

Least Squares and the Pseudoinverse

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The goal of this is to explain how the (Moore-Penrose) pseudoinverse relates to the least squares problem. Specifically, the pseudoinverse allows one to compute the least-norm solution to the problem.

Notation

$\mathbf{A} \in \mathbb{R}^{m \times n}$ denotes an $m \times n$ matrix and \mathbf{A}^\dagger is its pseudoinverse. $\text{Range } \mathbf{A}$ is the vector space spanned by the columns of \mathbf{A} (the column space). As a consequence, $\text{Range } \mathbf{A}^\top$ is the span of the rows of \mathbf{A} (the row space). $\text{Null } \mathbf{A}$ is the null space of \mathbf{A} .

Fundamental Theorem of Linear Algebra

Theorem. *If $\mathbf{A} \in \mathbb{C}^{m \times n}$, then*

$$\text{Null}(\mathbf{A}) = \text{Range}(\mathbf{A}^*)^\perp \text{ and } \text{Null}(\mathbf{A}^*) = \text{Range}(\mathbf{A})^\perp$$

where \mathbf{B}^\perp denotes the orthogonal complement of \mathbf{B} in its containing vector space.

1 Least Squares

The ordinary least squares problem is the following.

Given a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and a vector $\mathbf{b} \in \mathbb{R}^n$, solve

$$\min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|^2.$$

The vector \mathbf{x} is called the solution to this least squares problem. Note that this solution may not be unique.

1.1 Pseudoinverse

First, let's discuss the pseudoinverse. It can be shown that there exists a unique $\mathbf{A}^\dagger \in \mathbb{R}^{n \times m}$ satisfying the Moore-Penrose conditions:

1. $\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}$
2. $\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger$
3. $(\mathbf{A}\mathbf{A}^\dagger)^\top = \mathbf{A}\mathbf{A}^\dagger$ (so $\mathbf{A}\mathbf{A}^\dagger$ is symmetric)
4. $(\mathbf{A}^\dagger\mathbf{A})^\top = \mathbf{A}^\dagger\mathbf{A}$ (so $\mathbf{A}^\dagger\mathbf{A}$ is symmetric)

Firstly, we show that $\mathbf{A}\mathbf{A}^\dagger$ is a projection matrix:

$$(\mathbf{A}\mathbf{A}^\dagger)(\mathbf{A}\mathbf{A}^\dagger) = (\mathbf{A}\mathbf{A}^\dagger\mathbf{A})\mathbf{A}^\dagger = \mathbf{A}\mathbf{A}^\dagger.$$

Because it is symmetric, it must also be an orthogonal projection onto its range.

Now, we claim that $\text{Range } \mathbf{A}^\dagger = \text{Range } \mathbf{A}^\top$. Because $\text{Range } \mathbf{A}^\top \perp \text{Null } \mathbf{A}$, this is equivalent to saying $\text{Range } \mathbf{A}^\dagger \perp \text{Null } \mathbf{A}$. Suppose $\mathbf{A}^\dagger \mathbf{x} \in \text{Range } \mathbf{A}^\dagger$ and $\mathbf{y} \in \text{Null } \mathbf{A}$. Then, to show they are orthogonal,

$$\begin{aligned} (\mathbf{A}^\dagger \mathbf{x})^\top \mathbf{y} &= \mathbf{x}^\top (\mathbf{A}^\dagger)^\top \mathbf{y} \\ &= \mathbf{x}^\top (\mathbf{A}^\dagger \mathbf{A} \mathbf{A}^\dagger)^\top \mathbf{y} && \text{(using property of pseudoinverse)} \\ &= \mathbf{x}^\top ((\mathbf{A}^\dagger \mathbf{A}) \mathbf{A}^\dagger)^\top \mathbf{y} \\ &= \mathbf{x}^\top (\mathbf{A}^\dagger)^\top (\mathbf{A}^\dagger \mathbf{A})^\top \mathbf{y} \\ &= \mathbf{x}^\top (\mathbf{A}^\dagger)^\top \mathbf{A}^\dagger \mathbf{A} \mathbf{y} && \text{(because } \mathbf{A}^\dagger \mathbf{A} \text{ is symmetric)} \\ &= \mathbf{0} && \text{(because } \mathbf{y} \in \text{Null } \mathbf{A}) \end{aligned}$$

An identical process shows that $\text{Null } \mathbf{A}^\dagger \perp \text{Range } \mathbf{A}$ and hence $\text{Null } \mathbf{A}^\dagger = \text{Null } \mathbf{A}^\top$.

1.2 Minimising the norm

The goal is to solve for \mathbf{x} which minimises

$$\frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|^2.$$

Looking only at the norm, we can decompose \mathbf{b} into two orthogonal vectors—one in $\text{Null } \mathbf{A}^\top$ and one in $\text{Range } \mathbf{A}$. This is done using the orthogonal projection \mathbf{AA}^\dagger we found earlier. It should be clear that this has not changed the equation.

$$\|\mathbf{Ax} - \mathbf{b}\|^2 = \|\mathbf{Ax} - (\mathbf{AA}^\dagger + (\mathbf{I} - \mathbf{AA}^\dagger))\mathbf{b}\|^2$$

Now, we expand and regroup terms to get

$$\|\mathbf{Ax} - \mathbf{b}\|^2 = \underbrace{\|(\mathbf{Ax} - \mathbf{AA}^\dagger \mathbf{b})\|^2}_{\in \text{Range } \mathbf{A}} + \underbrace{\|(\mathbf{I} - \mathbf{AA}^\dagger)\mathbf{b}\|^2}_{\in \text{Null } \mathbf{A}^\top}.$$

It is obvious why the left part is in $\text{Range } \mathbf{A}$. Recall that \mathbf{AA}^\dagger is an orthogonal projection onto $\text{Range } \mathbf{A}$. $\mathbf{I} - \mathbf{AA}^\dagger$ projects onto the orthogonal complement of this, which is the $\text{Null } \mathbf{A}^\top$.

Because $\text{Null } \mathbf{A}^\top \perp \text{Range } \mathbf{A}$, we can use Pythagoras' theorem to split the norm.

$$\|(\mathbf{Ax} - \mathbf{AA}^\dagger \mathbf{b}) + (\mathbf{I} - \mathbf{AA}^\dagger)\mathbf{b}\|^2 = \|\mathbf{Ax} - \mathbf{AA}^\dagger \mathbf{b}\|^2 + \|(\mathbf{I} - \mathbf{AA}^\dagger)\mathbf{b}\|^2$$

The rightmost component is a constant so we can't change it. In fact, if $\mathbf{Ax} = \mathbf{b}$ has no exact solution, it is precisely because this part is non-zero. For our purposes of least squares, we can ignore it because

$$\arg \min \|\mathbf{Ax} - \mathbf{b}\|^2 = \arg \min \|\mathbf{Ax} - \mathbf{AA}^\dagger \mathbf{b}\|^2$$

The value of the minimum is 0. It's important to note that this can be zero when the original least squares might not be 0. This is because \mathbf{AA}^\dagger is an orthogonal projection onto $\text{Range } \mathbf{A}$, so there always exists an \mathbf{x} such that $\mathbf{Ax} = \mathbf{AA}^\dagger \mathbf{b}$ and the norm is 0, namely $\mathbf{x} = \mathbf{A}^\dagger \mathbf{b}$.

Contrast this with the original $\|\mathbf{Ax} - \mathbf{b}\|$. If $\mathbf{b} \notin \text{Range } \mathbf{A}$, this will never be 0. However, we can minimise it, which is what we aim to do with least squares.

Finally, we want show that $\mathbf{x} = \mathbf{A}^\dagger \mathbf{b}$ is the solution with the smallest norm. Because $\mathbf{x} \in \text{Range } \mathbf{A}^\top$, \mathbf{x} has no components in the direction of the null space. This is shown by

$$\mathbf{x} = \mathbf{A}^\dagger \mathbf{b} = (\mathbf{A}^\dagger \mathbf{A})\mathbf{A}^\dagger \mathbf{b} + \underbrace{(\mathbf{I} - \mathbf{A}^\dagger \mathbf{A})\mathbf{A}^\dagger \mathbf{b}}_{=0}.$$

If we add some component from the null space, we will get other solutions (because $\mathbf{A}\mathbf{x}$ will not change). These extra solutions can be expressed as

$$\mathbf{x} = \mathbf{A}^\dagger \mathbf{b} + \underbrace{(\mathbf{I} - \mathbf{A}^\dagger \mathbf{A})\mathbf{y}}_{\in \text{Null } \mathbf{A}}, \quad \text{for any } \mathbf{y} \in \mathbb{R}^m.$$

Clearly, these solutions will have a larger norm than the original $\mathbf{A}^\dagger \mathbf{b}$, so we conclude $\mathbf{A}^\dagger \mathbf{b}$ is the solution with the smallest norm.

Corollary: If $\text{Null } \mathbf{A} = \{\mathbf{0}\}$, then $\mathbf{A}^\dagger \mathbf{b} = \mathbf{A}^{-1} \mathbf{b}$ is the unique solution.