

Hypothesis Testing and statistical preliminaries

Stony Brook University
CSE545, Spring 2019

Hypothesis Testing:

- Random Variables
- Distributions
- Hypothesis Testing Framework

Comparing Variables:

- Simple Linear Regression, Correlation, Multiple Linear Regression,
- Comparing Variables and Hypothesis Testing
- Regularized Linear Regression
- Multiple Hypothesis Testing

Random Variables

X : A mapping from Ω to \mathbb{R} that describes the question we care about in practice.



“sample space”, set of all possible outcomes.

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Example: $\Omega = 5$ coin tosses = $\{\langle \text{HHHHH} \rangle, \langle \text{HHHHT} \rangle, \langle \text{HHHTH} \rangle, \langle \text{HHHTH} \rangle \dots\}$

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We may just care about how many tails? Thus,

$$X(\langle \text{HHHHH} \rangle) = 0$$

$$X(\langle \text{HHHTH} \rangle) = 1$$

$$X(\langle \text{TTTHT} \rangle) = 4$$

$$X(\langle \text{HTTTT} \rangle) = 4$$

X only has 6 possible values: 0, 1, 2, 3, 4, 5

What is the probability that we end up with $k = 4$ tails?

$$\mathbf{P}(X = k) := \mathbf{P}(\{\omega : X(\omega) = k\}) \quad \text{where } \omega \in \Omega$$

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$X(\omega) = 4$ for 5 out of 32 sets in Ω . Thus, assuming a fair coin, $\mathbf{P}(X = 4) = 5/32$

(Not a “variable”, but a function that we end up notating a lot like a variable)

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X amount of inches in a snowstorm

$$X(\omega) = \omega$$

What is the probability we receive (at least) a inches?

$$P(X \geq a) := P(\{\omega : X(\omega) \geq a\})$$

What is the probability we receive between a and b inches?

$$P(a \leq X \leq b) := P(\{\omega : a \leq X(\omega) \leq b\})$$

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(probability of receiving exactly i inches of snowfall is zero)

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How to model?

s?

inches?

Continuous Random Variables

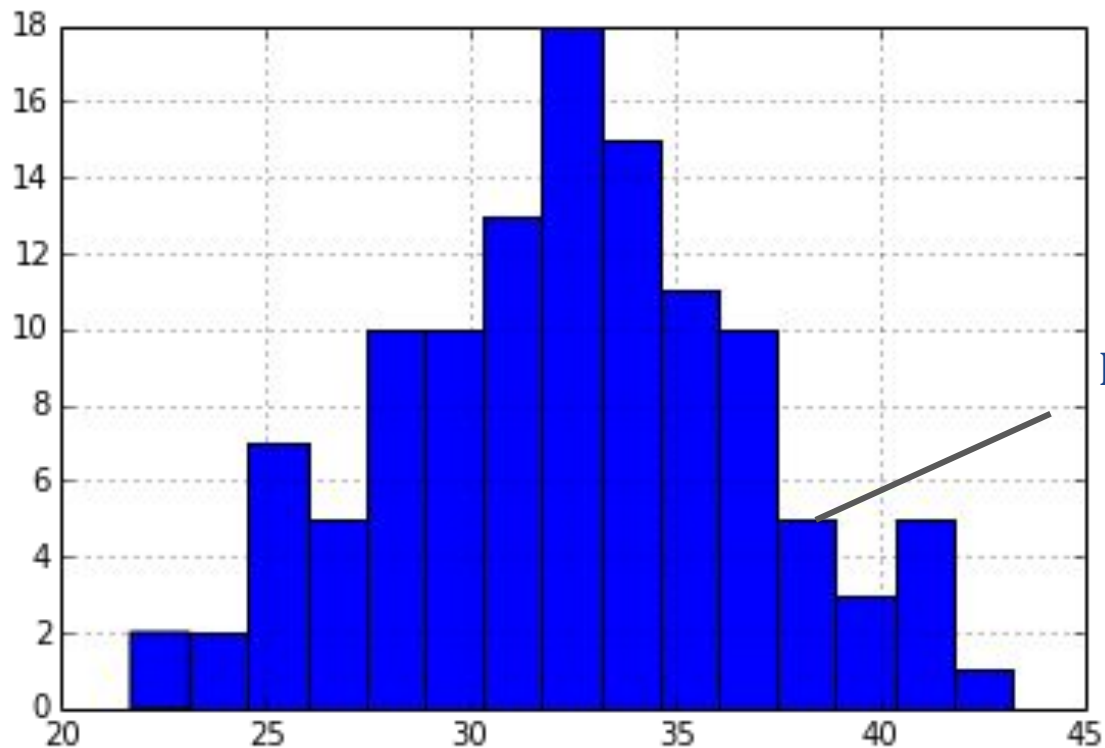


Discretize them!
(group into discrete bins)

How to model?

Continuous Random Variables

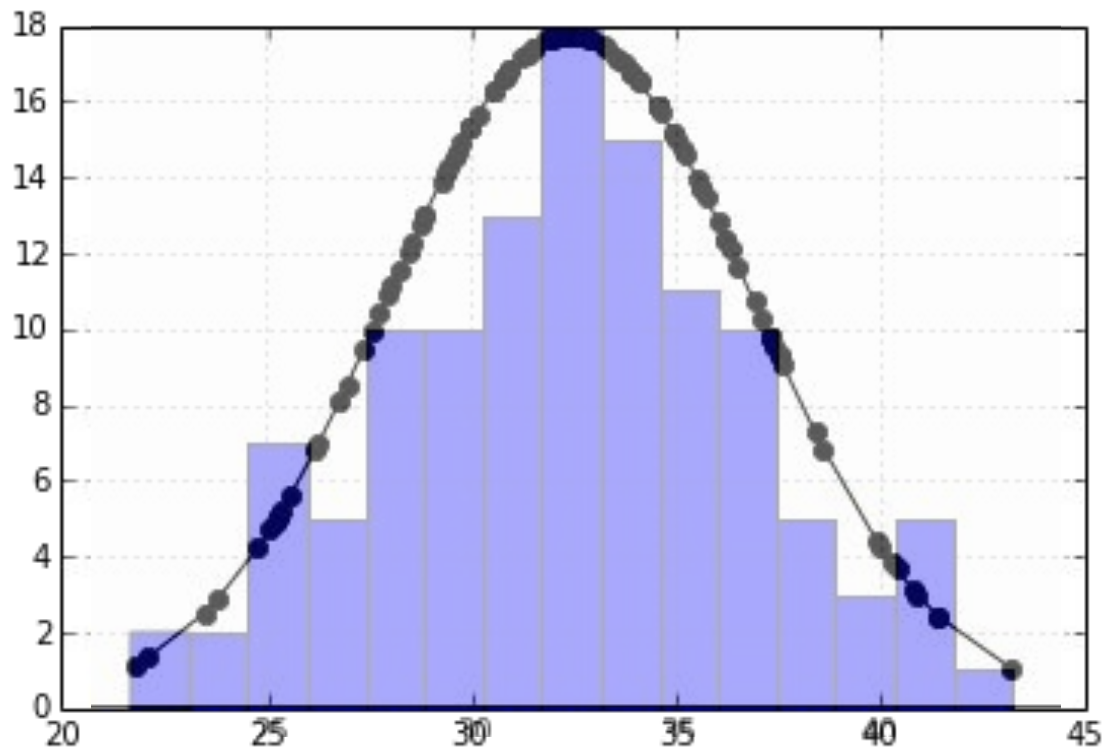
$$P(\text{bin}=8) = .32$$



$$P(\text{bin}=12) = .08$$

But aren't we throwing away information?

Continuous Random Variables



Continuous Random Variables

***X* is a *continuous random variable* if it can take on an infinite number of values between any two given values.**

X is a *continuous random variable* if there exists a function f_X such that:

$$f_X(x) \geq 0, \text{ for all } x \in X,$$
$$\int_{-\infty}^{\infty} f_X(x) dx = 1, \text{ and}$$
$$P(a < X < b) = \int_a^b f_X(x) dx$$

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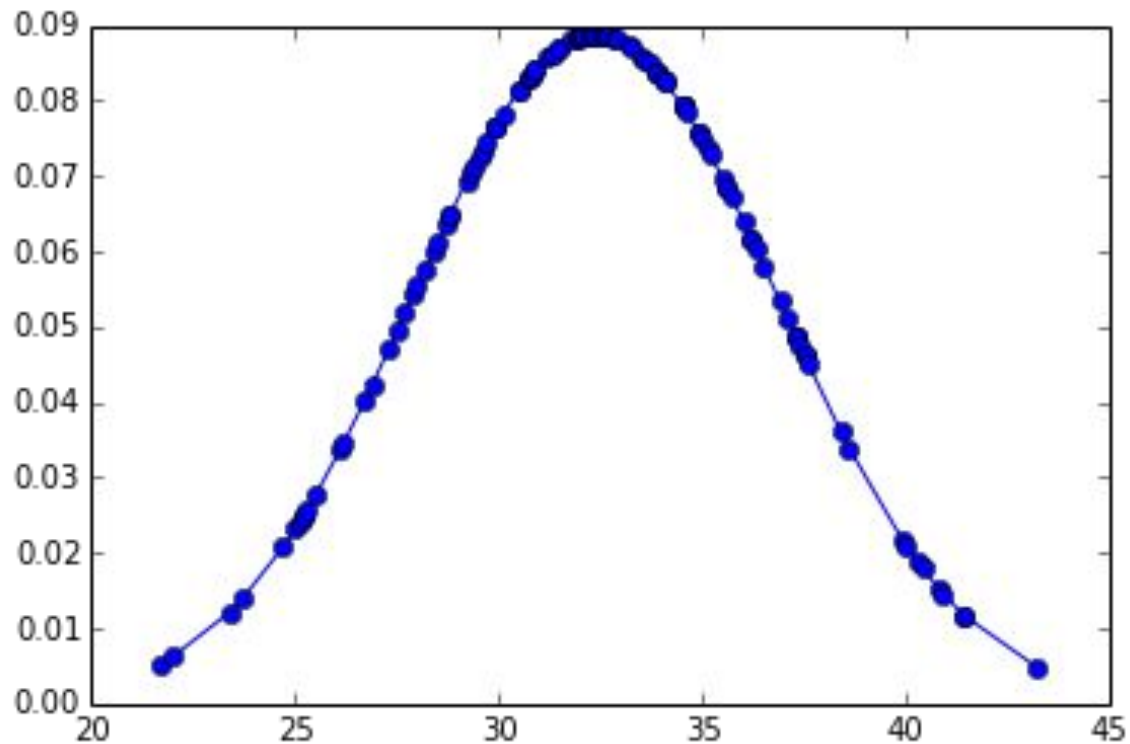
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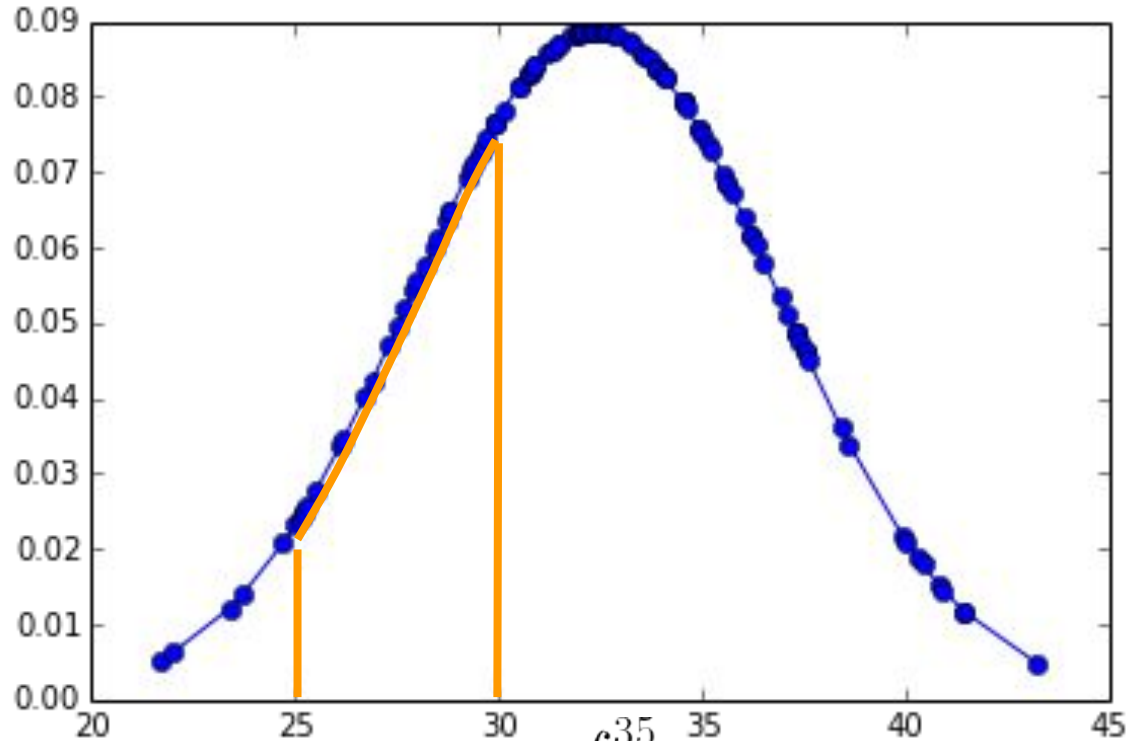
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f_X : “probability density function” (pdf)

Continuous Random Variables



Continuous Random Variables

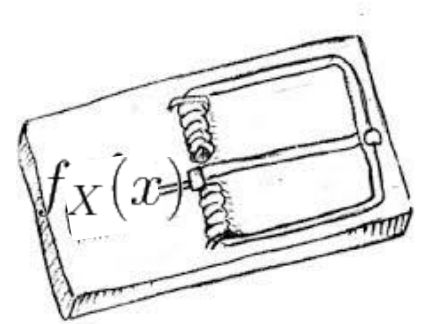


$$P(25 < X < 35) = \int_{25}^{35} f(x) dx$$

Continuous Random Variables

Common Trap

- $f_X(x)$ does not yield a probability
 - $\int_a^b f_X(x)dx$ does
 - x may be anything (\mathbb{R})
 - thus, $f_X(x)$ may be > 1



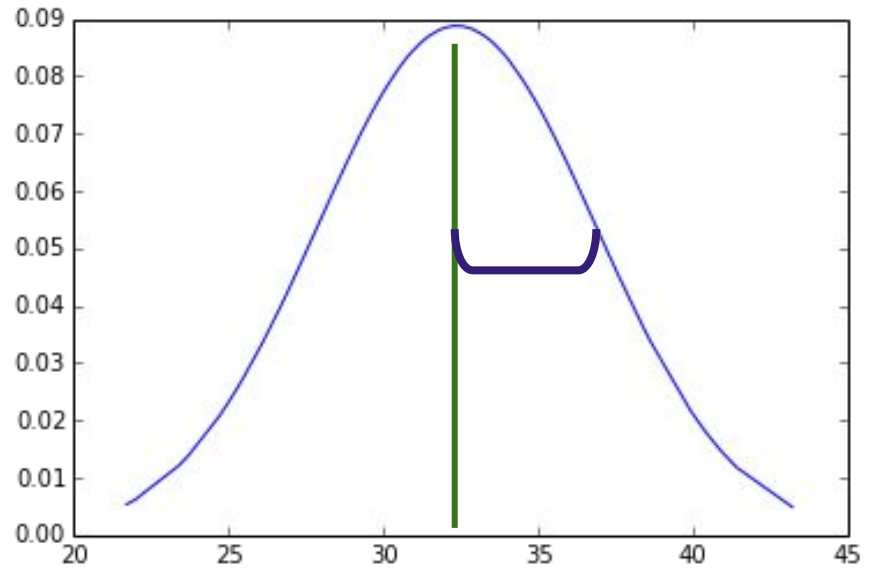
Continuous Random Variables

A Common Probability Density Function

Continuous Random Variables

Common *pdfs*: Normal(μ, σ^2)

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



Continuous Random Variables

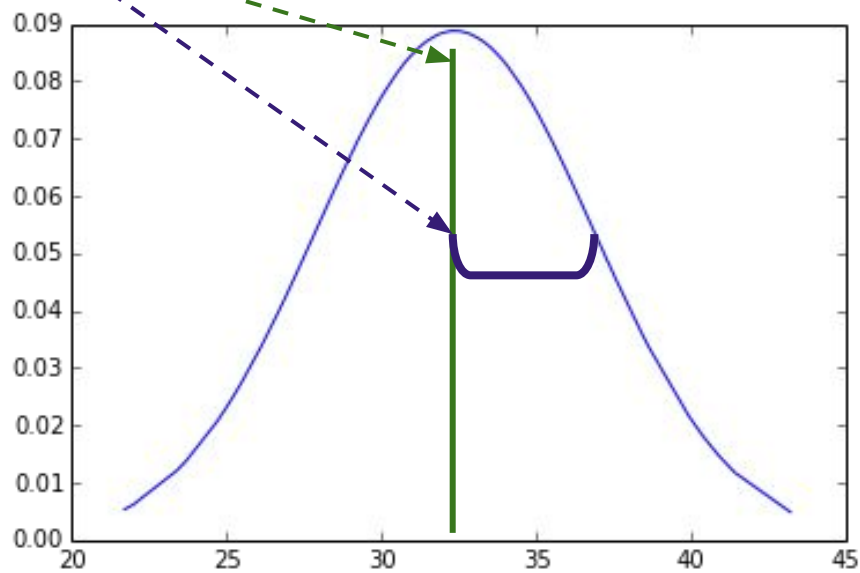
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μ : mean (or “center”)
= expectation

σ^2 : variance,

σ : standard deviation



Continuous Random Variables

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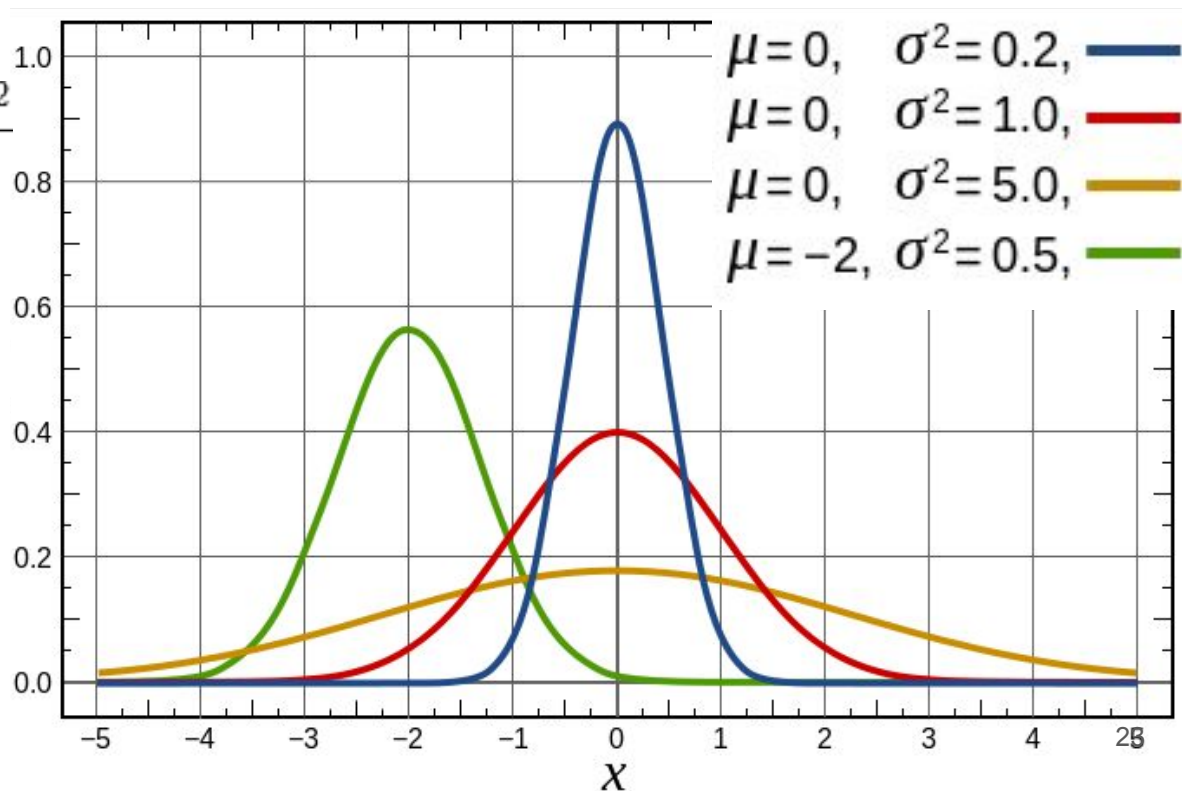
Credit: Wikipedia

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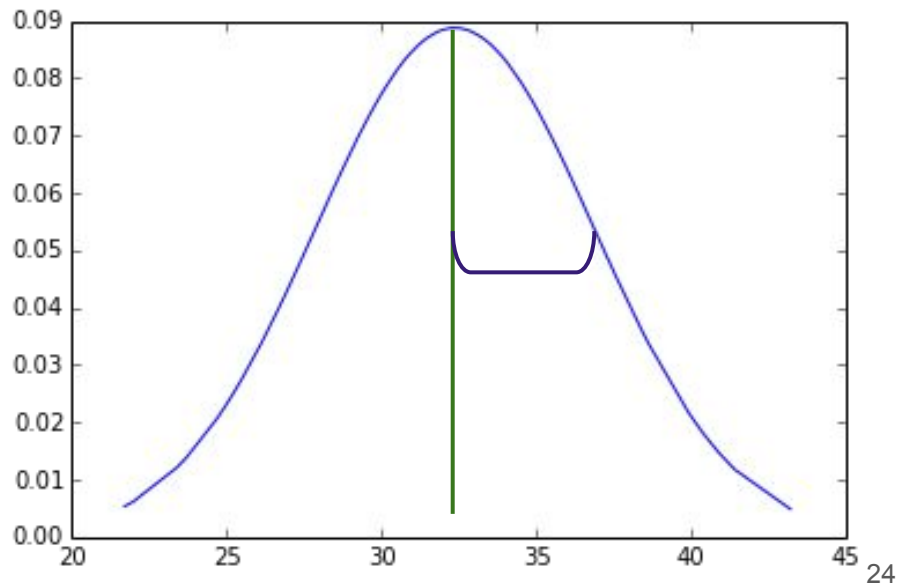


Continuous Random Variables

Common *pdfs*: Normal(μ, σ^2)

$X \sim \text{Normal}(\mu, \sigma^2)$, examples in real life:

- height
- intelligence/ability
- measurement error
- averages (or sum) of lots of random variables



Continuous Random Variables

Common *pdfs*: Normal(0, 1) (“standard normal”)

How to “standardize” any normal distribution:

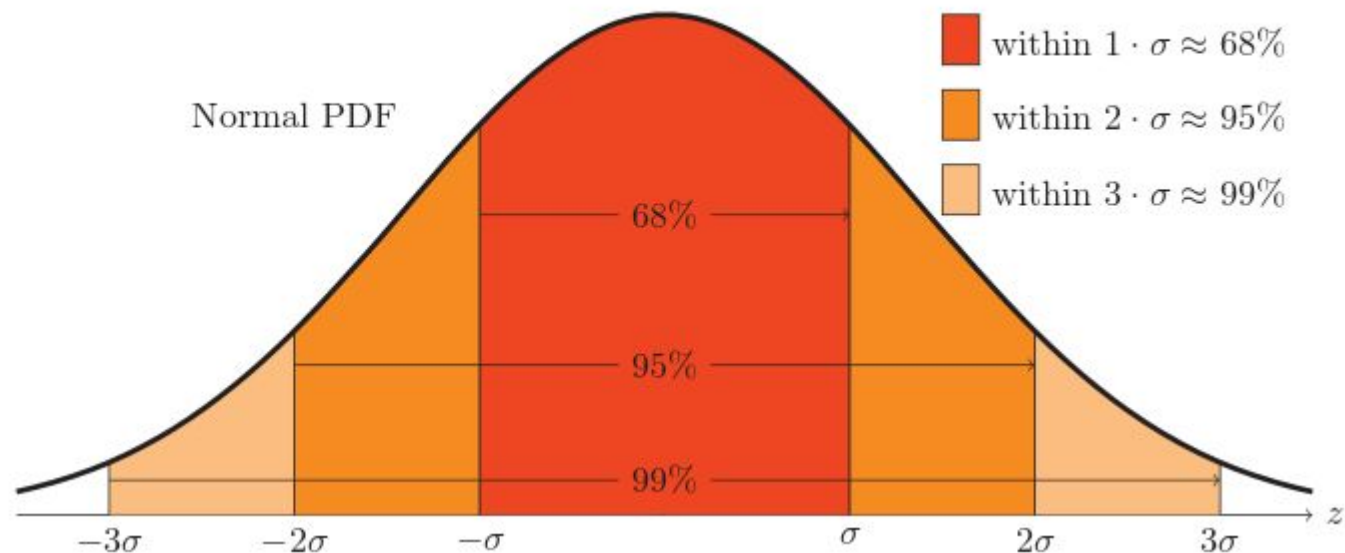
1. subtract the mean, μ (aka “mean centering”)
2. divide by the standard deviation, σ

$$z = (x - \mu) / \sigma, \text{ (aka “z score”)}$$

Continuous Random Variables

Common *pdfs*: Normal(0, 1)

$$P(-1 \leq Z \leq 1) \approx .68, \quad P(-2 \leq Z \leq 2) \approx .95, \quad P(-3 \leq Z \leq 3) \approx .99$$



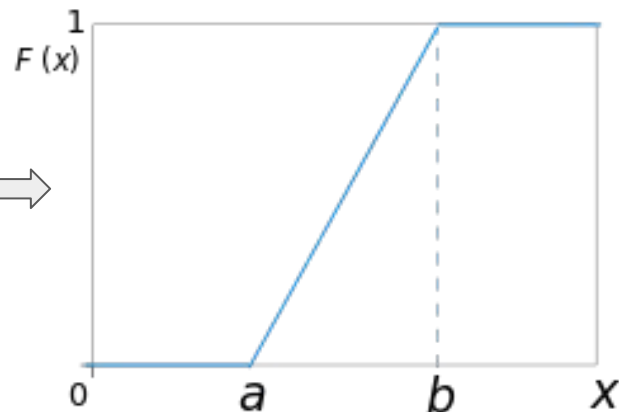
Cumulative Distribution Function

For a given random variable X , the *cumulative distribution function* (CDF),

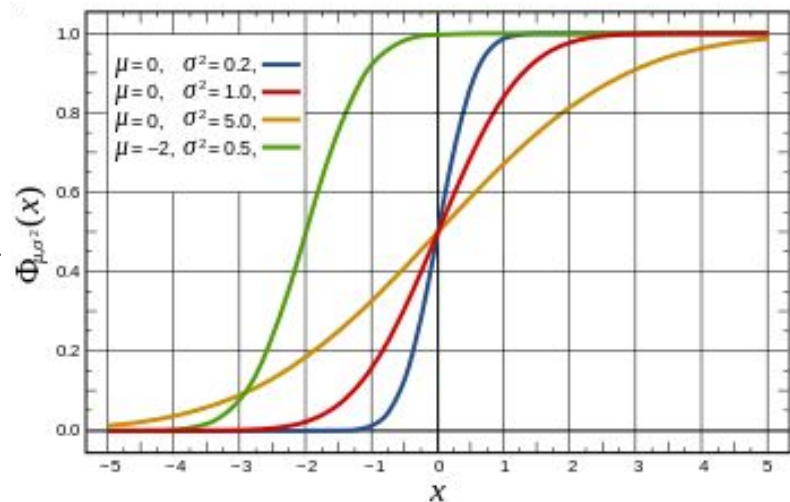
$F_X: \mathbb{R} \rightarrow [0, 1]$, is defined by:

$$F_X(x) = P(X \leq x)$$

Uniform \Rightarrow



Normal \Rightarrow



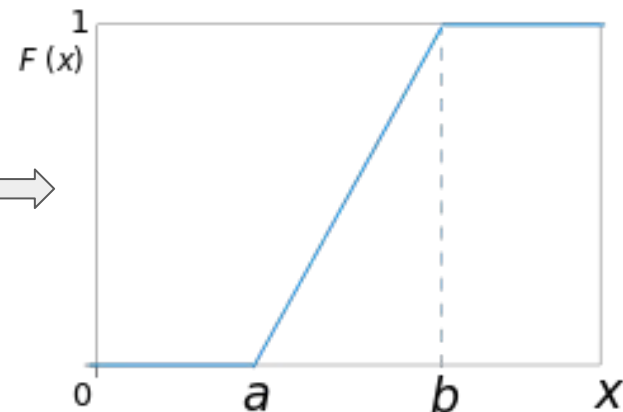
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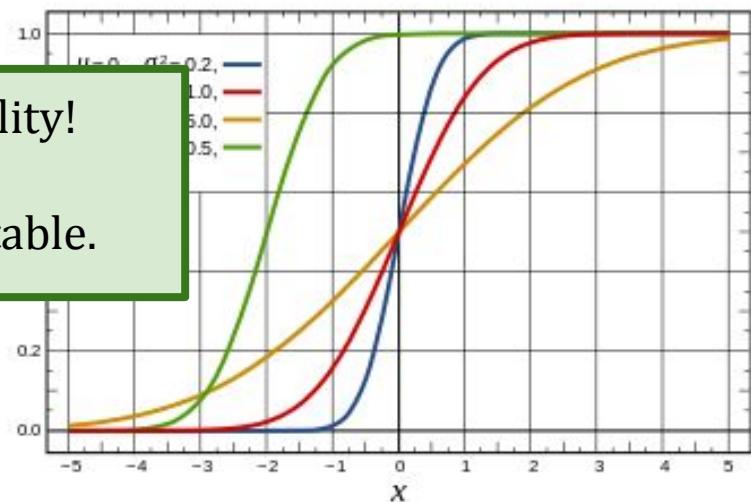
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Uniform \Rightarrow



Pro: $F_X(x)$ yields a probability!

Con: Not intuitively interpretable.



Random Variables, Revisited

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Discrete Random Variables

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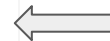
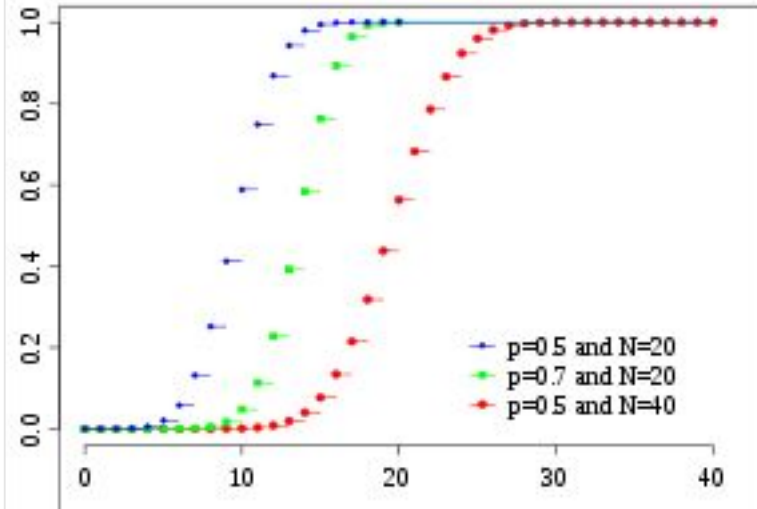
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Binomial (n, p)

(like normal)

Discrete Random Variables

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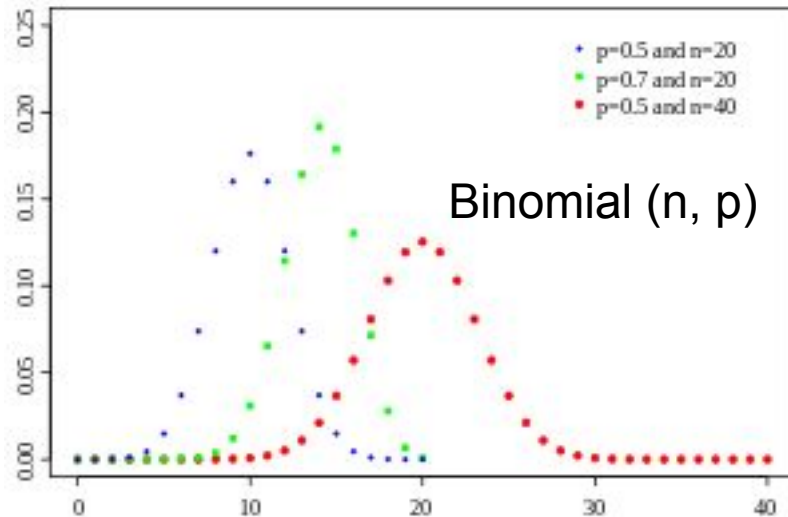
$F_X: \mathbb{R} \rightarrow [0, 1]$, is defined by:

$$F_X(x) = P(X \leq x)$$

For a given *discrete* random variable X , *probability mass function (pmf)*,

$f_X: \mathbb{R} \rightarrow [0, 1]$, is defined by:

$$f_X(x) = P(X = x)$$



X is a *discrete random variable* if it takes only a countable number of values.

$$\sum_i f_X(x) = 1$$

$$F_X(x) = P(X \leq x) = \sum_{x_i \leq x} f_X(x)$$

Discrete Random Variables

Two Common **Discrete** Random Variables

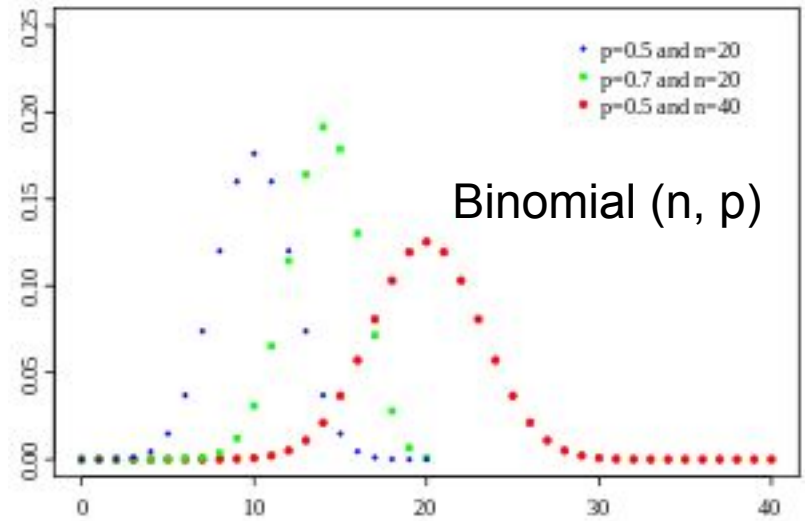
- Binomial(n, p)

$$f_X(x) = \binom{n}{x} p^x (1-p)^{n-x}, \text{ if } 0 \leq x \leq n \text{ (0 otherwise)}$$

example: number of heads after n coin flips (p, probability of heads)

- Bernoulli(p) = Binomial(1, p)

example: one trial of success or failure



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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% chance that alternative is true).

Hypothesis Testing

Example: Hypothesize a coin is biased.

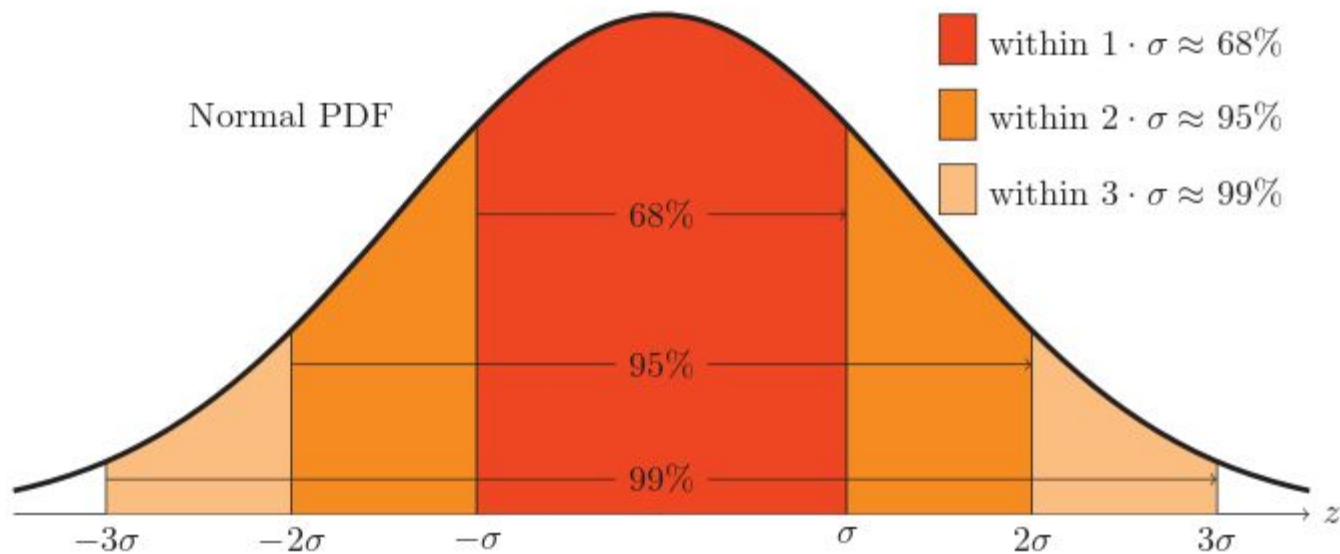
H_0 : the coin is not biased

(i.e. flipping n times results in a Binomial(n , 0.5))

H_1 : the coin is biased (i.e. flipping n times does not result in a Binomial(n , 0.5))

Hypothesis Testing

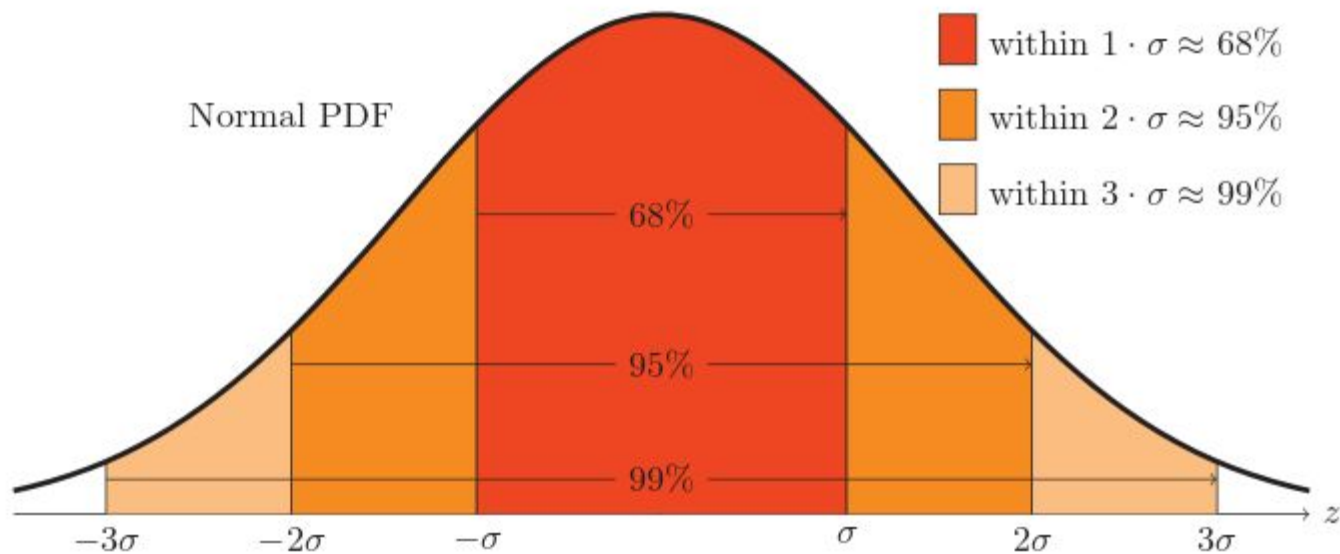
More formally: Let X be a random variable and let R be the range of X .
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Hypothesis Testing

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alpha : size of rejection region (e.g. 0.05, 0.01, .001)

In the biased coin example,

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

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A general framework for answering (yes/no) questions!

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- *Is my deep predictive model better than the state of the art?*

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A general framework for answering (yes/no) questions!

- *Are height and baldness related?*
- *Is my deep predictive model better than the state of the art?*
- *Is the heat index of a community related to poverty?*
- *Is the heat index of a community related to poverty **controlling for education rates?***
- *Does my website receive a higher average number of monthly visitors?*

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Hypothesis Testing

Why?

Failing to “reject the null” does not mean the null is true. However, if the sample is large enough, it may be enough to say that the effect size (correlation, difference value, etc...) is not very meaningful.

A general framework for answering (yes/**maybe**) questions!

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Hypothesis Testing

Important logical question:

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



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

Statistical Considerations in Big Data

1. Average multiple models (ensemble techniques)
2. Correct for multiple tests (Bonferonni's Principle)
3. Smooth data
4. "Plot" data (or figure out a way to look at a lot of it "raw")
5. Interact with data
6. Know your "real" sample size
7. Correlation is not causation
8. Define metrics for success (set a baseline)
9. Share code and data
10. The problem should drive solution

Measures for Comparing Random Variables

- Distance metrics
- **Linear Regression**
- Pearson Product-Moment Correlation
- Multiple Linear Regression
- (Multiple) Logistic Regression
- Ridge Regression (L2 Penalized)
- Lasso Regression (L1 Penalized)

Linear Regression

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 function r

The **expected** value of Y , given that the random variable X is equal to some specific value, x .

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

goal: find β_0, β_1 such that $r(x) \approx E(Y|X = x)$

Linear Regression

Simple Linear Regression $Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$

where $\mathbf{E}(\epsilon_i|X_i) = 0$ and $\mathbf{V}(\epsilon_i|X_i) = \sigma^2$

more precisely

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

Linear Regression

intercept

slope

error

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expected variance

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expected variance

Estimated intercept and slope

$$\hat{r}(x) = \hat{\beta}_0 + \hat{\beta}_1 x \quad \hat{Y}_i = \hat{r}(X_i)$$

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

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

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

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

Linear Regression

via Gradient Descent

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

Repeat until convergence:

Calculate all \hat{Y}_i

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

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

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Learning rate

Based on derivative of *RSS*

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via Direct Estimates (normal equations)

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

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$$

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

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

Pearson Product-Moment Correlation

Covariance

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

**via Direct Estimates
(normal equations)**

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

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$$

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Correlation

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

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If one standardizes X and Y (i.e. subtract the mean and divide by the standard deviation) before running linear regression, then:

$$\hat{\beta}_0 = 0 \quad \text{and} \quad \hat{\beta}_1 = r \quad \text{--- i.e. } \hat{\beta}_1 \text{ is the Pearson correlation!}$$

Measures for Comparing Random Variables

- Distance metrics
- Linear Regression
- Pearson Product-Moment Correlation
- Multiple Linear Regression
- (Multiple) Logistic Regression
- Ridge Regression (L2 Penalized)
- Lasso Regression (L1 Penalized)

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Multiple Linear Regression

Suppose we have multiple X that we'd like to fit to Y at once:

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

If we include and $X_{0i} = 1$ 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 β and ϵ are vectors and X is a matrix.

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Estimating β :

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

Multiple Linear Regression

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

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

$$s^2 = \frac{RSS}{df}$$

To test for significance of individual coefficient, j :

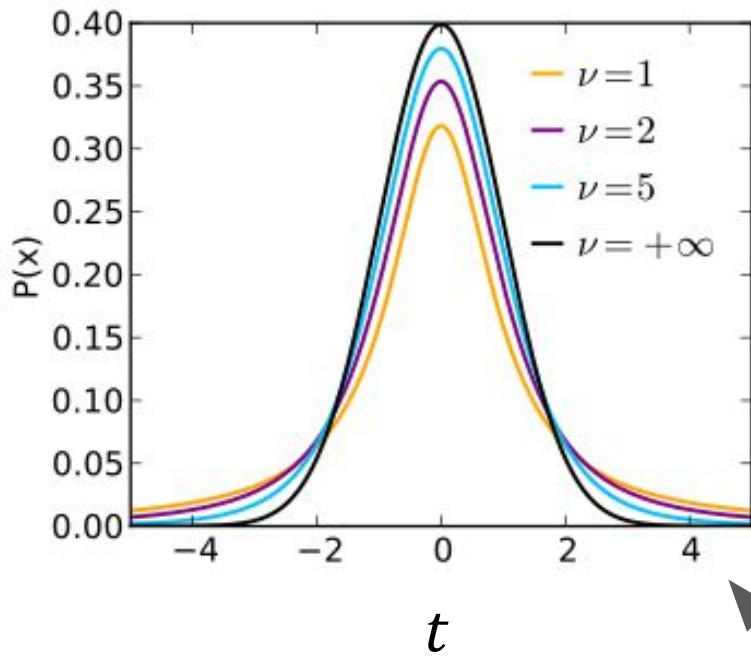
$$t = \frac{\hat{\beta}_j}{SE(\hat{\beta}_j)} = \frac{\hat{\beta}_j}{\sqrt{\frac{s^2}{\sum_{i=1}^n (X_{ij} - \bar{X}_j)^2}}}$$

T-Test for significance of hypothesis:

- 1) Calculate t
- 2) Calculate degrees of freedom:

$$df = N - (m+1)$$

- 3) Check probability in a t distribution:



$$\beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_m X_{im} + \epsilon_i$$

T-Test for significance of hypothesis:

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Hypothesis Testing

Important logical question:

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



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

Type I, Type II Errors

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

(Orloff & Bloom, 2014)

Power

significance level (“p-value”) = $P(\text{type I error}) = \mathbf{P(\text{Reject } H_0 \mid H_0)}$
(probability we are incorrect)

power = $1 - P(\text{type II error}) = \mathbf{P(\text{Reject } H_0 \mid H_1)}$
(probability we are correct)

	H_0	H_A
<u>Reject H_0</u>	$\mathbf{P(\text{Reject } H_0 \mid H_0)}$	$\mathbf{P(\text{Reject } H_0 \mid H_1)}$

		True state of nature	
		H_0	H_A
Our decision	Reject H_0	Type I error	correct decision
	‘Accept’ H_0	correct decision	Type II error

(Orloff & Bloom, 2014)

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

How to fix?



Multi-test Correction

How to fix?



What if all tests are independent?
=> “Bonferroni Correction” (α/m)

Better Alternative: False Discovery Rate
(Benjamini Hochberg)

Logistic Regression

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

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

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Note: this is a probability here.

In simple linear regression we wanted an expectation:

$$r(x) = \mathbf{E}(Y | X = x)$$

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Note: this is a probability here.

In simple linear regression we wanted an expectation:

$$r(x) = \mathbf{E}(Y | X = x)$$

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

Logistic Regression

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

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

Logistic Regression

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$\mathbf{P}(Y_i = 0 | X = x)$

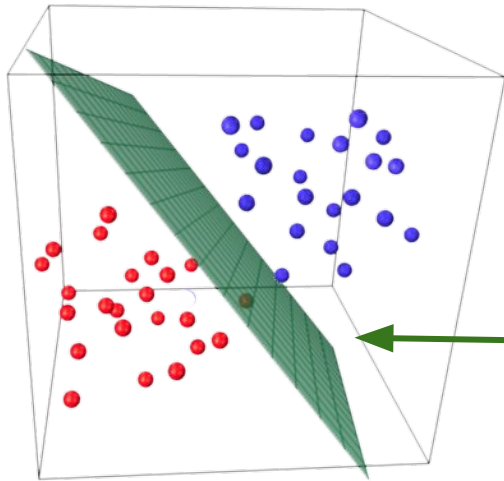
Thus, 0 is class 0

and 1 is class 1.

Logistic Regression

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

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

We're still learning a linear *separating hyperplane*, but fitting it to a *logit* outcome.

Logistic Regression

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

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

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

To estimate β ,
one can use
reweighted least squares:

(Wasserman, 2005; Li, 2010)

- 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 $\text{element}(i, i) = p_i(1 - p_i)$.
 2. Set $z_i = \text{logit}(p_i) + \frac{Y_i - p_i}{p_i(1 - p_i)} = X\hat{\beta} + \frac{Y_i - p_i}{p_i(1 - p_i)}$
 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.

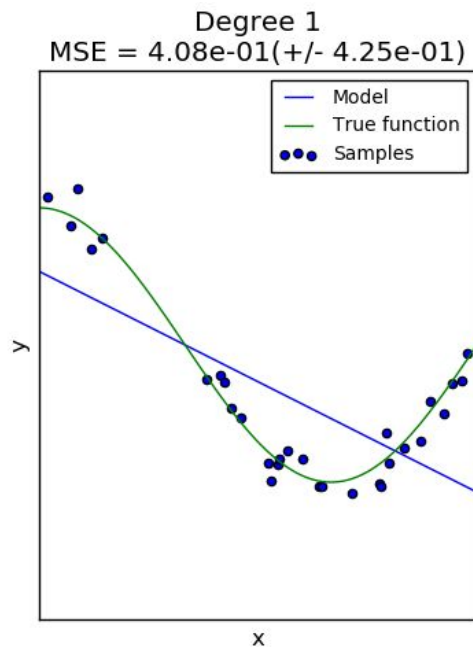
Uses of linear and logistic regression

1. Testing the relationship between variables given other variables. β is an “effect size” -- a score for the magnitude of the relationship; can be tested for significance.
2. Building a predictive model that generalizes to new data. \hat{Y} is an estimate value of Y given X .

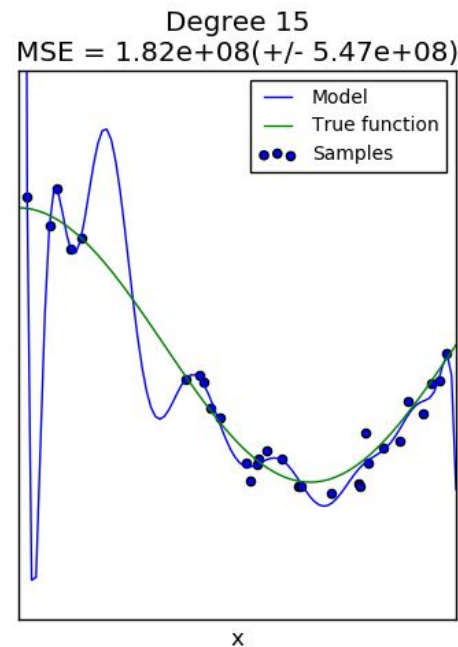
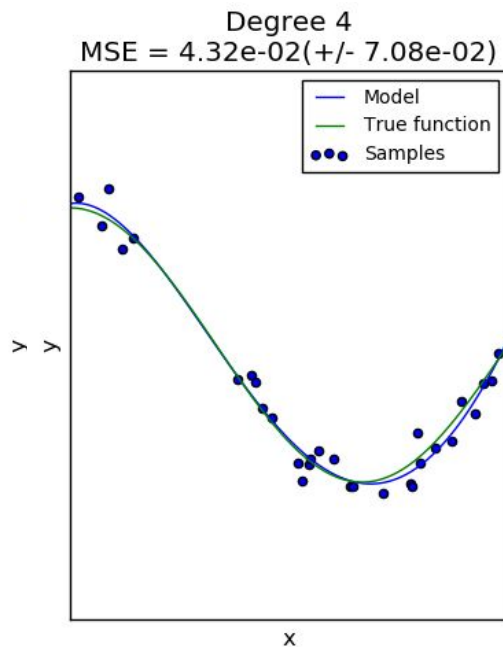
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2. Building a predictive model that generalizes to new data.
 \hat{Y} is an estimate value of Y given X .
However, unless $|X| \ll \text{observations}$ then the model might “overfit”.

Overfitting (1-d non-linear example)



Underfit
High Bias



Overfit
High Variance

(image credit: Scikit-learn; in practice data are rarely this clear)

Overfitting (5-d linear example)

$$Y = X$$

1	0.5	0	0.6	1	0	0.25
1	0	0.5	0.3	0	0	0
0	0	0	1	1	1	0.5
0	0	0	0	0	1	1
1	0.25	1	1.25	1	0.1	2

Overfitting (5-d linear example)

$$Y = X$$

1	0.5	0	0.6	1	0	0.25
1	0	0.5	0.3	0	0	0
0	0	0	1	1	1	0.5
0	0	0	0	0	1	1
1	0.25	1	1.25	1	0.1	2

$$\text{logit}(Y) = 1.2 + -63*X_1 + 179*X_2 + 71*X_3 + 18*X_4 + -59*X_5 + 19*X_6$$

Overfitting (5-d linear example)

Do we really think we found something generalizable?

Y	=	X					
1		0.5	0	0.6	1	0	0.25
1		0	0.5	0.3	0	0	0
0		0	0	1	1	1	0.5
0		0	0	0	0	1	1
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$$\text{logit}(Y) = 1.2 + -63*X_1 + 179*X_2 + 71*X_3 + 18*X_4 + -59*X_5 + 19*X_6$$

Overfitting (2-d linear example)

Do we really think we found something generalizable?

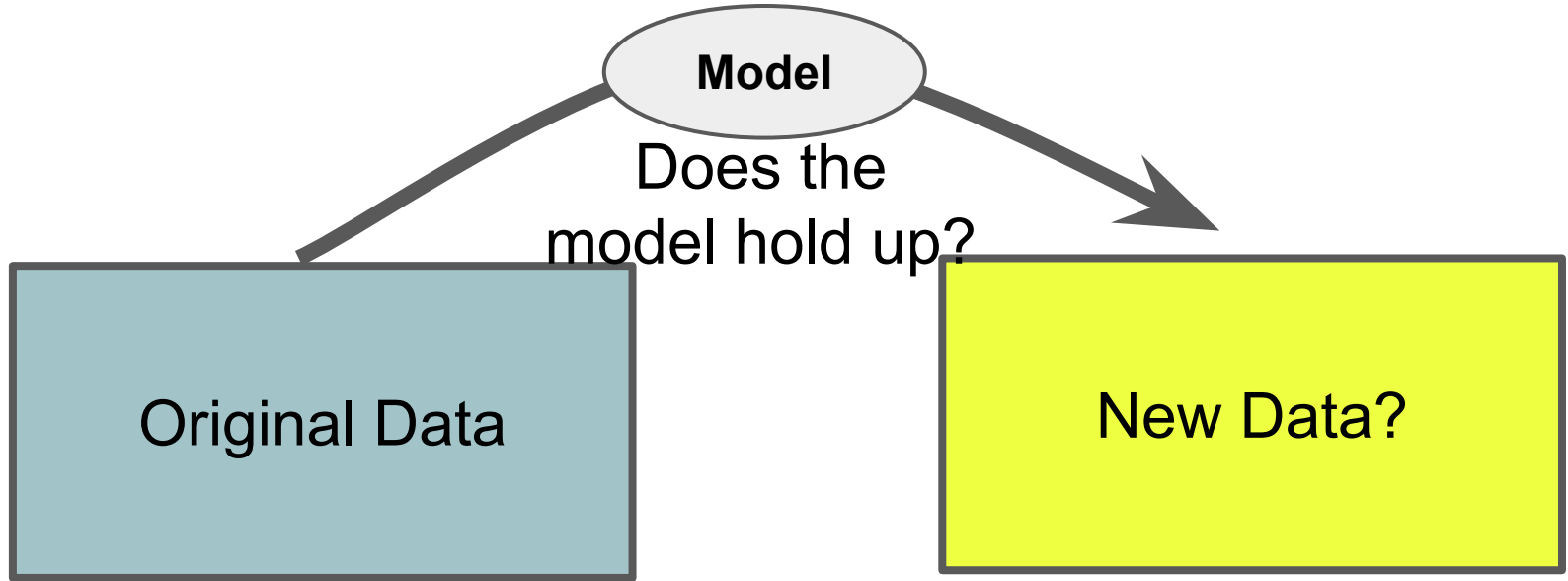
$$Y = X$$

1	0.5	0
1	0	0.5
0	0	0
0	0	0
1	0.25	1

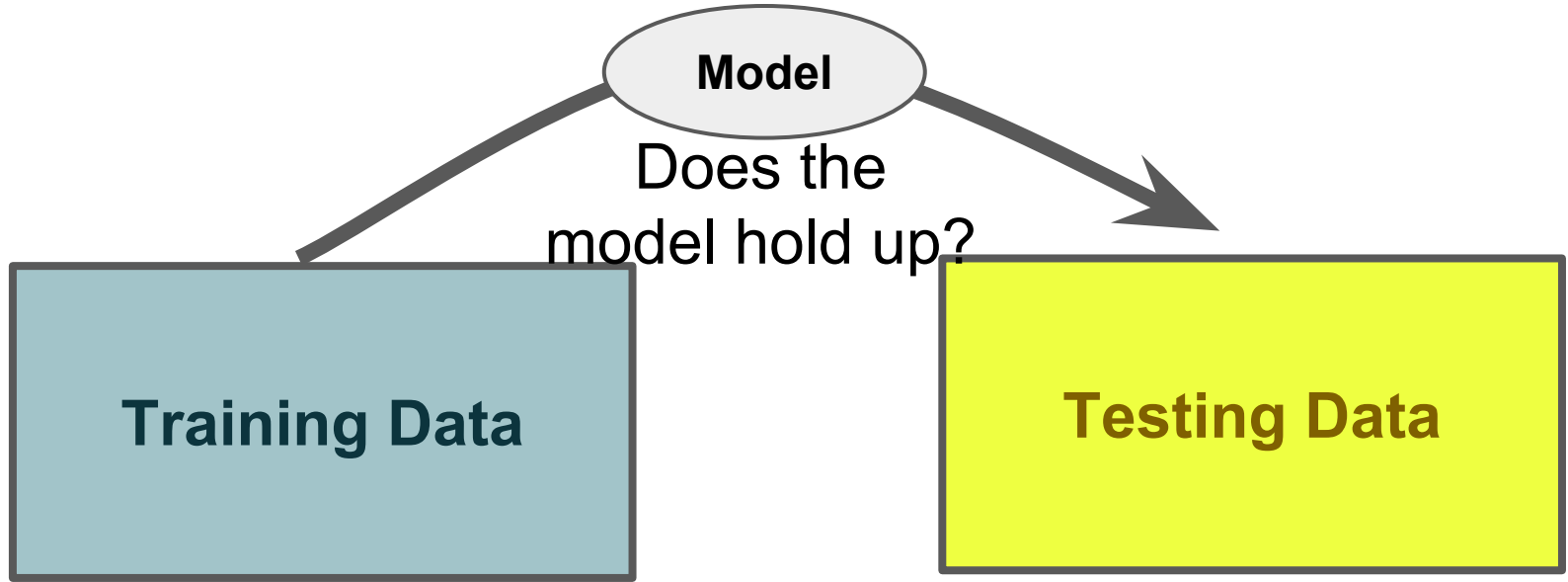
What if only 2 predictors?

$$\text{logit}(Y) = 0 + 2 * X_1 + 2 * X_2$$

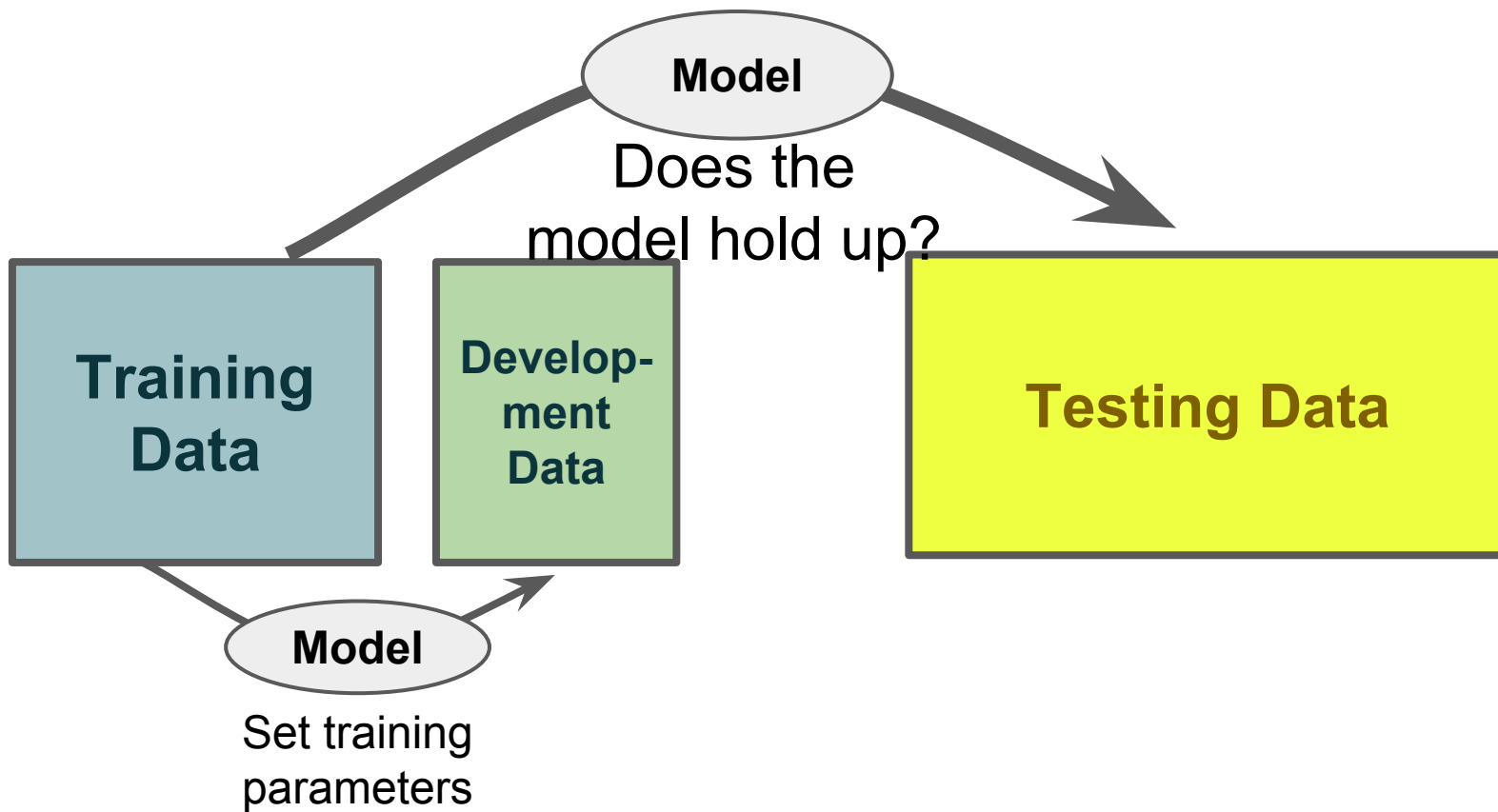
Common Goal: Generalize to new data



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Common Goal: Generalize to new data



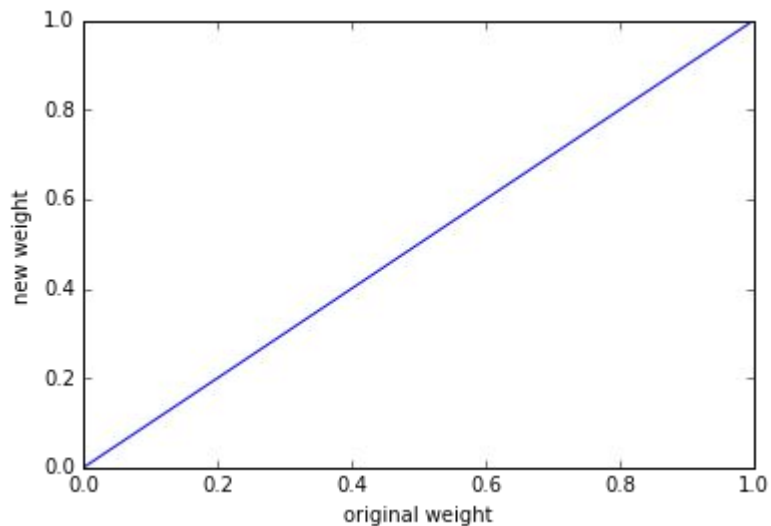
Feature Selection / Subset Selection

(bad) solution to overfit problem

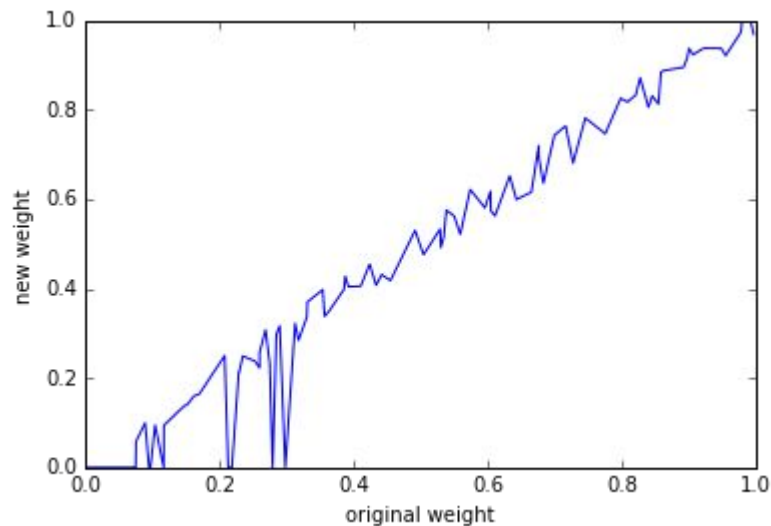
Use less features based on Forward Stepwise Selection:

- start with `current_model` just has the intercept (mean)
`remaining_predictors = all_predictors`
for `i` in range(`k`):
 #find best `p` to add to `current_model`:
 for `p` in `remaining_predictors`
 refit `current_model` with `p`
 #add best `p`, based on RSS_p to `current_model`
 #remove `p` from `remaining predictors`

Regularization (Shrinkage)



No selection (weight= β)



forward stepwise

Why just keep or discard features?

Regularization (L2, Ridge Regression)

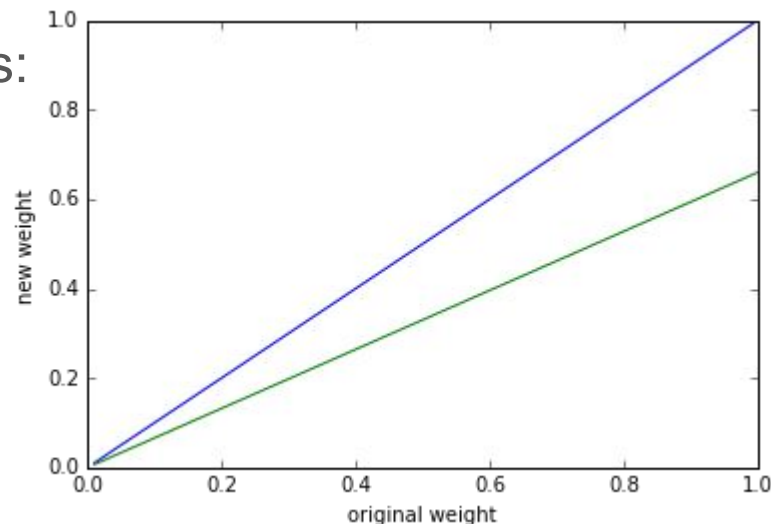
Idea: Impose a penalty on size of weights:

Ordinary least squares objective:

$$\hat{\beta} = \operatorname{argmin}_{\beta} \left\{ \sum_{i=1}^N (y_i - \sum_{j=1}^m x_{ij} \beta_j)^2 \right\}$$

Ridge regression:

$$\hat{\beta}^{\text{ridge}} = \operatorname{argmin}_{\beta} \left\{ \sum_{i=1}^N (y_i - \sum_{j=1}^m x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^m \beta_j^2 \right\}$$



Regularization (L2, Ridge Regression)

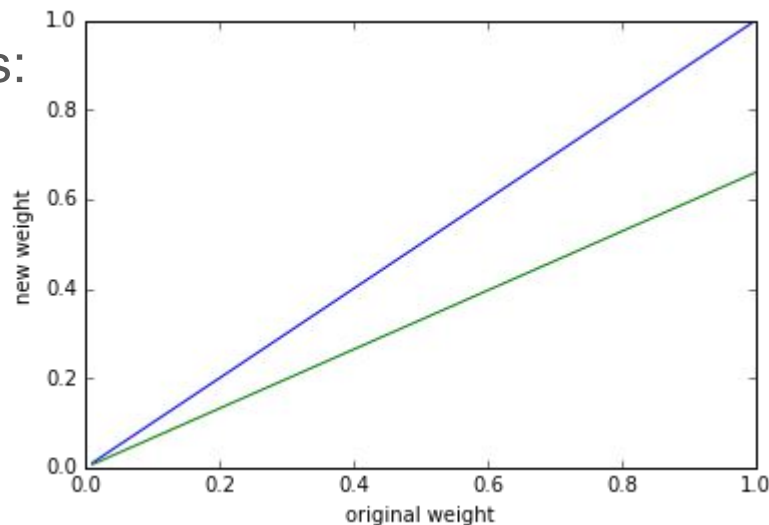
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$$\lambda \|\beta\|_2^2$$

Regularization (L2, Ridge Regression)

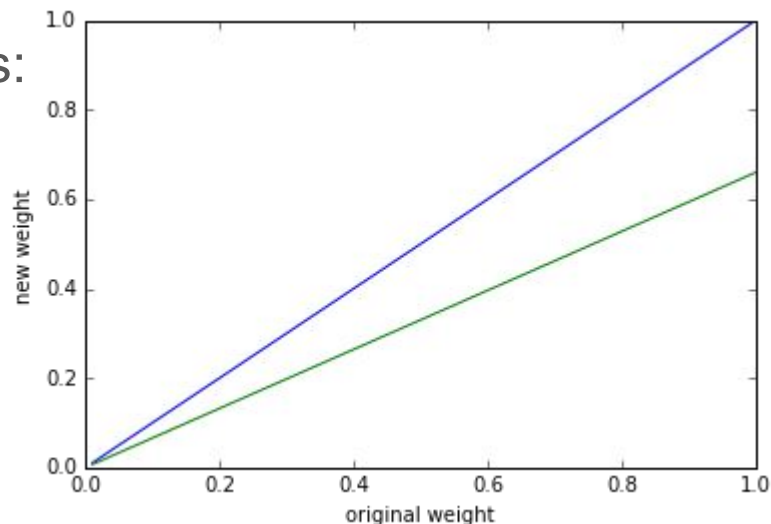
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In Matrix Form:

$$\text{RSS}(\lambda) = (y - X\beta)^T (y - X\beta) + \lambda \beta^T \beta$$

$$\hat{\beta}^{\text{ridge}} = (X^T X + \lambda I)^{-1} X^T y$$

I : $m \times m$ identity matrix

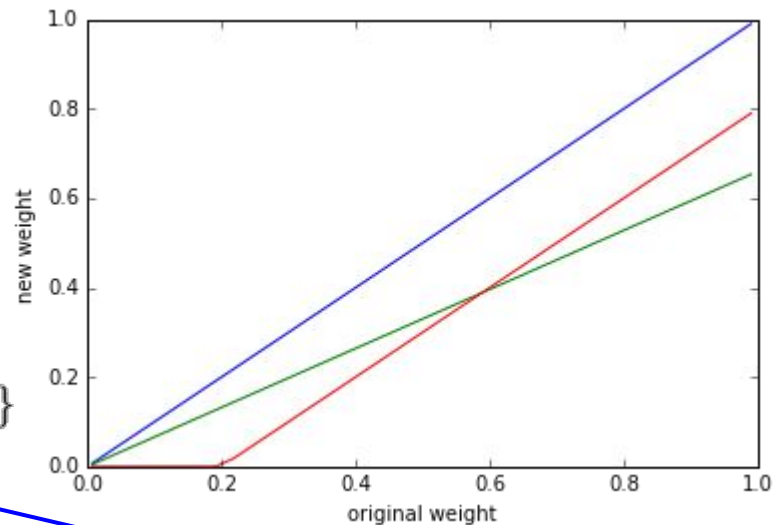
$$\lambda \|\beta\|_2^2$$

Regularization (L1, The “Lasso”)

Idea: Impose a penalty and zero-out some weights

The Lasso Objective:

$$\hat{\beta}^{lasso} = \underset{\beta}{\operatorname{argmin}} \left\{ \frac{1}{2} \sum_{i=1}^N (Y_i - \sum_{j=1}^m x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^m |\beta_j| \right\}$$



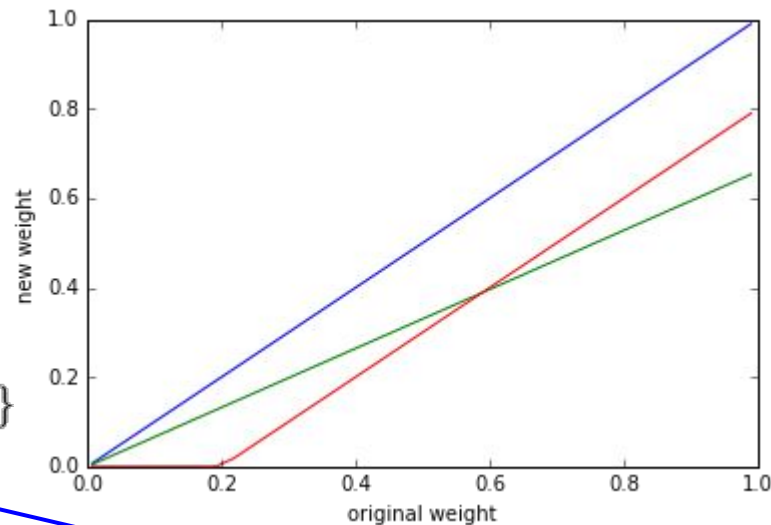
$$\lambda \|\beta\|_1$$

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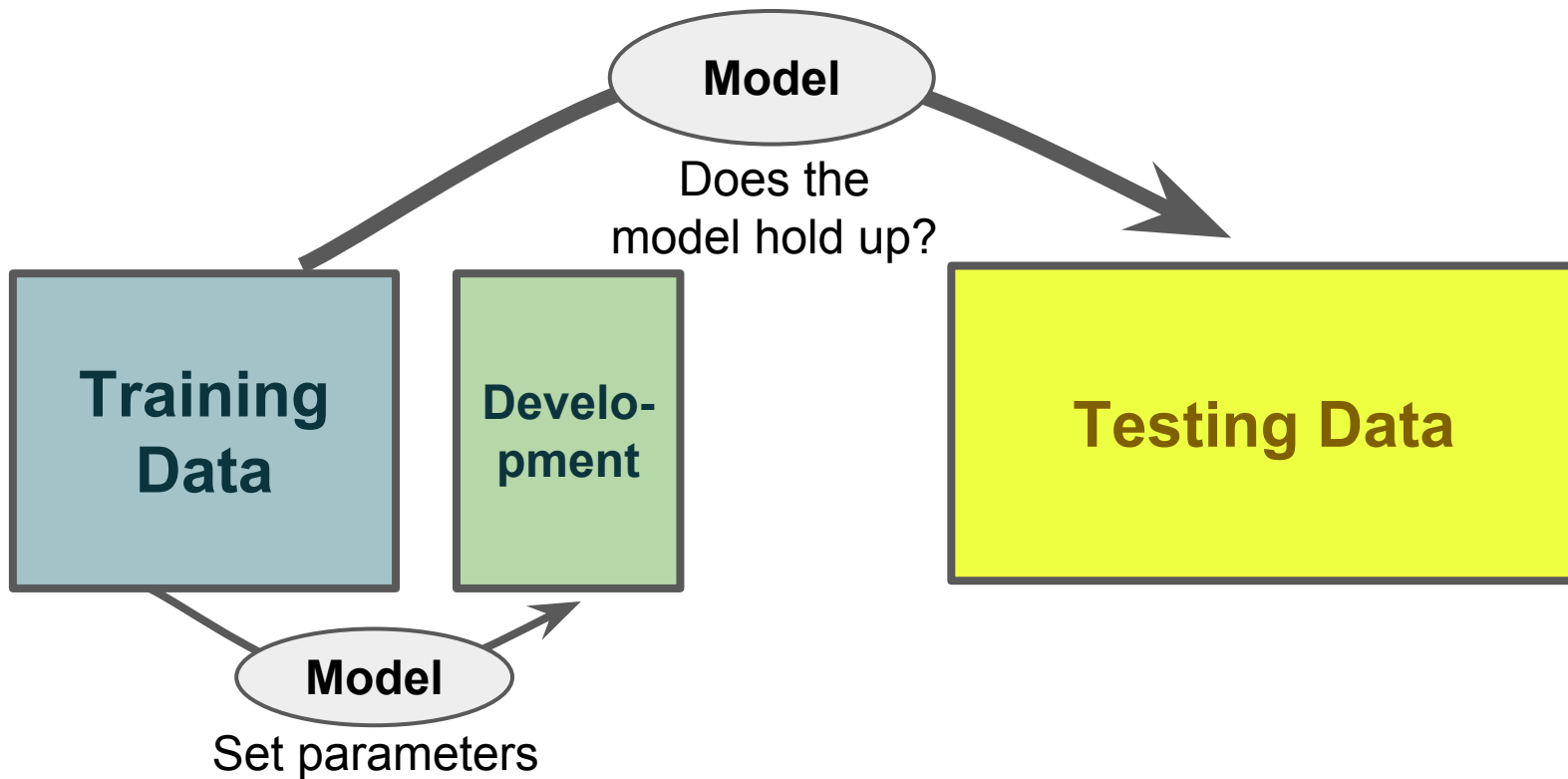


No closed form matrix solution, but often solved with coordinate descent.

$$\lambda \|\beta\|_1$$

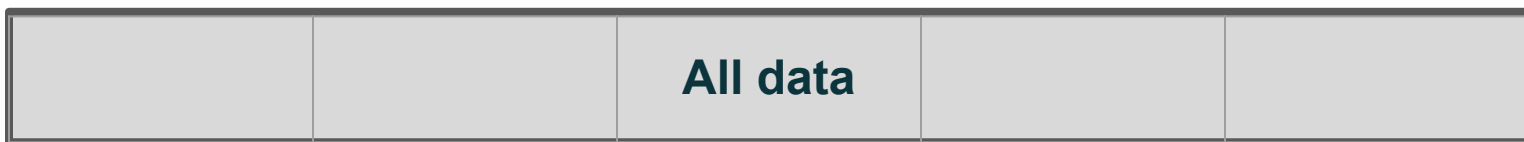
Application: $p \approx n$ or $p \gg n$ (p : features; n : observations)

Common Goal: Generalize to new data



N-Fold Cross-Validation

Goal: Decent estimate of model accuracy



Iter 1



Iter 2



Iter 3



....

...

Summary

Hypothesis Testing:

A framework for deciding which differences/relationships matter.

- Random Variables
- Distributions
- Hypothesis Testing Framework

Comparing Variables:

Metrics to quantify the difference or relationship between variables.

- Simple Linear Regression, Correlation, Multiple Linear Regression,
- Comparing Variables and Hypothesis Testing
- Regularized Linear Regression
- Multiple Hypothesis Testing