Lecture 05
Geometry of Least Squares

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STAT 312/612

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Goals for today

1. Geometry of least squares
2. Projection matrix P and annihilator matrix M
3. Application to

Geometry of Least Squares

Last time, we established that the least squares solution to the model:

$$y = X\beta + \epsilon$$

Yields the solution:

$$\widehat{\beta} = (X^t X)^{-1} X^t y$$

As long as the matrix $X^t X$ is invertable.

Define the column space of the matrix X as:

$$\mathcal{R}(X) = \{\theta : \theta = X\beta,\ \beta \in \mathbb{R}^p\} \subset \mathbb{R}^n$$

This is the space spanned by the p columns on X sitting in n-dimensional space.

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Notice that the least squares problem can be re-written as:

$$\widehat{\theta} = \arg\min_{\theta} \left\{ ||y - \theta||_2^2, \quad \text{s.t} \quad \theta = X\beta \right\}$$

Where $\widehat{\beta} = X\widehat{\theta}$.

Theorem 3.2 (p.g. 37, Rao & Toutenburg) The minimum, $\widehat{\theta}$ is attained when $(y - \widehat{\theta}) \perp \mathcal{R}(X)$. In other words, $(y - \widehat{\theta})$ is perpendicular to all vectors in $\mathcal{R}$.

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$$||y - \theta||^2 \quad = \quad (y - \widehat{\theta} + \widehat{\theta} - \theta)^t(y - \widehat{\theta} + \widehat{\theta} - \theta)$$

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||y - \theta||^2 &= (y - \widehat{\theta} + \widehat{\theta} - \theta)^t(y - \widehat{\theta} + \widehat{\theta} - \theta) \\
&= (y - \widehat{\theta})^t(y - \widehat{\theta}) + (\widehat{\theta} - \theta)^t(\widehat{\theta} - \theta) + 2(y - \widehat{\theta})^t(\widehat{\theta} - \theta)
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So, if such a $\widehat{\theta}$ exists it attains the minimum. To see that it does, write $\widehat{\theta} = X\widehat{\beta}$. Then:

$$\begin{aligned} X^t(y - \widehat{\theta}) \quad &= X^t(y - X\widehat{\beta}) \\ &= X^t y - X^t X\widehat{\beta} \end{aligned}$$

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&= X^t y - X^t y \\
&= 0
\end{aligned}$$

And therefore our proposed $\widehat{\theta} \in \mathcal{R}(X)$.

From this geometric interpretation of the least squares estimator, we introduce an important matrix P_X called the *projection matrix*.

$$P_X = X(X^tX)^{-1}X^t$$

I'll often drop the subscript as it should be understood that the projection is on the data matrix X.

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Py &= X(X^tX)^{-1}X^tXy \\
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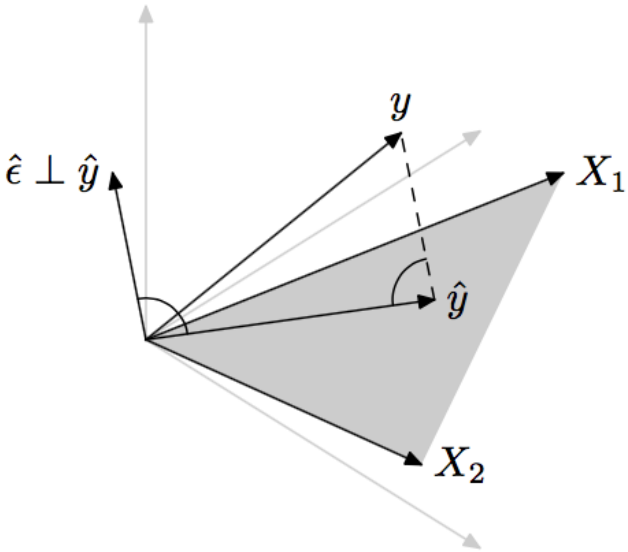
The projection matrix is sometimes called the *hat matrix*. Any thoughts as to why?



y
$\hat{\epsilon} \perp \hat{y}$
X_1
$\hat{y}$
X_2

A closely related matrix to P is the *annihilator matrix* M:

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$$M = I_n - P$$

It gets its name because $MX = 0$.

The matrix $P = X(X^tX)^{-1}X^t$ is clearly symettric. It is also idempotent:

$$\begin{aligned} P^2 &= X(X^tX)^{-1}X^tX(X^tX)^{-1}X^t \\ &= X(X^tX)^{-1}(X^tX)(X^tX)^{-1}X^t \\ &= X(X^tX)^{-1}X^t \\ &= P \end{aligned}$$

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These properties both make sense given the geometric interpretation of P and M as projections; into the column space of X and the compliment of the columns space of X.

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The matricies P and M not only help make the derivation easier, they also give geometric insight into what we are doing.

One particularly useful formula will be writing the squared residuals as:

$$\begin{aligned} ||r||_2^2 &= ||M\epsilon||_2^2 \\ &= \epsilon^t M^t M\epsilon \\ &= \epsilon^t M\epsilon \end{aligned}$$

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So the matrix M translates the sum of squared residuals into the sum of the square errors, which are estimated by the residuals.

Applications