 4 \end{cases}$$

Let $A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}, \vec{b} = \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix}$.

which clearly has no solutions.

Now compute!

$$A^T A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix} \text{ and } A^T \vec{b} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 8 \\ 18 \end{bmatrix}.$$

Performing some elementary row operations we deduce that

$$\left[\begin{array}{cc|c} 3 & 6 & 8 \\ 6 & 14 & 18 \end{array}\right] \sim \left[\begin{array}{cc|c} 1 & 0 & \frac{2}{3} \\ 0 & 1 & 1 \end{array}\right]$$

and thus $b = \frac{2}{3}$ and $m = 1$; so $y = \frac{2}{3} + x$ is the "best fit" line.