Advanced Section #1: Linear Algebra and Hypothesis Testing

CS109A Introduction to Data Science

Pavlos Protopapas, Kevin Rader and Chris Tanner

Presentation prepared by Will Claybaugh for CS109A 2018

Advanced Section 1

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.

Advanced Section 1

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: 75 minutes

- 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

LINEAR ALGEBRA

(THE HIGHLIGHTS)

Interpreting the dot product

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

2	-1	3
1	5	2
-1	1	3
6	4	9
2	2	1

5 by 3

•

3	1
-2	7
4	-2

3 by 2

=

20	-11
1	32
7	0
46	16
6	14

5 by 2

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

$(2,2,1) \cdot (1,7,-2)$

Matrix multiplication is a bunch of dot products

- In fact, it is every possible dot product, nicely organized
- Matrices being multiplied must have the shapes $(n, m) x\ (m, p)$ and the result is of size (n, p)
  - (the middle dimensions have to match, and then drop out)

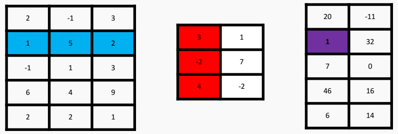
Column by Column

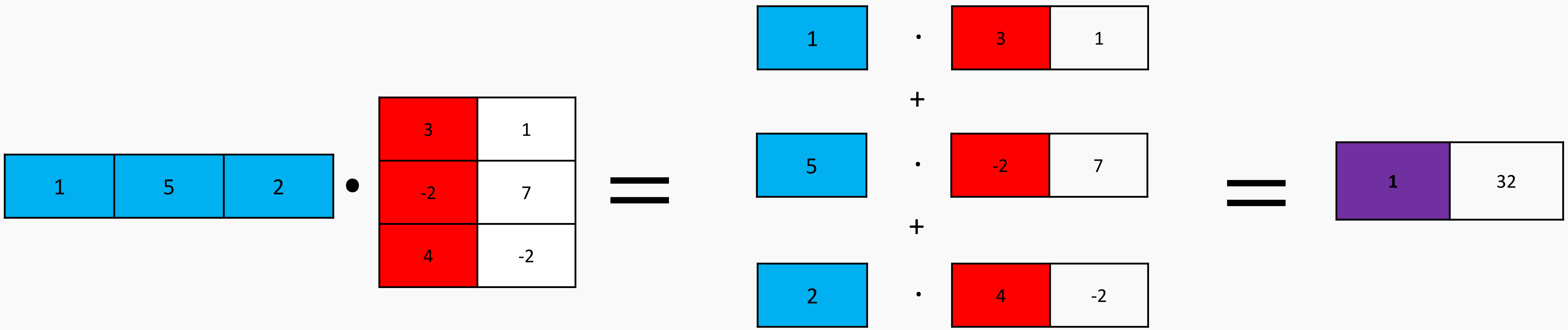
$$\begin{bmatrix} 2 & -1 & 3 \\ 1 & 5 & 2 \\ -1 & 1 & 3 \\ 6 & 4 & 9 \\ 2 & 2 & 1 \end{bmatrix} \begin{bmatrix} 3 & 1 \\ -2 & 7 \\ 4 & -2 \end{bmatrix} \begin{bmatrix} 20 & -11 \\ 1 & 32 \\ 7 & 0 \\ 46 & 16 \\ 6 & 14 \end{bmatrix}$$

$$\begin{bmatrix} 2 & -1 & 3 \\ 1 & 5 & 2 \\ -1 & 1 & 3 \\ 6 & 4 & 9 \\ 2 & 2 & 1 \end{bmatrix} \bullet \begin{bmatrix} 3 \\ -2 \\ 4 \end{bmatrix} = 3 \cdot \begin{bmatrix} 2 \\ 1 \\ -1 \\ 6 \\ 2 \end{bmatrix} + -2 \cdot \begin{bmatrix} -1 \\ 5 \\ 1 \\ 4 \\ 2 \end{bmatrix} + 4 \cdot \begin{bmatrix} 3 \\ 2 \\ 3 \\ 9 \\ 1 \end{bmatrix} = \begin{bmatrix} 20 \\ 1 \\ 7 \\ 46 \\ 6 \end{bmatrix}$$

- 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?

Row by Row





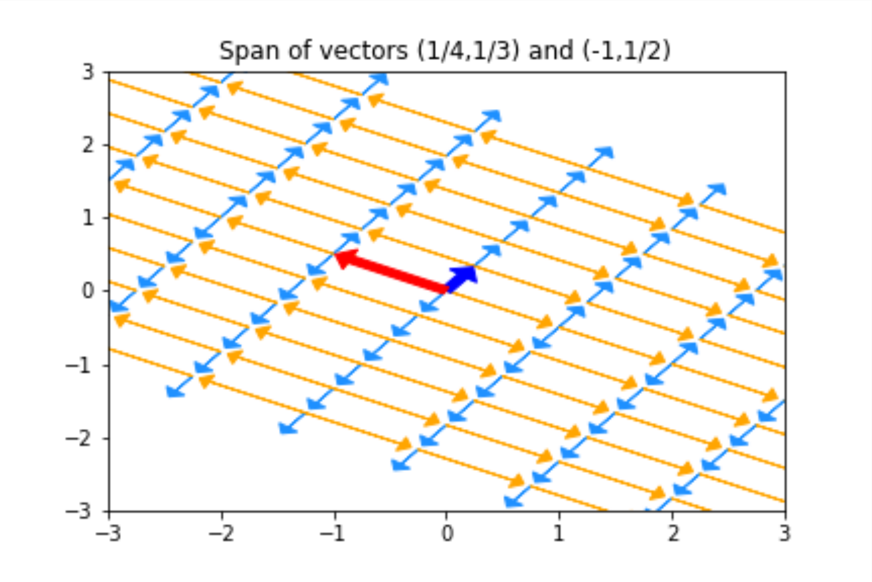
- Apply a row of A as weights on the rows B to get a row of output

Span

LINEAR ALGEBRA **(THE HIGHLIGHTS)**

Span and Column Space

$$\beta_1 \cdot \begin{bmatrix} 2 \\ 1 \\ -1 \\ 6 \\ 2 \end{bmatrix} + \beta_2 \cdot \begin{bmatrix} -1 \\ 4 \\ 1 \\ 4 \\ 2 \end{bmatrix} + \beta_3 \cdot \begin{bmatrix} 3 \\ 2 \\ 3 \\ 9 \\ 1 \end{bmatrix}$$



- **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

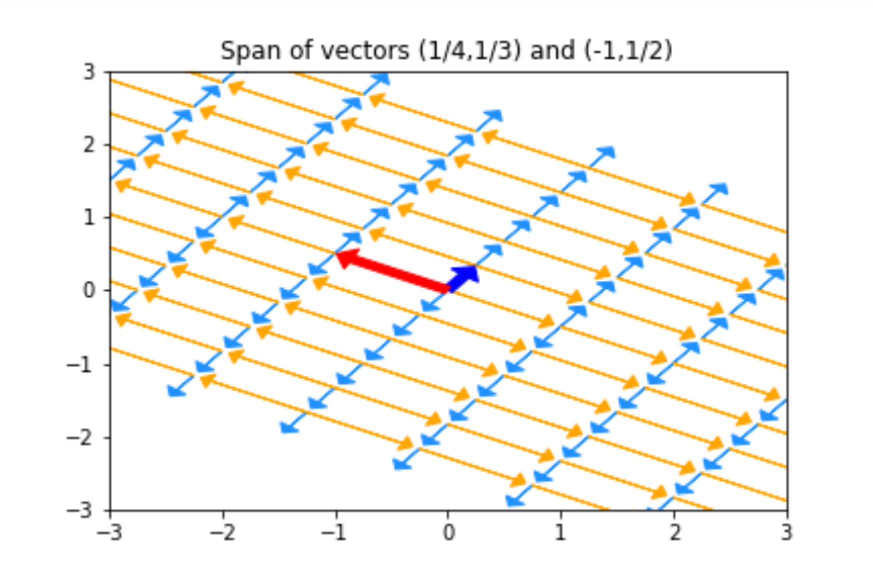
- Q: what is the span of {(-2,3), (5,1)}? What is the span of {(1,2,3), (-2,-4,-6), (1,1,1)}

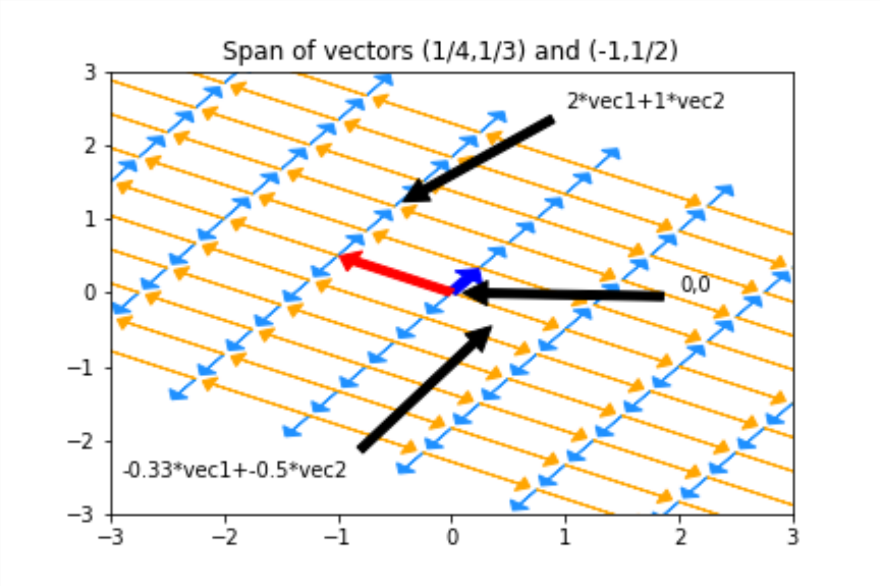
Bases

LINEAR ALGEBRA

(THE HIGHLIGHTS)

Basis Basics

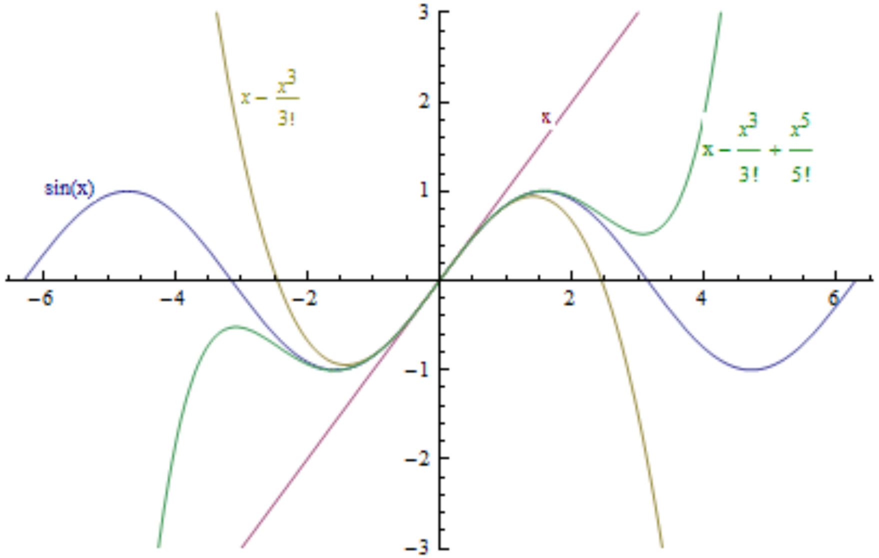




- Given a space, we'll often want to come up with a set of vectors that span it
- If we give a <u>minimal</u> set of vectors, we've found a **basis** for that space
- <u>A basis is a coordinate system for a space</u>
    - Any element in the space is a weighted sum of the basis elements
    - Each element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

Function Bases

- Bases can be quite abstract:
  - Taylor polynomials express any analytic function in the infinite basis $(1, x, x^2, x^3, \ldots)$
  - 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, $\sin(x) = (0,1,0,\frac{1}{6},0,\frac{1}{120},\ldots)$
- Bases become super important in feature engineering
  - Y may depend on some transformation of x, but we only have x itself
  - We can include features $(1, x, x^2, x^3, \ldots)$ to approximate



Taylor approximations to y=sin(x)

Interpreting Transpose and Inverse

LINEAR ALGEBRA

(THE HIGHLIGHTS)

Transpose

$x =$

3
2
3
9

$x^T =$

3	2	3	9

$A =$

3	1
2	-1
3	2
9	7

$A^T =$

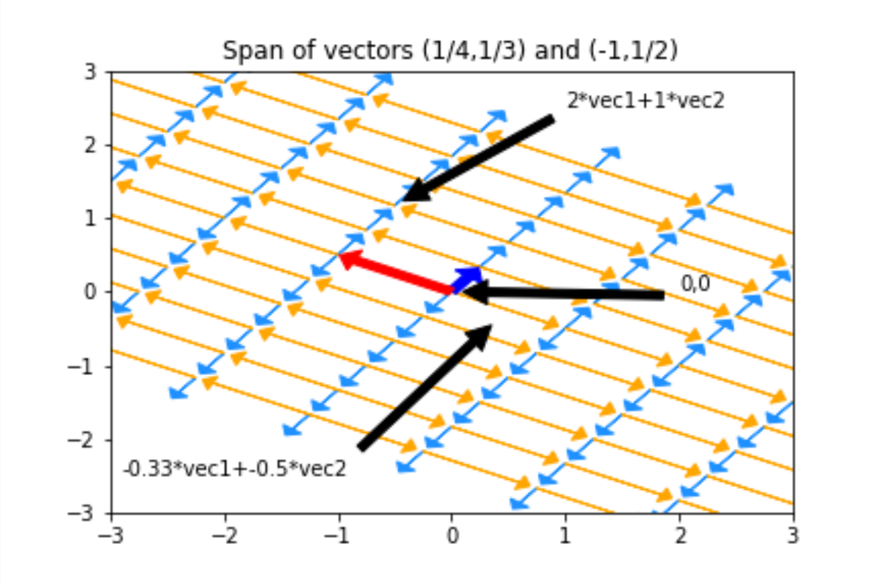
3	2	3	9
1	-1	2	7

- 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:

$$(AB)^T = B^T A^T \qquad (A+B)^T = A^T + B^T \qquad (A^T)^T = A$$

Inverses

- 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: [Invertible Matrix Theorem]



How do we write (-2,1) in this basis?

Just multiply A^{-1} by (-2,1)

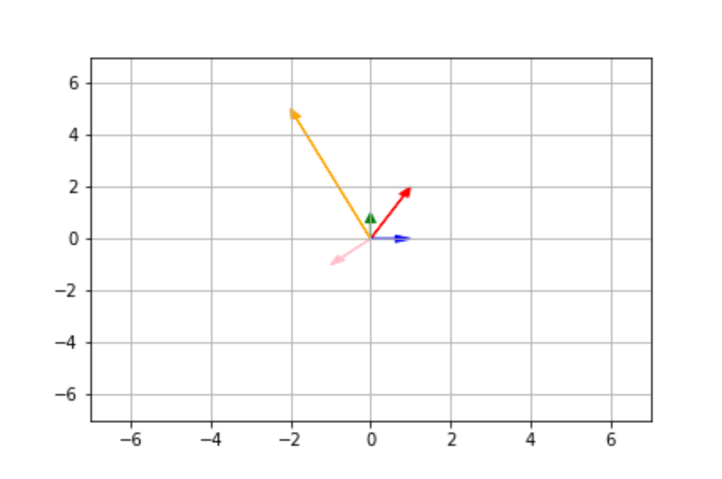
Eigenvalues and Eigenvectors

LINEAR ALGEBRA (THE HIGHLIGHTS)

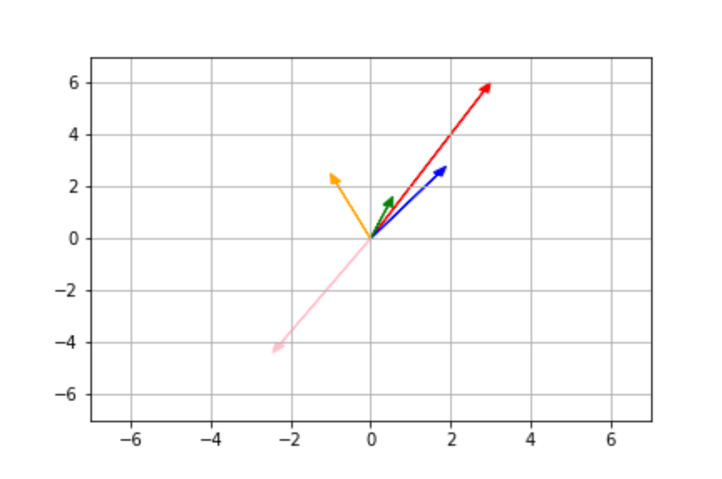
Eigenvalues

- 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:

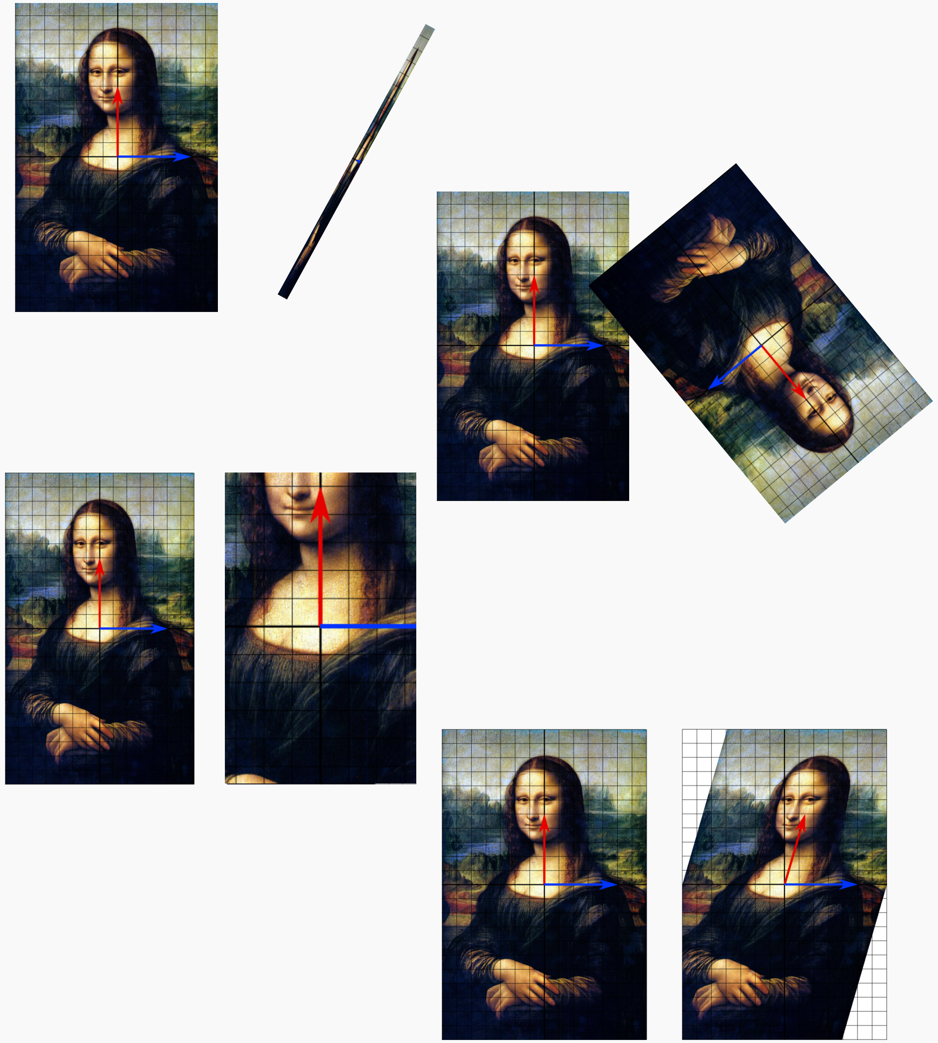


Interpreting Eigenthings

Warnings and Examples:

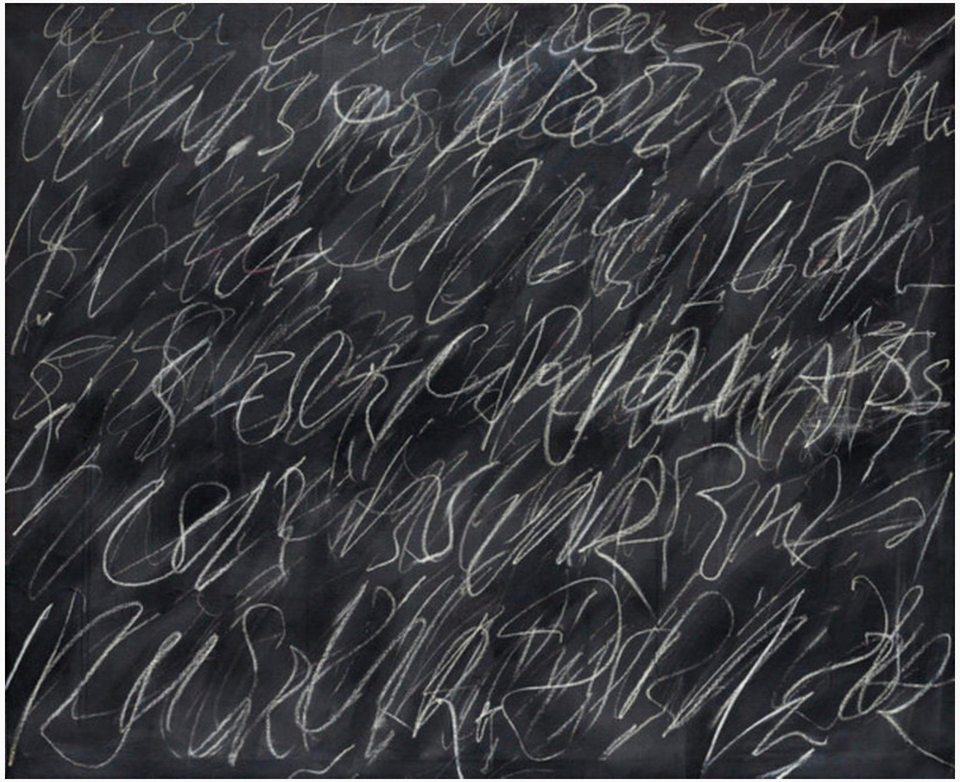
- Eigenvalues/Eigenvectors only apply to square matrices
- Eigenvalues may be 0 (indicating some axis is removed entirely)
- Eigenvalues may be complex numbers (indicating the matrix applies a rotation)
- Eigenvalues may be repeat, with one eigenvector per repetition (the matrix may scales some n-dimension subspace)
- Eigenvalues may repeat, with some eigenvectors missing (shears)

- If we have a full set of eigenvectors, we know everything about the given matrix S, and $S = QDQ^{-1}$
    - 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_n 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 this produces a polynomial in λ which can be solved to find eigenvalues



- Eigenvectors matching known eigenvalues can be found by solving $(\mathrm{A} - \lambda I_n)x = 0$ for x

Matrix Decomposition

LINEAR ALGEBRA (THE HIGHLIGHTS)

Matrix Decompositions

- **Eigenvalue Decomposition**: <u>Some</u> <u>square</u> matrices can be decomposed into scalings along particular axes
  - Symbolically: $S = QDQ^{-1}$; *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, Σ diagonal (though not square)*

Where we've been

Vector and Matrix dot product

2	-1	3
1	5	2
-1	1	3
6	4	9
2	2	1

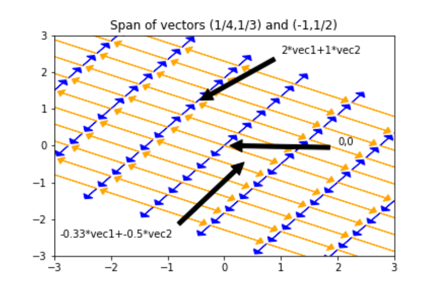
3	1
-2	7
4	-2

20	-11
1	32
7	0
46	16
6	14

Span

$$\beta_1 \cdot \begin{bmatrix} 2 \\ 1 \\ -1 \\ 6 \\ 2 \end{bmatrix} + \beta_2 \cdot \begin{bmatrix} -1 \\ 4 \\ 1 \\ 4 \\ 2 \end{bmatrix} + \beta_3 \cdot \begin{bmatrix} 3 \\ 2 \\ 3 \\ 9 \\ 1 \end{bmatrix}$$

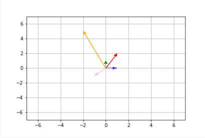
Basis as a coordinate system for a space



Invertibility

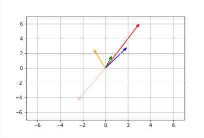
$$Ax = b \; ; x = A^{-1}b$$

Eigenvalues



$$Ax = \lambda x$$

$$S = QDQ^{-1}$$



Other decompositions

M = UP or M=PU

$$M = U\Sigma V^T$$

Reading

- What about all the facts about inverses and dot products I've forgotten since undergrad? [*Matrix Cookbook*] [*Linear Algebra Formulas*]

LINEAR ALGEBRA (SUMMARY)

Notes

- **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^{-1} 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

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

$$response = \beta_1 feature_1 + \beta_2 feature_2 + \beta_3 feature_3 + \ldots$$
$$y = X\beta$$

- 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 β (Matrix Cookbook (69) and (81): derivative of $\beta^T a$ is a^T, …)
    5. Simplify and solve for beta

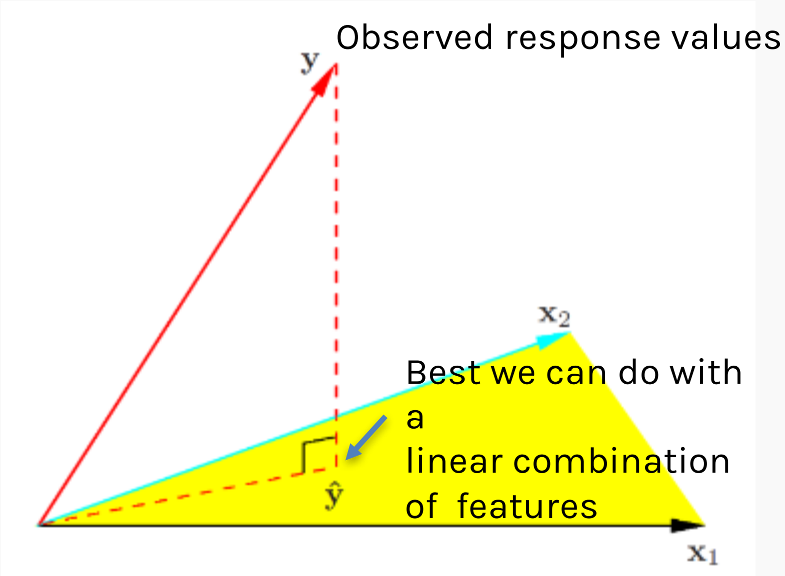
Interpreting LR: Algebra

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

- The best possible betas, $\hat{\beta} = (X^T X)^{-1} X^T y$ can be viewed in two parts:
  - Numerator ($X^T y$): columns of X dotted with (the) column of y; how related are the feature vectors and y?
  - Denominator ($X^T X$): columns of X dotted with columns of X; how related are the different features?
  - If the variables have mean zero and variances are ones, “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



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

- 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: HYPOTHESIS TESTING

OR: WHAT PARAMETERS EXPLAIN THE DATA

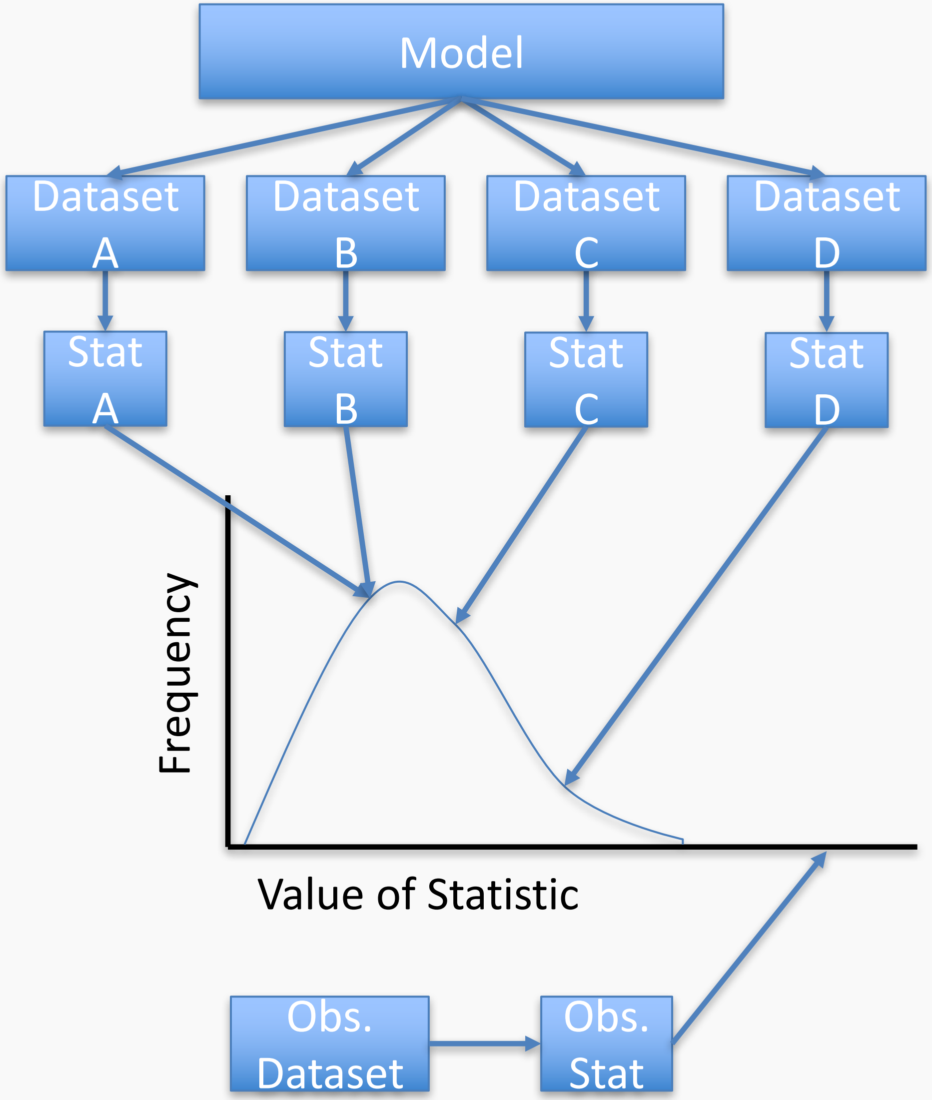
A Popper's Grave

- 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 we often simplify the problem 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 could produce 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 and observe, 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 data, we reject the model



Recap: How to understand any statistical test

- A statistical test typically specifies:
  1. A 'hypothesized' (probabilistic) data generating process *(Jargon: the null hypothesis)*
  2. A summary we'll use to compress/summarize a dataset *(Jargon: a statistic)*
  3. A rule for comparing the observed and the simulated summaries

- Example: *t*-test
  1. The y data are generated via the estimated line/plane, plus Normal(0, σ^2) noise,

     EXCEPT a particular coefficient is assumed to actually be zero!
  2. The coefficient we'd calculate for that dataset (minus 0), over the SE of the coefficient

$$t \text{ statistic} = \frac{\hat{\beta}_{\text{observed}} - 0}{\widehat{SE}(\hat{\beta}_{\text{observed}})}$$

  3. Declare the model bad if the observed result is in the top/bottom $\alpha/2$ of simulated results (commonly top/bottom 2.5%)

The t-test

Walkthrough:

- We set a particular β (or set of β's) we care about to zero (call them β_{null}).
- We simulate 10,000 new datasets using β_{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).
    - Plotting the *t* statistic in each simulation is a little nicer
- The *t* statistic calculated from the observed data was 17.8. *Do we think the proposed model generated our data?*
- One more thing: Amazingly, 'Student' knew what results we'd get from the simulation. He must have drunk a lot of Guinness.

T-test for β_2 = 0

$\beta_{MLE} = [2.2, 5, 3, 1.6]$

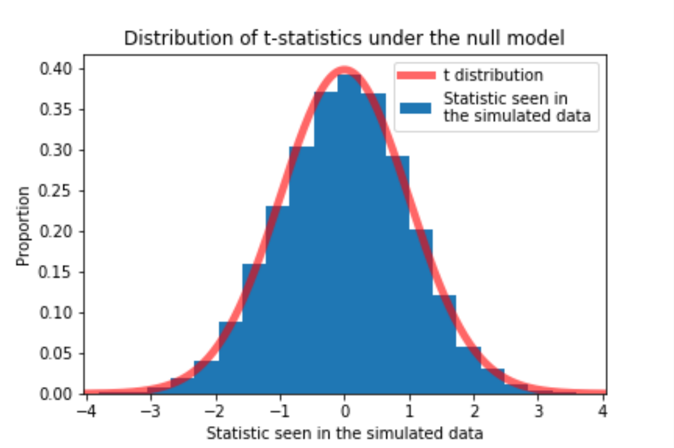
$\beta_{null} = [2.2, 5, 0, 1.6]$ σ_{MLE} X_{obs}

Simulate y values y=N($X\beta$, σ)

y_{sim1} y_{sim2} y_{sim3} … $y_{sim10,000}$

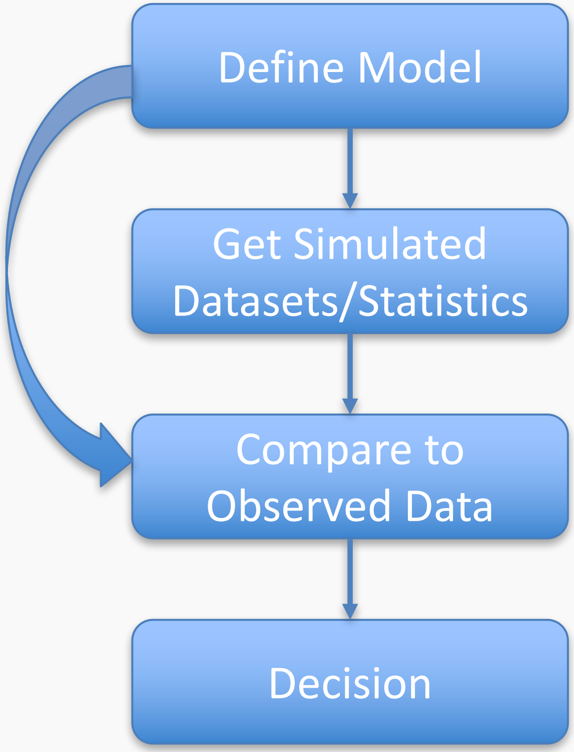
Fit linear regression y_sim = XB

β_{sim1} β_{sim2} β_{sim3} … $\beta_{sim10,000}$



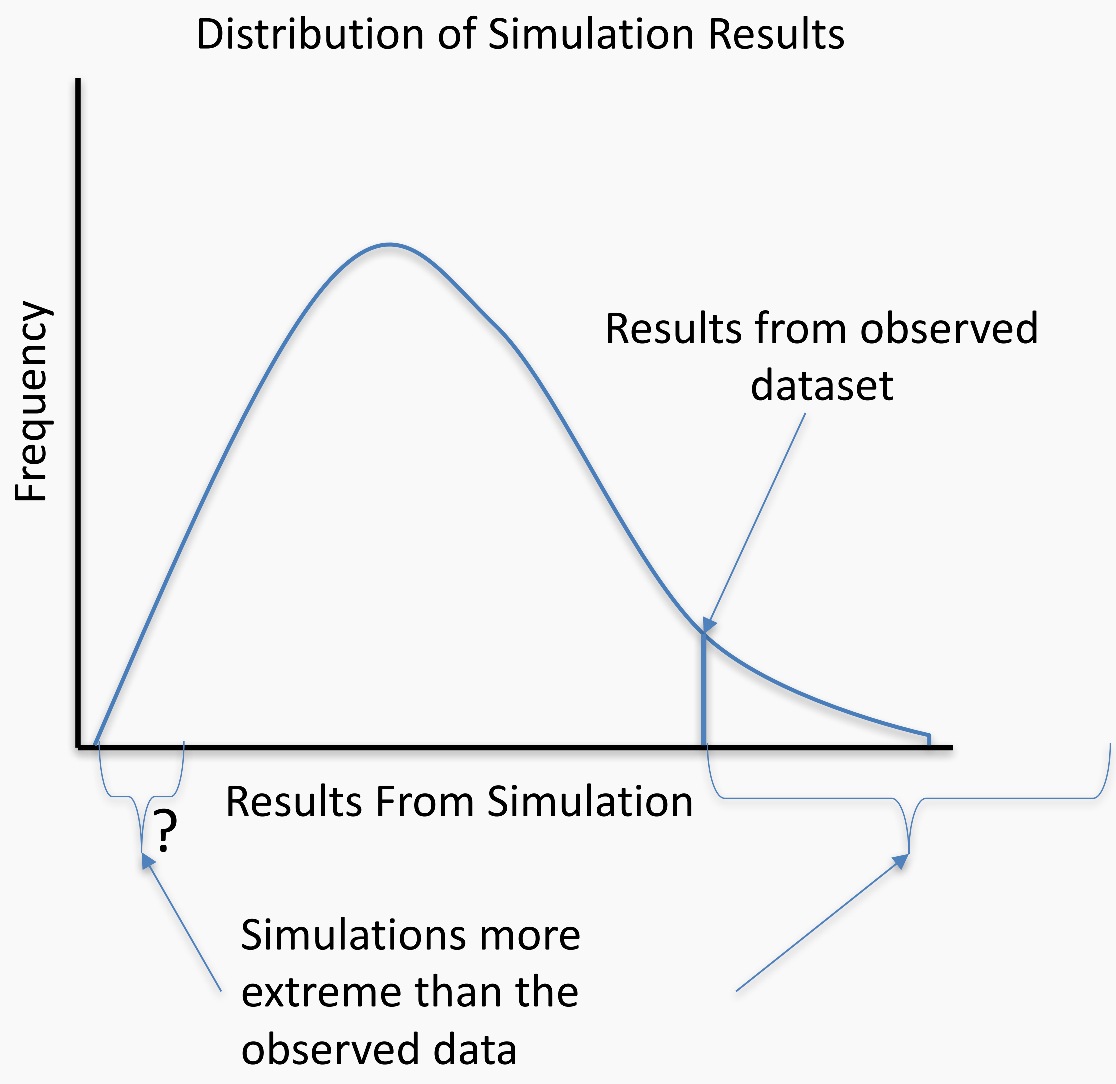
The Value of Assumptions

- Student’s clever set-up let’s 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 specific value
- 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=0.031 means that your observed data is in the top 3.1% of extreme results under this model (using our statistic)
    - There is some ambiguity about what 'extreme' should mean



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

p Value Warnings

- p values are just one possible measure of the evidence against a model
- Rejecting a model when $p<\text{threshold}$ is only one possible decision rule
  - 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 just suggests it.
  - It does mean that anyone who wants to believe in the null must explain with why something unlikely happened

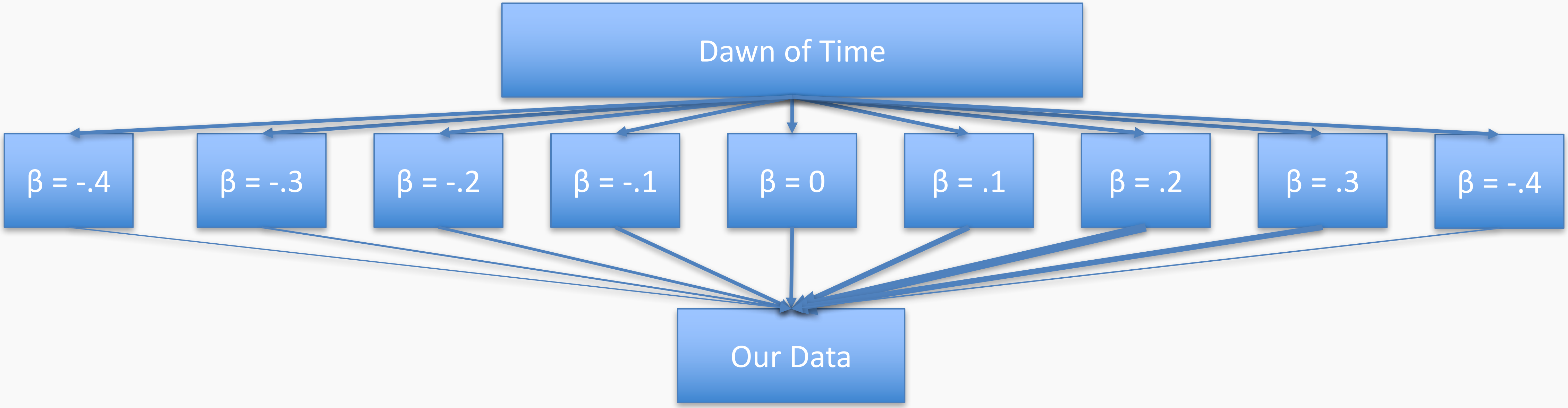
Recap

- We can't rule models in (it's difficult); we can only rule them out (much easier)
- 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] *sampling distribution* of statistics the null model produces
    - We rule out the null model if the observed data doesn't seem to come from the model (disagrees with the sampling distribution).
- A p value summarizes the level of evidence against a particular null

STATISTICS: HYPOTHESIS TESTING

CONFIDENCE INTERVALS AND COMPOSITE HYPOTHESES

Recap

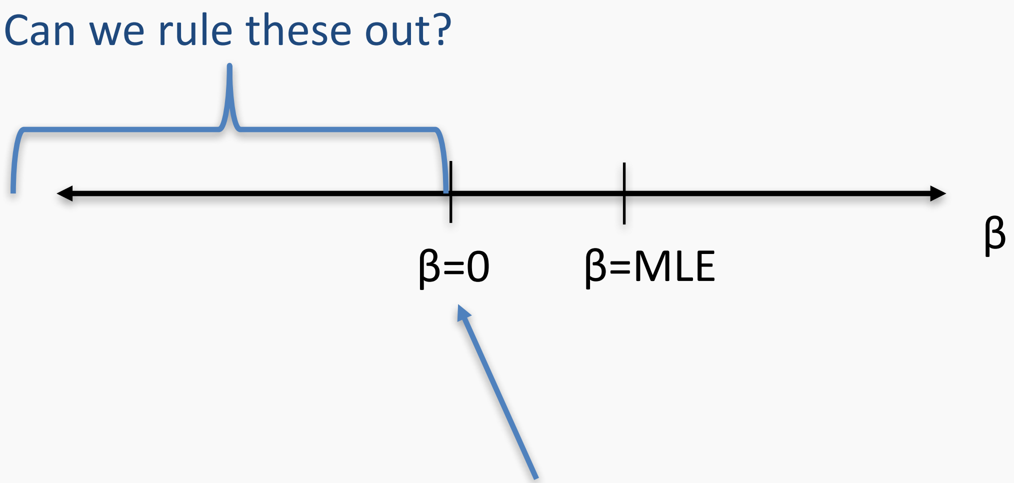


- Let's talk about what we just did
  - That t-test was ONLY testing the model where the coefficient in question is set to zero
  - Ruling out this model makes it more likely that other models are true, but doesn't tell us which ones
  - If the null is $\beta = 0$, getting $p<.05$ only rules out THAT 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…)

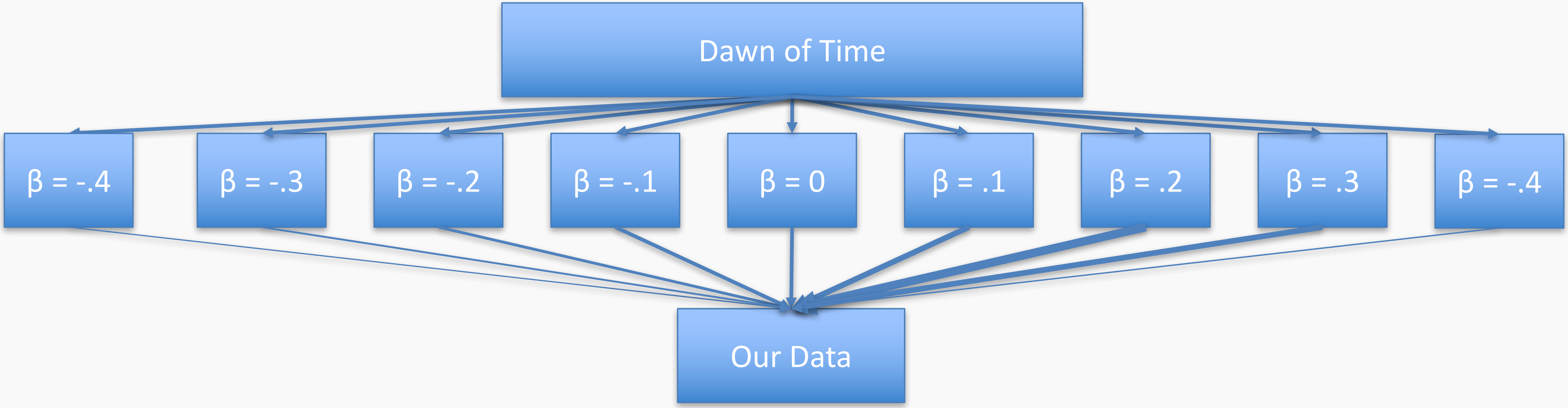
- Sometimes, ruling out the nearest model is enough; we know that the other models have to be worse
- If a method claims it can test θ<0, this is how



β=0 will be closer to matching the data (in terms of t statistic) than any other model in the set*; we only need to test β=0

* Non-trivial; true for student's t but not for other measures

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 from probability theory
- 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 do not 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 only promise**: if you were to repeatedly re-collect the data and build 95% CIs, (assuming our story about data generation is correct) 95% of the intervals would contain the true value

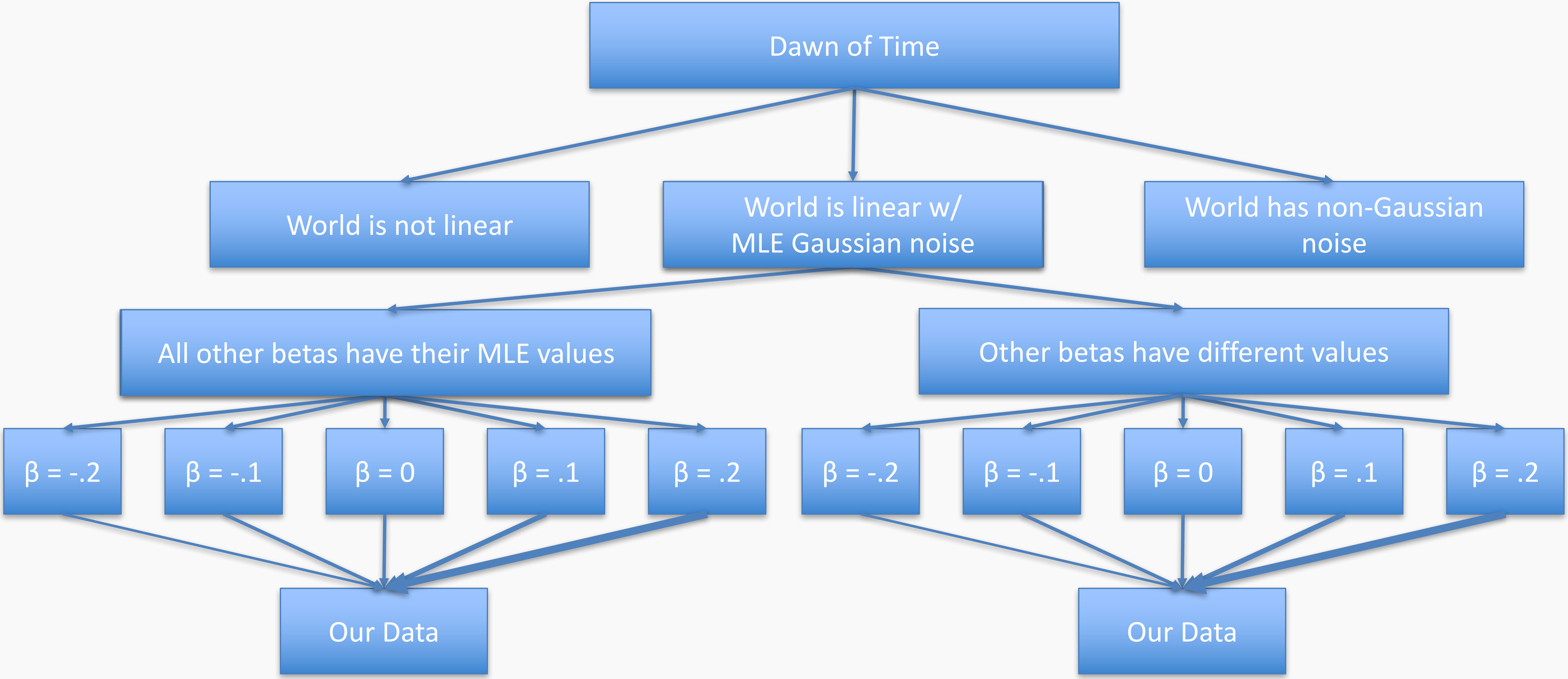
Confidence Interval Warnings

- 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

HW Preview

- 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?



- We rejected the null model(s) as tested, not the *idea* that β=0 – assumptions matter

Review

- 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

Going forward

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