# Quantitative Research Methods

Probability and Statistics for Data Science CSE594 - Spring 2016

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Probability and Statistics for Data **Science**CSE594 - Spring 2016

# The Scientific Method

#### Develop General Theories

General theories must be consistent with most or all available data and with other current theories.

### Gather Data to Test Predictions

Relevant data can come from the literature, new observations or formal experiments. Thorough testing requires replication to verify results.

#### Make Observations

What do I see in nature?
This can be from one's
own experiences, thoughts
or reading.

Refine, Alter,
Expand or Reject

Hypotheses

Develop Testable
Predictions

If my hypothesis is correct, then I expect a, b, c, ... Think of Interesting Questions

Why does that pattern occur?

# Formulate Hypotheses

What are the general causes of the phenomenon I am wondering about?

(Garland, 2015)

Hypothesis -- something one asserts to be true.

Classical Approach:

*H<sub>0</sub>: null hypothesis* -- some "default" value (usually that one's hypothesis is false)

 $H_1$ : the alternative -- usually that one's "hypothesis" is true

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Goal: Use probability to determine if we can "reject the null"  $(H_0)$  in favor of  $H_1$ . "There is less than a 5% chance that the null is true" (i.e. 95% alternative is true).

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 $H_0$ : the coin is not biased (i.e. flipping n times results in a Binomial(n, 0.5))



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More formally: Let X be a random variable and let R be the range of X.  $R_{reject} \subseteq R$  is the rejection region. If  $X \in R_{reject}$  then we reject the null.

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in the example, if n = 1000, then then  $R_{reject}$  = [0, 469]  $\cup$  [531, 1000]

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Assignment 1, Programming Problem "C) 9."



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(assuming independent, same variance) t statistic for 2 samples

#### **Degrees of Freedom:** the number of values that are free to vary

The number of observations available to measure a parameter in a distribution. In other words, what is the minimum *i*, such that given *i* observations one could determine the parameter?

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Statistical test is asking about generalizability to the population (or if we had infinite data).

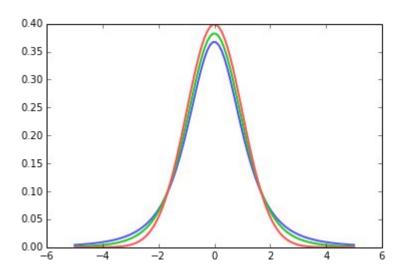
Examples: mean, variance

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{S_{X_1 X_2} \cdot \frac{1}{n_1} + \frac{1}{n_2}}}$$

(assuming independent, same variance) t statistic for 2 samples

t-test: comparing means of distributions

Remember, t identifies an x in a distribution (Student's t distribution) P(T < t; df)





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t-test: comparing means of distributions

$$df = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)}{\frac{(s_1^2/n_1)^2}{df_1} + \frac{(s_1^2/n_1)^2}{df_2}}$$
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(assuming independent, different variance)

$$t = \frac{\bar{X}_1 - \mu_0}{\frac{s_1}{\sqrt{n_1}}}$$

(compared to theoretical mean)

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{S_{X_1 X_2} \cdot \frac{1}{n_1} + \frac{1}{n_2}}}$$

(assuming independent, same variance)

#### Important logical question:

Does failure to reject the null mean the null is true?



#### Important logical question:

Does failure to reject the null mean the null is true? no.



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Traditionally, one of the most common reasons to fail to reject the null: n is too small (not enough data)

Thought experiment: If we have infinite data, can the null ever be true?



#### Important logical question:

Does failure to reject the null mean the null is true?

no.



Thought experiment: If we have infinite data, can the null ever be true?

Big Data problem: "everything" is significant. Thus, consider "effect size"



		True state of nature		
		$H_0$	$H_A$	
Our	Reject $H_0$	Type I error	correct decision	
decision	'Accept' $H_0$	correct decision	Type II error	

(Orloff & Bloom, 2014)

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(Orloff & Bloom, 2014)

Which is worse?



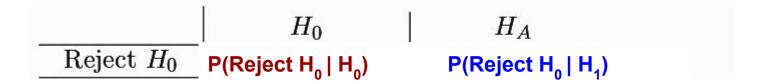
#### Quantitative Research Review: 3-1

- The Scientific Method
- Null Hypotheses, Alternative Hypotheses
- Defining a rejection region based on hypothesis
- T-tests
- Degrees of Freedom
- Error types

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		$H_0$	$H_A$	ff & Bloom, 20
	Reject $H_0$	P(Reject H <sub>0</sub>   H <sub>0</sub> )	P(Reject H <sub>0</sub>   H <sub>1</sub> )	
	'Accept' $H_0$	P(Fail to Reject H <sub>0</sub>	H <sub>0</sub> ) P(Fail to Re	ject H <sub>0</sub>
	\$ <del>-</del>	H <sub>4</sub> )	<del>V.C.</del>	-



#### Power

```
significance level ("p-value") = P(type I error) = P(Reject H_0 | H_0) (probability we are incorrect)

power = 1 - P(type II error) = P(Reject H_0 | H_1) (probability we are correct)
```

$$\begin{array}{c|cccc} & H_0 & H_A \\ \hline \hline \text{Reject } H_0 & \text{P(Reject } H_0 | H_0) & \text{P(Reject } H_0 | H_1) \\ \end{array}$$

#### Power

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power = 1 - P(type II error) =  $P(Reject H_0 | H_1)$ (probability we are correct)

Formally, a power function of a test with rejection region, *R*, is:

$$\beta(\theta) = P_{\theta}(X \in R)$$

where  $\theta$  is the parameters of the distribution over which R is defined. (e.g. p, n for a binomial distribution)

### **Multi-test Correction**

If alpha = .05, and I run 40
variables through significance
tests, then, by chance, how many
are likely to be significant?

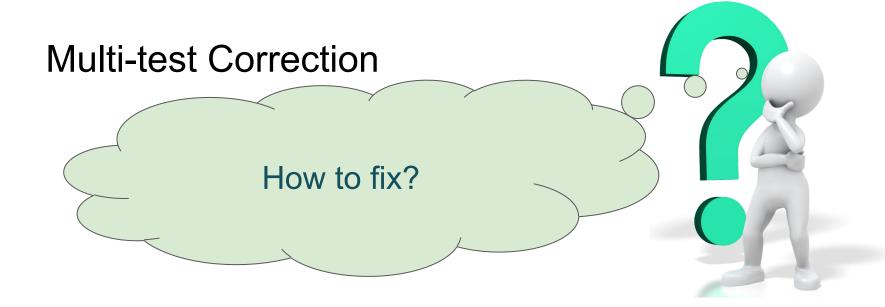


### **Multi-test Correction**

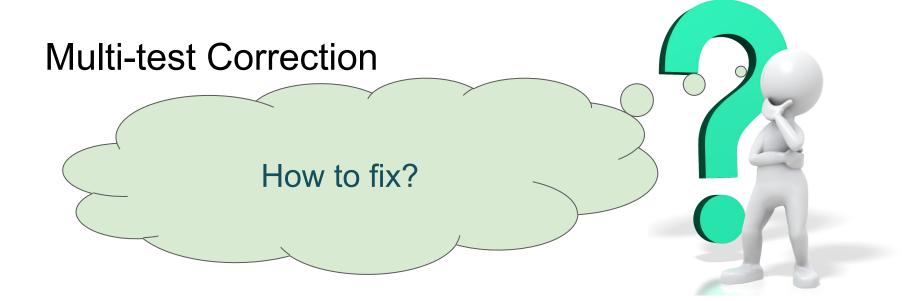
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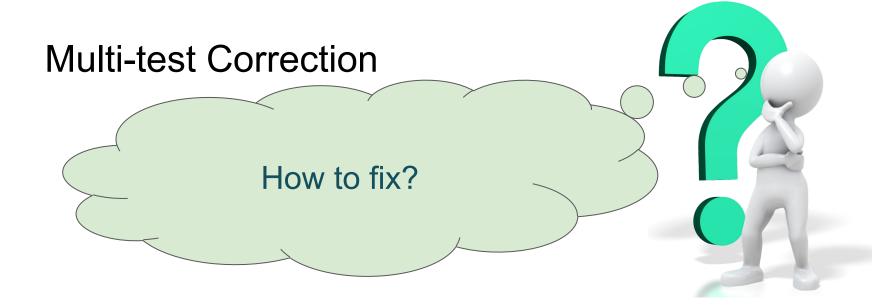
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What if all tests are independent?

=> "Bonferroni Correction" (α/m)





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But this may over-correct.

#### **Multi-test Correction**

### Benjamini-Hochberg Correction Procedure

- 1. Let  $P_{(1)} < ... < P_{(m)}$  denote ordered p-values
- 2. Define:  $\ell_i = \frac{ia}{C_m m}, \text{ and } R = max\left\{i: P_(i) < \ell\right\}$ where  $C_m = 1$  if p-values are independent,  $C_m = \sum_{i=1}^m \frac{1}{i}$  otherwise
- 3. Let  $T = P_{(R)}$ , the "rejection threshold"
- 4. Reject all  $H_{(0)}$  for which  $P_i \leq T$  (Weiss, 2005)

But this may over-correct.

## The Scientific Method

#### Develop General Theories

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#### Make Observations

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This can be from one's own experiences, thoughts or reading.

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If my hypothesis is correct, then I expect a, b, c, ...

#### Think of Interesting Questions

Why does that pattern occur?

# Formulate Hypotheses

What are the general causes of the phenomenon I am wondering about?

## The Scientific Method

Which steps are most subjective?

#### Develop General Theories

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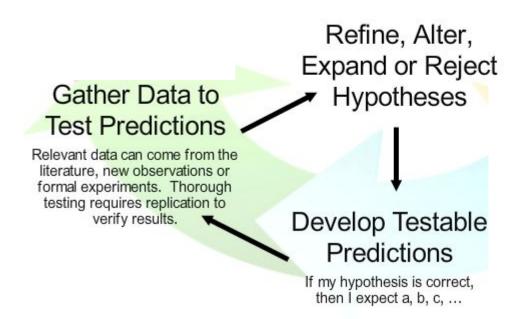
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Why does that pattern occur?

# Formulate Hypotheses

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# The Scientific Method Potential Effect from Big Data



### Hypothesis Testing

Terminology: "tails" -- is the rejection region made up of one or two sides of the rejection region?

Example: Comparing two means:

- two-tailed p-value: P(T > |t| or T < -|t|) = 2\*P(T > |t|)?
   (when there is no assumption of direction of difference)
- one-tailed p-value: P(T > t)? (when  $H_a$  posits the second mean is greater) P(T < t)? (when  $H_a$  posits the second mean is less)

#### Resampling Techniques

"nonparametric" tests

#### The permutation test:

- t<sub>obs</sub> = Compute observed score
- passes = 0
- for 1 to *B*:
  - o randomly permute the data, keeping the same sizes per class
  - $\circ$   $t_{B}$  = compute score on permuted data
  - $\circ$  if  $t_B > (or <) t_{obs}$ : passes+=1
- p\_value = passes/B

Application: comparing two distributions, especially when they are unknown.

Finding a linear function based on X to best yield Y.

X = "covariate" = "feature" = "predictor" = "regressor" = "independent variable"

Y = "response variable" = "outcome" = "dependent variable"

Regression: r(x) = E(Y|X = x)

goal: estimate the function r

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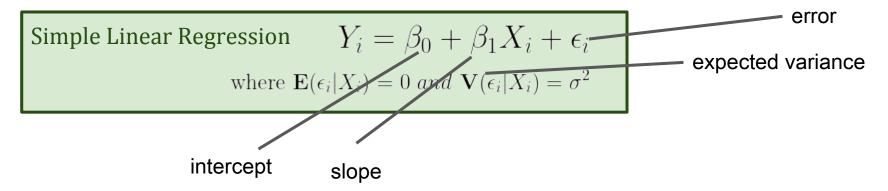
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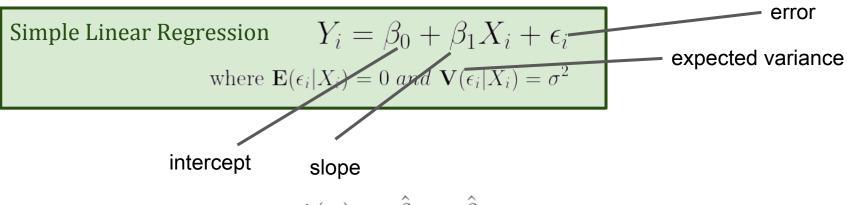
Linear Regression (univariate version):  $r(x) = \beta_0 + \beta_1 x$ 

goal: find  $\beta_0$ ,  $\beta_1$  such that  $r(x) \approx \mathrm{E}(Y|X=x)$ 

Simple Linear Regression 
$$Y_i=\beta_0+\beta_1X_i+\epsilon_i$$
 where  $\mathbf{E}(\epsilon_i|X_i)=0$  and  $\mathbf{V}(\epsilon_i|X_i)=\sigma^2$ 

$$r(x) = \beta_0 + \beta_1 x$$



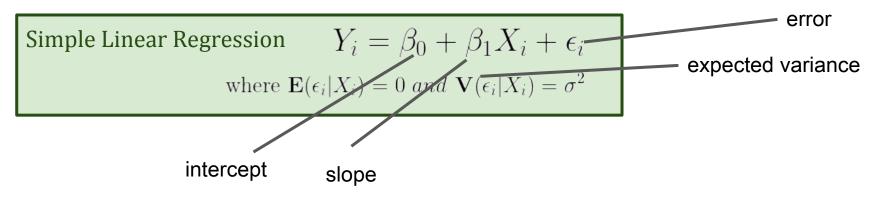


Estimated intercept and slope:  $\hat{r}(x) = \hat{eta}_0 + \hat{eta}_1 x$ 

$$\hat{Y}_i = \hat{r}(X_i)$$

Residual: —  $\hat{\epsilon}_i = Y_i - \hat{Y}_i$ 





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**Least Squares Estimate.** Find  $\hat{\beta}_0$  and  $\hat{\beta}_1$  which minimizes the residual sum of squares:

$$RSS = \sum_{i=1}^{n} \hat{\epsilon}_i^2 = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)^2$$

#### via Gradient Descent

Start with 
$$\hat{\beta}_0 = \hat{\beta}_1 = \mathbf{0}$$

Repeat until convergence:

Calculate all  $\hat{Y}_i$ 

$$\hat{\beta}_0 = \hat{\beta}_0 - \alpha \left(\sum_{i=1}^n \hat{Y}_i - Y_i\right)$$

$$\hat{\beta}_1 = \hat{\beta}_1 - \alpha (\sum_{i=1}^n X_i (\hat{Y}_i - Y_i))$$

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Learning rate

Based on derivative of RSS

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$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^n (X_i - \bar{X})^2}$$

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#### Pearson Product-Moment Correlation

#### Covariance

$$\begin{aligned} Cov(X,Y) &= \mathbf{E}(XY) - \mathbf{E}(X)\mathbf{E}(Y) \\ &= \mathbf{E}\left((X - \bar{X})(Y - \bar{Y})\right) \end{aligned}$$

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$$r = r_{X,Y} = \frac{Cov(X,Y)}{s_X s_Y}$$
$$= \frac{1}{n-1} \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{s_X}\right) \left(\frac{Y_i - \bar{Y}}{s_Y}\right)$$

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$$\hat{\beta}_{0} = \bar{Y} - \hat{\beta}_{1}\bar{X}$$

If one standardizes X and Y (i.e. subtract the mean and divide by the standard

deviation) before running linear regression, then:  $\hat{\beta}_0 = 0$  and  $\hat{\beta}_1 = r$ 

Suppose we have multiple independent variables that we'd like to fit to our dependent variable:  $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + ... + \beta_m X_{m1} + \epsilon_i$ 

If we include and  $X_{oi} = 1$  for all i (i.e. adding the intercept to X). Then we can say:

$$Y_i = \sum_{j=0}^m \beta_j X_{ij} + \epsilon_i$$

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 Or in vector notation across all i:  $Y = X\beta + \epsilon$ 

Where  $\beta$  and  $\epsilon$  are vectors and X is a matrix.

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Estimating  $\beta$ :

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To test for significance of individual Coefficient, *j*:

$$t = \frac{\hat{\beta}_{j}}{SE(\hat{\beta}_{j})} = \frac{\hat{\beta}_{j}}{\sqrt{\frac{s^{2}}{\sum_{i=1}^{n} (X_{ij} - \bar{X}_{j})^{2}}}}$$

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What if  $Y_i \in \{0, 1\}$ ? (i.e. we want "classification")

$$p_i \equiv p_i(\beta) \equiv \mathbf{P}(Y_i = 1|X = x) = \frac{e^{\beta_0 + \sum_{j=1}^m \beta_j x_{ij}}}{1 + e^{\beta_0 + \sum_{j=1}^m \beta_j x_{ij}}}$$

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Note: this is a probability here. In simple linear regression we wanted an expectation:

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(i.e. if p > 0.5 we can confidently predict  $Y_i = 1$ )

What if  $Y_i \in \{0, 1\}$ ? (i.e. we want "classification")

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$$logit(p_i) = log\left(\frac{p_i}{1 - p_i}\right) = \beta_0 + \sum_{j=1}^{m} \beta_j x_{ij}$$

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$$logit(p_i) = log\left(\frac{p_i}{1 - p_i}\right) = \beta_0 + \sum_{j=1}^m \beta_j x_{ij}$$

To estimate  $\beta$  , one can use

reweighted least squares:

set 
$$\hat{\beta}_0 = \dots = \hat{\beta}_m = 0$$
 (remember to include an intercept)

1. Calculate  $p_i$  and let W be a diagonal matrix where element  $(i, i) = p_i(1 - p_i)$ .

2. Set 
$$z_i = logit(p_i) + \frac{\hat{Y}_i - p_i}{p_i(1 - p_i)} = X\hat{\beta} + \frac{Y_i - p_i}{p_i(1 - p_i)}$$

- 3. Set  $\hat{\beta} = (X^T W X)^{-1} X^T W z$  //weighted lin. reg. of Z on Y.
- 4. Repeat from 1 until  $\hat{\beta}$  converges.

(Wasserman, 2005; Li, 2010)

#### Review: 3-3, 3-10

- Power
- Multi-test Correction: Bonferroni and Benjamini-Hochberg
- The Permutation Test
- "Tails"
- Regression goal and terminology
- Simple Linear Regression (Residual Sum of Squares)
- Multiple Linear Regression
- P-values for linear regression coefficients
- Logistic Regression: reweighted least squares

A lot can be answered with multiple linear regression

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_m X_{m1} + \epsilon_i$$

#### Mediation

Path Analyses (a type of "structured equation modeling")

How much does M mediate the effect of X on Y?

$$Y = \beta_{0c'b} + c'X + bM + \epsilon_{c'b}$$

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_m X_{m1} + \epsilon_i$$

#### Mediation

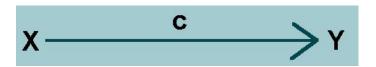
Path Analyses (a type of "structured equation modeling")

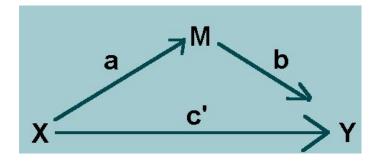
How much does M mediate the effect of X on Y?

$$Y = \beta_{0c} + cX + \epsilon_c$$

$$X = \beta_{0a} + aM + \epsilon_a$$

$$Y = \beta_{0c'b} + c'X + bM + \epsilon_{c'b}$$





(Kenney, 2015) http://davidakenny.net/cm/mediate.htm

#### Mediation

Path Analyses (a type of "structured equation modeling")

How much does M mediate the effect of X on Y?

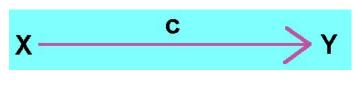
$$Y = \beta_{0c} + cX + \epsilon_c$$

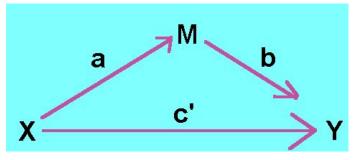
$$X = \beta_{0a} + aM + \epsilon_a$$

$$Y = \beta_{0c'b} + c'X + bM + \epsilon_{c'b}$$

Effect size: often reported as c - c'.

Used for \*basic\* causal inference.

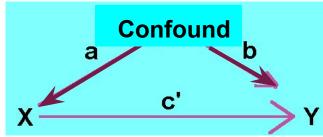




(Kenney, 2015) http://davidakenny.net/cm/mediate.htm

Problem: Sometimes variables at one unit of analysis are confounded by a

variable at another level.



Problem: Sometimes variables at one unit of analysis are *confounded* by a

Confound

variable at another level.

#### Examples:

Pot heads are more likely to say "hella"

but really californians are more like to say "hella" and be potheads.

X = use of "hella"

Y = pot-head or not

Confound = from california?

Problem: Sometimes variables at one unit of analysis are *confounded* by a variable at another level.

Confound

#### Examples:

Pot heads are more likely to say "hella"

but really californians are more like to say "hella" and be potheads.

Females are more likely to post pictures of food but really both food posts and females are more common on Pinterest.

Problem: Sometimes variables at one unit of analysis are *confounded* by a variable at another level.

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Solution: include aggregate confounding variable as a covariate in multiple linear regression. (also useful for prediction)

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_m X_{m1} + \epsilon_i$$

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Confound

$$Y = \beta_0 + \beta_1 X_1 + \beta_A A + \epsilon$$

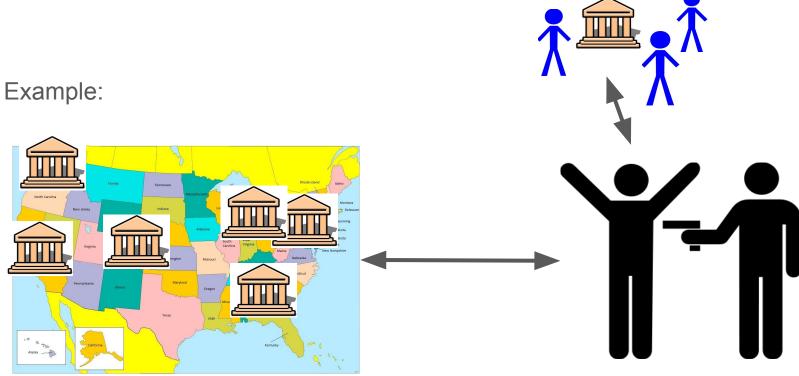
A : aggregate indicator variable (is in region or not? Pinterest usage).

Solution: include aggregate confounding variable as a covariate in multiple linear regression. (also useful for prediction)

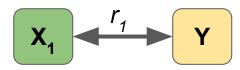
## **Ecological Fallacy**

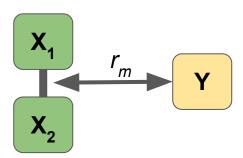
The assumption that an effect at one unit of analysis will hold for a smaller or

larger unit of analysis.



# Moderation (interaction)





When  $r_1 \neq r_m$ ,  $X_2$  moderates the relationship between  $X_1$  and Y.

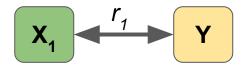
#### Examples:

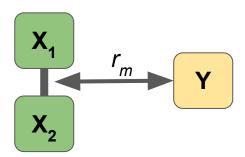
Y: Attend church?  $X_1$ : Agreeableness,  $X_2$ : From US?

#### Movie Reviews:

Y: Rated Depressing,  $X_1$ : "death" in review,  $X_2$ : Silly Horror Movie?

# Moderation (interaction)





When  $r_1 \neq r_m$ ,  $X_2$  moderates the relationship between  $X_1$  and Y.

More precisely moderation analyses fit the model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_M X_1 X_2 + \beta_2 X_2 + \epsilon$$

 $X_1X_2$ : The interaction term. (Element-wise multiplication)

 $\beta_{\rm M}$  can then be tested for significance using the same t-test we use for any individual coefficient in multiple linear regression

# Mediation, Moderation Code Examples



### Review: 3-22

- Mediation, path models
- HLM
- Moderation
- Ecological Fallacy

Examples:

Single class:

•  $X_1$ : Smoker or not(0/1)  $X_2$ : has cancer? (0/1)

• Y: Picture of goat? (0/1)  $\hat{Y}$ : prediction from a logistic model (0/1) or any model (e.g. a gradient boosting deep bayes neural forest)

#### Multi-class

• Y: word is subject, direct object, or indirect object (1, 2, or 3 but order means nothing)

 $\hat{Y}$ : prediction from a multi-class model

(a "multinomial" distribution)

- Chi-Square test for independence
- (true|false) (positive|negative) based metrics:

### Single class:

•  $X_1$ : Smoker or not(0/1)  $X_2$ : has cancer? (0/1)

N = 100 people sampled from cancer screening center population

	no cancer	cancer	
not smoker	60	10	
smoker	22	8	

### Single class:

•  $X_1$ : Smoker or not(0/1)  $X_2$ : has cancer? (0/1)

N = 100 people sampled from cancer screening center population

	no cancer	cancer	
not smoker	60	10	
smoker	22	8	

# Chi-Squared Test for Independence

 $H_0$ : Y and Z are independent  $H_1$ : Y and Z are dependent

$$U = \sum_{i=0}^{classes_{x1}} \sum_{j=0}^{classes_{x2}} \frac{(X_{ij} - E_{ij})^2}{E_{ij}}$$
where  $E_{ij} = \frac{X_{i*}X_{*j}}{n}$ 

	no cancer cancer		
not smoker	60	10	70
smoker	22	8	30
	82	18	100

## Chi-Squared Test for Independence

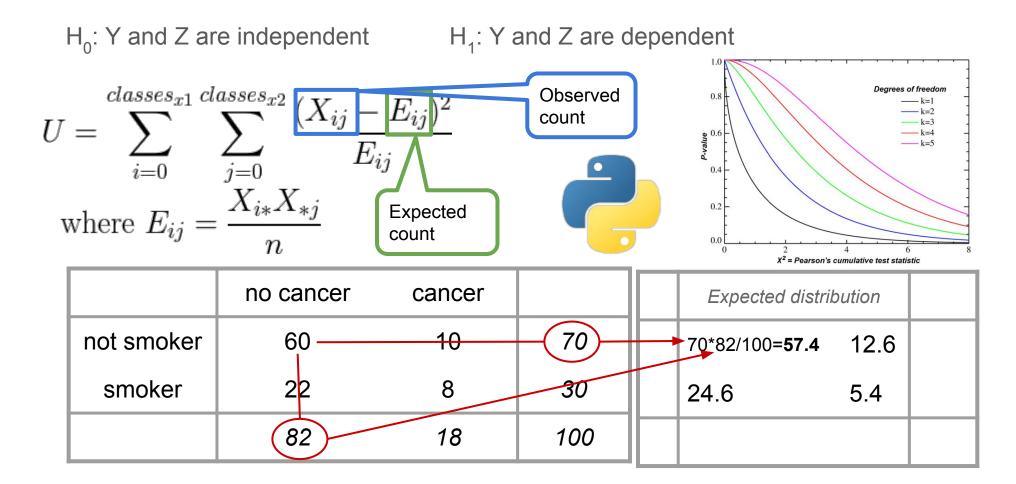
 $H_0$ : Y and Z are independent  $H_1$ : Y and Z are dependent

$$U = \sum_{i=0}^{classes_{x1}} \sum_{j=0}^{classes_{x2}} \underbrace{(X_{ij} - E_{ij})^2}_{E_{ij}}$$
 Observed count where  $E_{ij} = \frac{X_{i*}X_{*j}}{n}$  Expected count

	no cancer	cancer		Expected distribution		
not smoker	60	10	70	70*82/100 <b>=57.4</b>	12.6	
smoker	22	8	30	24.6	5.4	
	82	18	100			

# Chi-Squared Test for Independence

k = df (degrees of freedom) =  $(classes_{x1} - 1)(classes_{x2} - 1)$ 



- Chi-Square test for independence
- (true|false) (positive|negative) based metrics:

- Chi-Square test for independence
- (true|false) (positive|negative) based metrics:

		True condition		(Thank you,	
	Total population	Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Wikipedia!)
Predicted condition	Predicted condition positive	True positive	False positive (Type I error)	Positive predictive value (PPV), Precision $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Test outcome positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Test outcome positive}}$
	Predicted condition negative	False negative (Type II error)	True negative	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Test outcome negative}}$	Negative predictive value (NPV) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Test outcome negative}}$
	Accuracy (ACC) =	True positive rate (TPR), Sensitivity, Recall $= \frac{\sum \text{True positive}}{\sum \text{Condition positive}}$	False positive rate (FPR), $Fall-out$ $= \frac{\sum False\ positive}{\sum Condition\ negative}$	Positive likelihood ratio (LR+) $= \frac{TPR}{FPR}$	Diagnostic odds ratio (DOR)
	$\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	False negative rate (FNR), Miss rate $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) $= \frac{\sum \text{True negative}}{\sum \text{Condition negative}}$	Negative likelihood ratio $(LR-) = \frac{FNR}{TNR}$	$= \frac{LR+}{LR-}$

- Chi-Square test for independence
- (true|false) (positive|negative) based metrics:

		True condition			
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