Projection matrices and least squares

Projections

Last lecture, we learned that $P = A(A^TA)^{-1}A^T$ is the matrix that projects a vector $\mathbf{b}$ onto the space spanned by the columns of A. If $\mathbf{b}$ is perpendicular to the column space, then it's in the left nullspace $N(A^T)$ of A and $P\mathbf{b} = \mathbf{0}$. If $\mathbf{b}$ is in the column space then $\mathbf{b} = A\mathbf{x}$ for some $\mathbf{x}$, and $P\mathbf{b} = \mathbf{b}$.

A typical vector will have a component $\mathbf{p}$ in the column space and a component $\mathbf{e}$ perpendicular to the column space (in the left nullspace); its projection is just the component in the column space.

The matrix projecting $\mathbf{b}$ onto $N(A^T)$ is $I - P$:

$$\begin{aligned} \mathbf{e} &= \mathbf{b} - \mathbf{p} \\ \mathbf{e} &= (I - P)\mathbf{b}. \end{aligned}$$

Naturally, $I - P$ has all the properties of a projection matrix.

Least squares

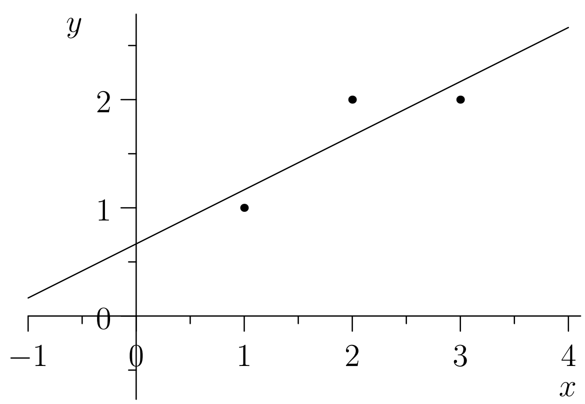

Figure 1: Three points and a line close to them.

We want to find the closest line $b = C + Dt$ to the points $(1, 1)$, $(2, 2)$, and $(3, 2)$. The process we're going to use is called *linear regression*; this technique is most useful if none of the data points are *outliers*.

By "closest" line we mean one that minimizes the error represented by the distance from the points to the line. We measure that error by adding up the squares of these distances. In other words, we want to minimize $||A\mathbf{x} - \mathbf{b}||^2 = ||\mathbf{e}||^2$.

If the line went through all three points, we'd have:

$$\begin{aligned} C+D &= 1 \\ C+2D &= 2 \\ C+3D &= 2, \end{aligned}$$

but this system is unsolvable. It's equivalent to $A\mathbf{x} = \mathbf{b}$, where:

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}, \mathbf{x} = \begin{bmatrix} C \\ D \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}.$$

There are two ways of viewing this. In the space of the line we're trying to find, e_1, e_2 and e_3 are the vertical distances from the data points to the line. The components p_1, p_2 and p_3 are the values of $C + Dt$ near each data point; $\mathbf{p} \approx \mathbf{b}$.

In the other view we have a vector $\mathbf{b}$ in $\mathbb{R}^3$, its projection $\mathbf{p}$ onto the column space of A, and its projection $\mathbf{e}$ onto $N(A^T)$.

We will now find $\hat{\mathbf{x}} = \begin{bmatrix} \hat{C} \\ \hat{D} \end{bmatrix}$ and $\mathbf{p}$. We know:

$$\begin{aligned} A^T A\hat{\mathbf{x}} &= A^T\mathbf{b} \\ \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix} \begin{bmatrix} \hat{C} \\ \hat{D} \end{bmatrix} &= \begin{bmatrix} 5 \\ 11 \end{bmatrix}. \end{aligned}$$

From this we get the *normal equations*:

$$\begin{aligned} 3\hat{C} + 6\hat{D} &= 5 \\ 6\hat{C} + 14\hat{D} &= 11. \end{aligned}$$

We solve these to find $\hat{D} = 1/2$ and $\hat{C} = 2/3$.

We could also have used calculus to find the minimum of the following function of two variables:

$$e_1^2 + e_2^2 + e_3^2 = (C + D - 1)^2 + (C + 2D - 2)^2 + (C + 3D - 2)^2.$$

Either way, we end up solving a system of linear equations to find that the closest line to our points is $b = \frac{2}{3} + \frac{1}{2}t$.

This gives us:

i	p_i	e_i
1	$7/6$	$-1/6$
2	$5/3$	$1/3$
3	$13/6$	$-1/6$

or $\mathbf{p} = \begin{bmatrix} 7/6 \\ 5/3 \\ 13/6 \end{bmatrix}$ and $\mathbf{e} = \begin{bmatrix} -1/6 \\ 2/6 \\ -1/6 \end{bmatrix}$. Note that $\mathbf{p}$ and $\mathbf{e}$ are orthogonal, and also that $\mathbf{e}$ is perpendicular to the columns of A.

The matrix $A^T A$

We've been assuming that the matrix $A^T A$ is invertible. Is this justified?

If A has independent columns, then $A^T A$ is invertible.

To prove this we assume that $A^T A\mathbf{x} = \mathbf{0}$, then show that it must be true that $\mathbf{x} = \mathbf{0}$:

$$\begin{aligned} A^T A\mathbf{x} &= \mathbf{0} \\ \mathbf{x}^T A^T A\mathbf{x} &= \mathbf{x}^T\mathbf{0} \\ (A\mathbf{x})^T (A\mathbf{x}) &= \mathbf{0} \\ A\mathbf{x} &= \mathbf{0}. \end{aligned}$$

Since A has independent columns, $A\mathbf{x} = \mathbf{0}$ only when $\mathbf{x} = \mathbf{0}$.

As long as the columns of A are independent, we can use linear regression to find approximate solutions to unsolvable systems of linear equations. The columns of A are guaranteed to be independent if they are *orthonormal*, i.e. if they are perpendicular unit vectors like $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$, or like $\begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}$ and $\begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}$.

Exercises on projection matrices and least squares

Problem 16.1: (4.3 #17. *Introduction to Linear Algebra:* Strang) Write down three equations for the line $b = C + Dt$ to go through $b = 7$ at $t = -1$, $b = 7$ at $t = 1$, and $b = 21$ at $t = 2$. Find the least squares solution $\hat{\mathbf{x}} = (C, D)$ and draw the closest line.

Problem 16.2: (4.3 #18.) Find the projection $\mathbf{p} = A\hat{\mathbf{x}}$ in the previous problem. This gives the three heights of the closest line. Show that the error vector is $\mathbf{e} = (2, -6, 4)$. Why is $P\mathbf{e} = \mathbf{0}$?

Problem 16.3: (4.3 #19.) Suppose the measurements at $t = -1, 1, 2$ are the errors 2, -6, 4 in the previous problem. Compute $\hat{\mathbf{x}}$ and the closest line to these new measurements. Explain the answer: $\mathbf{b} = (2, -6, 4)$ is perpendicular to __________ so the projection is $\mathbf{p} = \mathbf{0}$.

Problem 16.4: (4.3 #20.) Suppose the measurements at $t = -1, 1, 2$ are $\mathbf{b} = (5, 13, 17)$. Compute $\hat{\mathbf{x}}$ and the closest line and $\mathbf{e}$. The error is $\mathbf{e} = \mathbf{0}$ because this $\mathbf{b}$ is __________.

Problem 16.5: (4.3 #21.) Which of the four subspaces contains the error vector $\mathbf{e}$? Which contains $\mathbf{p}$? Which contains $\hat{\mathbf{x}}$? What is the nullspace of A?

Problem 16.6: (4.3 #22.) Find the best line $C + Dt$ to fit $b = 4, 2, -1, 0, 0$ at times $t = -2, -1, 0, 1, 2$.

Exercises on projection matrices and least squares

Problem 16.1: (4.3 #17. *Introduction to Linear Algebra:* Strang) Write down three equations for the line $b = C + Dt$ to go through $b = 7$ at $t = -1$, $b = 7$ at $t = 1$, and $b = 21$ at $t = 2$. Find the least squares solution $\hat{\mathbf{x}} = (C, D)$ and draw the closest line.

Solution: $\begin{bmatrix} 1 & -1 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 7 \\ 7 \\ 21 \end{bmatrix}.$

The solution $\hat{\mathbf{x}} = \begin{bmatrix} \mathbf{9} \\ \mathbf{4} \end{bmatrix}$ comes from $\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 35 \\ 42 \end{bmatrix}.$

Problem 16.2: (4.3 #18.) Find the projection $\mathbf{p} = A\hat{\mathbf{x}}$ in the previous problem. This gives the three heights of the closest line. Show that the error vector is $\mathbf{e} = (2, -6, 4)$. Why is $P\mathbf{e} = \mathbf{0}$?

Solution: $\mathbf{p} = A\hat{\mathbf{x}} = (5, 13, 17)$ gives the heights of the closest line. The error is $\mathbf{b} - \mathbf{p} = (2, -6, 4)$. This error $\mathbf{e}$ has $P\mathbf{e} = P\mathbf{b} - P\mathbf{p} = \mathbf{p} - \mathbf{p} = \mathbf{0}$.

Problem 16.3: (4.3 #19.) Suppose the measurements at $t = -1, 1, 2$ are the errors 2, -6, 4 in the previous problem. Compute $\hat{\mathbf{x}}$ and the closest line to these new measurements. Explain the answer: $\mathbf{b} = (2, -6, 4)$ is perpendicular to __________ so the projection is $\mathbf{p} = \mathbf{0}$.

Solution: If $\mathbf{b} =$ error $\mathbf{e}$ then $\mathbf{b}$ is perpendicular to the column space of A. Projection $\mathbf{p} = \mathbf{0}$.

Problem 16.4: (4.3 #20.) Suppose the measurements at $t = -1, 1, 2$ are $\mathbf{b} = (5, 13, 17)$. Compute $\hat{\mathbf{x}}$ and the closest line and $\mathbf{e}$. The error is $\mathbf{e} = \mathbf{0}$ because this $\mathbf{b}$ is __________.

Solution: If $\mathbf{b} = A\hat{\mathbf{x}} = (5, 13, 17)$ then $\hat{\mathbf{x}} = (9, 4)$ and $\mathbf{e} = \mathbf{0}$ since $\mathbf{b}$ is *in the column space of* A.

Problem 16.5: (4.3 #21.) Which of the four subspaces contains the error vector $\mathbf{e}$? Which contains $\mathbf{p}$? Which contains $\hat{\mathbf{x}}$? What is the nullspace of A?

Solution: $\mathbf{e}$ is in $\mathbf{N}(A^T)$; $\mathbf{p}$ is in $\mathbf{C}(A)$; $\hat{\mathbf{x}}$ is in $\mathbf{C}(A^T)$; $\mathbf{N}(A) = \{\mathbf{0}\}$ = zero vector only.

Problem 16.6: (4.3 #22.) Find the best line $C + Dt$ to fit $b = 4, 2, -1, 0, 0$ at times $t = -2, -1, 0, 1, 2$.

Solution: The least squares equation is $\begin{bmatrix} 5 & \mathbf{0} \\ \mathbf{0} & 10 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 5 \\ -10 \end{bmatrix}$.
Solution: $C = 1$, $D = -1$. Line $1 - t$. Symmetric t's $\Rightarrow$ diagonal $A^T A$