Lecture #9: Probability and the MLE

aka STAT109A, AC209A, CSCIE-109A

CS109A Introduction to Data Science

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Lecture Outline: Probability

- Today's Example
- Review
- Probability and Random Variables
- Normal Distribution
- Binomial Distribution
- Likelihood

Today's Data Science Example

Recall the data science process:

Today's question: how much are your professors' homes worth?

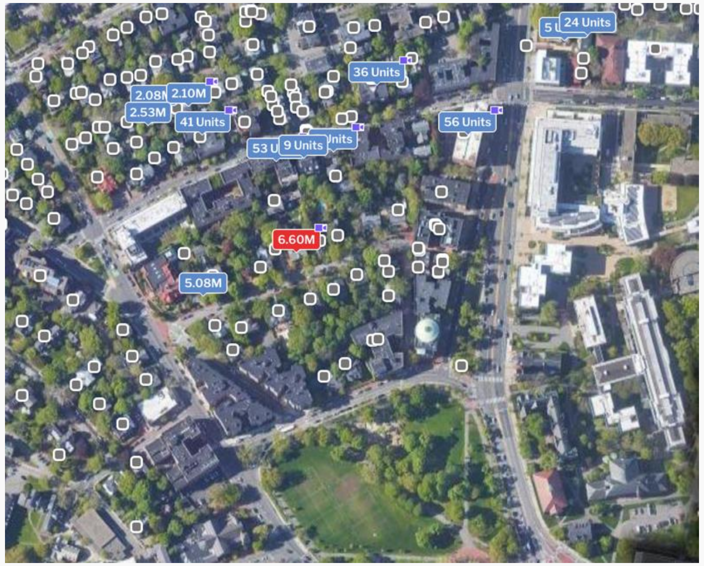
Related question: what variables are associated with selling prices of homes in the Cambridge-Somerville* area?

*Both Pavlos and Kevin live in Somerville

- Ask an interesting question
- Get the Data
- Explore the Data
- Model the Data
- Communicate/Visualize the Results

Today's Data Science Example

Today's Data are from Redfin.com:



A place to find historical selling prices of homes in any location (and plotted on a map). Today we're looking at the Cambridge & Somerville area, residential properties, that have sold in the last 12 months.

Address	Location	Price	Beds	Baths	Sq.Ft.	$/Sq.Ft.	On Redfin
20A Lafayette S...	East Arlington	$1,425,000	4	4.5	2,503	$569	—
45 Marlboro St	Belmont	$1,590,000	5	4	4,194	$379	—
28 Betts Rd	Belmont	$1,250,000	3	3	1,913	$653	—
97 Shaw Rd	Shaw Estates	$2,186,000	4	2.5	2,844	$769	—

Ask an interesting question

Get the Data

Explore the Data

Model the Data

Communicate/Visualize the Results

*Note: Kevin did a *little* preprocessing

Today’s Data Science Example

- **Response (y):**
  - Selling price (in \$) for $n = 592$ homes around Cambridge and Somerville
- **Predictors (X):**
  - Condo, single family, multi-family, or townhouse
  - Number of bedrooms
  - Number of bathrooms
  - Floor space in square feet
  - Lot size in square feet
  - The year the home was built
  - Distance to Harvard Sq T-stop (in km)

```
print(homes.dtypes)
```

```
date              object
type              object
address           object
city              object
zip                int64
price              int64
beds               int64
baths            float64
neighborhood      object
sqft               int64
lotsize          float64
year             float64
hoa              float64
url               object
mls                int64
latitude         float64
longitude        float64
dist             float64
dtype: object
```

- Ask an interesting question
- Get the Data
- Explore the Data
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Today's Data Science Example

Explore the Data

Notice anything concerning?
What does this indicate? What should we do?

```
homes["zip"]=homes["zip"].astype(str)
homes.describe().round(5)
```

	price	beds	baths	sqft	lotsize	year	hoa	mls	latitude	longitude	dist
count	5.920000e+02	592.00000	592.00000	592.00000	183.00000	591.00000	402.00000	5.920000e+02	592.00000	592.00000	592.00000
mean	1.244197e+06	2.92568	2.05828	1690.04561	3860.93989	1926.58545	352.30100	7.308775e+07	42.38443	-71.11148	2.17682
std	7.810677e+05	1.56242	0.96753	953.69978	1858.56503	46.57422	262.84504	3.623761e+04	0.01220	0.01653	0.88593
min	1.227940e+05	0.00000	1.00000	336.00000	1007.00000	1828.00000	1.00000	7.291816e+07	42.35605	-71.16066	0.44139
25%	8.000000e+05	2.00000	1.00000	1000.00000	2557.50000	1900.00000	200.00000	7.305637e+07	42.37497	-71.12367	1.50989
50%	1.028000e+06	3.00000	2.00000	1407.00000	3580.00000	1910.00000	286.00000	7.309318e+07	42.38459	-71.10973	2.07152
75%	1.450000e+06	3.00000	2.50000	2162.00000	4562.50000	1947.50000	443.50000	7.311370e+07	42.39333	-71.10031	2.82374
max	7.500000e+06	9.00000	7.00000	7530.00000	10454.00000	2024.00000	2984.00000	7.316201e+07	42.41408	-71.07172	4.60435

Today's Data Science Example

Explore the Data

```
homes['lotsize'] = homes['lotsize'].fillna(0)
homes['hoa'] = homes['hoa'].fillna(0)
homes['price'] = homes['price']/1000
```

What did we do? Is this reasonable?

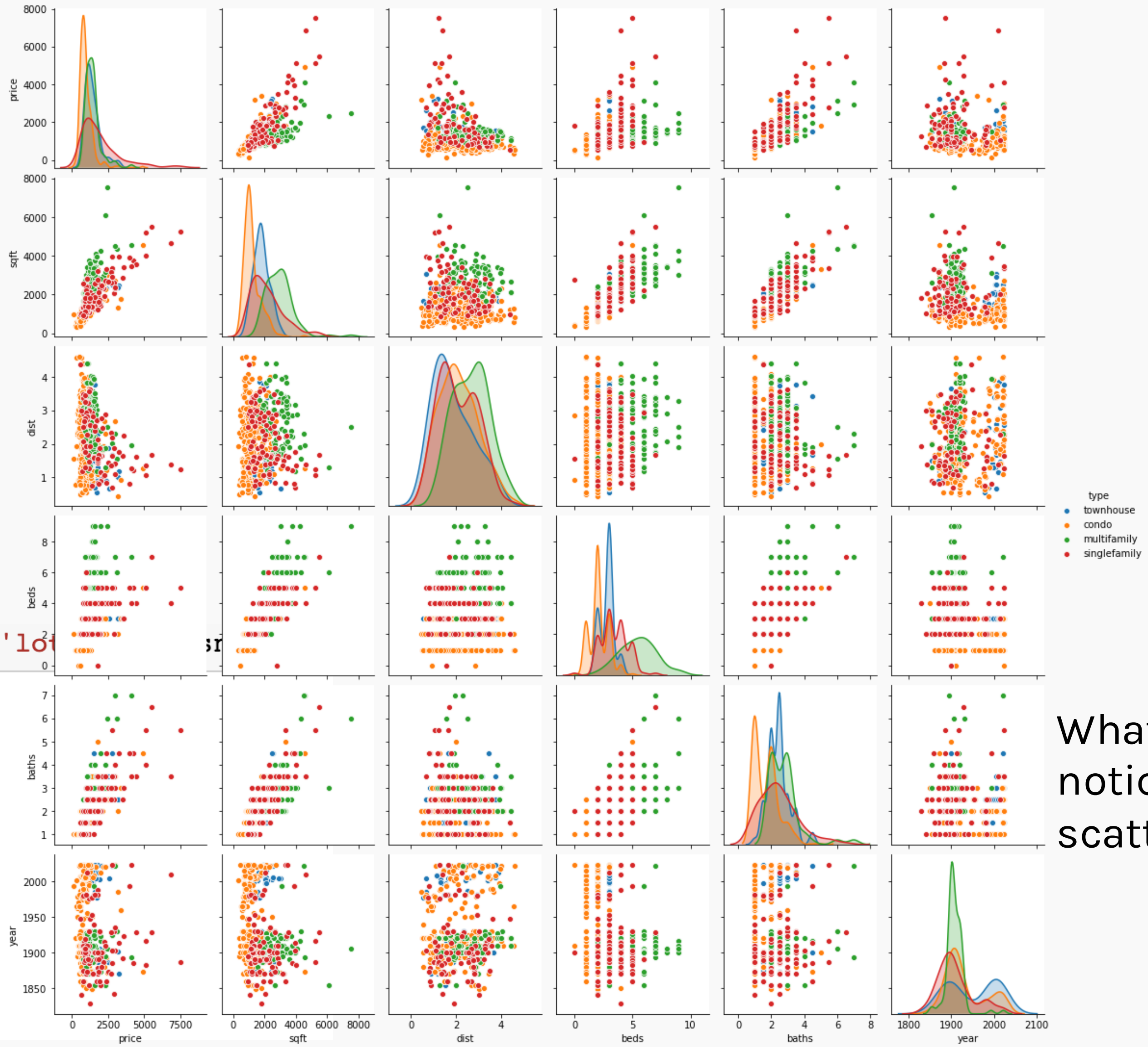
```
pd.crosstab(homes['type'],homes['hoa'].isnull())
```

hoa type	False	True
condo	334	7
multifamily	0	92
singlefamily	1	90
townhouse	67	1

```
pd.crosstab(homes['type'],homes['lot
```

lotsize type	False	True
condo	0	341
multifamily	92	0
singlefamily	91	0
townhouse	0	68

```
sns.pairplot(homes[['price','sqft', 'type',  'dist' , 'beds' , 'baths' , 'year']], hue="type");
```

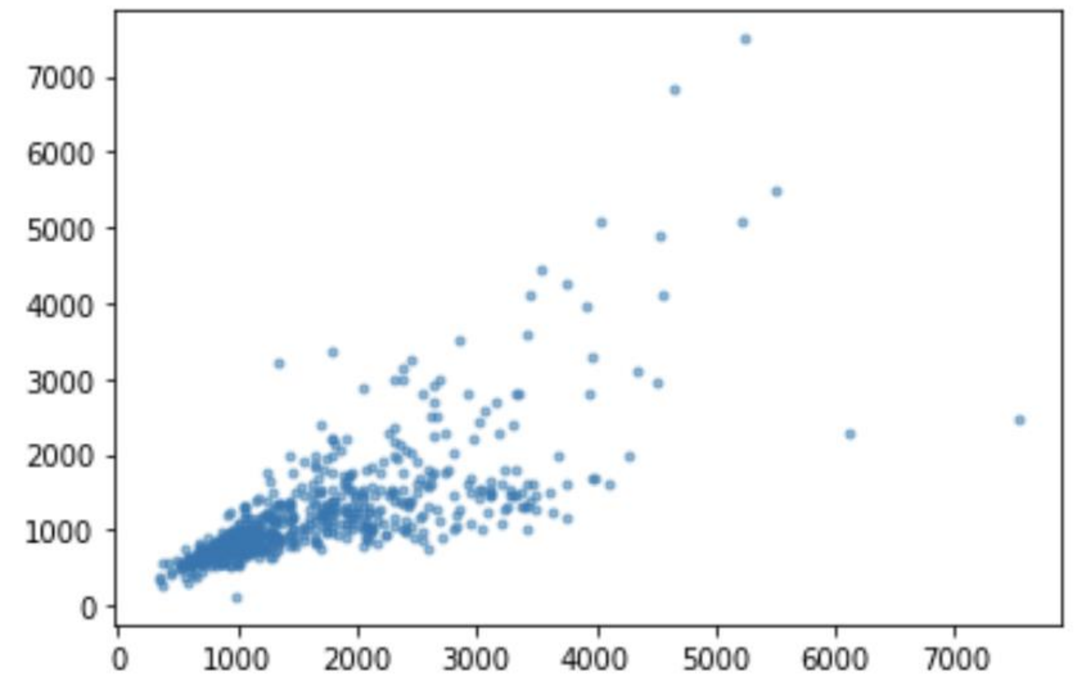


What do you notice in the scatterplots?

Today's Data Science Example

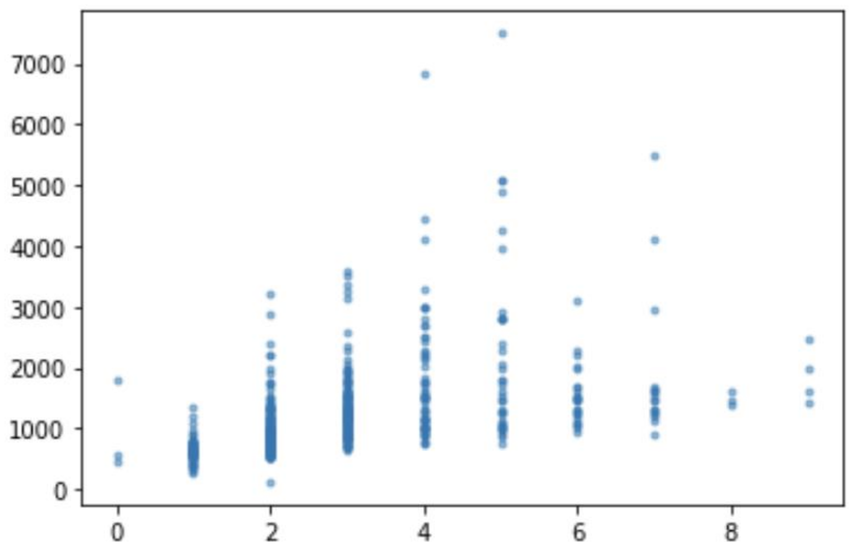
Explore the Data

```
plt.scatter(x = homes['sqft'], y = homes['price'],
            alpha = 0.5, marker = '.');
```

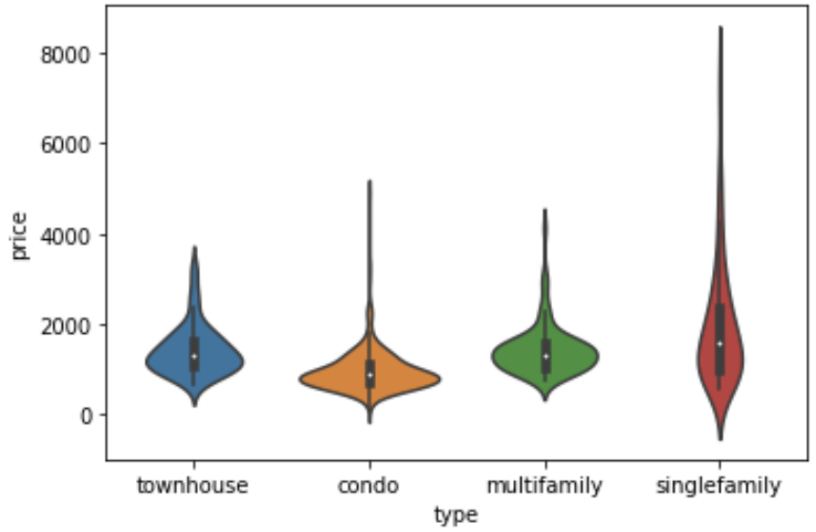


What do you notice? Any causes for concern?

```
plt.scatter(x = homes['beds'], y = homes['price'],
            alpha = 0.5, marker = '.');
```




```
sns.violinplot(x = homes['type'], y = homes['price']);
```



Today's Data Science Example

How should we model the data? Key: **price** (in thousands of $) is the response variable.

Linear Regressions make sense. Why?

Let's ask lots of questions ☺ Like…

- What associations do we care about?
- What predictors/features are likely to be strongly associated with the response?
- What might be nonlinear?
- What interactions are likely to be present?
- What other data considerations should we make?

Ask an interesting question

Get the Data

Explore the Data

Model the Data

Communicate/Visualize the Results

Today's Data Science Example

Model the Data

What are the coefficient interpretations?

Notice anything interesting? What does this indicate?

```
type_dummies = pd.get_dummies(homes['type'], drop_first=True)
homes=pd.concat([homes,type_dummies],axis=1)
```

```
X_full = homes[['multifamily', 'singlefamily', 'townhouse',
                'sqft',  'dist', 'beds', 'baths', 'year']]
regress_full = sk.linear_model.LinearRegression().fit(X = X_full, y = homes['price'])

pd.DataFrame({'coef': np.append(regress_full.intercept_,regress_full.coef_)},
             index = np.append("intercept",X_full.columns))
```

	coef
intercept	-1949.067039
multifamily	-452.235208
singlefamily	335.761220
townhouse	-76.437171
sqft	0.641074
dist	-173.542970
beds	-89.934486
baths	198.464604
year	1.229999

```
regress_sqft = sk.linear_model.LinearRegression().fit(X = homes[['sqft']], y = homes['price'])
print("Intercept =",regress_sqft.intercept_.round(2),", Slope =",regress_sqft.coef_[0].round(4))

regress_beds = sk.linear_model.LinearRegression().fit(X = homes[['beds']], y = homes['price'])
print("Intercept =",regress_beds.intercept_.round(2),", Slope =",regress_beds.coef_[0].round(4))
```

```
Intercept = 247.44 , Slope = 0.5898
Intercept = 570.39 , Slope = 230.3084
```

Today's Data Science Example

Model the Data

The library **`statsmodels`** makes our life WAY simpler (my R is showing):

```
import statsmodels.api as sm
import statsmodels.formula.api as smf
```

```
fullmodel_sm = smf.ols(formula = "price ~ sqft + type + dist + beds + baths + year",
                       data = homes).fit()
fullmodel_sm.params
#fullmodel_sm.summary()
```

```
Intercept               -1927.782817
type[T.multifamily]      -455.751842
type[T.singlefamily]      332.773270
type[T.townhouse]         -78.756789
sqft                        0.641839
dist                     -173.274319
beds                      -90.246936
baths                     199.724130
year                        1.218183
dtype: float64
```

Lecture Outline: Probability

- Today’s Example
- **Review**
- Probability and Random Variables
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- Likelihood

When do we use cross-validation?

Options

A. To choose the best k in a k-NN model.

B. To choose the best λ in a Ridge/LASSO model.

C. To choose the best predictors in a linear regression model.

D. To choose between families of models.

When should we standardize predictors?

Options

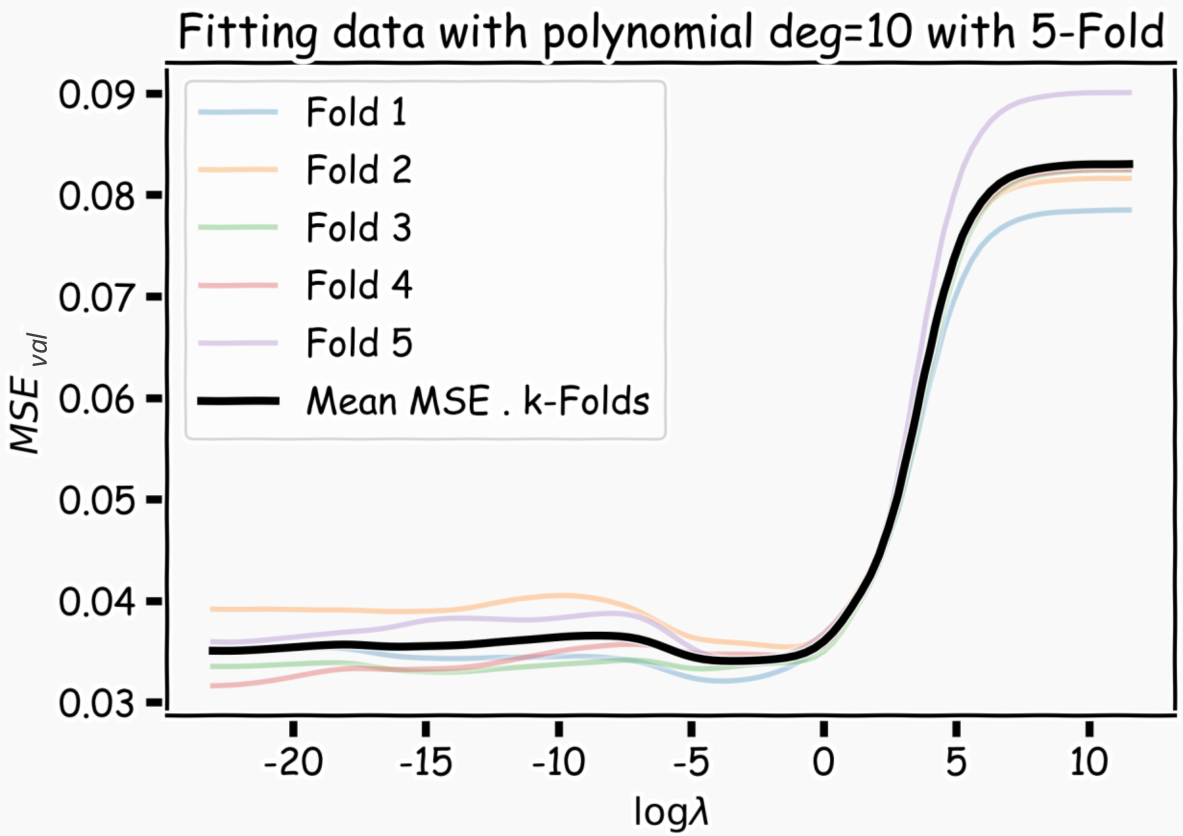
A. Always.

B. Whenever we use k-NN.

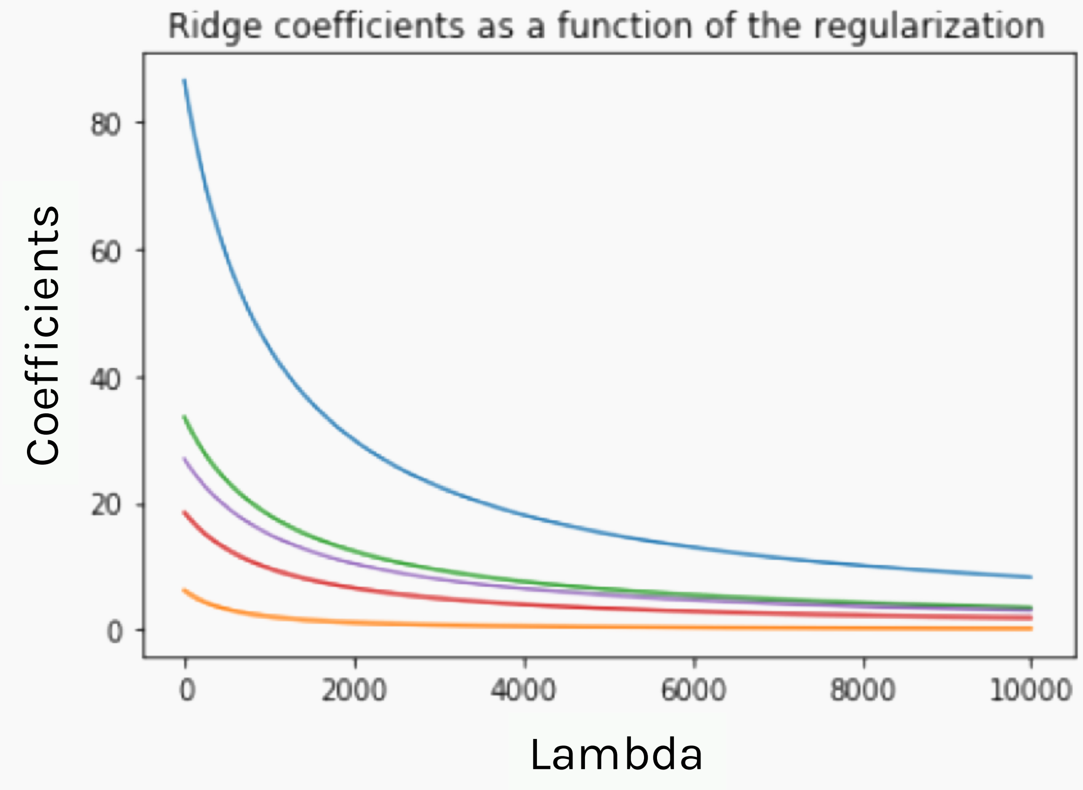
C. Whenever we use a Ridge/LASSO model.

D. Whenever we want to treat the transformed predictors more equally.

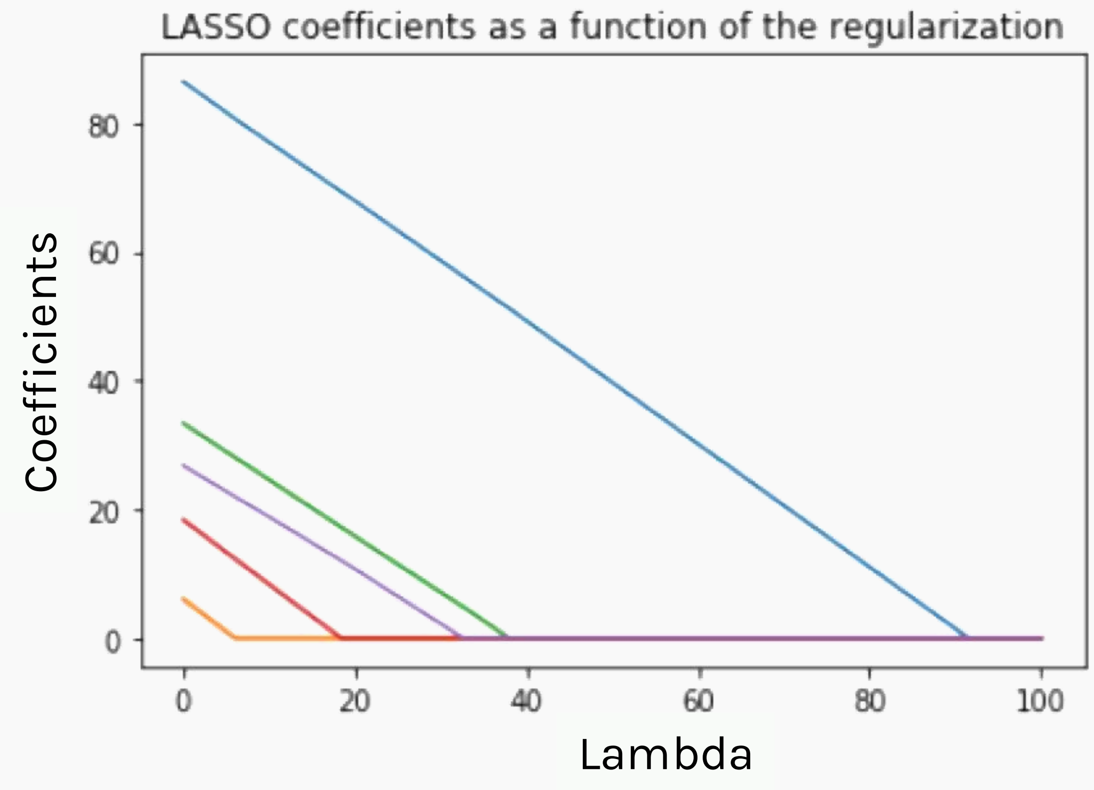
Ridge regularization with **cross-validation** only: step by step



Ridge and LASSO visualized

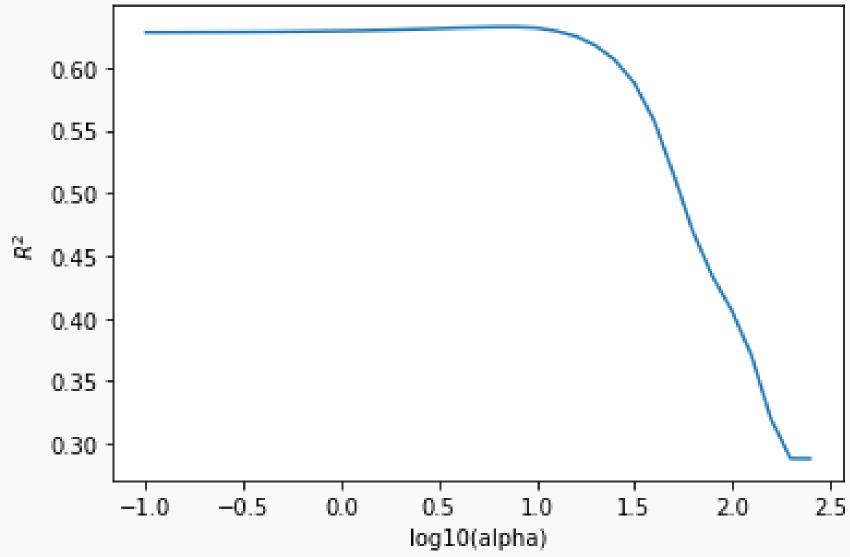


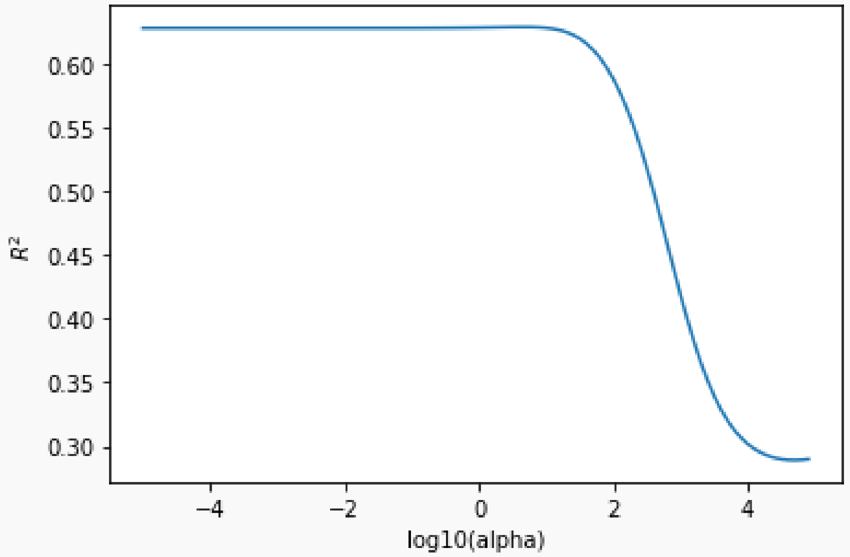
The values of the coefficients decrease as lambda increases, but they are not nullified.

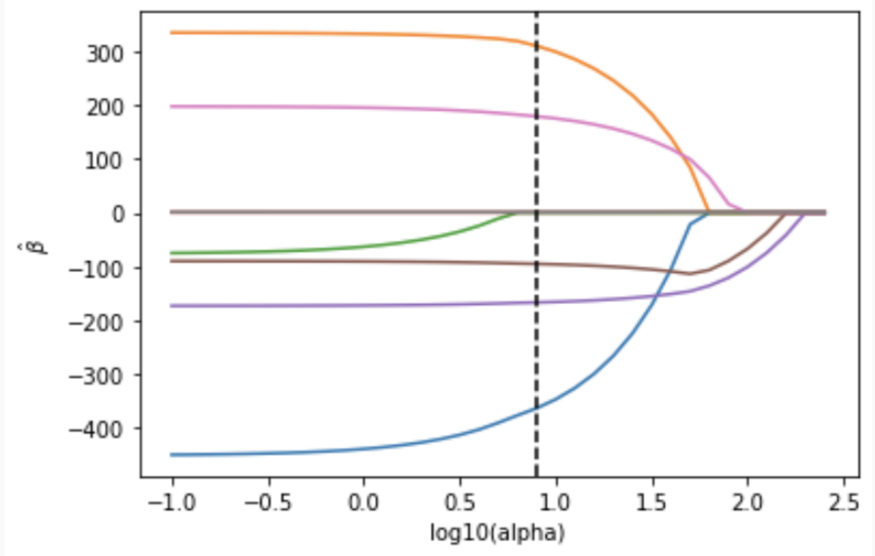


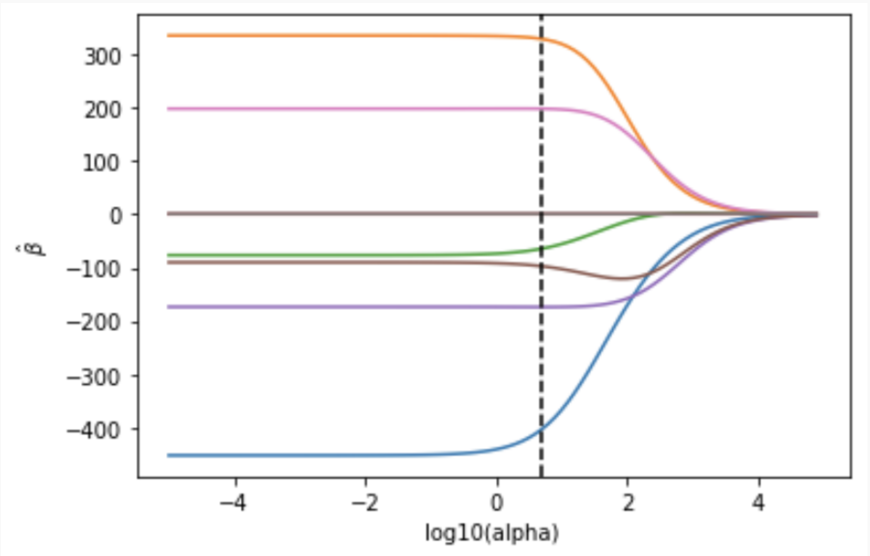
The values of the coefficients decrease as lambda increases and are nullified fast.

Ridge and LASSO: 2 real *trajectory* plots



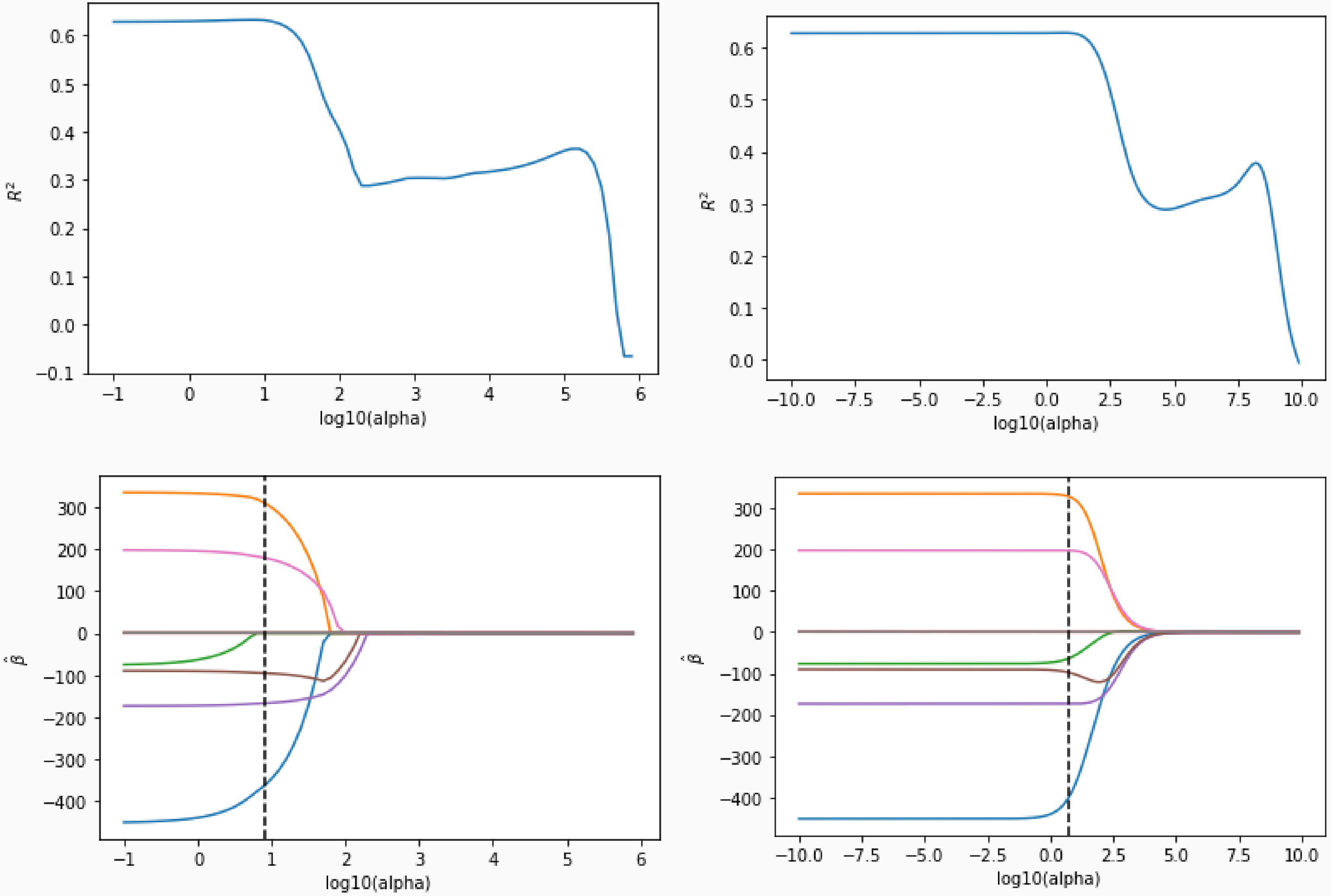






- Which is Ridge vs. Lasso?
- Which is the better predictive model?
- Which variable is least important? 2nd least?
- What is MSE in the OLS model? What about the intercept only model?
- Is there evidence of overfitting? Of multicollinearity?

Ridge and LASSO: 2 real *trajectory* plots



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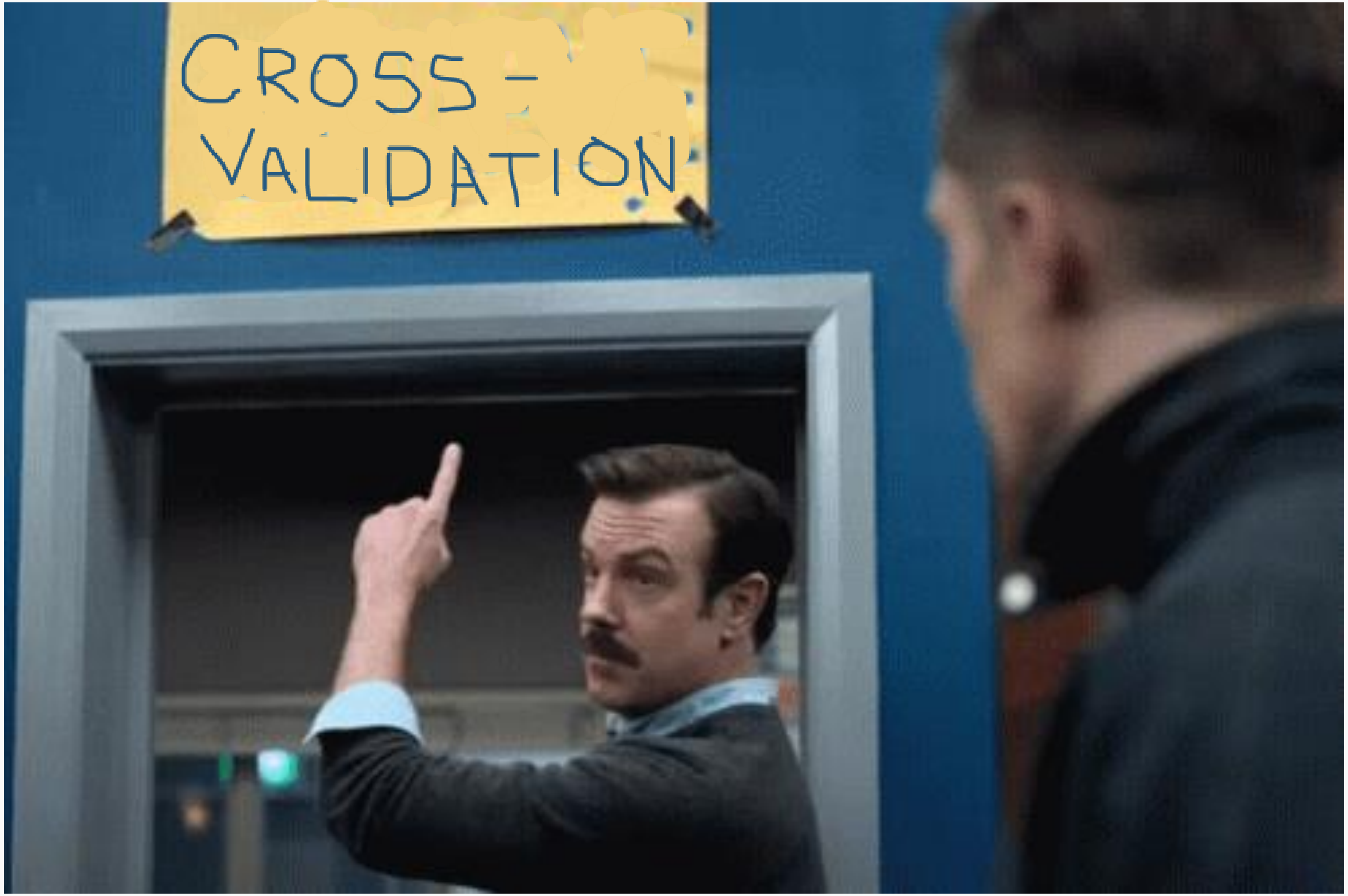

CROSS-
VALIDATION

Lecture Outline: Probability

- Today's Example
- Review
- **Probability and Random Variables**
- Normal Distribution
- Binomial Distribution
- Likelihood

What is probability?

Q: What is probability?

A: A common definition: the long-run, relative frequency* of a random phenomenon/experiment/event.

Q: What values can probabilities take on?

A: Any value between 0 and 1 (including the endpoints).

Q: Why do we care?

A: Because data can be thought of as random realizations of a *data generating process* (whether though sampling or a theoretical construct).

*Note: this ignores the Bayesian definition of probability: a measure of belief.

What is a random variable?

In the context of data, we often describe their potential **numeric** outcomes (before collecting the data) as random variables. That is:

Let's perform a survey of Harvard students and ask the question: do you primarily use a Mac (vs. PC vs. Linux/Ubuntu, etc.)?

Let X_1 be the observed response for the first person we are going to ask. Then X_1 can be thought of as a random variable. ($X_1 = 1$ implies 'Mac', $X_1 = 0$ implies anything else).

*Technically a random variable is a function that takes possible outcomes of random phenomenon (responses of 'Mac', 'PC', etc.) and maps them to numeric values.

What is a probability distribution?

A **probability distribution** is any function (formula, table, or graph) that assigns probabilities (or relative frequencies) to all the possible outcomes of a random variable.

Typically they are written as a formula (called a probability mass function or probability density function, or as its cumulative distribution function).

In our 'Mac' example, we could define the probability distribution as a table:

x	$P(X = x)$
0	$1 - p$
1	p

Which could be summarized as the formula, for $x \in \{0,1\}$:

$$P(X = x) = p^x(1 - p)^{1-x}$$

The goal of our study would be to estimate p.

Discrete vs. Continuous

There are two major types of random variables: **discrete** (can only take on specific values) and **continuous** (can take on any value within a range).

The probability distribution function is defined differently for these two types:

A **probability mass function** (PMF) is a function that gives the probability of getting a specific value for a discrete random variable.

A **probability density function** (PDF) is a function that gives the relative likelihood of a specific value for a continuous random variable (the height of the curve). This is usually written as $f(x)$

*Note: probabilities for a continuous random variable can be represented as areas under the curve, and thus $P(X = x) = 0$ since there is no width.

Joint Distributions

What happens to these probability distributions (PMFs and PDFs) when there are multiple random variables involved (aka, multiple observations in a data set)?

Let $f(x_1, x_2, \dots, x_n)$ be the **joint distribution** of n separate random variables. If they all come from the same generative marginal distribution, $f(x_i)$, and are **independent**, what is the resulting distribution?

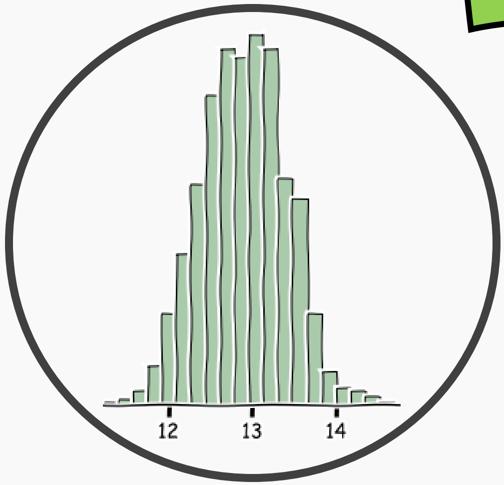
$$f(x_1, x_2, \dots, x_n) = f(x_1) \cdot f(x_2) \cdots f(x_n) = \prod_{i=1}^{n} f(x_i)$$

What does independent data mean, anyway? When does this breakdown?

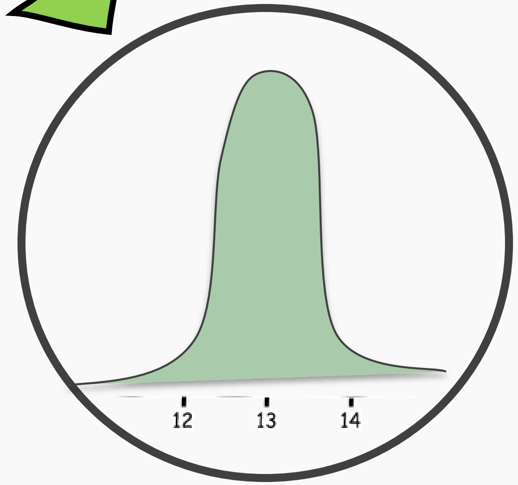
PDF vs PMF

Random Variable

X



Discrete Random Variable



Continuous Random Variable

Lecture Outline: Probability

- Today's Example
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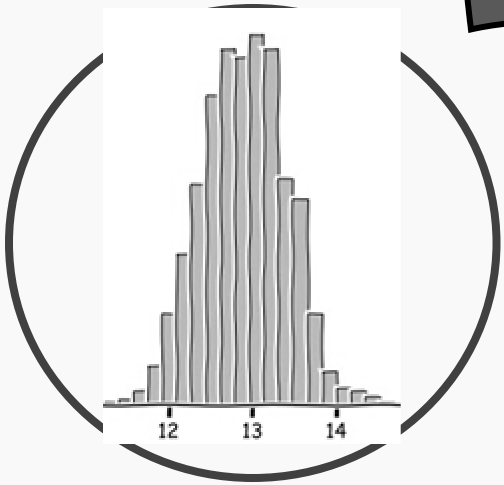
- **Normal Distribution**
- Binomial Distribution
- Likelihood

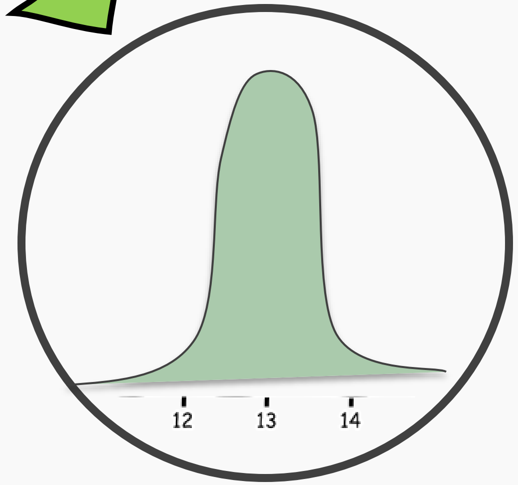
PDF vs PMF

Random Variable

X



~~Discrete Random Variable~~



Continuous Random Variable

The Normal Distribution

Let X be a **normally distributed** random variable. Then $X \sim N(\mu, \sigma^2)$, and X has probability density function (PDF):

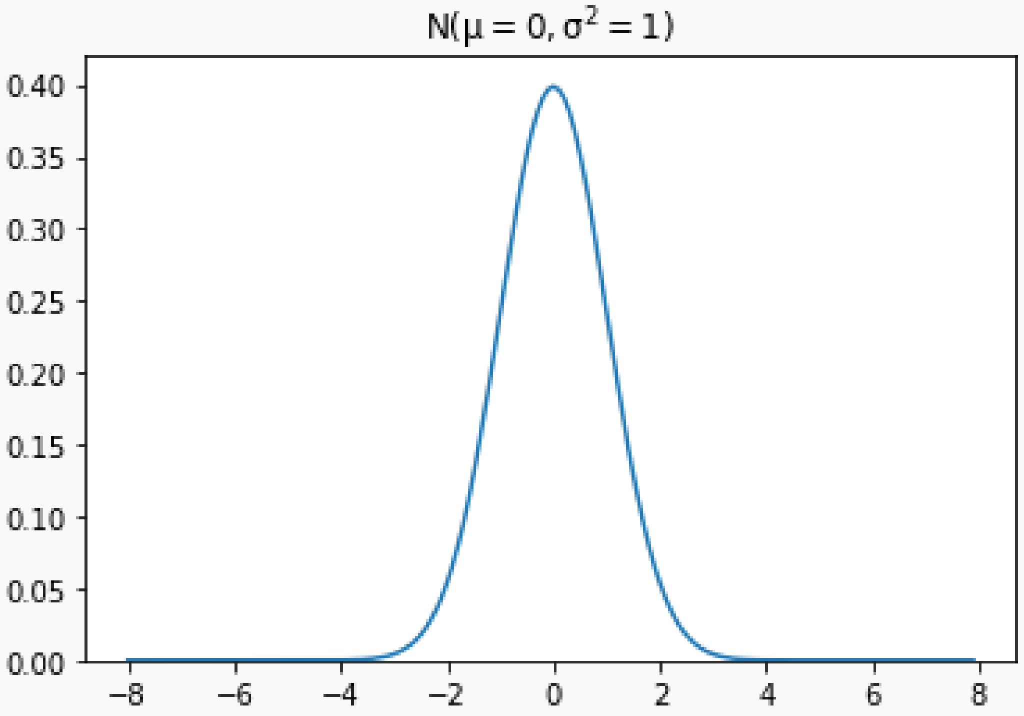
$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

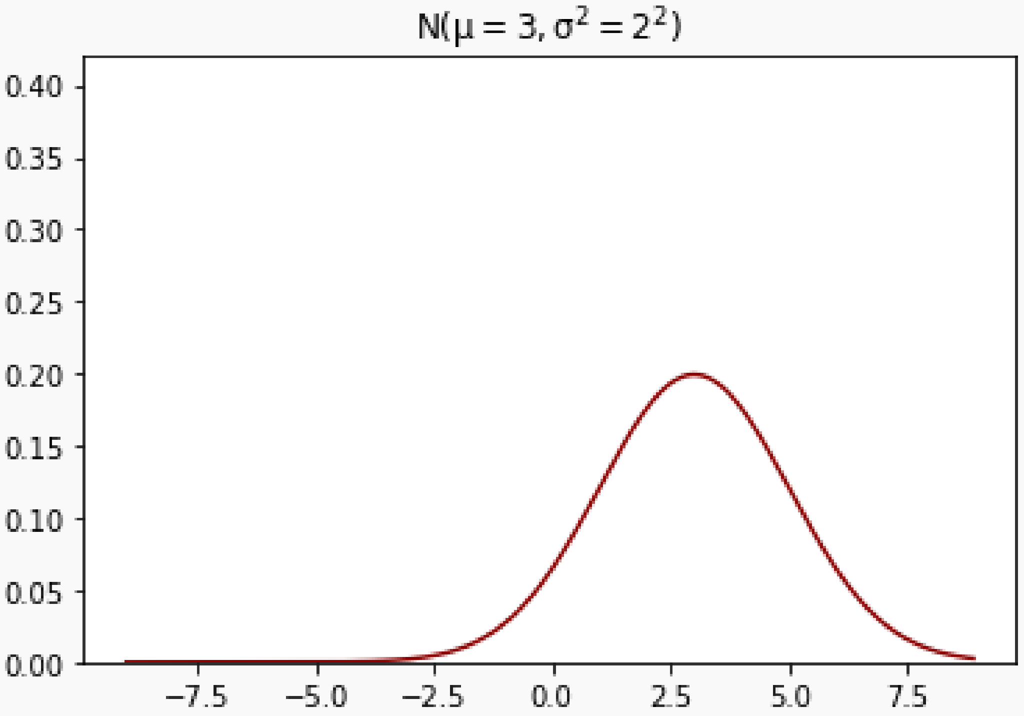
The normal distribution (sometimes called the Gaussian) is often referred to as the bell-shaped curve. But the normal distribution isn't the only one that is bell-shaped: t distributions are also bell-shaped, for example.

The standard normal distribution is a special case: $Z \sim N(0,1)$.

Any normal random variable can be standardized using the formula $Z = \frac{X-\mu}{\sigma}$.

The Normal Distribution Examples





A normal distribution has mean μ and standard deviation σ.

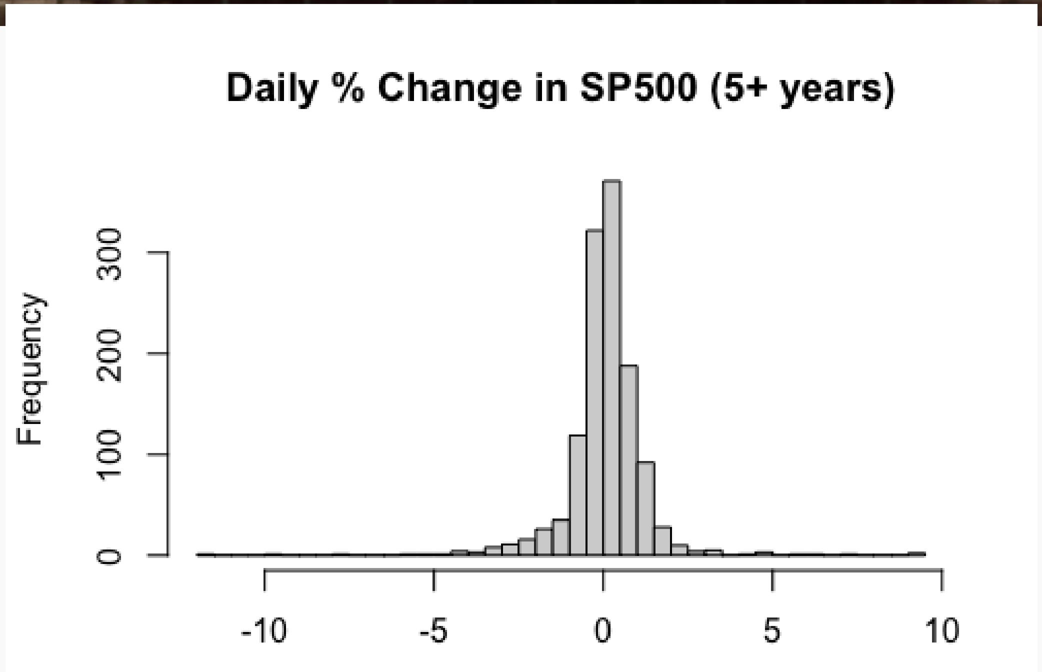
Central Limit Theorem

Why is the normal distribution used so often? The **Central Limit Theorem**: random variables that are averages or sums of many other random variables will be approximately normally distributed.

More specifically: if $X_1, X_2, \ldots, X_n$ are independent random variables (representing individual observations of data) with mean μ and standard deviation σ (not necessarily normal themselves), then the sample mean $\bar{X} = \frac{X_1+X_2+\cdots+X_n}{n}$ will have approximate distribution:

$$\bar{X} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

I See Normal Distributions



Lecture Outline: Probability

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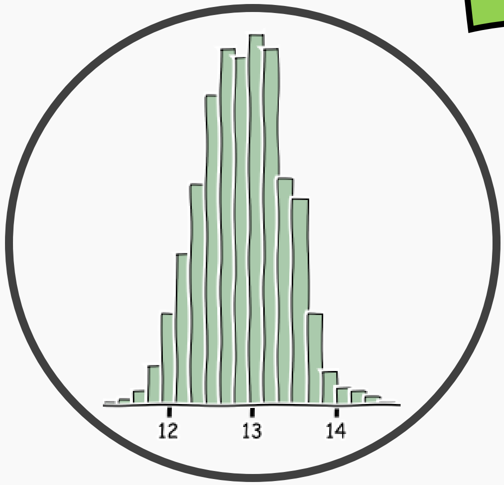
- **Binomial Distribution**
- Likelihood

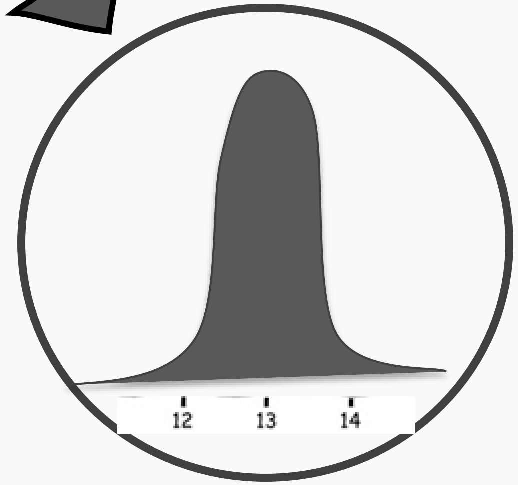
PDF vs PMF

Random Variable

X



Discrete Random Variable



Continuous Random Variable

The Binomial Distribution

Let X be a random variable that counts the number of successes in a fixed number of independent trials (n) with fixed probability of success (p) in each trial. Then X is said to have a **binomial distribution**. This is often written as: $X \sim Binom(n, p)$, and X has probability mass function (PMF):

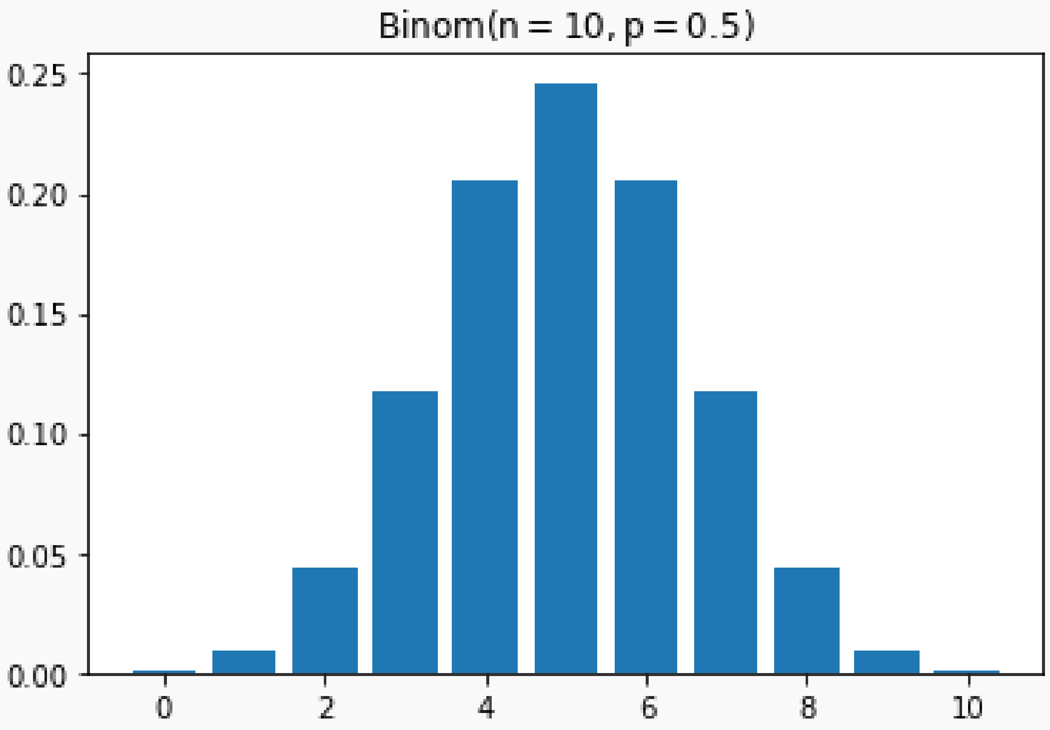
$$P(X = x) = \binom{n}{x} p^x (1-p)^{n-x}$$

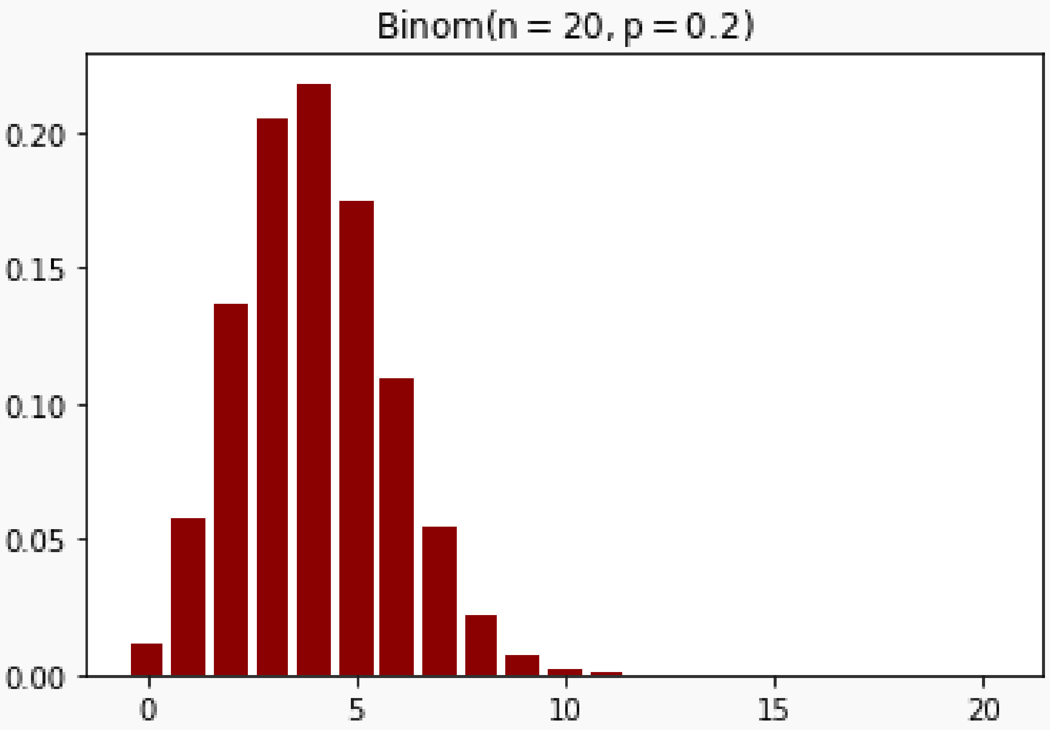
Think counting the number of heads when flipping a biased coin n times.

The binomial distribution is useful to describe polling data (proportion of people who will vote for Biden), survey data (will you take CS109B next year?), or any data that are binary!

The **Bernoulli distribution** is a special case when n = 1. This is the distribution that describes our `Mac` example.

Binomial Distribution Examples





A binomial distribution has mean np and standard deviation $\sqrt{np(1-p)}$.

Lecture Outline: Probability

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- **Likelihood: a roadmap for statistical inference**

The Probability of Data

In a typical probability problem (like in Stat 104 or 110), you would be told something like "20% of Harvard College students are collegiate athletes. What is the probability that there are 50 athletes in a random sample of 200 students from Harvard College?"

$$P(X = 50) = \binom{200}{50}(0.20)^{50}(0.80)^{150} = 0.0149$$

$$P(X \geq 50) = \sum_{50}^{200}\binom{200}{x}(0.20)^{x}(0.80)^{200-x} = 0.0494$$

<u>An alternative question</u>: what is more likely to occur: 50 athletes or 40 athletes in a sample of 200 students? How can we make the determination?

Inference: the inverse of probability

In the last problem, how did we know that the statement "20% of Harvard College students are collegiate athletes" is accurate? Where did this come from?

In most applications, the true population parameter (here, the proportion in all of Harvard College) is unknown. What we get to observe is the data, and we want to make a statement about the unknown parameter. So a more poignant question would be:

"There are 50 athletes in a random sample of 200 students from Harvard College. Is a binomial distribution with $p = 0.2$ or $p = 0.25$ more reasonable?"

This approach of using the data to make a statement about a parameter (in a statistical model) is called **inference**.

The idea of likelihood

The **likelihood** approach to inference is based on exactly what was presented in the last slide: given observed values of data (summarized by specific sample statistics), what values of the model's parameters are likely?

It simply just flips a PDF or PMF on its head: instead of writing this function with the data (X) as the unknown, it uses the same function but uses the parameter(s) as the unknown(s). The **likelihood function**, $\mathcal{L}$, measures how well a model (and its set of parameters) describes the observed data.

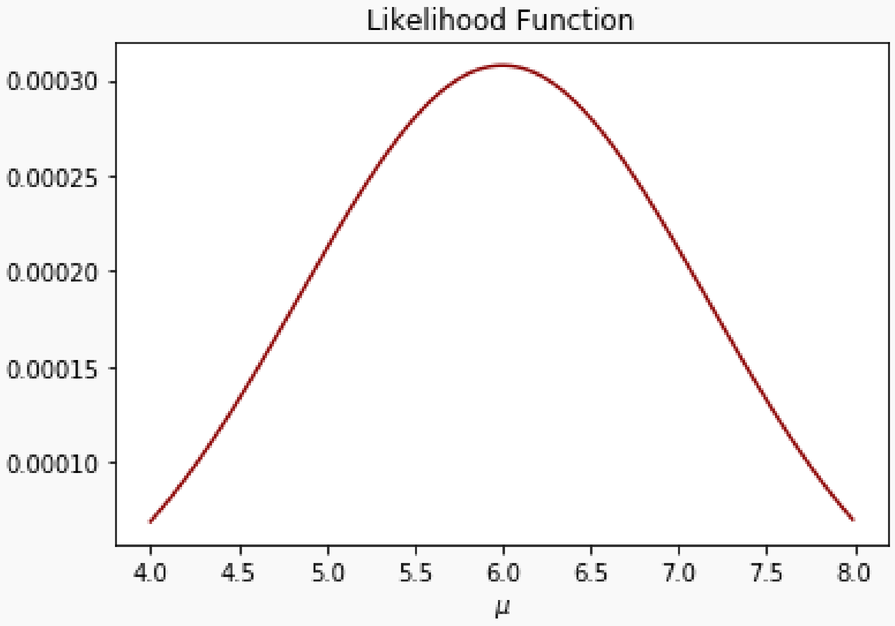
For a set of independent and normally distributed random variables, $X_i \sim N(\mu, \sigma^2)$:

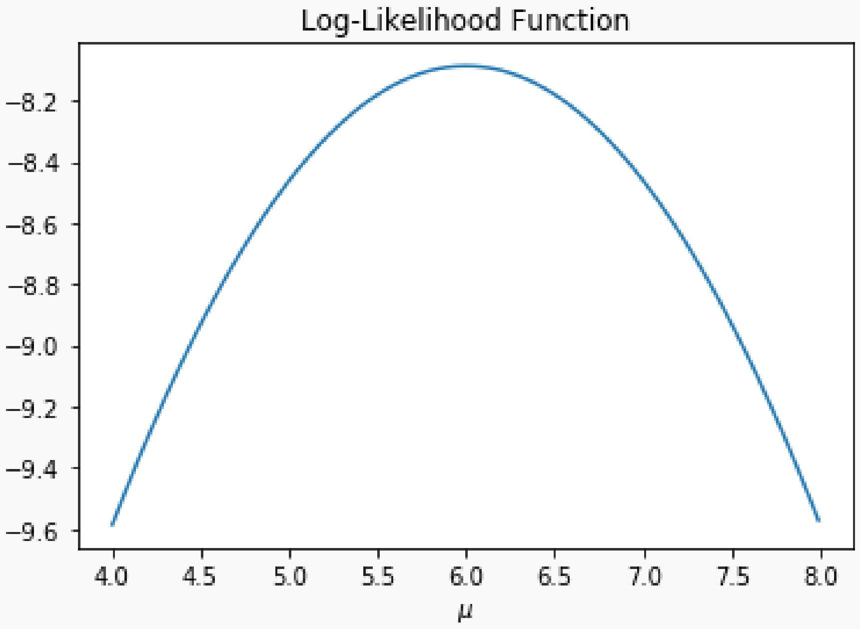
$$\mathcal{L}(\mu, \sigma^2 | x_1, \dots, x_n) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x_i - \mu}{\sigma}\right)^2}$$

Likelihood function example

3 observations are collected [3, 5, 10] that are thought to come from a normal distribution with unknown mean, μ, but is known to have a variance of $\sigma^2 = 2^2$ (yes, this is **very** contrived).

Let's plot the likelihood and log-likelihood functions:





Maximizing the likelihood

In order to choose the best Normal distribution to describe a set of data, we should maximize the likelihood that chooses the best set of parameters given the data.

The **maximum likelihood estimates** for a statistical model are those that maximize the likelihood function given the observed data.

How do we do this mathematically? How could we do this computationally?

With Math: ____

With Computers:_____________________________________

The Simple Linear Regression Model

We've defined the linear regression model to predict the i-th observation's response, Y_i, from a predictor, X_i, to be:

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

For any random variable, ϵ, that has zero mean, then:

$$E(Y_i) = \beta_0 + \beta_1 X_i$$

The error term, ϵ_i, represents the distance the observation lies from the line in the vertical distance (direction of Y).

The Probabilistic Regression Model

If we assume that $\epsilon_i \sim N(0, \sigma^2)$

This regression model can be rewritten as:

$$Y_i | X_i \sim N(\beta_0 + \beta_1 X_i, \sigma^2)$$

The likelihood of a measurement having value Y_i given X_i for a model β_0, β_1:

$$L(\beta_0, \beta_1, \sigma^2 | Y_i, X_i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{Y_i - (\beta_0 + \beta_1 X_i)}{\sigma}\right)^2}$$

The Probabilistic Regression Model

The likelihood of a measurement having value Y_i given X_i for a model β_0, β_1

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This formulation allows us to write out the **joint** likelihood function for this probability model.

The joint likelihood function for this probability model becomes:

$$L(\beta_0, \beta_1, \sigma^2 | \boldsymbol{Y}, \boldsymbol{X}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{Y_i-(\beta_0+\beta_1 X_i)}{\sigma}\right)^2}$$

The Likelihood of Linear Regression

What does this function look eerily similar to? What does maximize this function lead to with regards to the best estimates of β_0, β_1?

The joint likelihood function for this probability model becomes:

$$L(\beta_0, \beta_1, \sigma^2 | \boldsymbol{Y}, \boldsymbol{X}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{Y_i - (\beta_0 + \beta_1 X_i)}{\sigma}\right)^2}$$

Which leads to the log-likelihood:

$$l(\beta_0, \beta_1, \sigma^2 | \boldsymbol{Y}, \boldsymbol{X}) = \ln(L(\beta_0, \beta_1, \sigma^2 | \boldsymbol{Y}, \boldsymbol{X})) = -\sum_{i=1}^{n} \ln\left(\sqrt{2\pi\sigma^2}\right) - \frac{1}{2}\sum_{i=1}^{n}\left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma}\right)^2$$

What should we do with this log-likelihood?

The Likelihood of Linear Regression

Instead of maximizing the log-likelihood we can minimize the ***negative-log-likelihood:***

$$-l(\beta_0, \beta_1, \sigma^2 | \boldsymbol{Y}, \boldsymbol{X}) = \sum_{i=1}^{n} \ln\left(\sqrt{2\pi\sigma^2}\right) + \frac{1}{2}\sum_{i=1}^{n}\left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma}\right)^2$$

Which is equivalent to minimizing

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma}\right)^2$$

A look ahead: likelihood for binary outcomes

Let $Y \sim Bern(p)$. What is the joint likelihood function? What is the log-likelihood?

Likelihood:

$$L(p|\,\boldsymbol{Y}) = \prod_{i=1}^{n} p^{Y_i}(1-p)^{1-Y_i}$$

log-likelihood:

$$l(p|\,\boldsymbol{Y}) = \sum_{i=1}^{n} Y_i \ln(p) + \sum_{i=1}^{n} (1-Y_i)\ln(1-p)$$

Why do we care?

What if we let $p_i = \frac{1}{1+e^{-(\beta_0+\beta_1 X_1+\cdots)}}$? This is logistic regression!

Take home message

By taking a probabilistic approach to linear regression and assuming the residuals are normally distributed, we see that **maximizing the likelihood** for this model is equivalent to **minimizing mean squared error** around the line!

So, if we believe our residuals are normally distributed, then minimizing mean square error is a natural choice.

But by choosing this specific probability model, we get much more than simply motivation for our loss function. We get *instructions* on how to perform inferences as well ☺

We will see this in more details in next lecture!

CS109A
GAME Time

What is the goal of visualization?

Options

A. To explore the distributions of variables.

B. To explore the data to build hypotheses.

C. To communicate results of your models.

D. To trick and manipulate your audience.