Data, Environment and Society: Lecture 9: Intro to regression

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September 20, 2018

Announcements

Today

- Review bias-variance tradeoff
- Regression
  - K-nearest neighbors
  - Linear least squares

Reading

- Today's lecture draws from DS100 Ch10, ISLR Ch 2, ISLR Ch 3.1
- For next week
  - Read Alstone *et al* for next Tuesday – in class discussion
  - Review ISLR Ch 3.1-3.2

(review) Error or residual?

$y_i = f(x_i) + \epsilon_i$ the "true" model, if one exists.

$y_i = \hat{f}(x_i) + e_i$ the relationship between the data and the estimate.

(review) Error or residual?

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$$y_i = \hat{f}(x_i) + e_i \qquad \text{the relationship between the data and the estimate.}$$

So:

$$\epsilon_i \qquad \text{variation in } y \text{ that is uncorrelated with } x.$$
$$e_i = y_i - \hat{f}(x_i) \qquad \text{the “residual” between the data and the estimate.}$$

(Review) How to evaluate how well a model performs?

Generic term: the *Cost function.*

- Cost functions can be used to describe how much of the variation in the data can be captured by the model.
- Example: The mean squared error:

$$MSE = \frac{1}{n}((y_1 - \hat{y}_1)^2 + (y_2 - \hat{y}_2)^2 + \cdots + (y_n - \hat{y}_n)^2)$$

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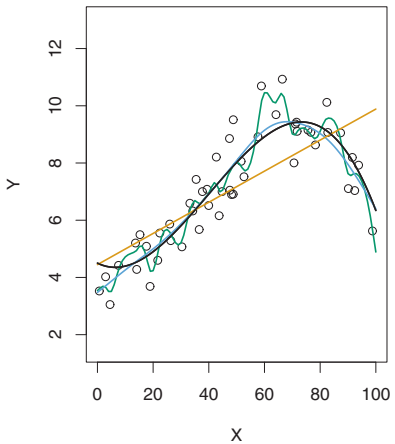
$$= \frac{1}{n}\sum_{i=1}^{n} e_i^2$$

(Review) A thought experiment from ISLR Ch 2

Suppose you have four different model forms to choose from. When you fit them to the data, you get this figure.

Which model should you choose?

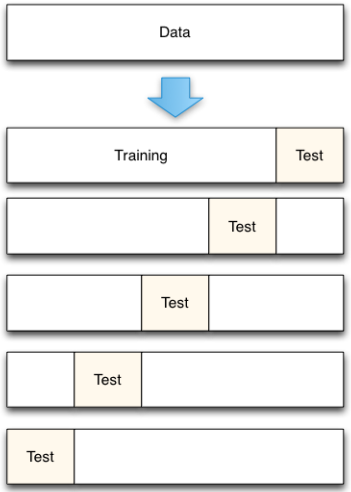
- The one that minimizes mean squared error?
- Careful! Doesn't the squiggly one minimize mean squared error?
- To do model selection we need to understand the concept of training and testing data.



(Review) Concept: Test and training data

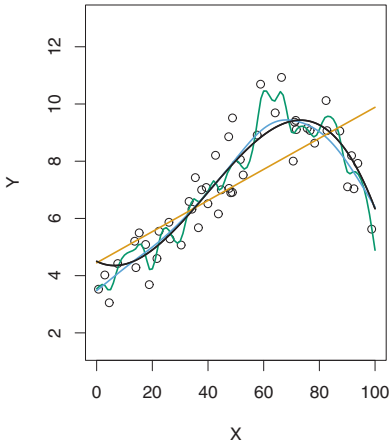
Choosing between different models can be done by partitioning your data in to “training” and “test” data.

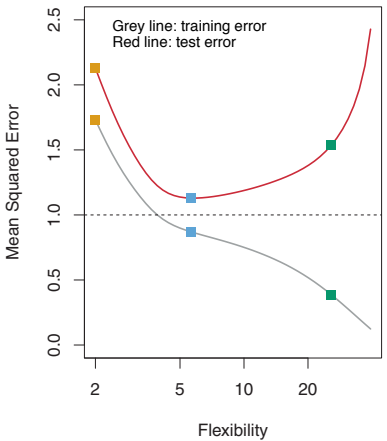
- “Training data”: The data we use to choose the parameters of an individual model.
- “Test data”: A set of data we withhold; it’s not for training. We use this data set to compare how different *models* perform relative to one another.



Source: kaggle.com

(Review) MSE for test and training data





What might a plot of MSE versus model "flexibility" look like?

Bias v. Variance

Bias:

- The propensity for a model to produce errors that are systematically high or low
- Bias can be positive in one range of the predictor and negative in another.

Variance

- The propensity for a model to make very different predictions if it is fit with two different training data sets that are sampled from the same population.

Total error can be decomposed:

$$\text{Avg } (y_0 - \hat{f}(x_0))^2 = \text{(variance in a prediction, across different training data)} + (\text{systematic bias})^2 + \text{(variance in } y \text{ that's uncorrelated with } x)$$

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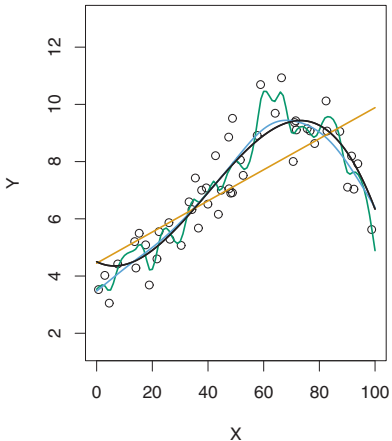
Bias v. Variance, ctd.



Which model has the greatest propensity for bias?

Which model has the greatest propensity for variance?

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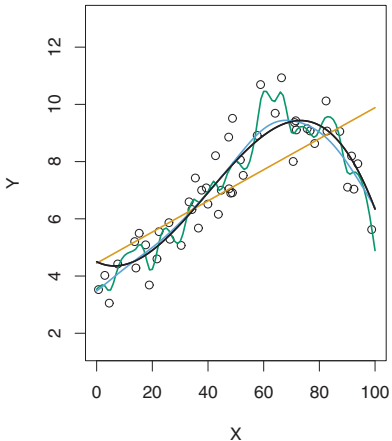

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- The linear one. In ranges of x, it systematically under- or over-estimates.

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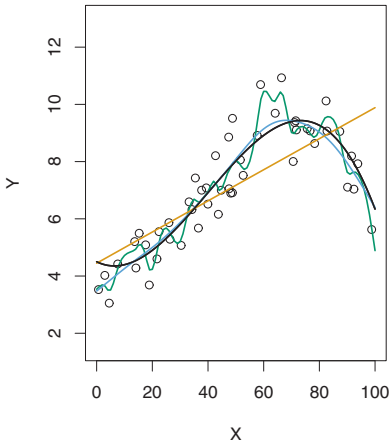

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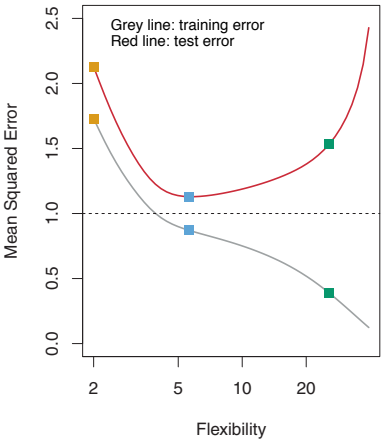
- The linear one. In ranges of x, it systematically under- or over-estimates.

Which model has the greatest propensity for variance?

- The squiggly one. If we drew another sample of data, we'd probably get very different squiggles.

Decomposing bias-variance



Take a moment to think about how bias and variance add up to make the red curve on the left. Try to draw bias and variance separately.

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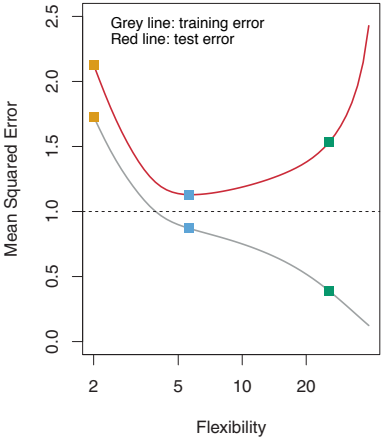

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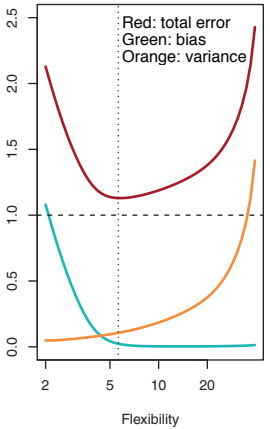

Parametric vs. non-parametric models

The model examples we discussed Tuesday were **parametric**, meaning they relate inputs to outputs with a mathematical function defined by parameters.

But **non-parametric** models are also possible.

- These don't use functions with coefficients
- Instead the data *become* the model

It's easiest to see this by example using the K-nearest neighbors algorithm.

K-nearest neighbors (KNN)

We'll work with just a one-dimensional independent variable. For example,

- y_i could be NOx emissions from a power plant,
- x_i could be its coal use;
- different i would correspond to different power plants in different years.

Definitions:

- First, define proximity between two points as $|x_i - x_j|$
- Next, define $\mathcal{N}_i$ as the set of K points closest to x_i

K-nearest neighbors

The basic idea behind using KNN for regression (i.e. predicting a continuous variable or set of variables) is simple:

$$\hat{y}_j = \frac{1}{K} \sum_{i \in \mathcal{N}_j} y_i$$

In other words, the prediction equals the average of the K nearest points.

If you're working with KNN, what is your most important decision?

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What is K?

Check of intuition: Would increasing K reduce or increase bias? **Increase!**

- Using a lower K would cause the estimates to more closely follow the underlying data.
- In the extreme, $K = 1$ would make the model equal the underlying data.
- At the other extreme, $K = n$ would make the model equal the sample mean.

Linear regression

Regression: A method to estimate the expected value of an output variable (y), *conditional* on one or more input values (x)

- KNN regression does this by averaging nearby values.
- Linear regression does this by fitting a linear function to the data.
- Broadly speaking, *regression* can be used for prediction.
- *Linear* regression specifically can also be used for inference.
- Many of the methods we'll work with later in the semester will be rooted in linear regression.

The basic model

- x_i: one dimensional independent variable
- y_i: one dimensional dependent variable

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 x_i + e_i$$
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

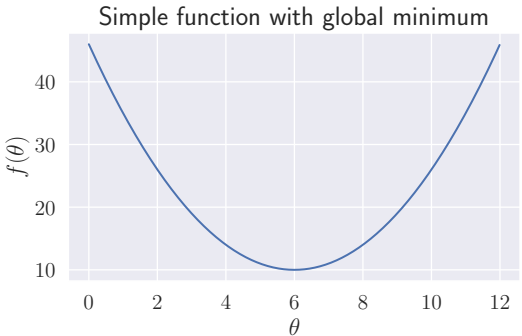
- We use the $\hat{}$ symbol to denote an estimate, or prediction

(extremely important) Side note: Optimality.

Define the "argument" that minimizes a function f with respect to θ as:

$$\theta^* = \arg\min_{\theta} f(\theta)$$

In the plot below, what's θ^*?



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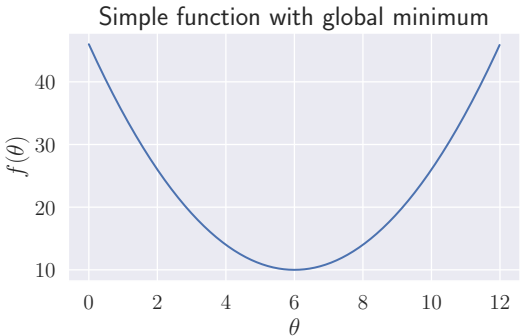

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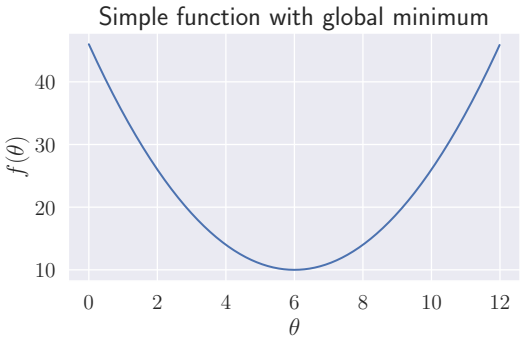

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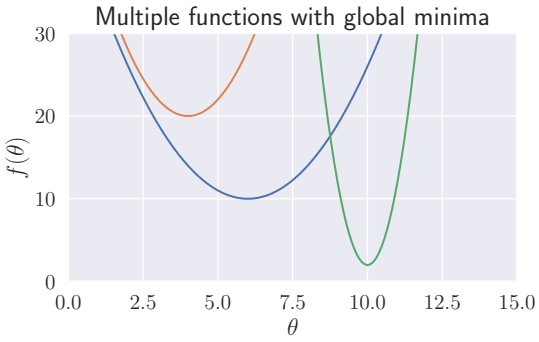
What do the minima share in common?



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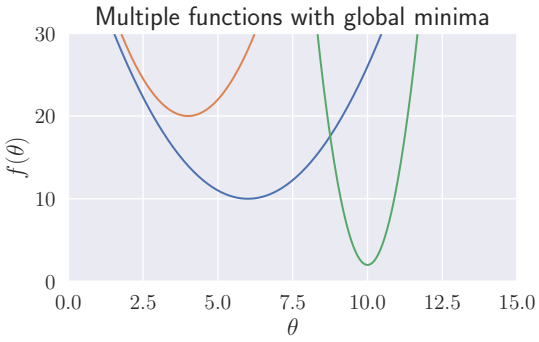
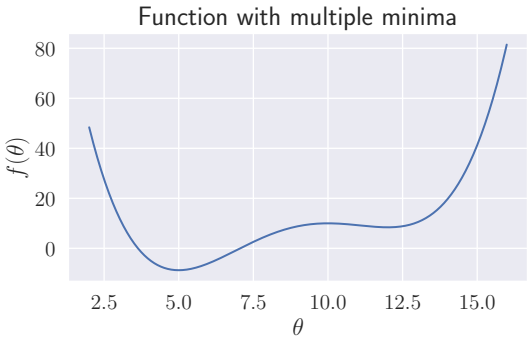


$$\left.\frac{\partial f(\theta)}{\partial \theta}\right|_{\theta^*} = 0$$

What's the challenge here?



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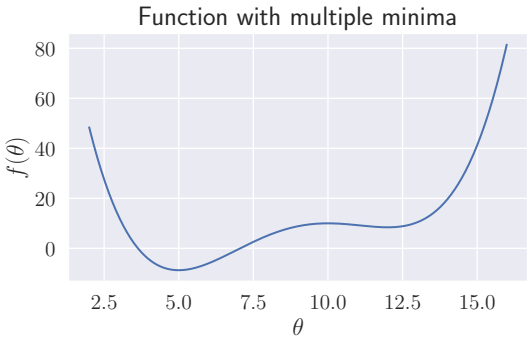

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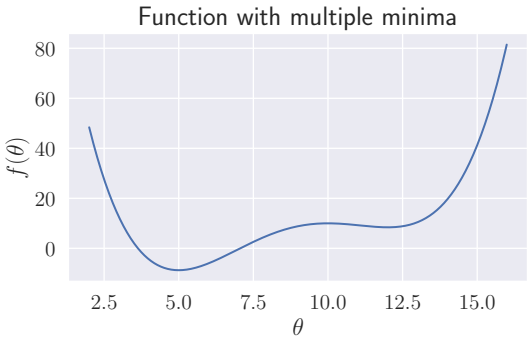

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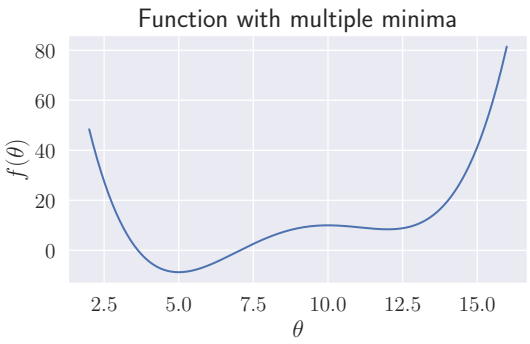

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The function is said to be "non-convex"

Which should we choose?

- We could enumerate all the solutions and choose the best.
- But that can get really tedious with complicated functions.

Estimation can be framed as an optimization problem

In many forms of estimation, we set up the problem as follows:

$$\{\hat{\beta}_0, \hat{\beta}_1\} = \arg\min_{\beta_0, \beta_1} J(\beta_0, \beta_1)$$

...where βs are the parameters we wish to identify.

In this course, we'll be looking at a broad variety of ways to define the *cost function*, J.

Linear regression as optimization

In “least squares” linear regression, the starting point for estimation is

$$\{\hat{\beta}_0, \hat{\beta}_1\} = \arg\min_{\beta_0,\beta_1} \sum_{i=1}^{n} (e_i)^2$$

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$$
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&= \arg\min_{\beta_0,\beta_1} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2
\end{aligned}
$$

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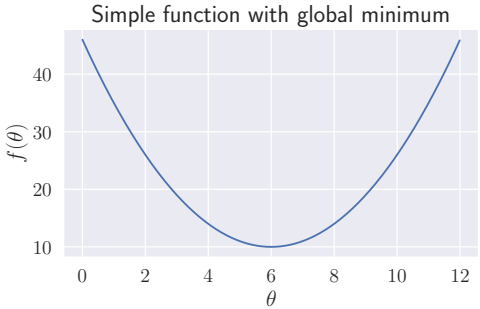
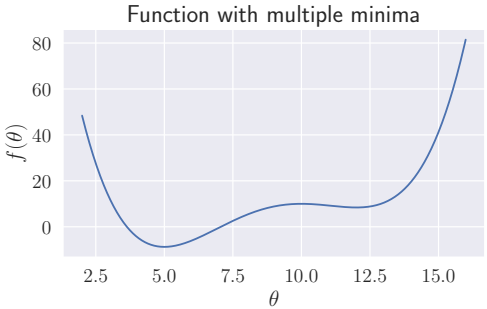
Hint:





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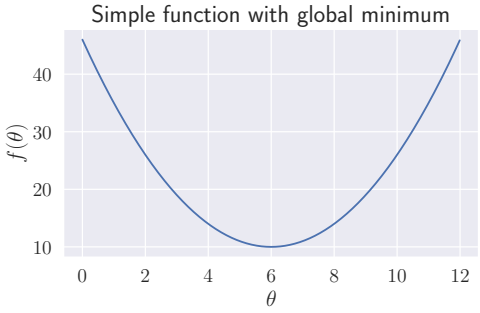

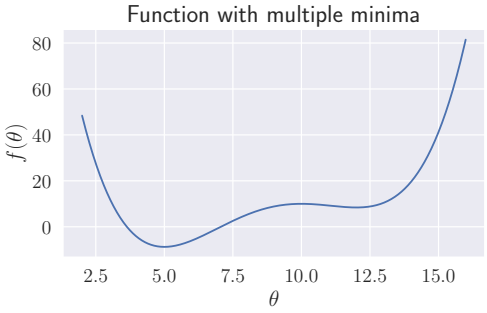

With least squares, the cost function

- Has one global minimum
- Is differentiable – we can write an equation for $\frac{\partial f(\theta)}{\partial \theta} = 0$

Solving the estimation problem

$$\{\hat{\beta}_0, \hat{\beta}_1\} = \arg\min_{\beta_0,\beta_1} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

So the optimal parameters must satisfy:

$$\frac{\partial \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2}{\partial \beta_0} = 0$$

$$\frac{\partial \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2}{\partial \beta_1} = 0$$

The solution:

$$\frac{\partial \sum_{i=1}^{n}(y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2}{\partial \hat{\beta}_0} = 0 \qquad \Rightarrow \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\frac{\partial \sum_{i=1}^{n}(y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2}{\partial \hat{\beta}_0} = 0 \qquad \Rightarrow \hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

Before moving on, a little linear algebra:

Here are two vectors:

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

$$\mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

Then the “dot” product of the two vectors is

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2$$

Next, a little more linear algebra:

We can also multiply *matrices* and vectors. Matrices are like column vectors stacked side by side

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

Then matrix multiplication gives us

$$\mathbf{Ab} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} a_{11}b_1 + a_{12}b_2 \\ a_{21}b_1 + a_{22}b_2 \end{bmatrix}$$

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Each element of the resulting matrix (or vector) is the dot product of a row of the first term (**A**) and a column of the second (**b**)

Therefore: the horizontal "dimension" of the first must be the same as the vertical "dimension" of the second.

Let's define matrices for our data:

Suppose we have n observations, (x_i, y_i). We'll arrange them all into a matrix form:

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Note: when we start working with more than one independent variable, X will have a new column for each new variable.

And then a lot more linear algebra:

Let's define the 'transpose':

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \quad \Rightarrow \quad X^T = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix}$$

And then a lot more linear algebra:

Let's define the 'transpose':

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \quad \Rightarrow \quad X^T = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix}$$

Now a challenge question: what's the product of these two matrices:

$$X^T X = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

Product of a matrix and its transpose

$$X^T X = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

Product of a matrix and its transpose

$$X^T X = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

$$= \begin{bmatrix} \text{1st row dot 1st col} & \text{1st row dot 2nd col} \\ \text{2nd row dot 1st col} & \text{2nd row dot 2nd col} \end{bmatrix}$$

Product of a matrix and its transpose

$$X^T X = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

$$= \begin{bmatrix} \text{1st row dot 1st col} & \text{1st row dot 2nd col} \\ \text{2nd row dot 1st col} & \text{2nd row dot 2nd col} \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{i=1}^{n} 1 \cdot 1 & \sum_{i=1}^{n} 1 \cdot x_i \\ \sum_{i=1}^{n} 1 \cdot x_i & \sum_{i=1}^{n} x_i \cdot x_i \end{bmatrix}$$

Product of a matrix and its transpose

$$X^T X = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

$$= \begin{bmatrix} \text{1st row dot 1st col} & \text{1st row dot 2nd col} \\ \text{2nd row dot 1st col} & \text{2nd row dot 2nd col} \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{i=1}^{n} 1 \cdot 1 & \sum_{i=1}^{n} 1 \cdot x_i \\ \sum_{i=1}^{n} 1 \cdot x_i & \sum_{i=1}^{n} x_i \cdot x_i \end{bmatrix} \quad = \begin{bmatrix} n & n\bar{x} \\ n\bar{x} & \sum_{i=1}^{n} x_i^2 \end{bmatrix}$$

Doing linear algebra in numpy:

See the in-class workbook!

Finally, the “normal equations”

We showed a way to compute β coefficients individually a few slides ago.

Finally, the "normal equations"

We showed a way to compute β coefficients individually a few slides ago.

However that can get tedious if you're doing *multiple* linear regression – i.e. if you have more than one independent variable.

The so-called "normal equations" give a nice, compact form to get the parameters.

$$\Theta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = (X^T X)^{-1} X^T Y$$

$$= \left(\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

A note for computing and linear algebra geeks

The normal equations are an efficient way to solve the least squares linear regression problem *when the number of independent variables is relatively small.*

But! Inverting a matrix (the $(\cdot)^{-1}$ part) is a heavy computational lift – especially as the size of the matrix gets big.

Later in the semester we'll talk about an alternative approach, called "gradient descent",

- It searches for the optimal point on the cost function in a more manual way.
- But it's actually faster than getting the solution using the normal equations.