LEAST SQUARES SOLUTIONS

Suppose that a linear system $Ax = b$ is inconsistent. This is often the case when the number of equations exceeds the number of unknowns (an overdetermined linear system). If a tall matrix $A$ and a vector $b$ are randomly chosen, then $Ax = b$ has no solution with probability 1.

In geometric terms, inconsistency means that $b$ is not in the image of $A$. If so, it may still be reasonable to look for $x$ such that $y = Ax$ is as close to $b$ as possible, i.e.,

$$\|Ax - b\|$$ is a minimum.

In other words, we are interested in a vector $x^*$ such that

$$Ax^* = \text{proj}_{\text{im}A} b.$$ Any such vector $x^*$ is called a least squares solution to $Ax = b$, as it minimizes the sum of squares

$$\|Ax - b\|^2 = \sum_k ((Ax)_k - b_k)^2.$$ For a consistent linear system, there is no difference between a least squares solution and a regular solution.

Consider the following derivation:

$$Ax^* = \text{proj}_{\text{im}A} b$$

$$b - Ax^* \perp \text{im}A \quad (b - Ax^* \text{ is normal to } \text{im} A)$$

$$b - Ax^* \text{ is in } \ker A^\top$$

$$A^\top(b - Ax^*) = 0$$

$$A^\top Ax^* = A^\top b \quad (\text{normal equation}).$$

Note that $A^\top A$ is a symmetric square matrix. If $A^\top A$ is invertible, and this is the case whenever $A$ has trivial kernel, then the least squares solution is unique:

$$x^* = (A^\top A)^{-1} A^\top b.$$ Moreover,

$$Ax^* = A(A^\top A)^{-1} A^\top b,$$

so $A(A^\top A)^{-1} A^\top$ is the standard matrix of the orthogonal projection onto the image of $A$. If $A^\top A$ is not invertible, there are infinitely many least squares solutions. They all yield the same $Ax^*$.

Here are some supporting propositions and examples.

**Proposition.** $Ax \cdot y = x \cdot A^\top y$

**Proof.** Exercise.
Proposition. \((\text{im } A)^\perp = \ker A^\top\)

Proof. Exercise.

Proposition. \(\ker A = \ker A^\top A\)

Proof. If \(Ax = 0\), then \(A^\top Ax = 0\). If \(A^\top Ax = 0\), \(\|Ax\|^2 = (Ax)^\top Ax = x^\top A^\top Ax = 0\). \(\square\)

Proposition. \(\text{im } A^\top = \text{im } A^\top A\)

Proof. \(\text{im } A^\top = (\ker A)^\perp = (\ker A^\top A)^\perp = (\text{im } A^\top A)^\perp = \text{im } A^\top A\) \(\square\)

Example. The linear system \[
\begin{pmatrix}
1 & 1 \\
1 & 1 \\
1 & 0
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
= \begin{pmatrix}
1 \\
2
\end{pmatrix}
\] is inconsistent.

The vector \(b = \begin{pmatrix} 1 \\ 2 \end{pmatrix}\) is not on the line \(\text{im } A = \text{span} \begin{pmatrix} 1 \\ 1 \end{pmatrix}\).

The associated normal equation is
\[
\begin{pmatrix}
2 & 2 \\
2 & 2
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
= \begin{pmatrix}
3 \\
3
\end{pmatrix}.
\]

The matrix \(A^\top A = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}\) is not invertible.

The least squares solutions are \(x^* = \begin{pmatrix} 1 \\ .5 \end{pmatrix} + \text{span} \begin{pmatrix} 1 \\ -1 \end{pmatrix}\).

The orthogonal projection of \(b\) onto \(\text{im } A\) is \(Ax^* = \begin{pmatrix} 1.5 \\ 1.5 \end{pmatrix}\).

Example. The linear system \[
\begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2 \\
x_3
\end{pmatrix}
= \begin{pmatrix}
0 \\
1 \\
1
\end{pmatrix}
\] is inconsistent.

The vector \(b = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}\) is not in the plane \(\text{im } A = \text{span} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\).

The associated normal equation is
\[
\begin{pmatrix}
3 & 2 \\
2 & 2
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
= \begin{pmatrix}
2 \\
1
\end{pmatrix}.
\]

The matrix \(A^\top A = \begin{pmatrix} 3 & 2 \\ 2 & 2 \end{pmatrix}\) is invertible, \((A^\top A)^{-1} = \frac{1}{2} \begin{pmatrix} 2 & -2 \\ -2 & 3 \end{pmatrix}\).

The least squares solution is unique, \(x^* = \begin{pmatrix} 1 \\ -.5 \end{pmatrix}\).

The orthogonal projection of \(b\) onto \(\text{im } A\) is \(Ax^* = \begin{pmatrix} .5 \\ .5 \end{pmatrix}\).

The matrix of the orthogonal projection onto \(\text{im } A\) is \(A(A^\top A)^{-1}A^\top = \begin{pmatrix} .5 & .5 & 0 \\ .5 & .5 & 0 \\ 0 & 0 & 1 \end{pmatrix}\).