6.5: Least Squares Problems

When we set up the equation:

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

we know there are three general outcomes: (1) A unique solution (found by inverting the matrix A), (2) An infinite number of solutions (found by reducing the augmented matrix $[A|b]$, and (3) No (exact) solution.

Today, we focus on the last issue.

Example

This is a common problem: Given points (x_1, t_1), (x_2, t_2), (x_3, t_3), up to (x_p, t_p), (t stands for "target") find a line:

$$y = mx + b$$

through the data.

The problem is, there is no line that goes through all the data *exactly*- If there were, we would only need two points, and solve for m, b directly. By setting up the matrix equation that we would get by using the data:

$$\begin{array}{rl} mx_1 + b & = t_1 \\ mx_2 + b & = t_2 \\ mx_3 + b & = t_3 \\ \vdots & \\ mx_p + b & = t_p \end{array} \quad \Rightarrow \quad \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ \vdots & \vdots \\ x_p & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots \\ t_p \end{bmatrix} \quad \Rightarrow \quad A\mathbf{c} = \mathbf{t}$$

To interpret this, we have the matrix equation with no (exact) solution. To solve this equation, and therefore to find the line of "best" fit, we will define an **error function**, and we will then find the **best approximate** solution.

The Error Function

If the matrix equation $A\mathbf{x} = \mathbf{b}$ does not have a solution, then in terms of our four fundamental subspaces $\mathbf{b}$ is not contained in the column space.

We seek to find $\hat{\mathbf{b}} \in \mathrm{Col}(A)$ that is the closest to $\mathbf{b}$:

$$E(\mathbf{x}) = \|\mathbf{b} - \hat{\mathbf{b}}\| = \|\mathbf{b} - A\mathbf{x}\|$$

and so we wish to find $\mathbf{x}$ that *minimizes the error.* The error is commonly referred to as the "least squared error", and so this problem is called *the general least squares problem.*

Solving the Line of Best Fit Using Calculus

Going back to the line of best fit problem, our error function is given by:

$$E(m,b) = \|\mathbf{t} - A\mathbf{c}\|^2 = \sum_{i=1}^{p} (t_i - mx_i - b)^2 =$$

$$(t_1 - (mx_1 + b))^2 + (t_2 - (mx_2 + b))^2 + (t_3 - (mx_3 + b))^2 + \cdots + (t_p - (mx_p + b))^2$$

This problem has one minimum (it is quadratic), and that point must occur at a critical point. The partial derivatives are nice and continuous, so the extreme point must be at the zeros of the partial derivatives.

$$\frac{\partial E}{\partial m} = 2(t_1 - mx_1 - b)(-x_1) + 2(t_2 - mx_2 - b)(-x_2) + 2(t_3 - mx_3 - b)(-x_3) + \cdots + 2(t_p - mx_p - b)(-x_p)$$

or more compactly:

$$\frac{\partial E}{\partial m} = \sum_{i=1}^{p} 2(t_i - mx_i - b)(-x_i) = 2\sum_{i=1}^{p} (-x_i t_i + mx_i^2 + bx_i)$$

Similarly, you can show that

$$\frac{\partial E}{\partial b} = \sum_{i=1}^{p} 2(t_i - mx_i - b)(-1) = 2\sum_{i=1}^{p} (-t_i + mx_i + b)$$

Set each of these to zero:

$$\begin{array}{lll} m\sum x_i^2 & +b\sum x_i & = \sum x_i t_i \\ m\sum x_i & +bp & = \sum t_i \end{array} \quad \Rightarrow \quad \begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & p \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} \sum x_i t_i \\ \sum t_i \end{bmatrix}$$

This is easily solved using the 2×2 inverse or by Cramer's Rule.

Solving the problem using the Fundamental Spaces

Given $A\mathbf{x} = \mathbf{b}$ has no solution, then the point in the column space closest to $\mathbf{b}$ will be defined as $\hat{\mathbf{b}}$, and the point $\hat{\mathbf{x}}$ that gives us $\hat{\mathbf{b}}$ is the **least squares solution.**

By the Best Approximation Theorem, we know that $\hat{\mathbf{b}}$ is the orthogonal projection of $\mathbf{b}$ into the column space, so

$$\mathbf{b} - \hat{b} \in \text{Null}(A^T)$$

(Draw a picture). In other words,

$$A^T(\mathbf{b} - \hat{\mathbf{b}}) = \vec{0} \quad \Rightarrow \quad A^T\mathbf{b} - A^T\hat{\mathbf{b}} = \vec{0}$$

Since $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$, we have: **The least squares solution solves the normal equations:** (Which is Theorem 13)

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

Connecting the two solutions

In the special case of the line of best fit, let's see what the normal equations will give us.

$$\begin{bmatrix} x_1 & x_2 & \dots & x_p \\ 1 & 1 & \dots & 1 \end{bmatrix} \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ \vdots & \vdots \\ x_p & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & \dots & x_p \\ 1 & 1 & \dots & 1 \end{bmatrix} \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots \\ t_p \end{bmatrix}$$

$$\begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & p \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} \sum x_i t_i \\ \sum t_i \end{bmatrix}$$

This is the exact same expression as before.

Continuing with the Normal Eqns

Continuing with the normal equations, we saw that the solution to the normal equations will give us the least square solution:

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

We might ask: When is this expression uniquely solvable?

That happens when $A^T A$ is invertible, or when A is "**full rank**". In that case, the least squares solution is given by:

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

(This is Theorem 14).

Special Case: A has orthogonal columns

Given $A\mathbf{x} = \mathbf{b}$ where the columns of A are orthogonal, then we can actually project $\mathbf{b}$ into the column space of A. Before we do that, recall that

$$A\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + \cdots + x_n\mathbf{a}_n$$

And the projection is:

$$\hat{\mathbf{b}} = \frac{\mathbf{b}\cdot\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_1}\mathbf{a}_1 + \frac{\mathbf{b}\cdot\mathbf{a}_2}{\mathbf{a}_2\cdot\mathbf{a}_2}\mathbf{a}_2 + \cdots + \frac{\mathbf{b}\cdot\mathbf{a}_n}{\mathbf{a}_n\cdot\mathbf{a}_n}\mathbf{a}_n$$

Comparing these two, we see that the projection gives us the solution.

$$x_1 = \frac{\mathbf{b}\cdot\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_1}, \text{ etc}$$

A (numerically) better solution

Finally, in the extra special case that $A = QR$, then $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$. **This technique is recommended for generating computer solutions. It is generally more stable than inverting A^TA.** In this case, we note that:

$$A\widehat{\mathbf{x}} = AR^{-1}Q^T\mathbf{b} = QRR^{-1}Q^T\mathbf{b} = QQ^T\mathbf{b}$$

Numerical Examples

1. (Exercise 4 in text) Find the least squares solution to $A\mathbf{x} = \mathbf{b}$ by using the normal equations. Also determine the error in the solution, and find the projection of $\mathbf{b}$ into the column space of A.

$$A = \begin{bmatrix} 1 & 3 \\ 1 & -1 \\ 1 & 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 5 \\ 1 \\ 0 \end{bmatrix}$$

SOLUTION: We note that the columns of A are not orthogonal, but they are linearly independent, so we can use the normal equations.

$$A^TA\mathbf{x} = \mathbf{b} \quad \Rightarrow \quad \begin{bmatrix} 3 & 3 \\ 3 & 11 \end{bmatrix}\mathbf{x} = \begin{bmatrix} 6 \\ 14 \end{bmatrix} \quad \Rightarrow \quad \mathbf{x} = \frac{1}{24}\begin{bmatrix} 11 & -3 \\ -3 & 3 \end{bmatrix}\begin{bmatrix} 6 \\ 14 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Further,

$$\hat{\mathbf{b}} = A\mathbf{x} = \begin{bmatrix} 4 \\ 0 \\ 2 \end{bmatrix}$$

and the error (the distance from the column space of A to $\mathbf{b}$) is:

$$\sqrt{(4-5)^2 + (0-1)^2 + (2-0)^2} = \sqrt{6}$$

2. (Exercise 6) This one is interesting because the columns of A are not linearly independent, but we can still solve the normal equations.

Find all least squares solutions of the equation $A\mathbf{x} = \mathbf{b}$. By the way, we know that $\mathbf{b}$ is not contained in the column space of A. If there are an infinite number of solutions, what does that say about which of the fundamental subspaces $\hat{\mathbf{x}}$ lies?

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix}$$

(We will form an augmented matrix: $[A^TA\,|\,A^Tb]$

$$\left[\begin{array}{ccc|c} 6 & 3 & 3 & 27 \\ 3 & 3 & 0 & 12 \\ 3 & 0 & 3 & 15 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 0 & 1 & 5 \\ 3 & 3 & 0 & 12 \\ 6 & 3 & 3 & 27 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 0 & 1 & 5 \\ 0 & 3 & -3 & -3 \\ 0 & 3 & -3 & -3 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 0 & 1 & 5 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

From this, we get the least squares solution:

$$\begin{array}{rrr} x_1 = & 5 & -x_3 \\ x_2 = & -1 & +x_3 \\ x_3 = & & x_3 \end{array} = \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix} + x_3 \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$$

As usual, note that the first vector is the particular solution and the second vector is in the null space of A. Therefore, when we compute $\hat{\mathbf{b}}$, we can ignore the second.

Here we compute the projection of $\mathbf{b}$ and the error associated with our solution set.

$$\hat{\mathbf{b}} = A \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix} = \begin{bmatrix} 4 \\ 4 \\ 4 \\ 5 \\ 5 \\ 5 \end{bmatrix} \qquad \|\mathbf{b} - \hat{\mathbf{b}}\| = \sqrt{16} = 4$$

3. (Exercise 10) This one is interesting because the columns of A are orthogonal.

$$A = \begin{bmatrix} 1 & 2 \\ -1 & 4 \\ 1 & 2 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 3 \\ -1 \\ 5 \end{bmatrix}$$

The solution is from the scalar projection of $\mathbf{b}$ into the columns of A:

$$x_1 = \frac{\mathbf{b}\cdot\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_1} = \frac{9}{3} = 3$$

$$x_2 = \frac{\mathbf{b}\cdot\mathbf{a}_2}{\mathbf{a}_2\cdot\mathbf{a}_2} = \frac{12}{24} = \frac{1}{2}$$

4. (Exercise 25) Describe all least squares solution of the system

$$\begin{aligned} x + y &= 2 \\ x + y &= 4 \end{aligned}$$

SOLUTION: Geometrically, it should be the line $x + y = 3$. It is! The matrix $[A^TA\,|\,A^T\mathbf{b}]$ is simply

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

5. Exercise 19 shows that the null spaces of $A^T A$ and A are the same. How does that prove the following:
$$\text{rank}(A^T A) = \text{rank}(A)$$

   SOLUTION: Let A be $m \times n$ with rank k. We note that $A^T A$ is $n \times n$ so the null space of it and the null space of A are both in $\mathbb{R}^n$.

   If the null spaces are the same, then the dimensions of the null spaces are the same.

   If the dimensions are the same, so are the dimensions of the row space of A and the row space of $A^T A$.

   The dimension of the row space is equal to the dimension of the column space, so the dimension of the column space of A is equal to the dimension of the column space of $A^T A$ (the dimensions are equal, even though they are in different vector spaces).

   The rank is the dimension of the column space, so the ranks are equal as well