Least squares solution

So far we've spent a lot of time trying to figure out solutions to $A\vec{x}=\vec{b}$. We're given the matrix A, we're given the vector $\vec{b}$, and we're trying to find any and all $\vec{x}$ that satisfy $A\vec{x}=\vec{b}$.

When $\vec{b}$ is in the column space of A, then there's a solution to $A\vec{x}=\vec{b}$. Because if $\vec{b}$ is in the column space of A, that means $\vec{b}$ can be made from a linear combination of the columns of A. The components of the solution $\vec{x}$ simply tell us how many of each of A's columns to use in the combination in order to get $\vec{b}$.

So, when $\vec{b}$ isn't in the column space of A, that means there's no linear combination of A's columns that can be used to get $\vec{b}$, which means there's no solution $\vec{x}$ that solves $A\vec{x}=\vec{b}$.

The least square solution

When there's no solution to $A\vec{x}=\vec{b}$, we're still interested in the next best thing. In general, we're interested in how close we can get to a solution, even when there isn't one.

The least squares solution of the matrix equation $A\vec{x}=\vec{b}$ is a vector $\vec{x}^*$ in $\mathbb{R}^n$, such that $A\vec{x}^*$ is as "close" to $\vec{b}$ as possible. By "close," we mean that we're minimizing the distance between $A\vec{x}^*$ and $\vec{b}$. In other words, $\vec{x}^*$ will tell us the combination of A's columns that we can use to get as close as possible to $\vec{b}$. The solution $\vec{x}^*$ will satisfy

$$A^TA\vec{x}^* = A^T\vec{b}$$

So to find the least squares solution, we need to find A^TA and $A^T\vec{b}$, and then solve for $\vec{x}^*$.

The reason we're talking about the least squares solution now is because this concept is directly related to what we just learned about the projection of a vector onto a subspace.

Think about the column space $C(A)$ as a subspace, maybe a plane. When there's a solution to $A\vec{x} = \vec{b}$, it means $\vec{b}$ is in the column space, so it's on the plane. But if there's no solution to $A\vec{x} = \vec{b}$, that means $\vec{b}$ sticks up out of the plane, and the closest $\vec{x}^*$ that we can find to $\vec{b}$ is the projection of $\vec{b}$ into the plane, or the projection of $\vec{b}$ onto the subspace.

So when we're solving for $\vec{x}^*$, we're really solving for the projection of $\vec{b}$ onto the column space $C(A)$, $\text{Proj}_{C(A)}\vec{b}$, which is as close as we can get to $\vec{b}$, even when $\vec{b}$ is not in the column space of A.

Let's do an example to see how this works.

Example

Find the least squares solution to the system.

$$x - y = 3$$

$$2x + y = 1$$

$$-x - 4y = 2$$

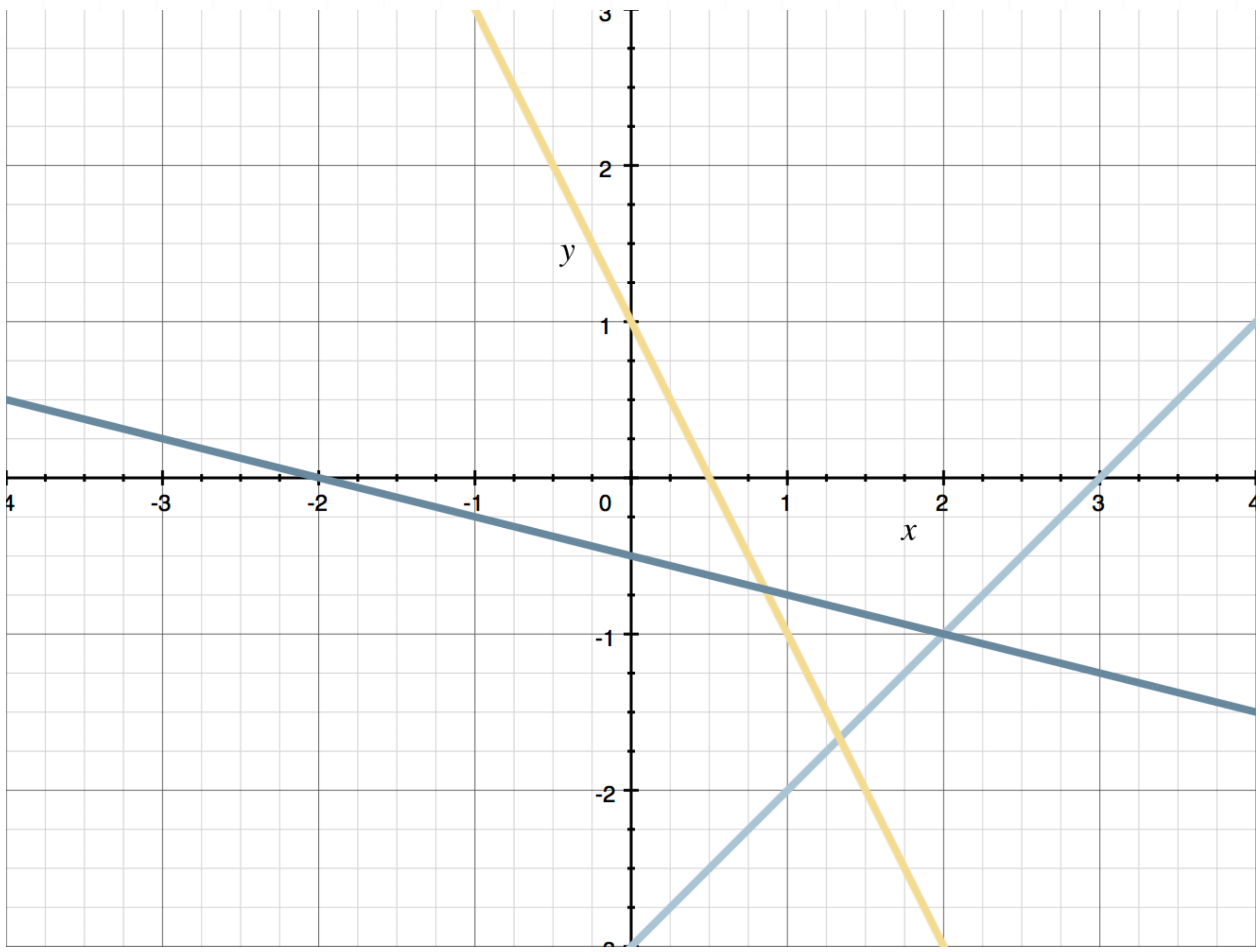
First, let's graph each line to confirm that the system does not have a solution. If we put each line in slope-intercept form,

$$y = x - 3$$

$$y = -2x + 1$$

$$y = -\frac{1}{4}x - \frac{1}{2}$$

then the graph of all three is



While there are three points at which two of the lines intersect one another, there's no single point where all three lines intersect, which means there's no solution to

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

$$\begin{bmatrix} 1 & -1 \\ 2 & 1 \\ -1 & -4 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}$$

In other words, $\vec{b} = (3,1,2)$ is not in the column space of A, and there's no vector $\vec{x} = (x, y)$ you can find that will make that equation true.

The next best thing we can do is find the point which minimizes the squared distances. By building the matrix equation, we've already found

$$A = \begin{bmatrix} 1 & -1 \\ 2 & 1 \\ -1 & -4 \end{bmatrix}$$

Now we'll find A^T.

$$A^T = \begin{bmatrix} 1 & 2 & -1 \\ -1 & 1 & -4 \end{bmatrix}$$

Then A^TA is

$$A^TA = \begin{bmatrix} 1 & 2 & -1 \\ -1 & 1 & -4 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 2 & 1 \\ -1 & -4 \end{bmatrix}$$

$$A^TA = \begin{bmatrix} 1(1) + 2(2) - 1(-1) & 1(-1) + 2(1) - 1(-4) \\ -1(1) + 1(2) - 4(-1) & -1(-1) + 1(1) - 4(-4) \end{bmatrix}$$

$$A^TA = \begin{bmatrix} 1 + 4 + 1 & -1 + 2 + 4 \\ -1 + 2 + 4 & 1 + 1 + 16 \end{bmatrix}$$

$$A^TA = \begin{bmatrix} 6 & 5 \\ 5 & 18 \end{bmatrix}$$

And $A^T\vec{b}$ is

$$A^T\vec{b}=\begin{bmatrix}1 & 2 & -1\\ -1 & 1 & -4\end{bmatrix}\begin{bmatrix}3\\ 1\\ 2\end{bmatrix}$$

$$A^T\vec{b}=\begin{bmatrix}1(3)+2(1)-1(2)\\ -1(3)+1(1)-4(2)\end{bmatrix}$$

$$A^T\vec{b}=\begin{bmatrix}3+2-2\\ -3+1-8\end{bmatrix}$$

$$A^T\vec{b}=\begin{bmatrix}3\\ -10\end{bmatrix}$$

Then we get

$$A^TA\vec{x}^*=A^T\vec{b}$$

$$\begin{bmatrix}6 & 5\\ 5 & 18\end{bmatrix}\vec{x}^*=\begin{bmatrix}3\\ -10\end{bmatrix}$$

Then to find $\vec{x}^*$, we'll put the augmented matrix into reduced row-echelon form.

$$\begin{bmatrix}6 & 5 & | & 3\\ 5 & 18 & | & -10\end{bmatrix}$$

$$\begin{bmatrix}1 & \frac{5}{6} & | & \frac{1}{2}\\ 5 & 18 & | & -10\end{bmatrix}$$

$$\begin{bmatrix}1 & \frac{5}{6} & | & \frac{1}{2}\\ 0 & \frac{83}{6} & | & -\frac{25}{2}\end{bmatrix}$$

$$\begin{bmatrix} 1 & \frac{5}{6} & | & \frac{1}{2} \\ 0 & 1 & | & -\frac{75}{83} \end{bmatrix}$$

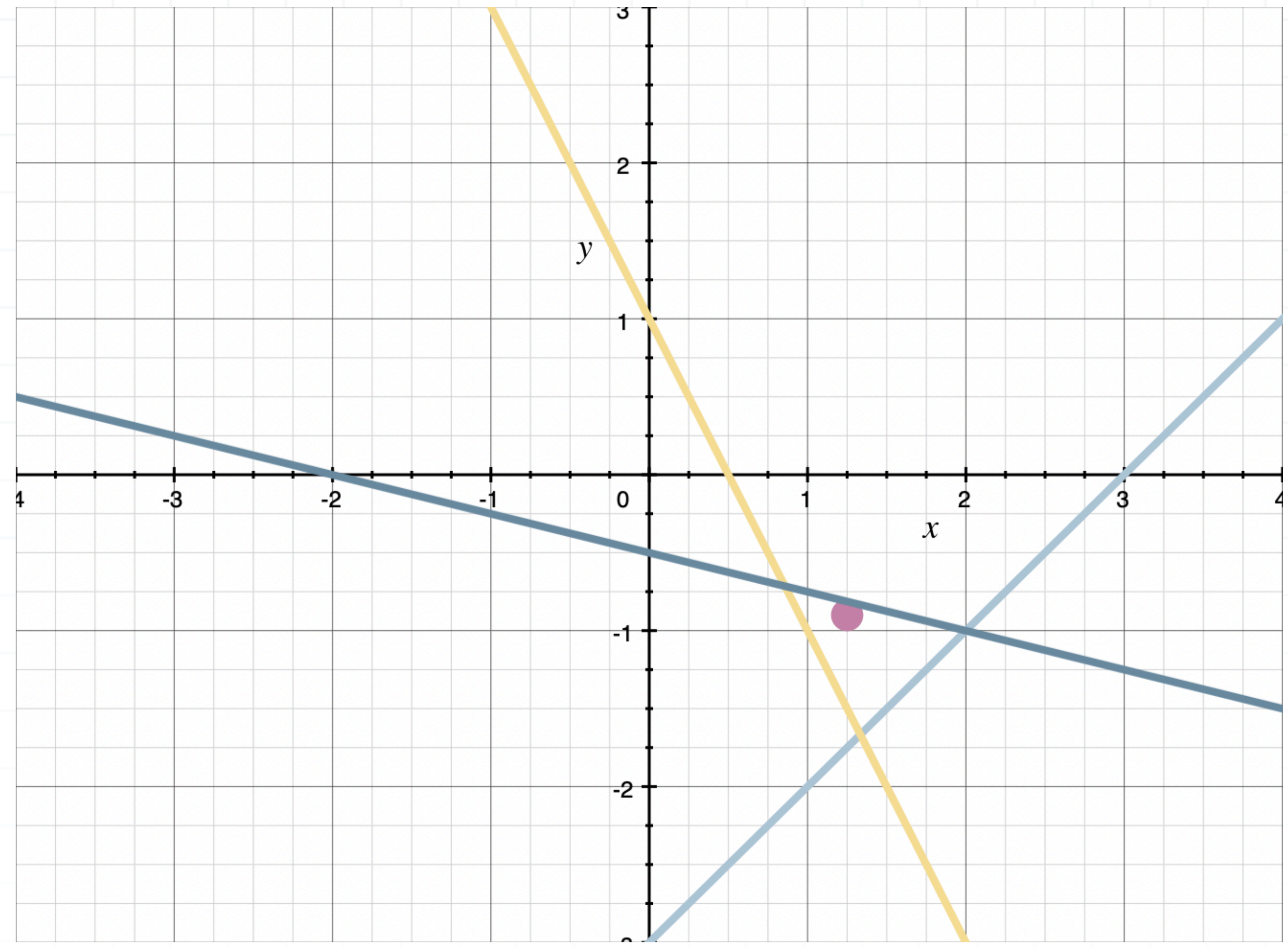
$$\begin{bmatrix} 1 & 0 & | & \frac{104}{83} \\ 0 & 1 & | & -\frac{75}{83} \end{bmatrix}$$

Then the least squares solution is given by the augmented matrix as

$$\vec{x}^* = \left(\frac{104}{83}, -\frac{75}{83}\right)$$

$$\vec{x}^* \approx (1.25, -0.90)$$

If we graph this solution, alongside the lines we sketched earlier, we can see that the solution is inside the triangle created by the points of intersection of the system.



y
x
3
2
1
0
-1
-2
-4
-3
-2
-1
1
2
3
4