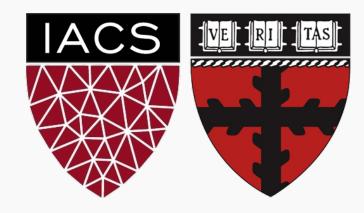
# Advanced Section #1: Linear Algebra and Hypothesis Testing

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#### CS109A Introduction to Data Science Pavlos Protopapas and Kevin Rader



#### WARNING

This deck uses animations to focus attention and break apart complex concepts.

Either watch the section video or read the deck in Slide Show mode.



Today's topics: Linear Algebra (Math 21b, 8 weeks) Maximum Likelihood Estimation (Stat 111/211, 4 weeks) Hypothesis Testing (Stat 111/211, 4 weeks) Our time limit: <u>90 minutes</u>

- We will move fast
- You are only expected to catch the big ideas
- Much of the deck is intended as notes
- I will give you the TL;DR of each slide
- We will recap the big ideas at the end of each section

- We'll work together
- I owe you this knowledge
- Come debt collect at OHs if I don't do my job today
- Let's do this : )



# LINEAR (THE HIGHLIGHTS) ALGEBRA

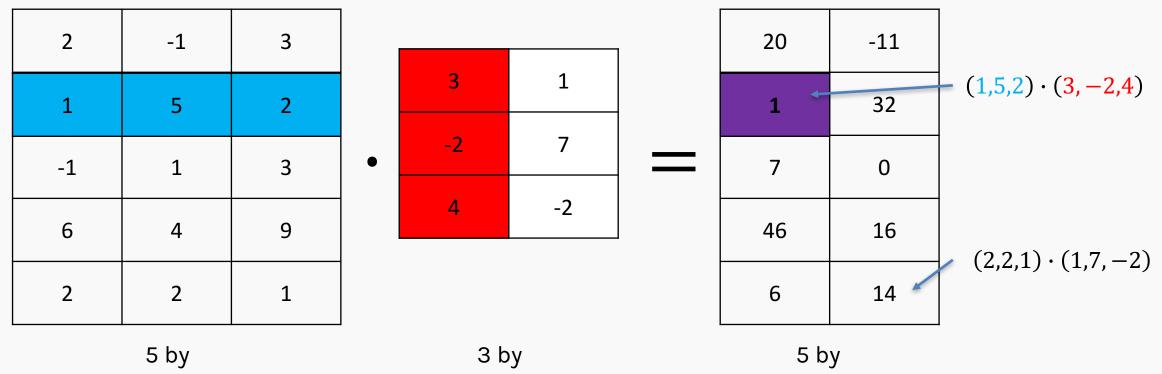
What does a dot product mean?

 $(1,5,2) \cdot (3,-2,4) = 1 \cdot (3) + 5 \cdot (-2) + 2 \cdot (4)$ 

- Weighted sum: We weight the entries of one vector by the entries of the other
  - Either vector can be seen as weights
  - Pick whichever is more convenient in your context
- **Measure of Length**: A vector dotted with itself gives the squared distance from (0,0,0) to the given point
  - $(1,5,2) \cdot (1,5,2) = 1 \cdot (1) + 5 \cdot (5) + 2 \cdot (2) = (1-0)^2 + (5-0)^2 + (2-0)^2 = 28$
  - (1,5,2) thus has length  $\sqrt{28}$
- **Measure of orthogonality**: For vectors of fixed length,  $a \cdot b$  is biggest when a and b point are in the same direction, and zero when they are at a 90° angle
  - Making a vector longer (multiplying all entries by c) scales the dot product by the same amount

**Question**: how could we get a true measure of orthogonality (one that ignores length?)

#### **Dot Product for Matrices**



Matrix multiplication is a bunch<sup>2</sup> of dot products

- In fact, it is every possible dot product, nicely organized
- Matrices being multiplied must have the shapes  $n, m \cdot m, p$  and the result is of size n, p

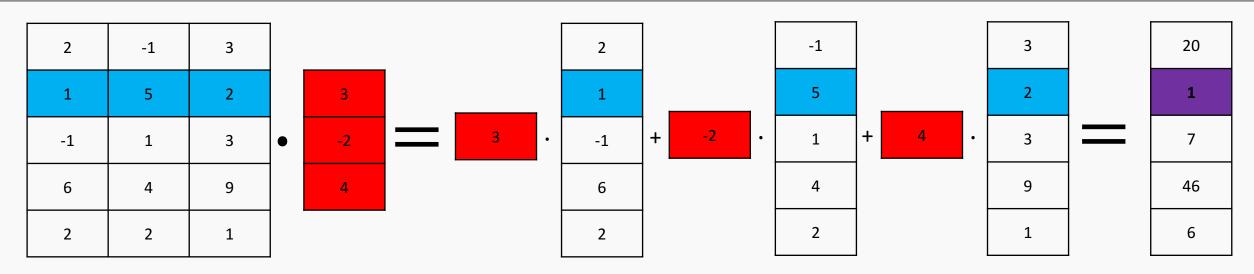
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• (the middle dimensions have to match, and then drop out)



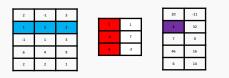
#### Column by Column

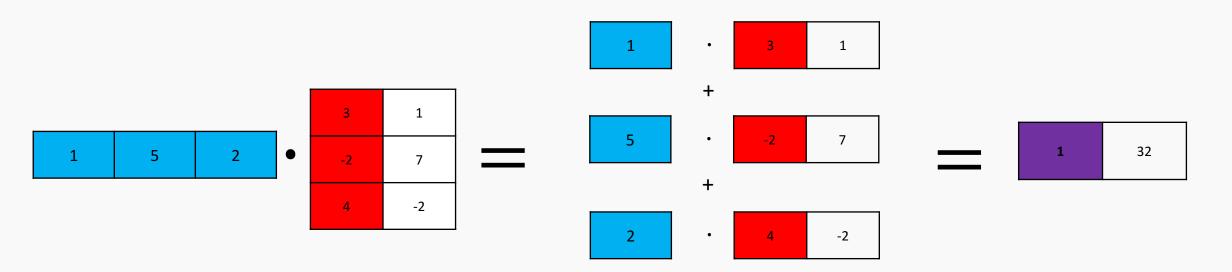




- Since matrix multiplication is a dot product, we can think of it as a weighted sum
  - We weight each column as specified, and sum them together
  - This produces the first column of the output
  - The second column of the output combines the same columns under different weights
- Rows?







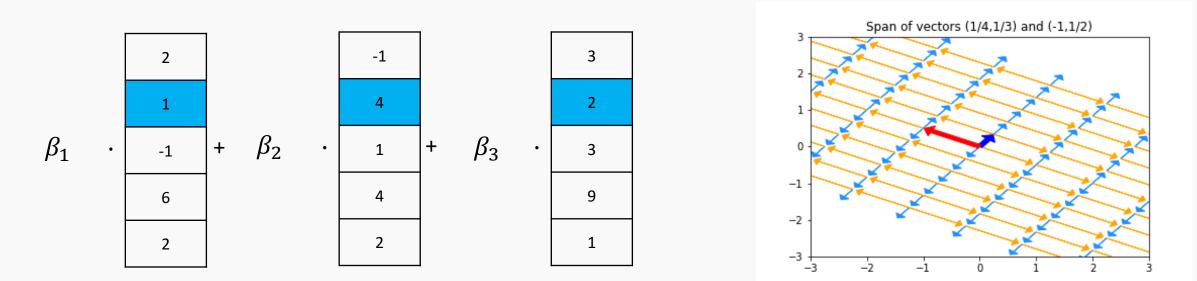
• Apply a row of A as weights on the rows B to get a row of output



# LINEAR (TI ALGEBRA

# (THE HIGHLIGHTS)

#### Span and Column Space

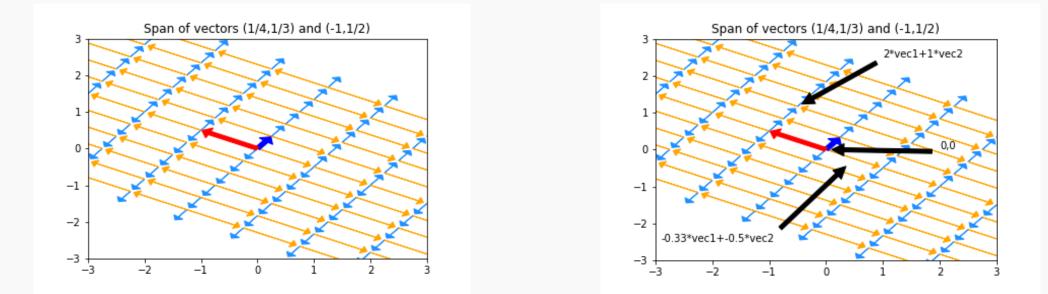


- **Span**: every possible linear combination of some vectors
  - If vectors are the columns of a matrix call it the **column space** of that matrix
  - If vectors are the rows of a matrix it is the **row space** of that matrix
- Q: what is the span of {(-2,3), (5,1)}? What is the span of {(1,2,3), (-2,-4,-6), (1,1,1)}



# LINEAR ALGEBRA

# (THE HIGHLIGHTS)



- Given a space, we'll often want to come up with a set of vectors that span it
- If we give a <u>minimal</u> set of vectors, we've found a **basis** for that space
- <u>A basis is a coordinate system for a space</u>
  - Any element in the space is a weighted sum of the basis elements
  - Each element has exactly one representation in the basis
- The same space can be viewed in any number of bases pick a good

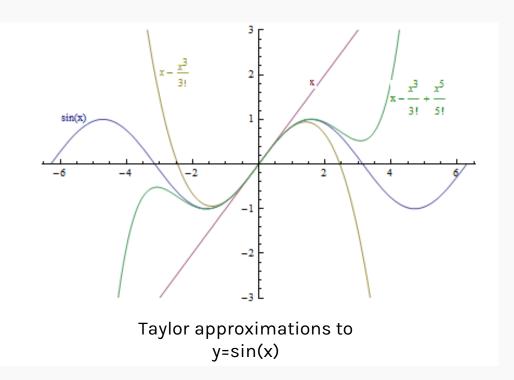


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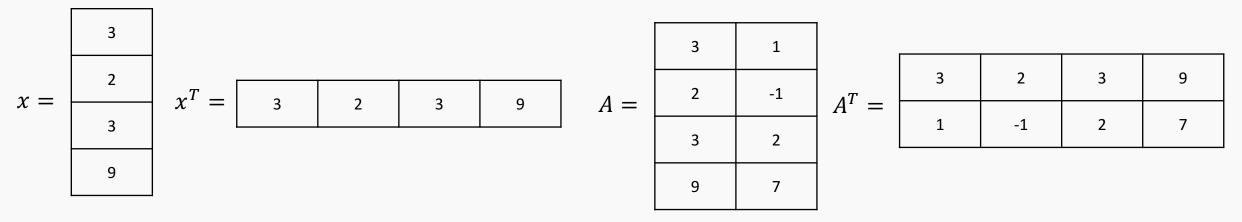
CS109A, Protopapas, Rader

## **Function Bases**

- Bases can be quite abstract:
  - Taylor polynomials express any analytic function in the infinite basis  $(1, x, x^2, x^3, ...)$
  - The Fourier transform expresses many functions in a basis built on sines and cosines
  - Radial Basis Functions express functions in yet another basis
- In all cases, we get an 'address' for a particular function
  - In the Taylor basis, sin(x) =۲  $(0,1,0,\frac{1}{6},0,\frac{1}{120},\dots)$
- Bases become super important in feature ۲ engineering
  - Y may depend on some transformation of x, but we only have x itself
  - We can include features  $(1, x, x^2, x^3, ...)$  to approximate



# LINEAR (THE HIGHLIGHTS)

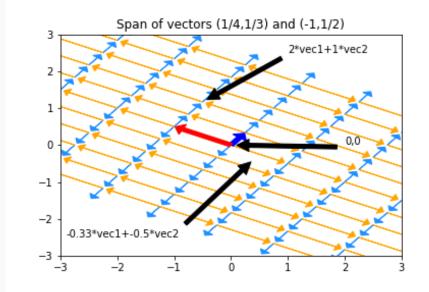


- Transposes switch columns and rows. Written  $A^T$
- Better dot product notation:  $a \cdot b$  is often expressed as  $a^T b$
- Interpreting: The matrix multiplilcation *AB* is rows of A dotted with columns of B
  - $A^T B$  is columns of A dotted with columns of B
  - $AB^T$  is rows of A dotted with rows of B
- Transposes (sort of) distribute over multiplication and addition:

$$(AB)^{T} = B^{T}A^{T}$$
  $(A+B)^{T} = A^{T} + B^{T}$   $(A^{T})^{T} = A$ 



- Algebraically,  $AA^{-1} = A^{-1}A = 1$
- Geometrically,  $A^{-1}$  writes an arbitrary point b in the coordinate system provided by the columns of A
  - Proof (read this later):
  - Consider Ax = b. We're trying to find weights x that combine A's columns to make b
  - Solution  $x = A^{-1}b$  means that when  $A^{-1}$ • multiplies a vector we get that vector's coordinates in A's basis
- Matrix inverses exist iff columns of the matrix form a basis
  - 1 Million other equivalents to invertibility: lacksquare**Invertible Matrix Theorem** CS109A, PROTOPAPAS, RADER



How do we write (-2,1) in this basis? Just multiply  $A^{-1}$  by (-2,1)

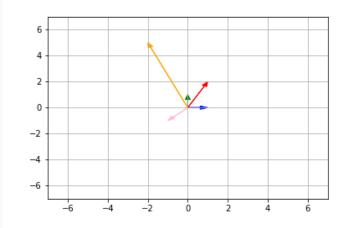


# LINEAR (THE HIGHLIGHTS)

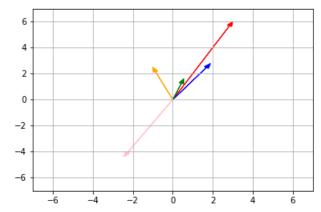
# Eigenvalues

- Sometimes, multiplying a vector by a matrix just scales the vector
  - The red vector's length triples
  - The orange vector's length halves
  - All other vectors point in new directions
- The vectors that simply stretch are called egienvectors. The amount they stretch is their eigenvalue
  - Anything along the given axis is an eigenvector; Here, (-2,5) is an eigenvector so (-4,10) is too
  - We often pick the version with length 1
- When they exist, eigenvectors/eigenvalues can be used to understand what a matrix does

#### Original vectors:



After multiplying by 2x2 matrix A:

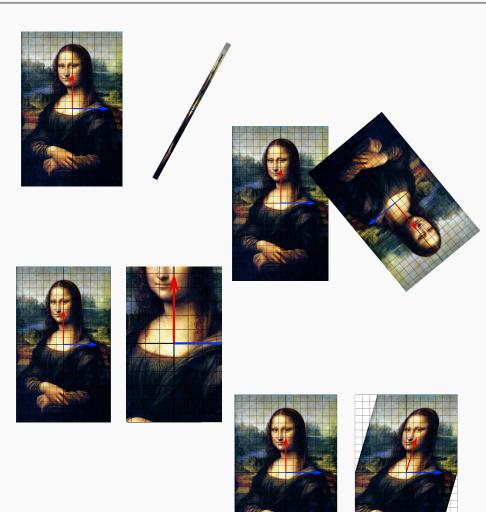




# Interpreting Eigenthings

Warnings and Examples:

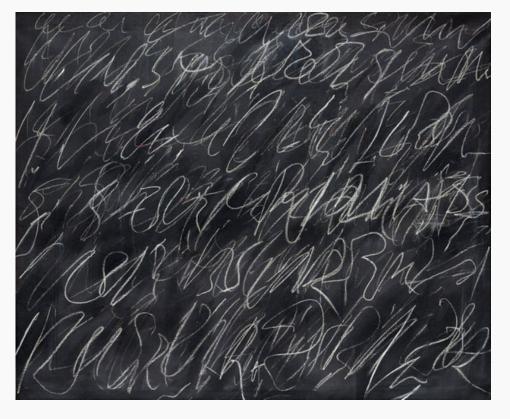
- Eigenvalues/Eigenvectors only apply to <u>square</u> matrices
- Eigenvalues may be 0 (indicating some axis is removed entirely)
- Eigenvalues may be complex numbers (indicating the matrix applies a rotation)
- Eigenvalues may be repeat, with one eigenvector per repetition (the matrix may scales some n-dimension subspace)
- Eigenvalues may repeat, with some eigenvectors missing (shears)
- <u>If</u> we have a full set of eigenvectors, we know everything about the given matrix S, and S = QDQ<sup>-1</sup>
  - Q's columns are eigenvectors, D is diagonal matrix of eigenvalues





# Calculating Eigenvalues

- Eigenvalues can be found by:
  - A computer program
- But what if we need to do it on a blackboard?
  - The definition  $Ax = \lambda x$ 
    - This says that for special vectors x, multiplying by the matrix A is the same as just scaling by λ (x is then an eigenvector matching eigenvalue λ)
  - The equation  $det(A \lambda I_n) = 0$ 
    - *I<sub>n</sub>* is the n by n identity matrix of size n by n. In effect, we subtract lambda from the diagonal of A
    - Determinants are tedious to write out, but
- Eigenvectors producting kolonomeigen values be found by solving  $(A \lambda I_n)x = 0$  for x be solved to find eigenvalues



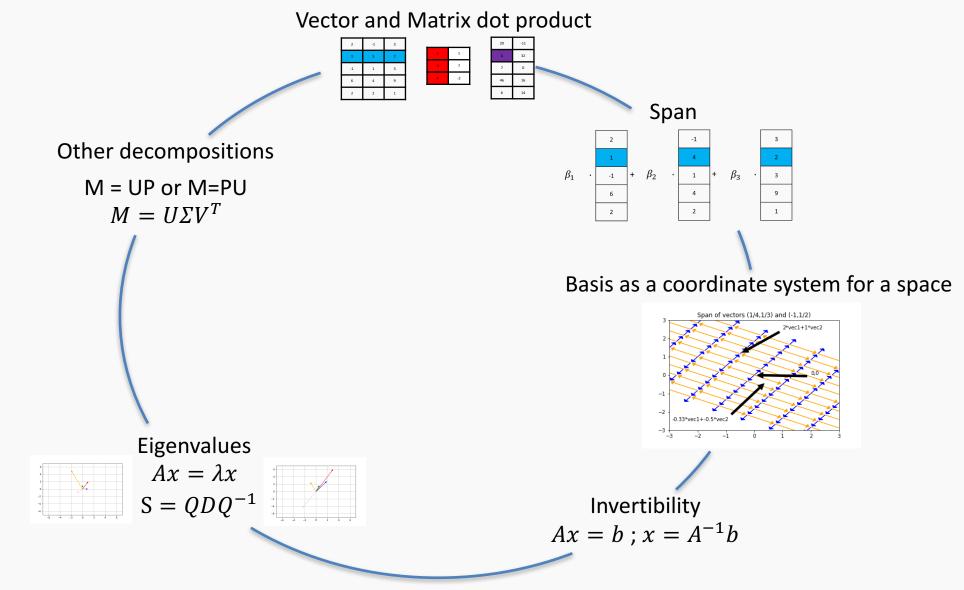
#### LINEAR Matrix Decomposition ALGEBRA

# (THE HIGHLIGHTS)

- **Eigenvalue Decomposition**: <u>Some square</u> matrices can be decomposed into scalings along particular axes
  - Symbolically: S = QDQ<sup>-1</sup>; D diagonal matrix of eigenvalues; Q made up of eigenvectors, but possibly wild (unless S was symmetric; then Q is orthonormal)
- **Polar Decomposition**: Every matrix M can be expressed as a rotation (which may introduce or remove dimensions) and a stretch
  - Symbolically: M = UP or M=PU; P positive semi-definite, U's columns orthonormal
- **Singular Value Decomposition**: Every matrix M can be decomposed into a rotation in the original space, a scaling, and a rotation in the final space
  - Symbolically:  $M = U\Sigma V^T$ ; U and V orthonormal,  $\Sigma$  diagonal (though not square)



#### Where we've been





- Simplify  $(A^TB)^T$ . What is in position 1,4? What does it mean if that value is large?
- What are the eigenvectors of  $A^2$ ? What are the eigenvalues?
- What does it mean when an entry of  $A^T A = 0$ ?
- What about all the facts about inverses and dot products I've forgotten since undergrad? [<u>Matrix Cookbook</u>] [<u>Linear Algebra Formulas</u>]



# LINEAR ALGEBRA

# (SUMMARY)

- Matrix multiplication: every dot product between rows of A and columns of B
  - Important special case: a matrix times a vector is a weighted sum of the matrix columns
- **Dot products** measure similarity between two vectors: 0 is extremely un-alike, bigger is pointing in the same direction and/or longer
  - Alternatively, a dot product is a weighted sum
- **Bases**: a coordinate system for some space. Everything in the space has a unique address
- Matrix Factorization: all matrices are rotations and stretches. We can decompose 'rotation and stretch' in different ways
  - Sometimes, re-writing a matrix into factors helps us with algebra
- Matrix Inverses don't always exist. The 'stretch' part may collapse a dimension.
   M<sup>-1</sup> can be thought of as the matrix that expresses a given point in terms of columns of M
- Span and Row/Column Space: every weighted sum of given vectors
- Linear (In)Dependence is just "can some vector in the collection be represented as a weighted sum of the others" if not, vectors are Linearly Independent

# LINEAR REGRESSION

AFTER A BREAK

## Review and Practice: Linear Regression

• In linear regression, we're trying to write our response data y as a linear function of our [augmented] features X

$$\begin{aligned} response &= \beta_1 feature_1 + \beta_2 feature_2 + \beta_3 feature_3 + \dots \\ y &= X\beta \end{aligned}$$

• Our response isn't actually a linear function of our features, so we instead find betas that produce a column  $\hat{y}$  that is as close as possible to y (in Euclidean distance)

$$\min_{\beta} \sqrt{(y - \hat{y})^T (y - \hat{y})} = \min_{\beta} \sqrt{(y - X\beta)^T (y - X\beta)}$$

- Goal: find that the optimal  $\beta = (X^T X)^{-1} X^T y$
- Steps:
  - 1. Drop the sqrt [why is that legal?]
  - 2. Distribute the transpose
  - 3. Distribute/FOIL all terms
  - 4. Take the derivative with respect to  $\beta$  (Matrix Cookbook (69) and (81): derivative of  $\beta^T a$  is  $a^T$ , ...)
  - 5. Simplify and solve for beta CS109A, PROTOPAPAS, RADER

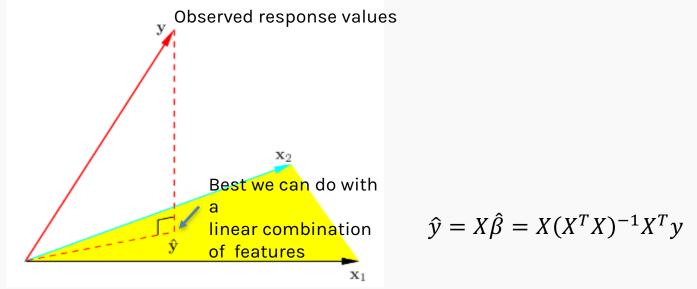
$$\hat{\beta} = (X^T X)^{-1} X^T y$$

• The best possible betas,  $\hat{\beta} = (X^T X)^{-1} X^T y$  can be viewed in two parts:

- Numerator (*X<sup>T</sup> y*): columns of X dotted with (the) column of y; how related are the feature vectors and y?
- Denominator (*X<sup>T</sup>X*): columns of X dotted with columns of X; how related are the different features?
- If the variables have mean zero, "how related" is literally "correlation"
- Roughly, our solution assigns big values to features that predict y, but punishes features that are similar to (combinations of) other features
- Bad things happen if  $X^T X$  is uninvertible (or nearly so)



### Interpreting LR: Geometry



- The only points that CAN be expressed as  $X\beta$  are those in the span/column space of X.
  - By minimizing distance, we're finding the point in the column space that is closest to the actual y vector
- The point  $X\hat{\beta}$  is the projection of the observed y values onto the things linear regression can express
- Warnings:
  - Adding more columns (features) can only make the span bigger and the fit better
  - If some features are very similar, results will be unstable



# STATISTICS

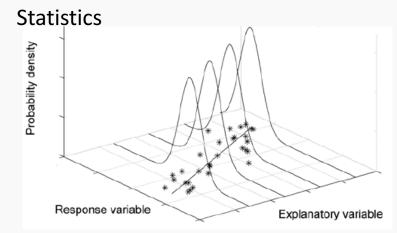
Linear Regression

#### ML to Statistics

- What we've done so far is the Machine Learning style of modeling:
  - Specify a loss function [Squared error] and a model format [y=Xβ]
  - Find the settings that minimize the loss function

- Statistics adds more assumptions and gets back richer results
  - Adds assumptions about where the data came from
  - We can ask "What about other beta values? On a different day, might we get that result instead?"
  - Statistics can answer yes/no via our assumptions about where the data come from

#### Machine Learning loss loss $-5 \times 10^7$ $-1 \times 10^8$ -400 $\beta_1$ 200 400 200 $\beta_2$ -200 -200 $\beta_2$ -200-20





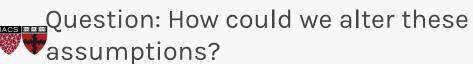
# Statistical Assumptions

What are Statistics' assumptions about the linear regression data?

- The observed X values simply are.
- The observed y come from a *Normal(mu(x), sigma)* distribution, mu(x) is linear, and each y is drawn independently from the others
  - For all observations i:  $y_i \sim N(x_i\beta, \sigma^2)$
  - Equivalently, column y  $y \sim N_{mv}(X\beta, \sigma^2 I_n)$

Why these assumptions?

- Any story about how the X data came to be is problem-dependent
- Makes the problem solvable using 1800s era tools



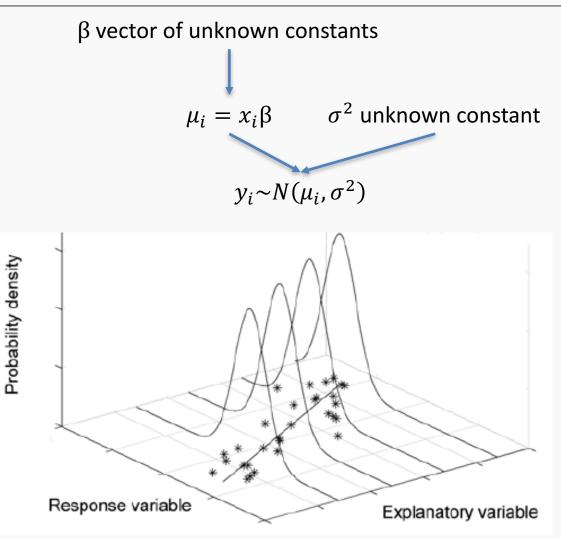


Image from: http://bolt.mph.ufl.edu/6050-6052/unit-4b/module-15/

#### Maximum Likelihood: the other ML

• We need to guess at the unknown values ( $\beta$  and  $\sigma^2$ )

Maximum Likelihood

- Rule: Guess whatever values of the unknowns make the observed data as probable as possible
  - As a loss function, we feel pain when the data surprise the model
- Only works if we have a likelihood function
  - Likelihood maps (dataset) -> (probability of seeing that dataset); uses parameter values (e.g.  $\beta$  and  $\sigma^2$ ) in the calculation
  - Actually maximizing can be hard
- But, Maximum Likelihood can be shown to be a very good guessing strategy, especially with lots of observations (see Stat 111 or 211)



#### Maximum Likelihood: the other ML

- Likelihood (Probability of seeing data y, given parameters X,  $\beta$ , and  $\sigma^2$ ):

$$P(Y = y | X, \beta, \sigma^2) = N(X\beta, \sigma^2 I_n) = \frac{1}{\sqrt{2\pi |\sigma^2 I_n|}} e^{-\frac{1}{2}(y - X\beta)^T (\sigma^2 I_n)^{-1} (y - X\beta)}$$

- Since X is constant, we're maximizing by choosing the vector  $\beta$  and scalar  $\sigma^2$
- Finding optimal  $\beta$  quickly reduces to the least squares problem we just saw:  $\min_{\beta} (y - X\beta)^T (y - X\beta)$
- Optimal  $\sigma^2 = \frac{\text{residuals under the optimal }\beta}{(\text{number of observations number of features})}$



- We actually get the joint distribution of the betas:  $\beta_{MLE} \sim N(\beta_{True}, \sigma^2 (X^T X)^{-1})$
- HW investigates the variance term: how well we can learn each beta, and whether one is linked to another
  - It depends on X!
  - It doesn't depend on y! (If our assumptions are correct
- Lets us attach error bars to our estimates, e.g.  $\beta_1 = 3 \pm .2$

• Main question: What can we do to our X matrix to



- We can add assumptions about where the data came from and get richer statements from our model
- A Likelihood is a function that tells us how likely any given dataset is. Plug in data, get a probability
- The MLE finds the parameter settings that make our data as likely as possible
- Finding the MLE parameter values can be hard, sometimes possible via calculus, often requires computer code



# **STATISTICS: HYPOTHESIS TESTING**

OR: WHAT PARAMETERS EXPLAIN THE DATA

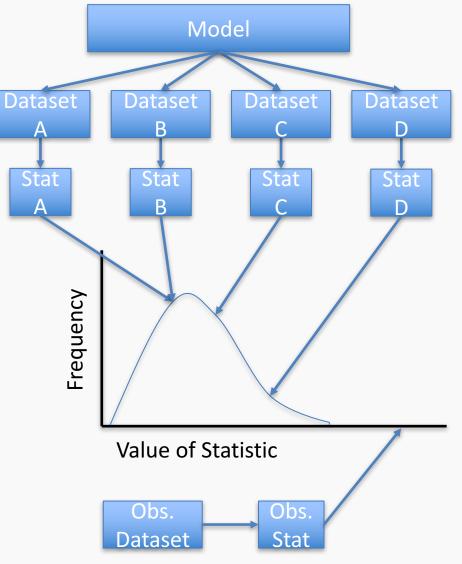
- It's impossible to prove a model is correct
  - In fact, there are many correct models
  - Can you prove increasing a parameter by .0000001% is incorrect?
- We can only rule models out.
- The great tragedy is that you have been taught to rule out just ONE model, and then quit





### Model Rejection

- Important: a 'model' is a (probabilistic) story about how the data came to be, complete with specified values of every parameter
  - The model produces many possible datasets
  - We only have one observed dataset
- How can we tell if a model is wrong?
  - If the model is unlikely to reproduce the aspects of the data that we care about, it has to go
  - Therefore, we have some real-number summary of the dataset (a 'statistic') by which we'll compare model-generated datasets and our observed dataset
  - If the statistics produced by the model are clearly different than the one from the real



#### Recap: How to understand any test

- Any model test specifies:
  - 1. A (probabilistic) data generating process
  - 2. A summary we'll use to compress a dataset
  - 3. A rule for comparing the observed and the simulated summaries
- Example: t-test
  - The y data are generated via the estimated line/plane, plus Normal(0,sigma) noise,

EXCEPT a particular coefficient is actually zero!

2. The coefficient we'd calculate for that dataset (minus 0), over the SE of the coefficient

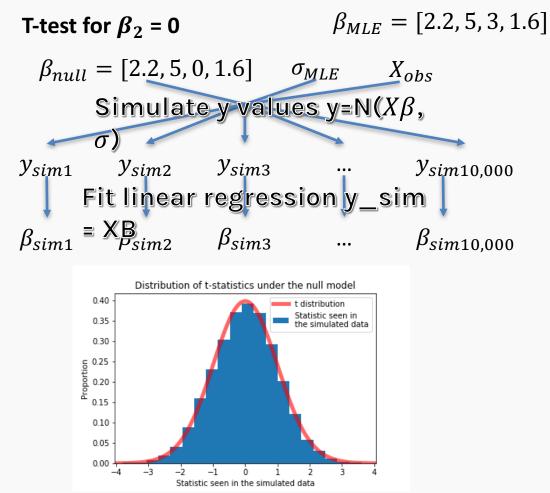
## t statistic = $\frac{\beta_{Simulated} - 0}{\widehat{SE}(\beta_{0bserved})}$

 Declare the model bad if the observed result is in the top/bottom α% of simulated results (commonly top/bottom 5%)



(Jargon: the null hypothesis) (Jargon: a statistic) Walkthrough:

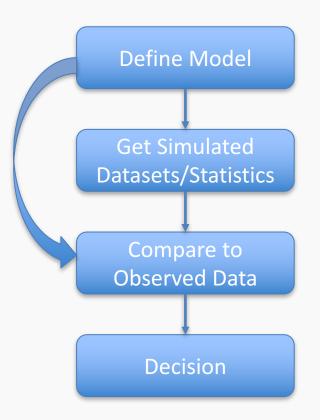
- We set a particular beta we care about to zero (call these betas  $\beta_{null}$ )
- We simulate 10,000 new datasets using  $\beta_{null}$  as truth
- In each of the 10,000 datasets, fit a regression against X and plot the values of the β we care about (the one we set to zero)
  - The plotting the t statistic in each simulation is a little prettier
- The t statistic calculated from the observed data was 17.8. Do we think the proposed model generated our data
- the proposed model generated our data?
  One more thing: Amazingly, 'Student' knew what results we'd get from the simulation





### The Value of Assumptions

- Student's clever set-up lets us skip the simulation
- In fact, all classical tests are built around working out what distribution the results will follow, without simulating
  - Student's work lets us take infinite samples at almost no cost
- These shortcuts were *vital* before computers, and are still important today
  - Even so, via simulation we're freer to test and reject more diverse models and use wilder summaries
  - However, the summaries and rules we choose still require thought: some are *much* better than others

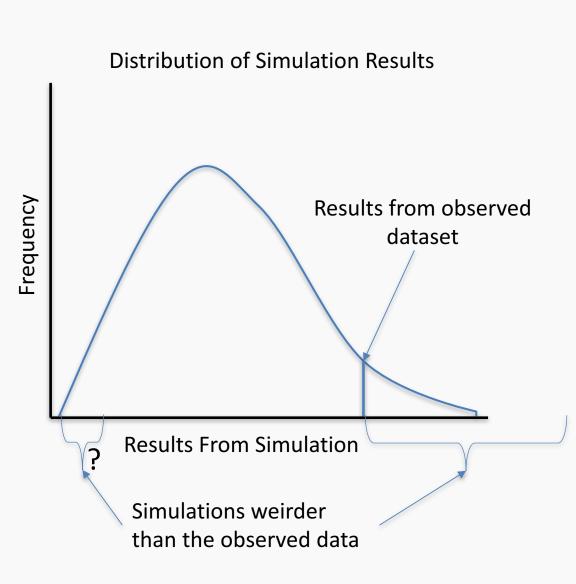


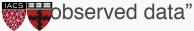


### p-values

- Hypothesis (model) testing leads to comparing a distribution against a point
- A natural way to summarize: report what percentage of results are more extreme than the observed data
  - Basically, could the model frequently produce data that looks like ours?
- This is the p value: p=.031 means that your observed data is in the top 3.1% of weird results under this model+statistic
  - There is some ambiguity about what 'weird' should mean

Jargon: p values are "The probability, assuming the null model is exactly true, of seeing a value of [your statistic] as extreme or more extreme than what was seen in the





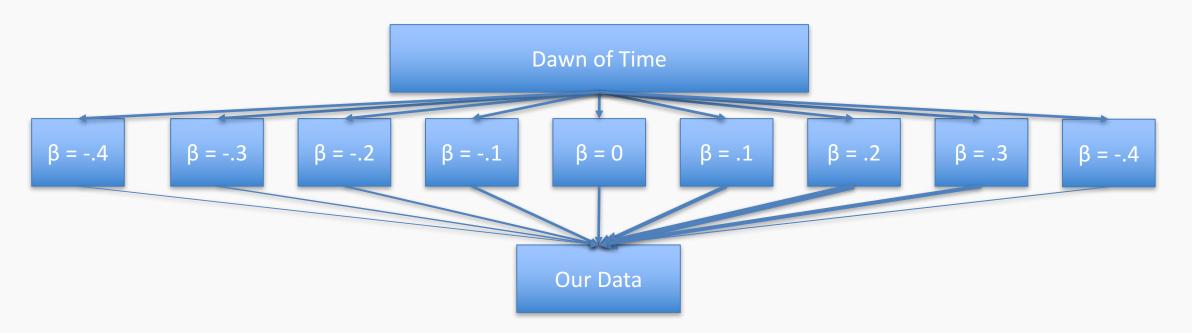
- p values are only one possible measure of the evidence against a model
- Rejecting a model when p<threshold is only one possible decision rule</li>
  - Get a book on Decision Theory for more
- Even if the null model is exactly true, 5% of the time, we'll get a dataset with p<.05
  - p<.05 doesn't prove the null model is wrong
  - It does mean that anyone who wants to believe in the null must explain with why something unlikely happened



- We can't rule models in; we can only rule them out
- We rule models out when the data they produce is different from the observed data
  - We pick a particular candidate (null) model
  - A statistic summarizes the simulated and observed datasets
  - We compare the statistic on the observed data to the simulated or theoretical distribution of statistics the null produces
  - We rule out the null if the observed data doesn't seem to come from the model
- A p value summarizes the level of evidence against a particular null
  - "The observed data are in the top 1% of results produced by this model... do you really think we hit those odds?"

# **STATISTICS: HYPOTHESIS TESTING**

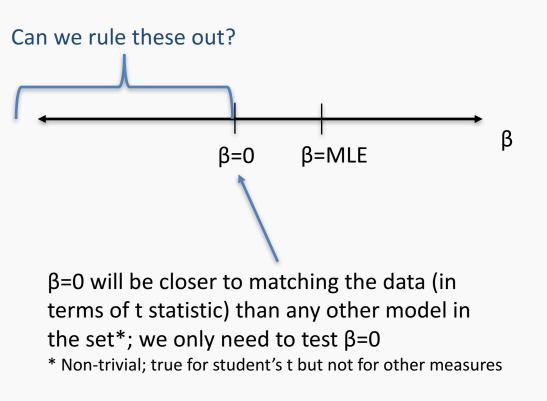
CONFIDENCE INTERVALS AND COMPOSITE HYPOTHESES



- Let's talk about what we just did
  - That t-test was ONLY testing the model where the coefficient in question is set to zero
  - Ruling out this model makes it more likely that other models are true, but doesn't tell us which ones
  - If the null is  $\beta$  = 0, getting p<.05 only rules out THAT ONE model
- When would it make sense to stop after ruling out  $\beta = 0$ , without testing  $\beta = .1$ ?

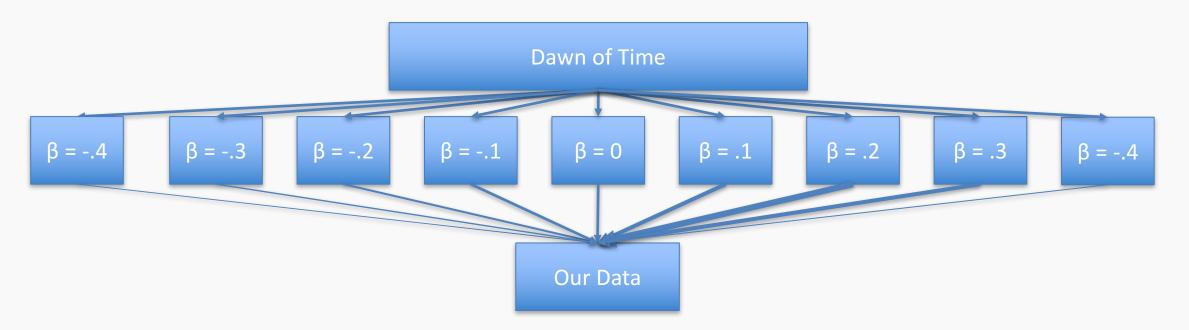
### Composite Hypotheses: Multiple Models

- Often, we're interested in trying out more than one candidate model
  - E.g. Can we disprove all models with a negative value of beta?
  - This amounts to simulating data from each of those models (but there are infinitely many...)
- Sometimes, ruling out the nearest model is enough; we know that the other models have to be worse
- If a method claims it can test θ<0, this is how





### THE Null vs A Null



- What if we tested LOTS of possible values of beta?
  - Special conditions must hold to avoid multiple-testing issues; again, the t test model+statistic pass them
- We end up with a set/interval of surviving values, e.g. [.1,.3]
  - Sometimes, we can directly calculate what the endpoints would be
- Since each beta was tested under the rule "reject this beta if the observed results are in the top 5% of weird datasets under this model", we have [.1,.3] as a 95% confidence
   interval



### Confidence Interval Warnings

- WARNING: This kind of accept/reject confidence interval is rare
  - Most confidence intervals <u>do not</u> map accept/reject regions of a (useful) hypothesis test
  - A confidence interval that excludes zero does not usually mean a result is statistically significant
    - Statistically significant: The data resulting from an experiment/data collection have p<.05 (or some other threshold) against a no-effect model, meaning we reject the no-effect model
  - It depends on how that confidence interval was built
- A confidence interval's <u>only</u> promise: if you were to repeatedly recollect the data and build 95% CIs, (assuming our story about data generation is correct) 95% of the intervals would contain the true value



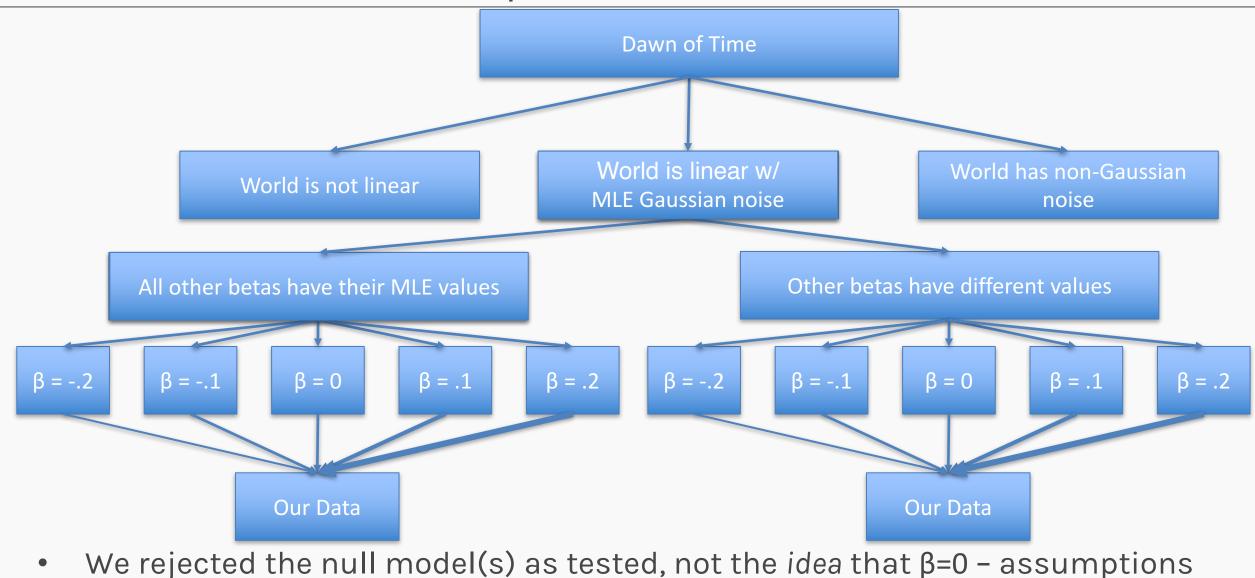
- WARNING: A 95% confidence interval DOES NOT have a 95% chance of holding the true value
  - There may be no such thing as "the true value", b/c the model is wrong
- Even if the model is true, a "95% chance" statement requires prior assumptions about how nature sets the true value
- Stick around after section for a heartbreaking demo of why a group of confidence intervals make 95% but any particular CI can be 0%, 100%, or anything in between

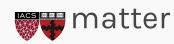


- The 209 homework touches on another kind of confidence interval
  - Class: "How well have I estimated beta?"
  - HW: "How well can I estimate the mean response at each X?"
  - Bonus: "How well can I estimate the possible responses at each X"?



#### Remember those assumptions?





- Ruling out a single model isn't much
- Sometimes, ruling out a single model is enough to rule out a whole class of models
- Assumptions our model makes are weak points that should be justified and checked for accuracy
- Confidence intervals give a reasonable idea of what some unknown value might be
- Any single confidence intervals cannot give a probability
- Statistical significance is 99% unrelated to confidence intervals



# **STATISTICS: REVIEW**

You made it!

#### Review

- To test a particular model (a particular set of parameters) we must:
  - 1. Specify a data generating process
  - 2. Pick a way to measure whether our data plausibly comes from the process
  - **3.** Pick a rule for when a model cannot be trusted (when is the range of simulated results too different from the observed data?)
- What features make for a good test?
  - We want to make as few assumptions as possible, and choose a measure that is sensitive to deviations from the model
  - If we're clever, we might get math that lets us skip simulating from the model
  - Tension: more assumptions make math easier, fewer assumptions make results broader
- There is no such thing as THE null hypothesis. It's only **A** null hypothesis.
  - A p value only tests one null hypothesis and is rarely enough

As the course moves on, we'll see

- Flexible assumptions about the data generating process
  - Generalized Linear Models
- Ways of making fewer assumptions about the data generating process:
  - Bootstrapping
  - Permutation tests
- Easier questions: Instead of 'find a model that explains the world', 'pick the model that predicts best'
  - Validation sets and cross validation





Office hours are:

Monday 6-7:30 (Camilo) Tuesday 6:30-8 (Will)



- Need a volunteer
  - I'll explain the rules and you'll write down some letter between A and H
- Everyone else: go to Random.org and get a random number between 1 and 10
- If your number was \_\_\_\_your wining letters are:
  1: G,H,I,J,A,B,C,D,E
  2: E,F,G,H,I,J,A,B,C
  3: D,E,F,G,H,I,J,A,B
  4: J,A,B,C,D,E,F,G,H
  5: B,C,D,E,F,G,H,I,J

