L21LeastSquares

April 23, 2015

1 Least Squares

Let's go back to week 1. A long time ago!

Recall Gauss's remarkable accomplishment in his early 20s. He took the set of measurements made by Piazzi of the dwarf planet Ceres and predicted where Ceres subsequently would appear in the sky (after it was lost behind the sun). This told Olbers exactly where to look, and lo and behold . . .

We can understand now a little better what Gauss had to do.

Kepler had discovered, and Newton had explained, that each planet orbits the sun following the path of an ellipse.

To describe the orbit of Ceres, Gauss had to construct the equation for its ellipse:

$$a_1x_1^2 + a_2x_2^2 + a_3x_1x_2 + a_4x_1 + a_5x_2 + a_6 = 0.$$

He had many measurements of (x_1, x_2) pairs and had to find the $a_1, \ldots, a_6$.

This is actually a linear system:

$$\begin{bmatrix} x_{11}^2 & x_{21}^2 & x_{11}x_{21} & x_{11} & x_{21} & 1 \\ x_{12}^2 & x_{22}^2 & x_{12}x_{22} & x_{12} & x_{22} & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{1n}^2 & x_{2n}^2 & x_{1n}x_{2n} & x_{1n} & x_{2n} & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{bmatrix} = \mathbf{0}$$

Now, according to Newton, this is a consistent linear system. The equation for the ellipse is exactly correct and all we need is six (x_1, x_2) sets of measurements to know the orbit of Ceres exactly.

What could go wrong? :)

Obviously, there may be measurement errors in Piazzi's observations. If we just solve the system using six measurements, we will probably get incorrect values for the coefficients $a_1, \ldots, a_6$.

A better idea is to use all of the n measurement data available, and try to find a way to cancel out errors.

So, using all the n data measurements available, we construct a linear system:

$$X\mathbf{a} = \mathbf{b}$$

where X is $n \times 6$ and $\mathbf{b} \in \mathbb{R}^n$.

But now, due to measurement errors, we can't expect $\mathbf{b}$ will lie in the column space of X. We have an incosistent system.

This system has **no solutions!**

What can we do if $A\mathbf{x} = \mathbf{b}$ has **no solutions?**

We now understand if A is $m \times n$ and $A\mathbf{x} = \mathbf{b}$ has no solutions, that is because the columns of A do not span $\mathbb{R}^m$, and $\mathbf{b}$ is not in the column space of A.

In many cases we will be quite satisfied to find an $\mathbf{x}$ that makes $A\mathbf{x}$ as close as possible to $\mathbf{b}$.

In other words, we are looking for an $\mathbf{x}$ such that $A\mathbf{x}$ makes a good **approximation** to $\mathbf{b}$.

We can think of the quality of the approximation of $A\mathbf{x}$ to $\mathbf{b}$ as the distance from $A\mathbf{x}$ to $\mathbf{b}$, which is

$$\|A\mathbf{x} - \mathbf{b}\|.$$

The **general least-squares problem** is to find an $\mathbf{x}$ that makes $\|A\mathbf{x} - \mathbf{b}\|$ as small as possible.

This is called "least squares" because it is equivalent to minimizing $\|A\mathbf{x} - \mathbf{b}\|^2$, which is the sum of squared differences.

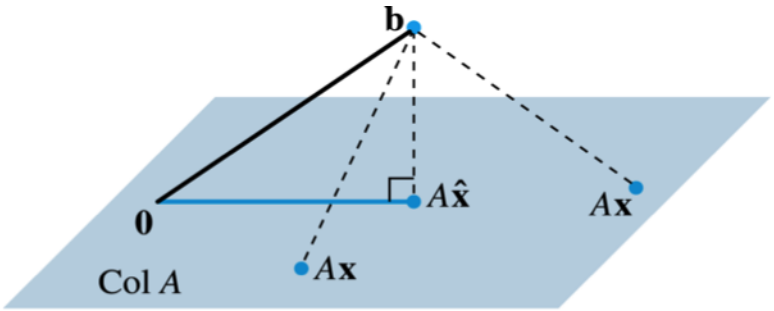
Definition. If A is $m \times n$ and $\mathbf{b}$ is in $\mathbb{R}^m$, a **least squares solution** of $A\mathbf{x} = \mathbf{b}$ is an $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ such that

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

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

The point to remember at all times is that no matter what $\mathbf{x}$ is, $A\mathbf{x}$ will be in the column space of A, Col A.

So $\mathbf{b}$ is outside Col A, and we are looking for $\mathbf{x}$ that specifies the closest point in Col A to $\mathbf{b}$.



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

Solving the General Least Squares Problem.

The last two lectures developed methods for finding the point in a subspace that is closest to a given point.

We know that the closest point to $\mathbf{b}$ in a subspace W is the **projection** of $\mathbf{b}$ onto W.

So the point we are looking for, $\hat{\mathbf{b}}$, is:

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

The key is that $\hat{\mathbf{b}}$ **is** in the column space of A. So this equation is consistent, and we can solve it:

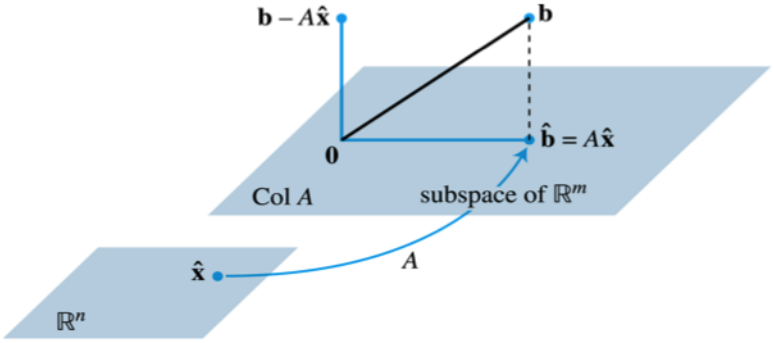
$$A\hat{\mathbf{x}} = \hat{\mathbf{b}}.$$

Since $\hat{\mathbf{b}}$ is the closest point in Col A to $\mathbf{b}$, a vector $\mathbf{x}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $\hat{\mathbf{x}}$ satisfies $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.

In other words, $\hat{\mathbf{x}}$ are the coordinates of $\hat{\mathbf{b}}$ in the basis given by the columns of A – it is the list of weights that will build $\hat{\mathbf{b}}$ out of the columns of A.

Note: we know that $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$ is consistent (by definition), so there exists at least one solution. However note that if A has free variables (the columns of A are not independent) then there would be many solutions of $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.

Here is another picture of what we are doing:



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

Now let's look at a specific case.

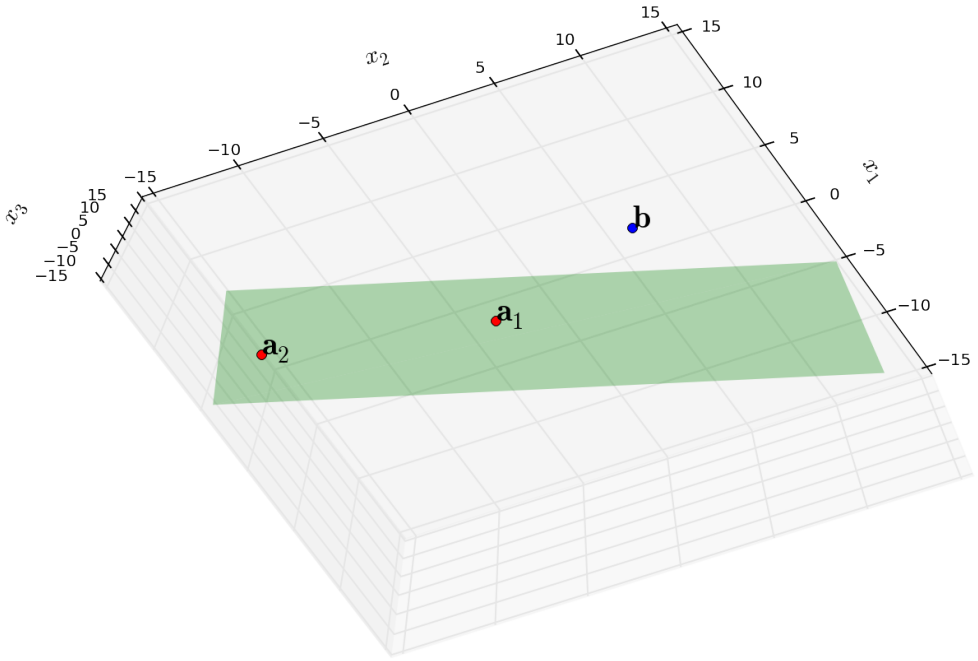
Say that

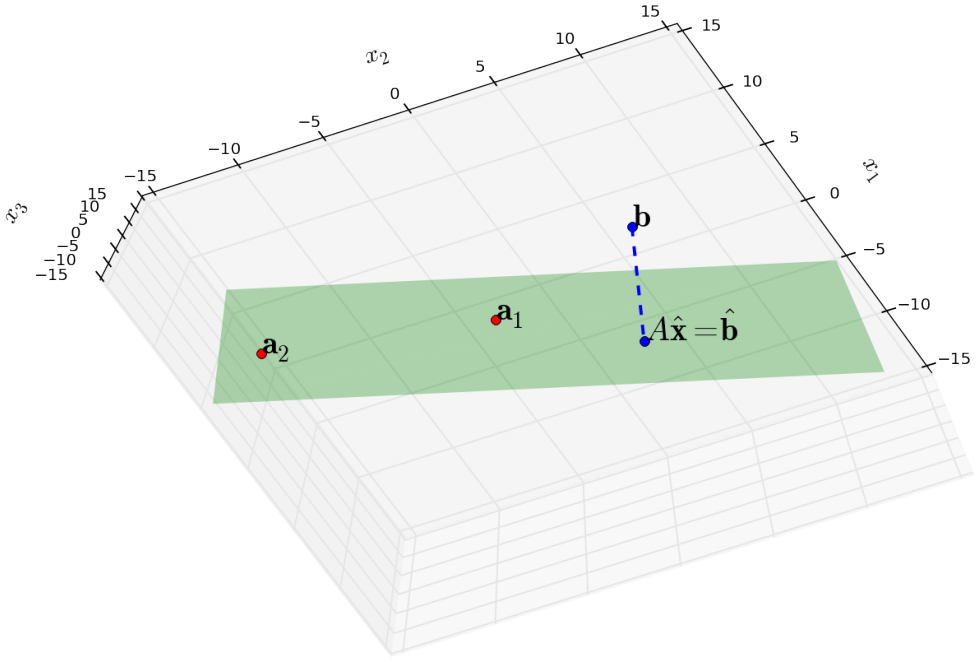
$$A = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \end{bmatrix} = \begin{bmatrix} 1 & 5 \\ -2 & -13 \\ 3 & -3 \end{bmatrix}$$

and

$$\mathbf{b} = \begin{bmatrix} 6 \\ 8 \\ -5 \end{bmatrix}$$

We have two columns $\mathbf{a}_1$ and $\mathbf{a}_2$ so the do not span $\mathbb{R}^3$. So $\mathbf{b}$ may not lie in Col A, and indeed it does not:


x_2
x_3
x_1
$\mathbf{b}$
$\mathbf{a}_1$
$\mathbf{a}_2$


x_2
x_3
x_1
$\mathbf{b}$
$\mathbf{a}_1$
$\mathbf{a}_2$
$A\hat{\mathbf{x}} = \hat{\mathbf{b}}$

OK, how are we going to find this projection $\hat{\mathbf{b}}$?

Here is the key idea: we know that the projection $\hat{\mathbf{b}}$ has the property that $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to Col A.

Suppose $\hat{\mathbf{b}}$ is $\text{proj}_{\text{Col } A}\mathbf{b}$, and that $\hat{\mathbf{x}}$ satisfies $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.

So $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to each column of A.

If $\mathbf{a}_j$ is any column of A, then

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

Now, each $\mathbf{a}_j^T$ is a row of A^T. We can collect all of the equations for all the $\mathbf{a}_j$ as:

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

So

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

So

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

Looking at this, we see that $A^T\mathbf{b}$ is a vector, and A^TA is a matrix, so this is a standard linear system.

This linear system is called the **normal equations** for $A\mathbf{x} = \mathbf{b}$.

It's solution is usually denoted $\hat{\mathbf{x}}$.

Theorem The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.

Proof.

(1) The set of solutions is nonempty. The matrix on the left has the same column space as A^T and the vector on the right is a vector in A^T.

And, by the arguments above, any least-squares solution of $A\mathbf{x} = \mathbf{b}$ must satisfy the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.

(2) Now let's show that any solution of $A^TA\mathbf{x} = A^T\mathbf{b}$ is a least squares solution of $A\mathbf{x} = \mathbf{b}$.

If $\hat{\mathbf{x}}$ satisfies $A^TA\mathbf{x} = A^T\mathbf{b}$, then $A^T(A\hat{\mathbf{x}} - \mathbf{b}) = \mathbf{0}$,

which shows that $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to the rows of A^T, and so is orthogonal to the columns of A.

So the vector $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to Col A.

So the equation

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

is a decomposition of $\mathbf{b}$ into the sum of a vector in Col A and a vector orthogonal to Col A.

Since the orthogonal decomposition is unique, $A\hat{\mathbf{x}}$ must tbe the orthogonal projection of $\mathbf{b}$ onto the column space of A.

So $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$ and $\hat{\mathbf{x}}$ is a least-squares solution.

Example. Find the least squares solution of the inconsistent system $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}.$$

Solution.

We will use the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.

$$A^TA = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$$

$$A^T\mathbf{b} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

So the normal equations are:

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

We can solve this using row operations, or by inverting A^TA.

$$(A^TA)^{-1} = \frac{1}{84} \begin{bmatrix} 5 & -1 \\ -1 & 17 \end{bmatrix}$$

And we can then solve $A^TA\mathbf{x} = A^T\mathbf{b}$ as

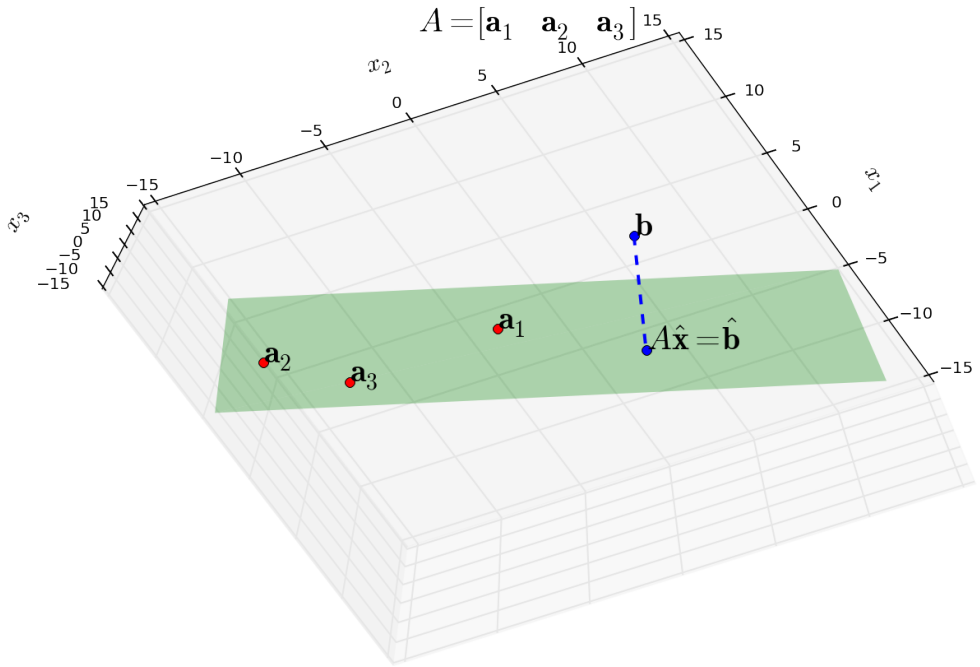
$$\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b}$$

$$= \frac{1}{84} \begin{bmatrix} 5 & -1 \\ -1 & 17 \end{bmatrix} \begin{bmatrix} 19 \\ 11 \end{bmatrix} = \frac{1}{84} \begin{bmatrix} 84 \\ 168 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

So we conclude that $\hat{\mathbf{x}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ is the vector that minimizes $\|A\mathbf{x} - \mathbf{b}\|$.

When there are multiple solutions.

We have seen that the normal equations always have a solution. Is there always a unique solution?
No, there can be multiple solutions that **all** minimize $\|A\mathbf{x} - \mathbf{b}\|$.
Let's remind ourselves of what is going on when a linear system has multiple solutions.
We know that a linear system has multiple solutions when there are columns that are not pivot columns.
Equivalently, whern there are multiple solutions the columns of A are linearly dependent.
Here is a picture of what is going on:



Example.
Find a least-squares solution for $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1 \end{bmatrix}.$$

Solution. Compute

$$A^TA = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{bmatrix}$$

$$A^T\mathbf{b} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} -3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ -4 \\ 2 \\ 6 \end{bmatrix}$$

To solve $A^TA\mathbf{x} = A^T\mathbf{b}$, we'll use row reduction. The augmented matrix $[A^TA\ A^T\mathbf{b}]$ is:

$$\begin{bmatrix} 6 & 2 & 2 & 2 & 4 \\ 2 & 2 & 0 & 0 & -4 \\ 2 & 0 & 2 & 0 & 2 \\ 2 & 0 & 0 & 2 & 6 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & 1 & 3 \\ 0 & 1 & 0 & -1 & -5 \\ 0 & 0 & 1 & -1 & -2 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Since there is a row of zeros, we know the columns of A^TA are linearly dependent. This occurs because the columns of A are linearly dependent.

The general solution is $x_1 = 3 - x_4$, $x_2 = -5 + x_4$, $x_3 = -2 + x_4$, and x_4 is free.

So the general least-squares solution of $A\mathbf{x} = \mathbf{b}$ has the form

$$\hat{\mathbf{x}} = \begin{bmatrix} 3 \\ -5 \\ -2 \\ 0 \end{bmatrix} + x_4 \begin{bmatrix} -1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Keep in mind that the orthogonal projection $\hat{\mathbf{b}}$ is always unique.

The reason that there are multiple solutions to this least squares problem is that there are **multiple ways** to construct $\hat{\mathbf{b}}$.

The reason that there are multiple ways to construct $\hat{\mathbf{b}}$ is that the columns of A are linearly dependent, so **any** vector in the column space of A can be constructed in multiple ways.

Here is a theorem that allows use to identify when there are multiple least-squares solutions.

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

1. The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each $\mathbf{b}$ in $\mathbb{R}^m$.
2. The columns of A are linearly independent.
3. The matrix A^TA is invertible.

When these statements are true, the least-squares solution $\hat{\mathbf{x}}$ is given by:

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

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

Finding $\hat{\mathbf{b}}$ directly.
When $A^T A$ is invertible, and $\hat{\mathbf{b}}$ is unique, we can put together the two equations

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

and

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

to get:

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

Let's stop and look at this another way. Up until now we have seen how to project a point onto a line, or on to a subspace with an orthogonal basis.

Now here is a formula for projection onto a subspace space given an **arbitrary** basis. This is a general formula that can be very useful.