§6.5 Least Squares Problems

<u>Motivation</u>: If A is an $m\times n$ matrix and b a vector in $\mathbb{R}^m$, sometimes the matrix equation $Ax=b$ is inconsistent, i.e. has no solution.

Even though there is no solution, can we find a vector $\hat{x}$ in $\mathbb{R}^n$ such that $A\hat{x} \approx b$. In other words, can we find a best approximation?

We aim to make the error $b-Ax$ as small as possible.

<u>Definition</u>
With the notation as above, we say $\hat{x}$ is a <u>least-squares solution</u> of $Ax=b$ if

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

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

How can we find such an $\hat{x}$?

We must find an $\hat{x}$ so that $A\hat{x}$ is as close to b as possible. We can use orthogonal projections!

Recall Ax is a vector in Col A for any x and $Ax = b$ has a solution if and only if b is in Col A.

If b is not in Col A, lets find the closest vector $\hat{b}$ in Col A to b. By the best approximation theorem (§6.3), we have

$$\hat{b} = \text{proj}_{\text{Col} A}\, b$$

With this $Ax = \hat{b}$ is consistent and hence has a solution $\hat{x}$ such that $A\hat{x} = \hat{b}$.

This $\hat{x}$ is exactly what we want, but could be difficult to find.

(unless we come up with a good process)

Write $a_1, \dots, a_n$ for the columns of A and suppose $A\hat{x} = \hat{b}$ where $\hat{b} = \text{proj}_{\text{Col}\,A} b$. By the orthogonal decomposition theorem, recall $b - \hat{b}$ is orthogonal to Col A, thus

$$0 = a_i \cdot (b - \hat{b}) = a_i \cdot (b - A\hat{x})$$

for all $i = 1, \dots, n$. Recall from the definition of $\bullet$ product ($u \cdot v = u^T v$) this means

$$a_i^T (b - A\hat{x}) = 0 \quad \text{hence} \quad A^T (b - A\hat{x}) = 0$$

since a_i^T is a row of A^T for $i = 1, \dots, n$.

Rearranging, we see

$$A^T b - A^T A x = 0 \implies A^T A \hat{x} = A^T b$$

Thus it suffices to find the solution(s) to

$$A^T A x = A^T b$$

We call the equations of $A^TAx = A^Tb$ the <u>normal equations</u> for $Ax=b$

<u>Example</u>

Find a least squares solution to $Ax=b$ where

$$A=\begin{bmatrix} -1 & 4 \\ 2 & -3 \\ -1 & 3 \end{bmatrix} \qquad b=\begin{bmatrix} 12 \\ 6 \\ 6 \end{bmatrix}$$

<u>Solution:</u>

$$A^TAx = A^Tb$$

$$\begin{bmatrix} -1 & 2 & -1 \\ 4 & -3 & 3 \end{bmatrix}\begin{bmatrix} -1 & 4 \\ 2 & -3 \\ -1 & 3 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -1 & 2 & -1 \\ 4 & -3 & 3 \end{bmatrix}\begin{bmatrix} 12 \\ 6 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} 6 & -13 \\ -13 & 34 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -6 \\ 48 \end{bmatrix}$$

$$\left[\begin{array}{cc|c} 6 & -13 & -6 \\ -13 & 34 & 48 \end{array}\right] \sim \left[\begin{array}{cc|c} 1 & -13/6 & -1 \\ 0 & 35/6 & 35 \end{array}\right] \sim \left[\begin{array}{cc|c} 1 & -13/6 & -1 \\ 0 & 1 & 6 \end{array}\right]$$

$$\sim \left[\begin{array}{cc|c} 1 & 0 & 12 \\ 0 & 1 & 6 \end{array}\right]$$

Thus $\hat{x} = \begin{bmatrix} 12 \\ 6 \end{bmatrix}$ is a least squares solution.

Remark

$A^T A x = A^T b$ is consistent, but this doesn't mean theres always one unique solution. Depending on free variables, sometimes there are infinitely many least squares solutions.

Example

Find all least squares solutions to $Ax = b$ where

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

solution:

$$A^T A x = A^T b$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 5 \\ 3 \\ 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 4 & 2 & 2 \\ 2 & 2 & 0 \\ 2 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 2 \\ 8 \end{bmatrix}$$

pivots

$$\left[\begin{array}{ccc|c} 4 & 2 & 2 & 10 \\ 2 & 2 & 0 & 2 \\ 2 & 0 & 2 & 8 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & \frac{1}{2} & \frac{1}{2} & \frac{5}{2} \\ 0 & 1 & -1 & -3 \\ 0 & -1 & 1 & 3 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & \frac{1}{2} & \frac{1}{2} & \frac{5}{2} \\ 0 & 1 & -1 & -3 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

x_3 free !

$$\sim \left[\begin{array}{ccc|c} 1 & 0 & 1 & 4 \\ 0 & 1 & -1 & -3 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

$$\begin{cases} x_1 + x_3 = 4 \\ x_2 - x_3 = -3 \end{cases}$$

$$\hookrightarrow \begin{cases} x_1 = 4 - x_3 \\ x_2 = -3 + x_3 \\ x_3 = x_3 \end{cases}$$

$$\hat{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ -3 \\ 0 \end{bmatrix} + x_3 \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$$

Thus $\hat{x}$ is a least squares solution for any value of x_3.

Theorem

Let A be an $m \times n$ matrix. The following are equivalent:

1) $Ax = b$ has a unique least squares solution $\hat{x}$ for all b in $\mathbb{R}^m$

2) The columns of A are linearly independent

3) $A^T A$ is invertible.

Proof

(1) $\Rightarrow$ (2): Suppose $Ax=b$ has a unique least squares solution for all b. Pick $b=0$ so $Ax=0$ has a unique least squares solution. Thus

$$A^T A x = A^T \cdot 0 = 0$$

has a unique solution. Obviously $x=0$ is a solution so it must be the unique solution. Thus we've shown if $Ax=0$, then $x=0$. Thus $\text{Null } A = 0$ which implies the columns of A are linearly independent.

(2) $\Rightarrow$ (3): Suppose the columns of A are linearly independent. Then $Ax=0$ has only the trivial solution $x=0$.

Since A^TA is a square matrix, A^TA is invertible if and only if $A^TAx=0$ has only the trivial solution $x=0$.

If $A^TAx=0$, then

$$0 = x^T(\underbrace{A^TAx}_{=0}) = x^TA^TAx = (Ax)^T(Ax) = Ax \cdot Ax$$

by the definition of $\cdot$ product. Now $Ax \cdot Ax = 0$ implies $Ax=0$, hence $x=0$ (linear independent columns). Thus $A^TAx=0$ has only the trivial solution so A^TA is invertible.

(3) $\Rightarrow$ (1): Suppose A^TA is invertible and consider the matrix equation $Ax=b$. A least squares solution to $Ax=b$ is a solution to

$$A^TAx = A^Tb$$

if A^TA is invertible, then $\hat{x} = (A^TA)^{-1}A^Tb$ is the unique least squares solution.

Theorem

Suppose A is an $m \times n$ matrix with linearly independent columns. Write $A = QR$ with Q and R as in §6.4

From the previous theorem $Ax = b$ has a unique least squares solution (columns are linearly independent). Moreover this solution is

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

Proof

We need only show $A\hat{x} = \hat{b}$ where $\hat{x}$ is as above.

$$A(R^{-1}Q^T b) = (QR)(R^{-1}Q^T b) = QRR^{-1}Q^T b = QQ^T b$$

Since the columns of Q are an orthonormal basis of $\mathrm{Col}\, A$, by the last theorem of §6.3

$$QQ^T b = \mathrm{proj}_{\mathrm{Col}\, A} b = \hat{b}$$