# YOU READY?

An Introduction to Data Science in RStudio

Andira Putri
GSU 2018 -- Xylem Inc.

Georgia State University

xylem

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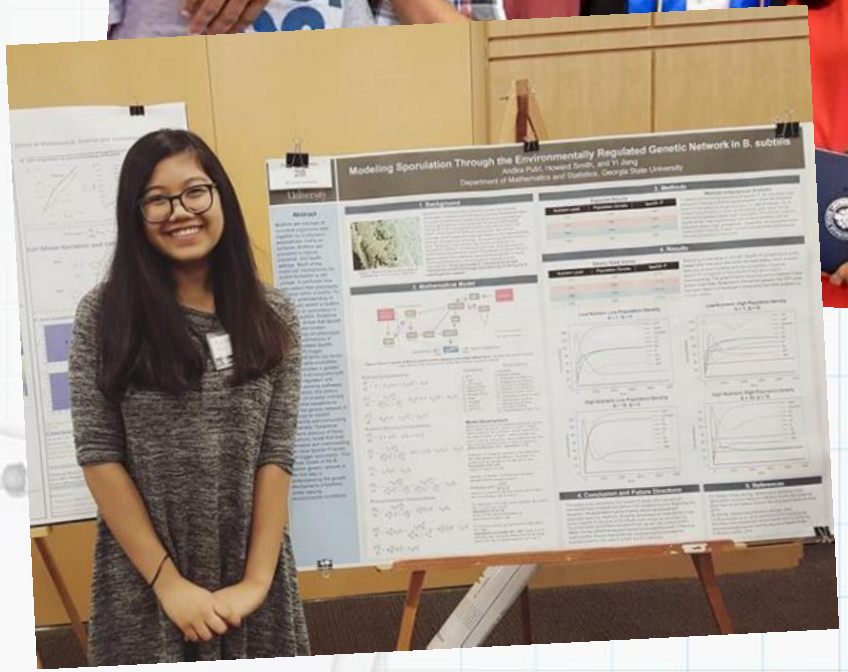
# WORKSHOP STRUCTURE

1. Introduction
    - About Me
    - What is Data Science?
2. Linear Regression
3. Logistic Regression
4. Resampling Methods
5. Case Study
6. Questions?

# INTRODUCTION

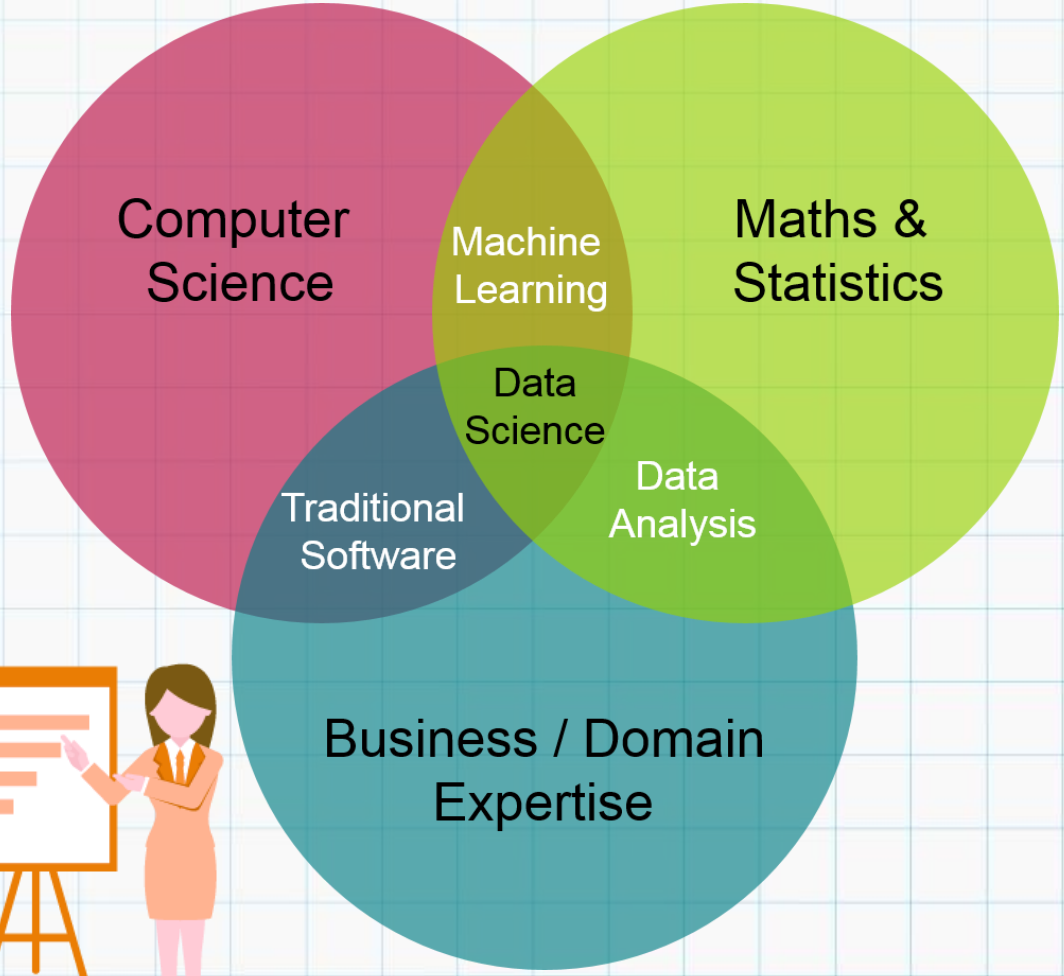
## About Me

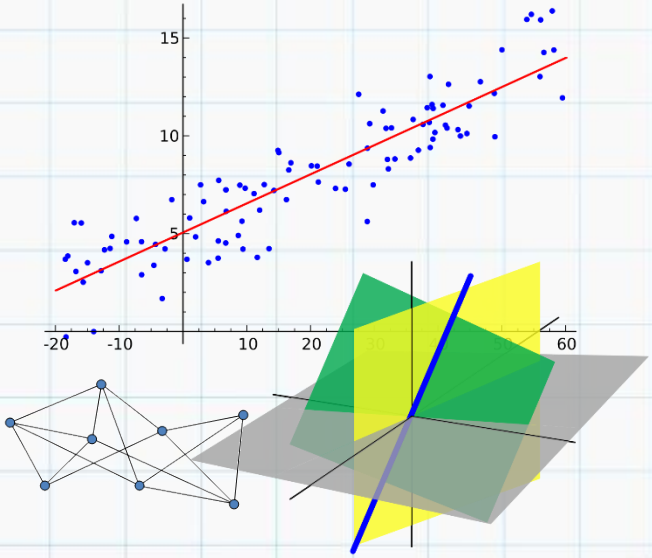



- Graduated from Georgia State in Spring 2018 – B.S. in Mathematics
- Data Scientist at Xylem Inc. in Research Triangle Park, NC
- Will be pursuing an M.S. in Statistics soon at North Carolina State University

# INTRODUCTION

## What is Data Science?

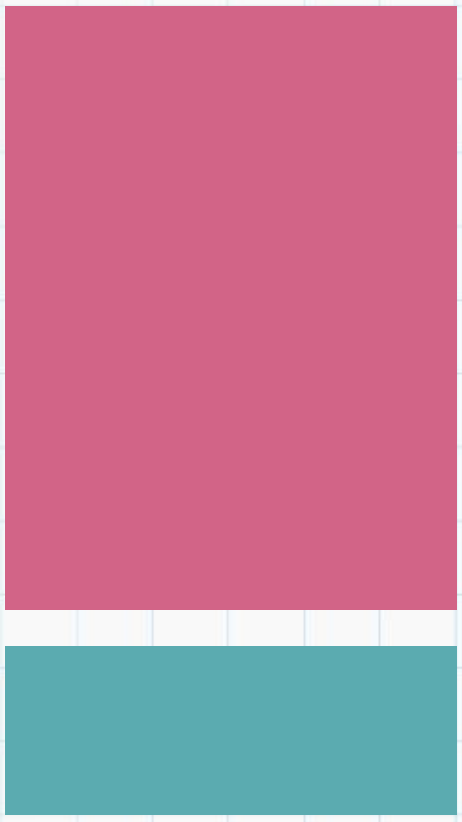



# INTRODUCTION

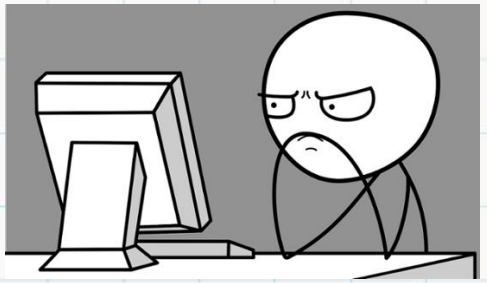
## The Perfect Data Scientist

# INTRODUCTION

## A Typical Project Breakdown



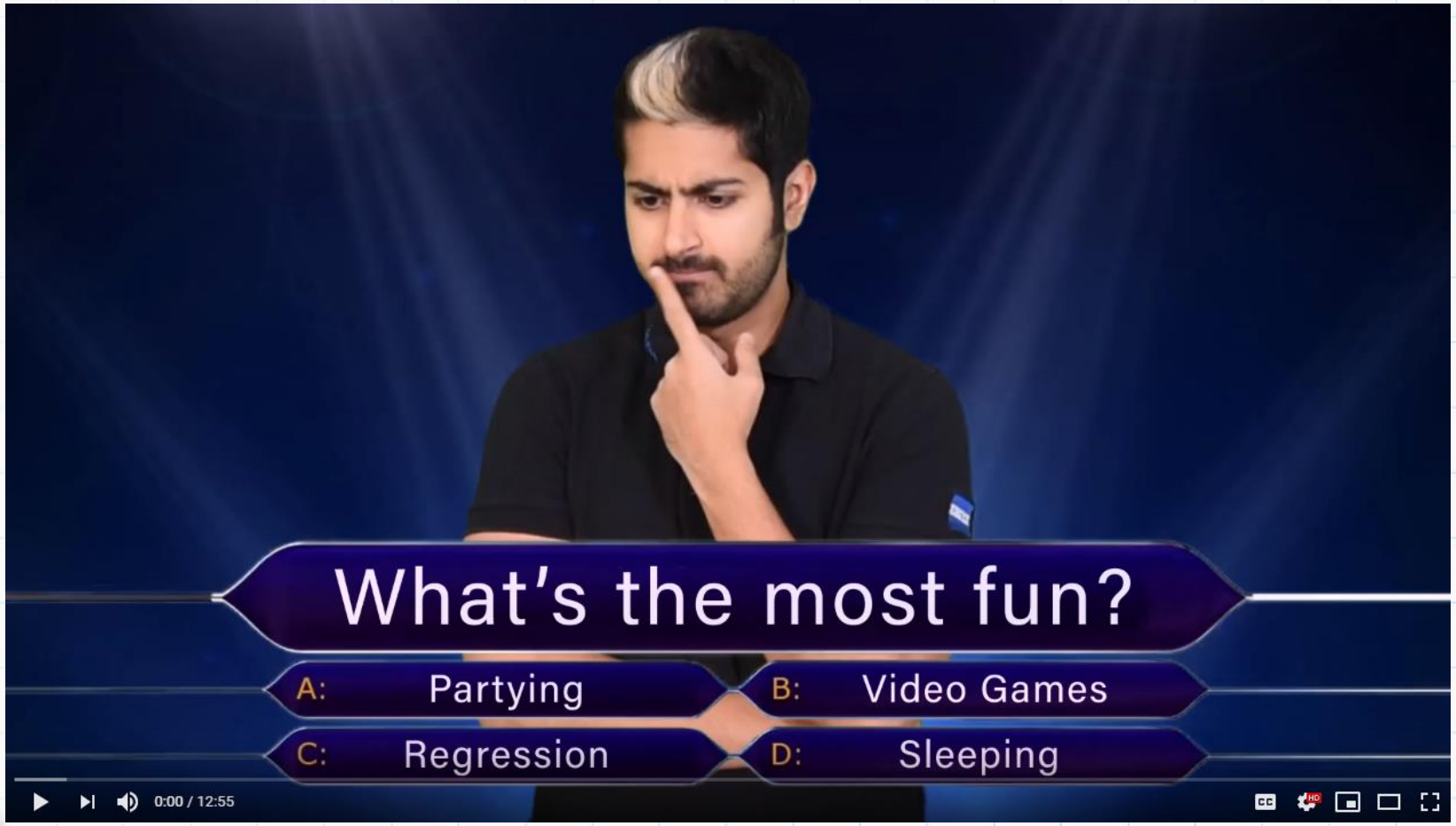
85% Data Mining



15% Applications,
Productizing, Writing

# REGRESSION

## You Must Know It!




Siraj Raval

# LINEAR REGRESSION

## A Foundation of Data Science

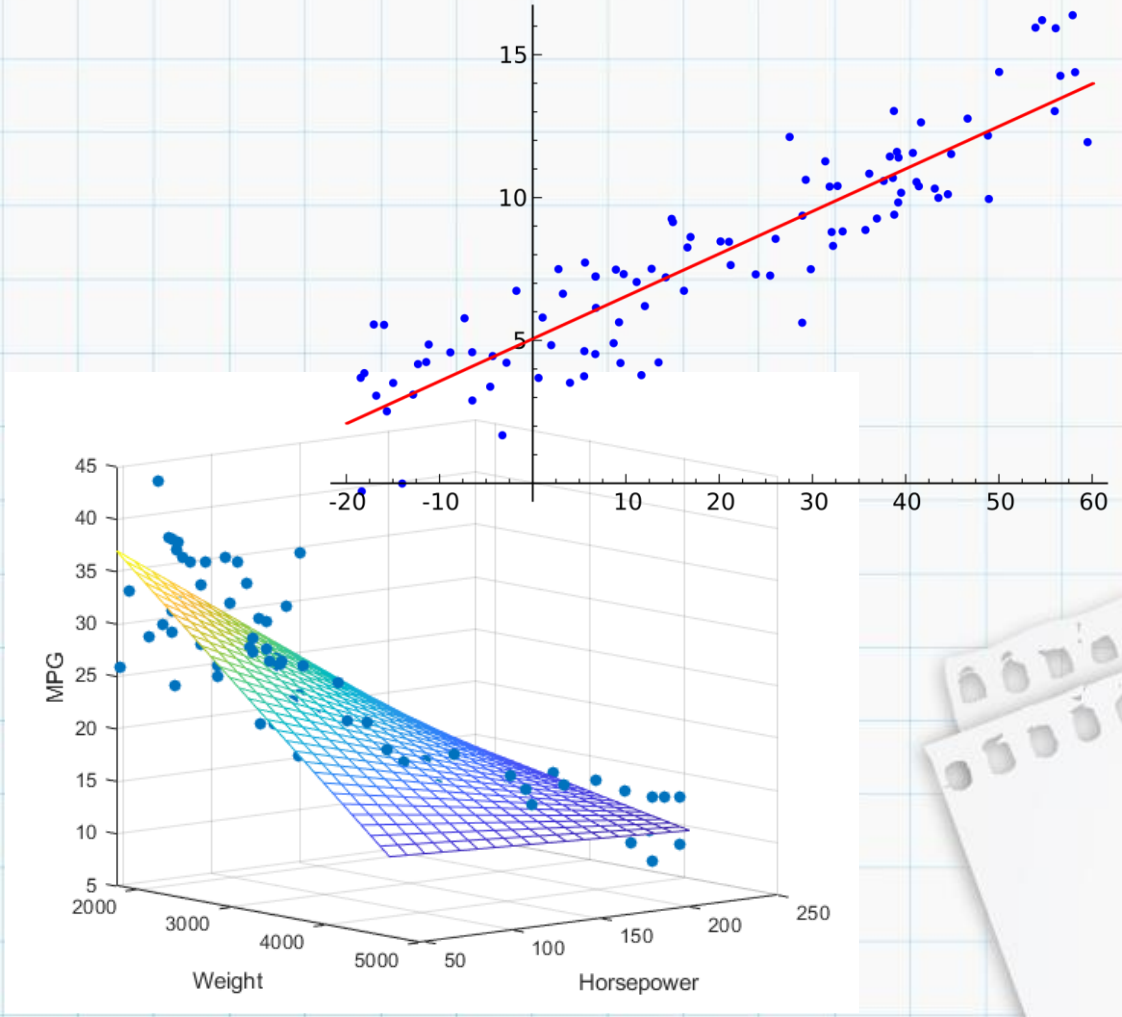
- Assumes a linear relationship between predictors $X_{1...n}$ and a response Y

$$Y = \beta_0 + \beta_1 X_1 + \varepsilon + \beta_2 X_2 + \ldots + \beta_n X_n$$

Simple

Multiple

- $\beta_0$, $\beta_1 \ldots \beta_n$ are known as regression coefficients
  - $\beta_0$ → expected mean when predictors = 0
  - $\beta_1 \ldots \beta_n$ → association between predictor and response
  - $\varepsilon$ → error (the residual)



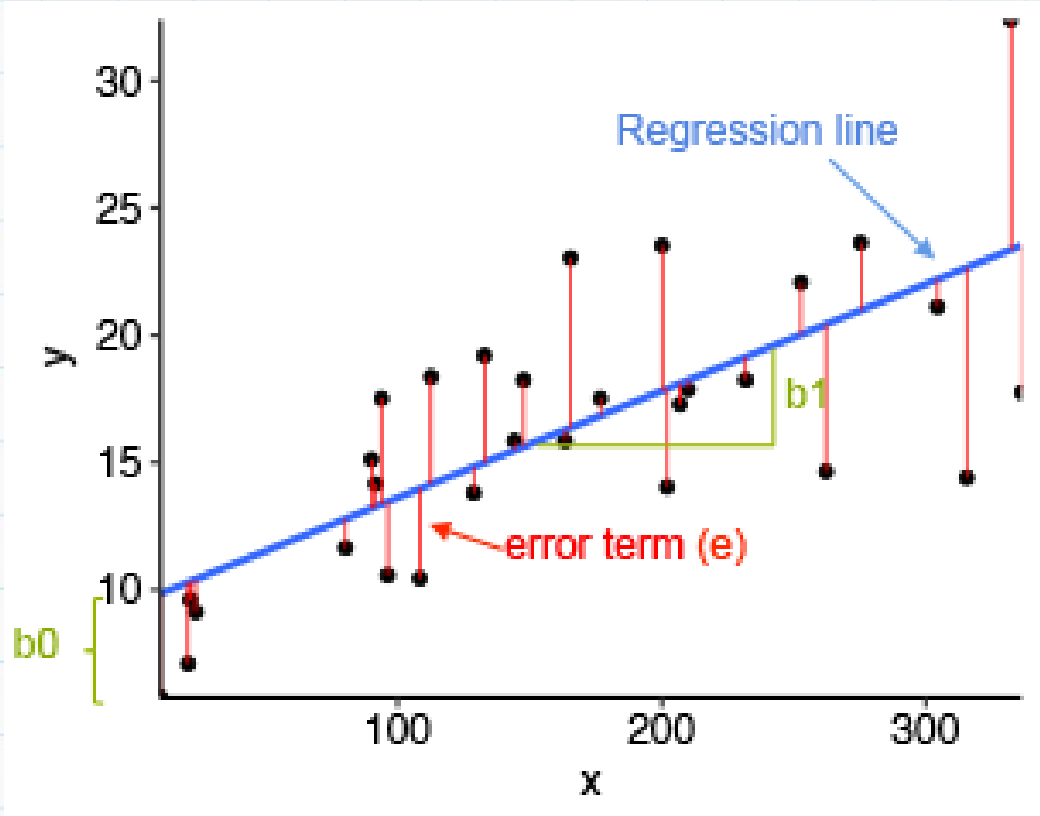
# LINEAR REGRESSION

## A Foundation of Data Science

- Coefficients are estimated by least squares method

- How accurate is our model? We can assess our model using:
  - R-Squared and Adjusted R-Squared
  - Residual Standard Error (RSE)
  - F-statistics

- All values can be called using the summary() function in R



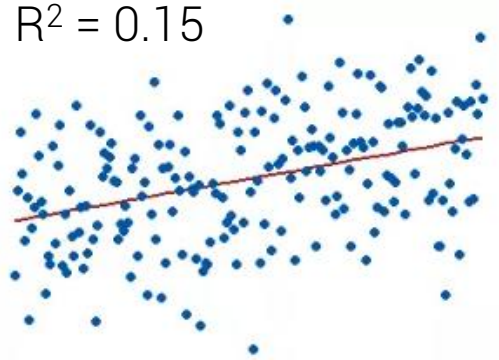
# LINEAR REGRESSION

## A Foundation of Data Science

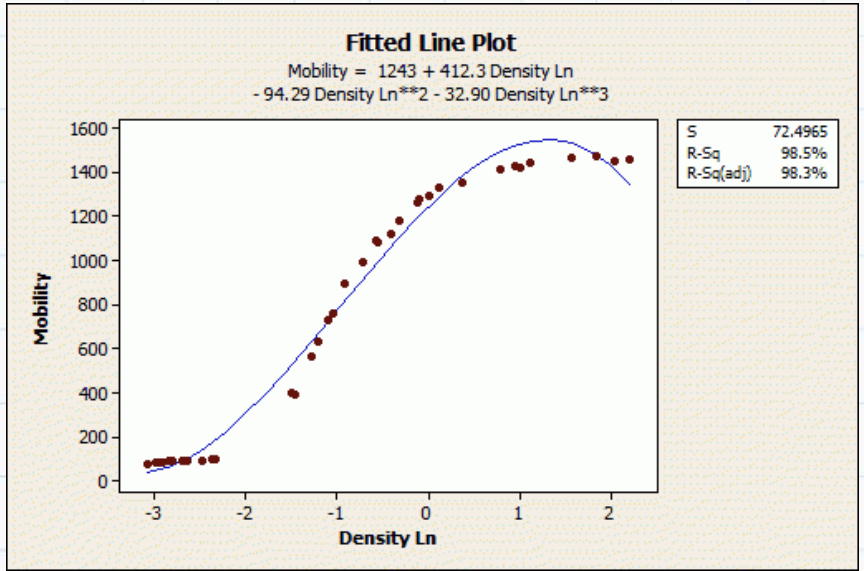
### $R^2$ and Adjusted-$R^2$ Values

- Represents the proportion of variation in the response that can be explained by the predictors
- $R^2 \in [0,1]$ ; the closer to 1, the better
- $R^2$ IS NOT ALWAYS RELIABLE
  It increases when you add more predictors – predictors could be weakly related to the response
- Adjusted- $R^2$ corrects for the additional predictors

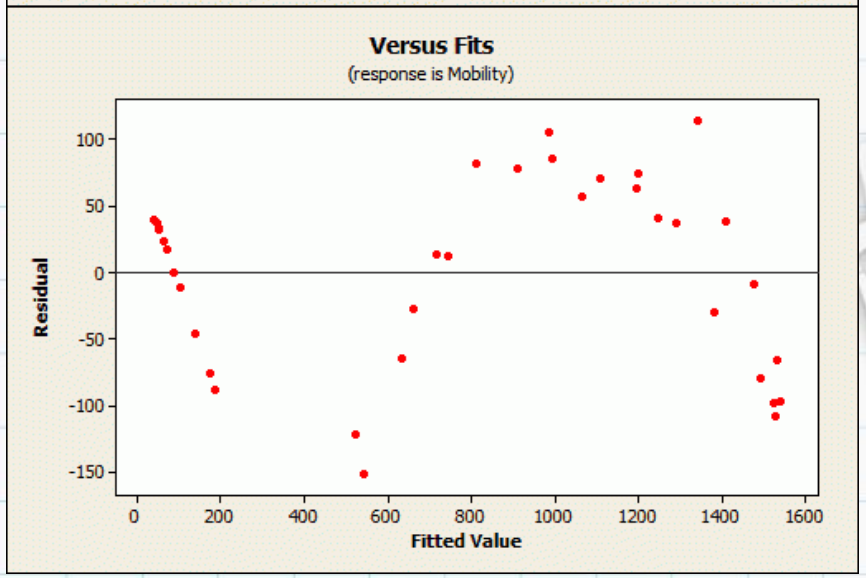
$R^2 = 0.15$



$R^2 = 0.85$




$R^2 = 0.99$



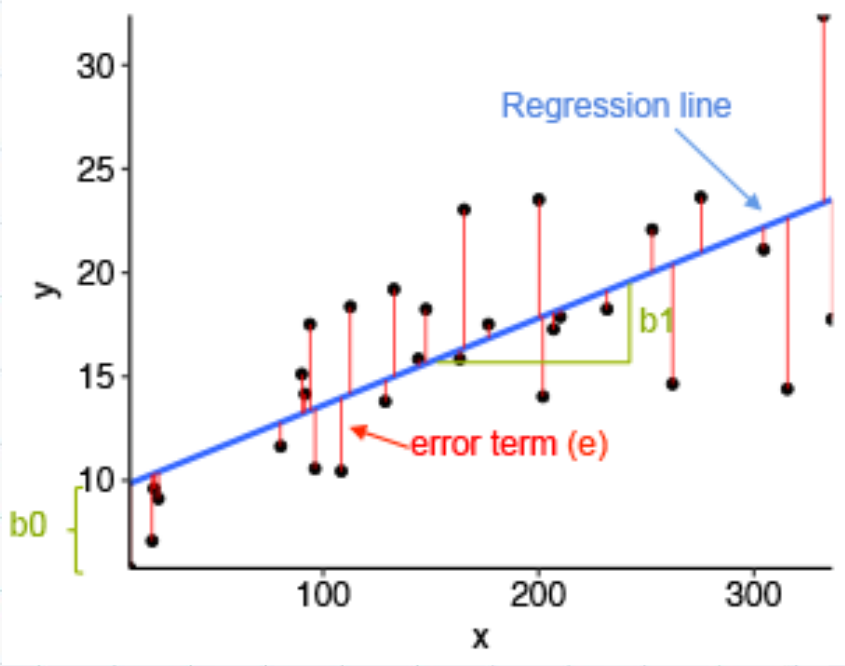

Bias!

# LINEAR REGRESSION

## A Foundation of Data Science

### Residual Standard Error (RSE)

- Represents roughly the average difference between the true response values and the predicted values by the model
- The smaller, the better!
- Dividing the RSE by the average value of the response will give you the prediction error rate

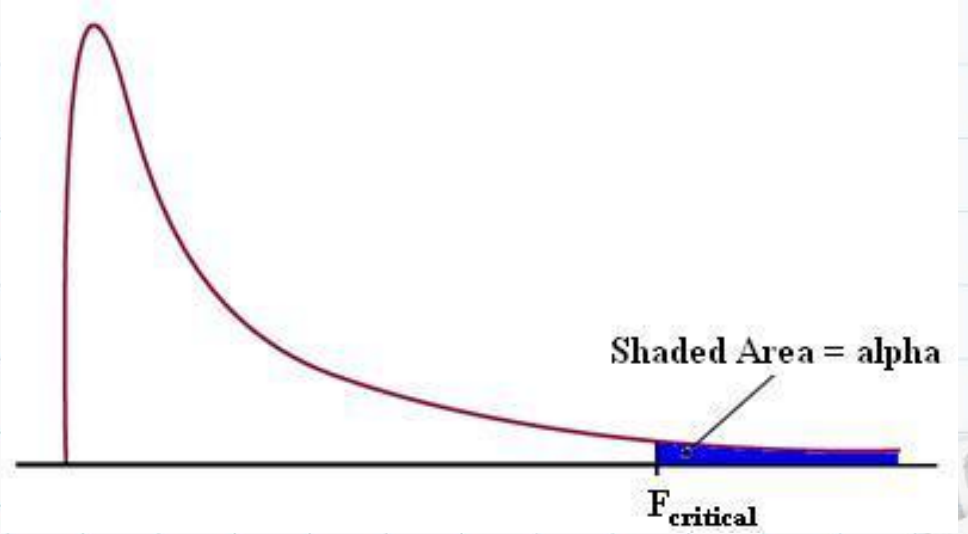


# LINEAR REGRESSION

## A Foundation of Data Science

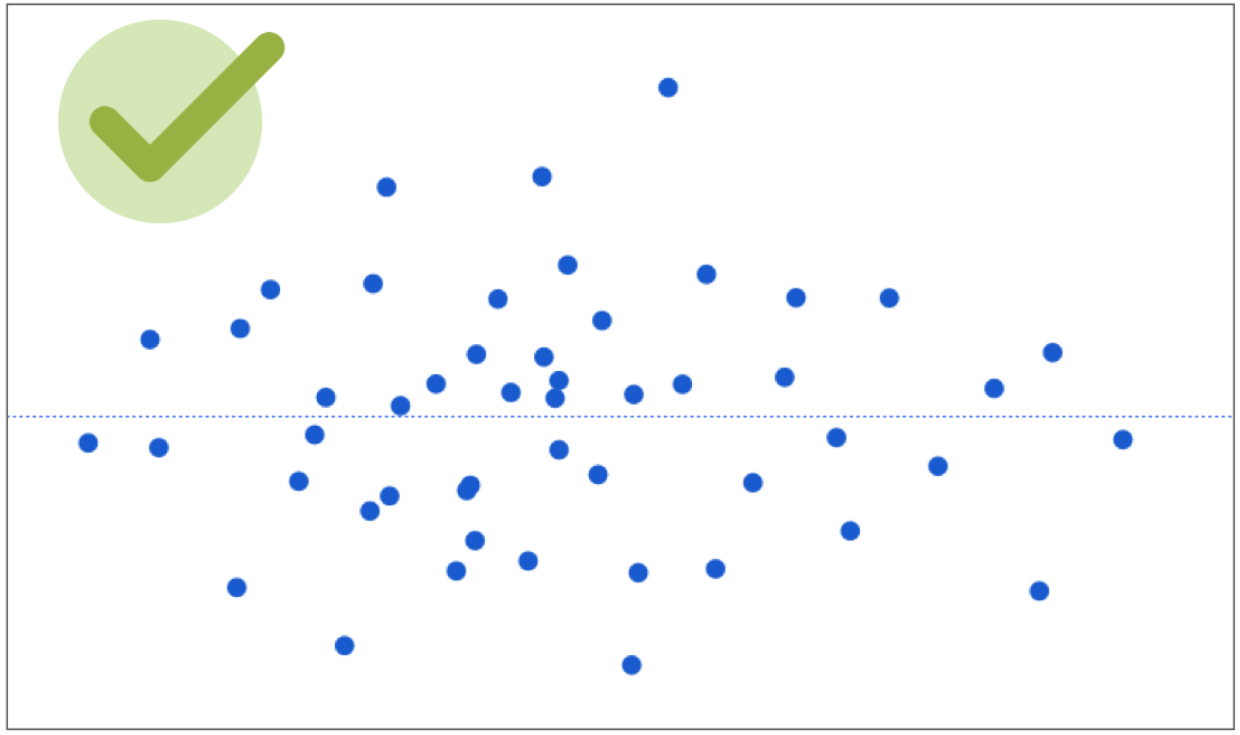
### F-statistic

- Gives the overall significance of the model - assesses whether at least one predictor variable has a non-zero coefficient
- Useful for multiple regression
- We want a large F-statistic, which gives a statistically significant p-value for a confidence level α (e.g. at α = 95%, we want $p < 0.05$)



# ASSUMPTIONS

1. The true relationship is linear
2. Errors are normally distributed
3. Homoscedasticity of errors
4. Observations are independent
5. Variables are not correlated with one another



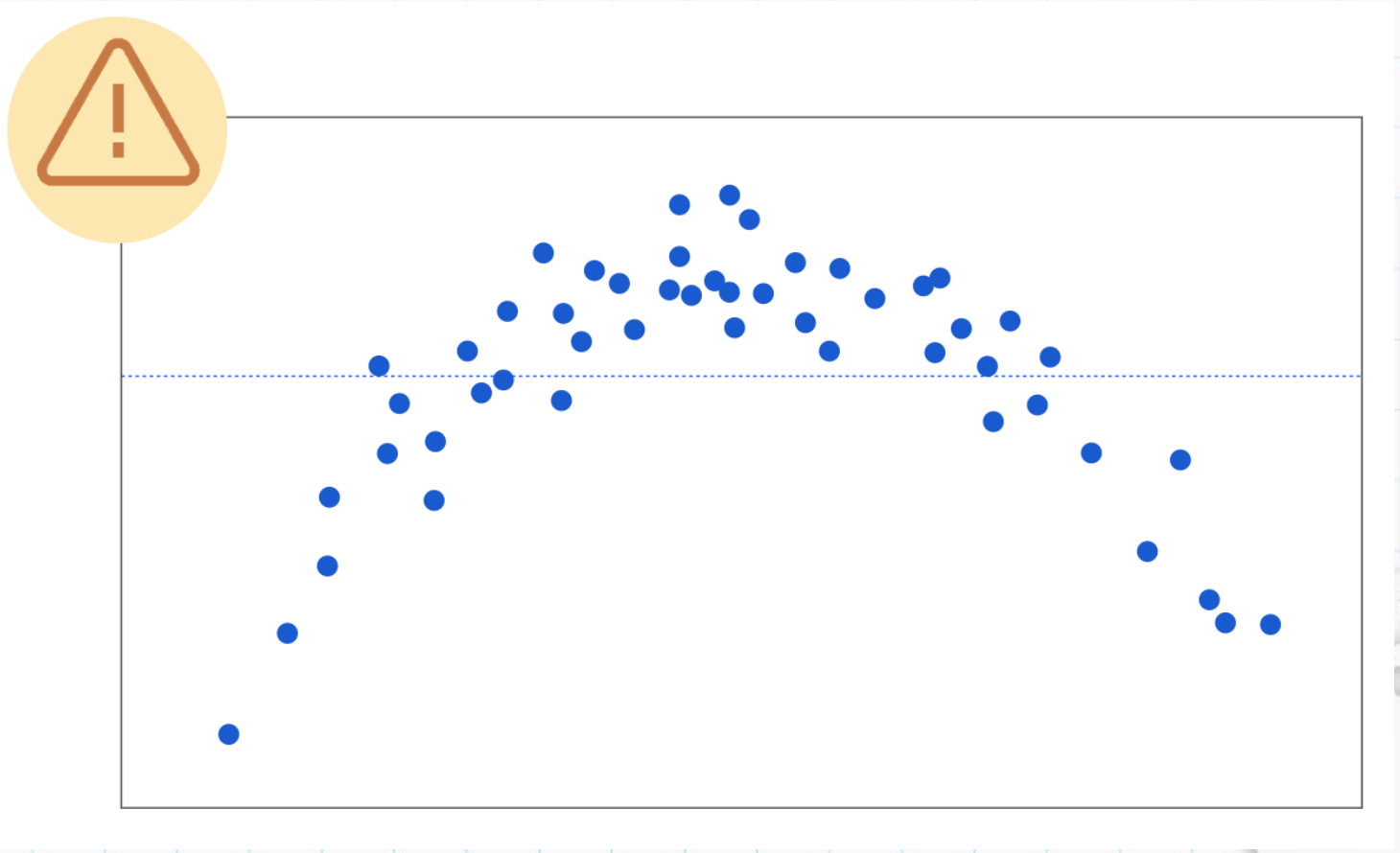
# ASSUMPTIONS

VIOLATION in this residual plot!

There is an obvious curvature in the plot → non-linear relationship

A nonlinear regression would be more informative than a linear one

Under-predicts and over-predicts values → model bias



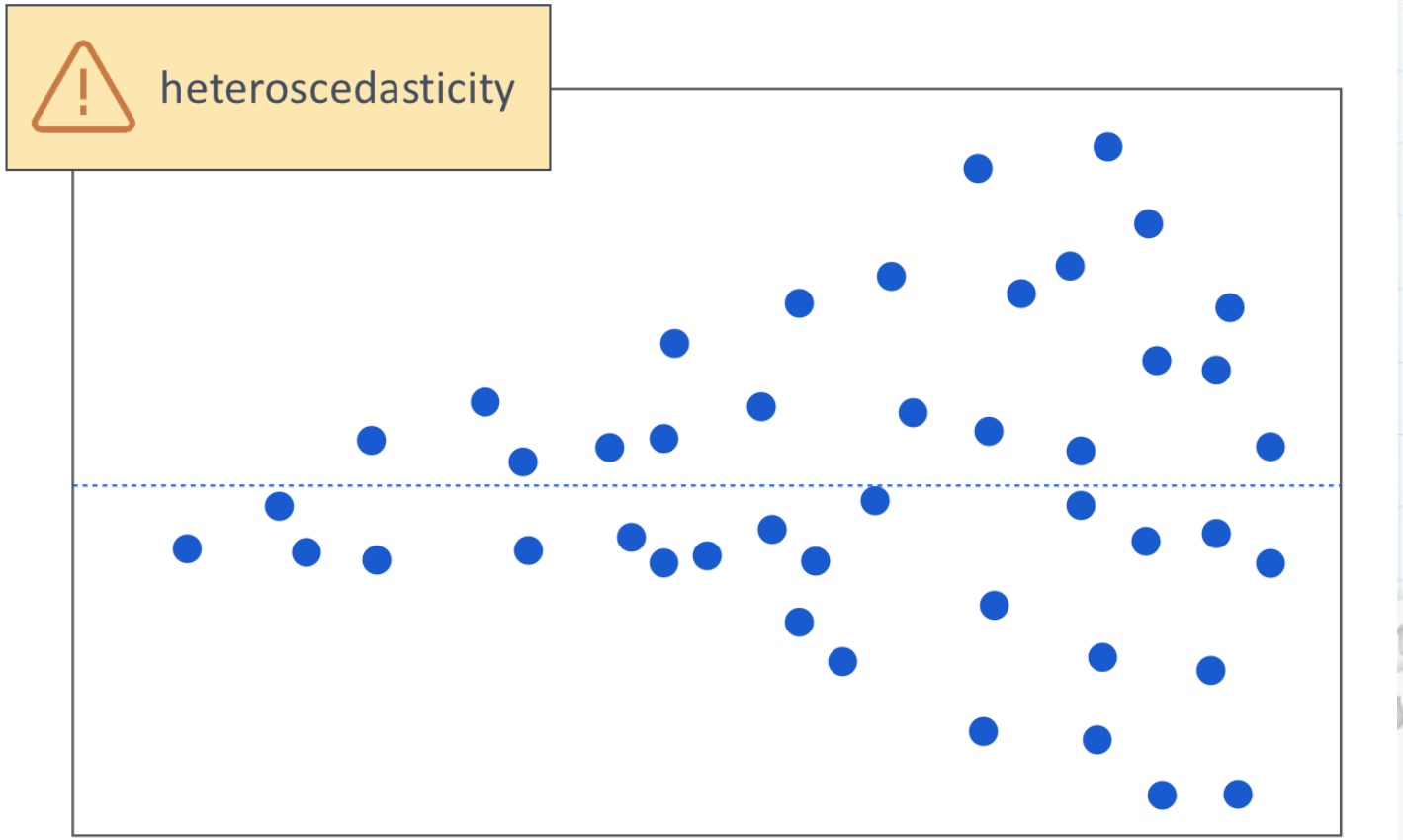
# ASSUMPTIONS

VIOLATION in this residual plot!

We have heteroscedasticity

Variance is unequal across the range of values

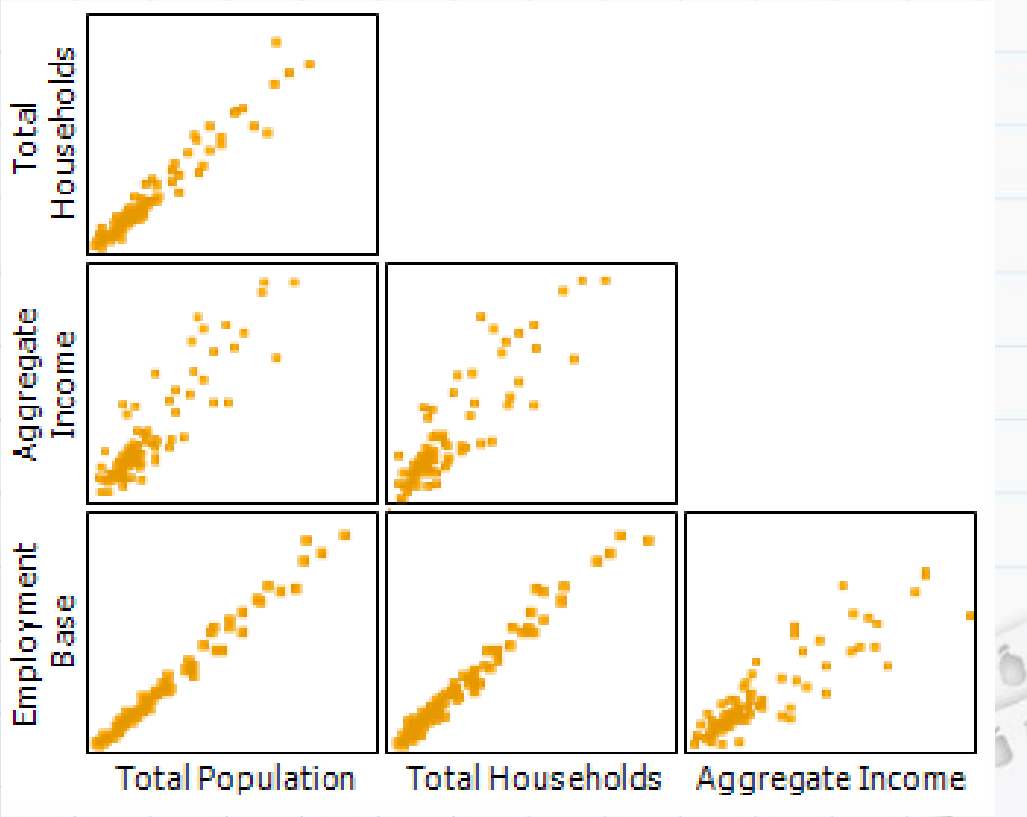
Predicting low values = high accuracy
High values = low accuracy
Model should not be trusted!



# ASSUMPTIONS

## Collinearity (violation)

- Occurs when predictors are highly correlated with each other
- Classic symptom:
  Small change in data can cause big change in coefficients
  OVERFITTING
- Tell-tale signs:
  High $R^2$ but low t-scores
  Variation Inflation Factor (VIF) > 5
- You may be able to ignore it if you are just worried about prediction accuracy



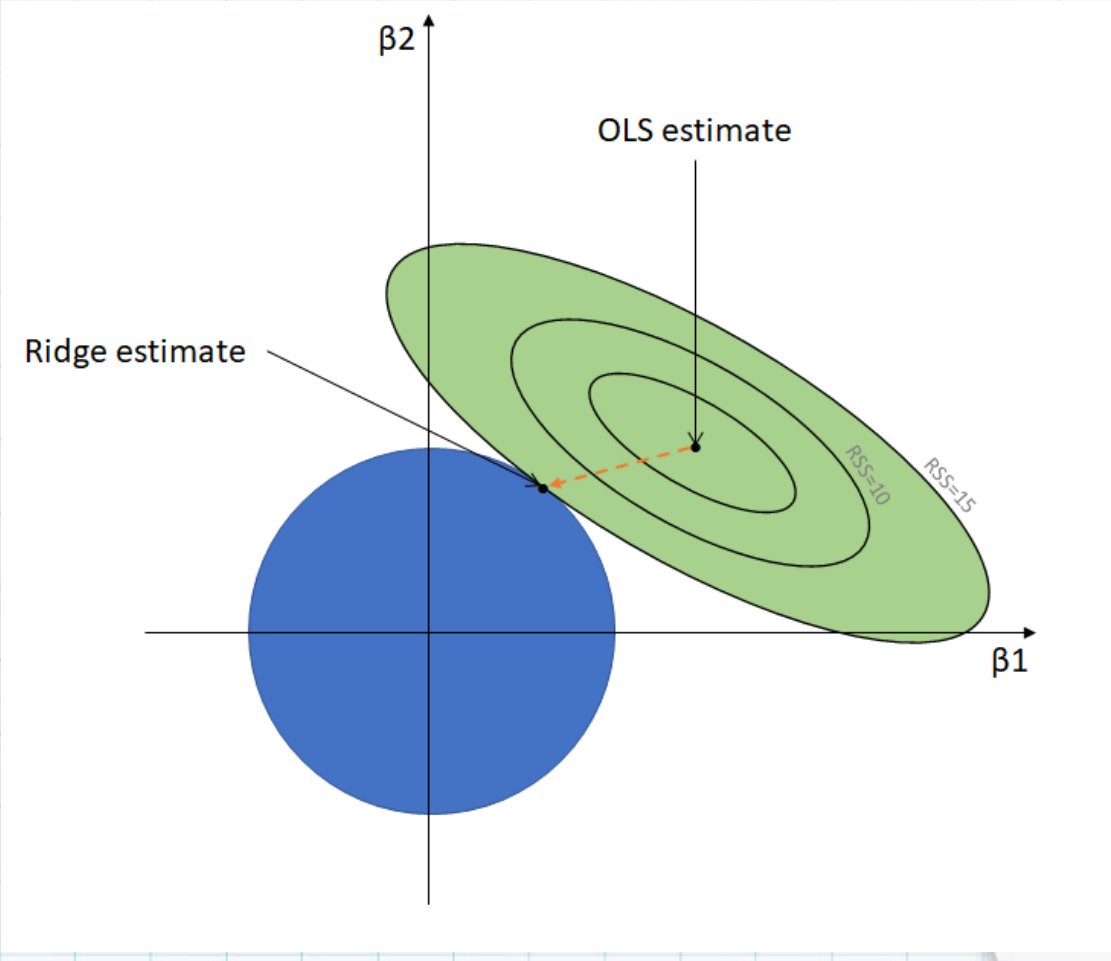
# RIDGE REGRESSION

- To address collinearity, ridge regression adds a bias term to our standard equation
  Reduces variance
  - Least squares will want to minimize residual sum of squares (RSS)

$$\text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2$$

The summation is called the shrinkage penalty

  - λ is the tuning parameter
    Higher λ → more shrinkage, and coefficients shrink towards 0
  - λ is determined through cross-validation



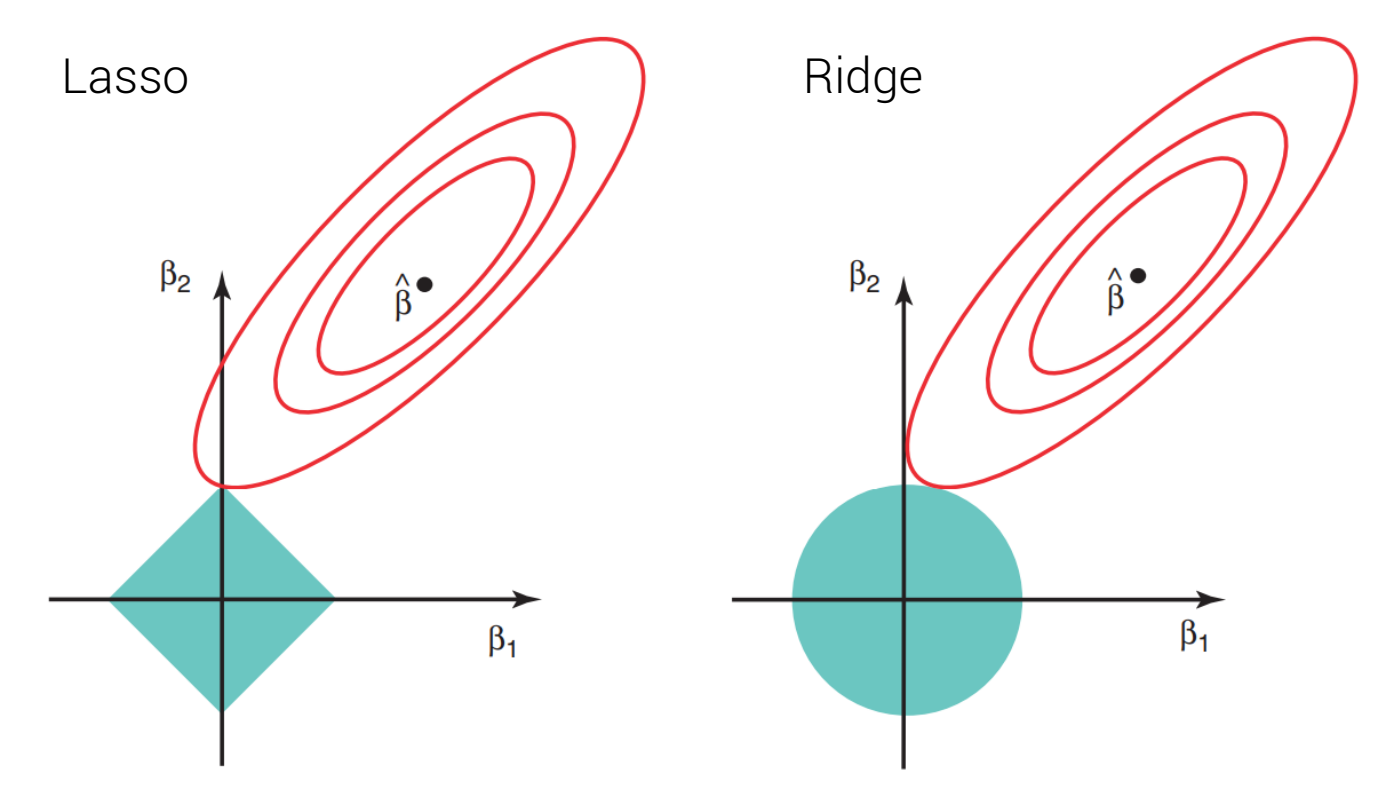
# THE LASSO

- Very similar to ridge regression except we have the ability to set coefficients to zero if irrelevant – HUGE effect on variance

- Bias term:

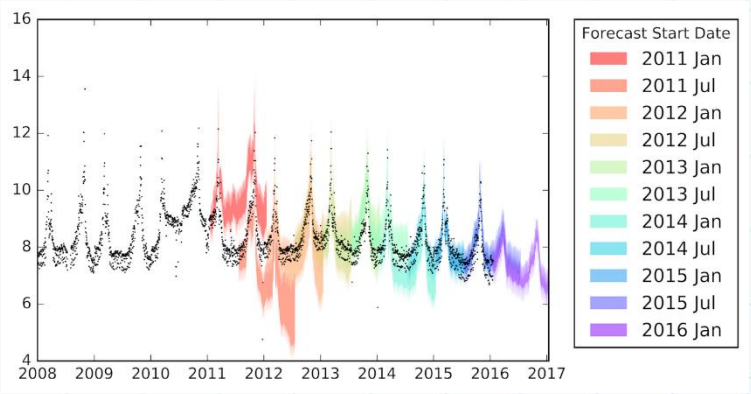
$$\text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|$$

- This is my preferred shrinkage method



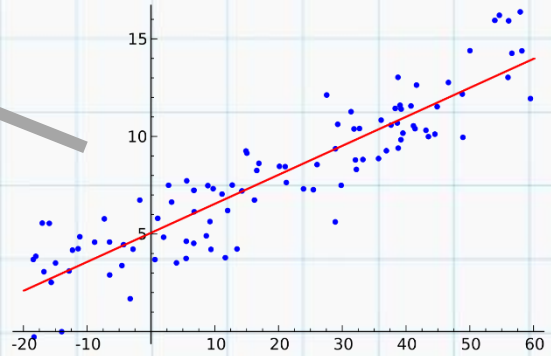
# LINEAR REGRESSION

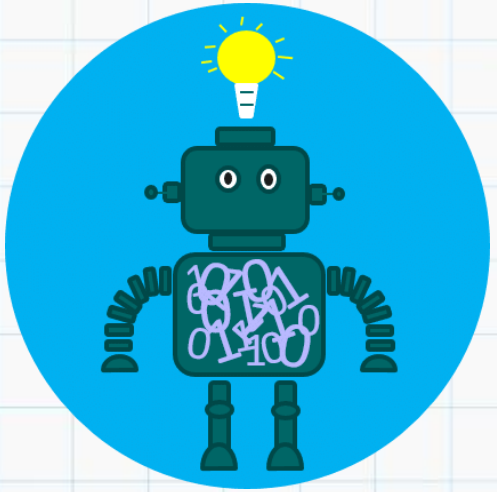
## A Foundation of Data Science




Time Series Analytics

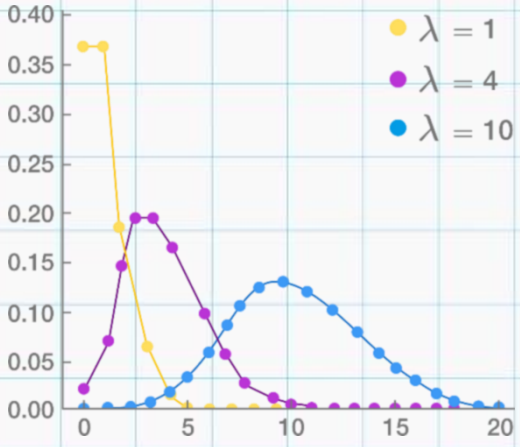
Linear Regression





Machine Learning

Neural Networks



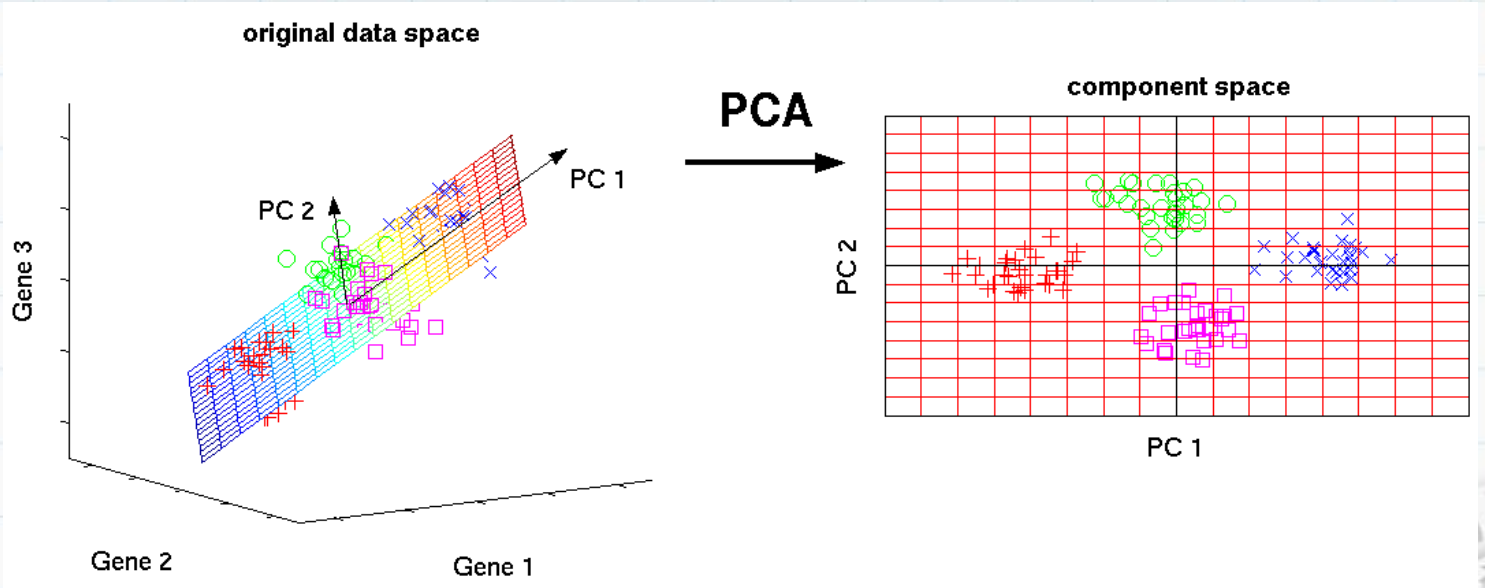

Count Data Analysis

# LINEAR REGRESSION

## A Foundation of Data Science

Additional *Important* Topics:

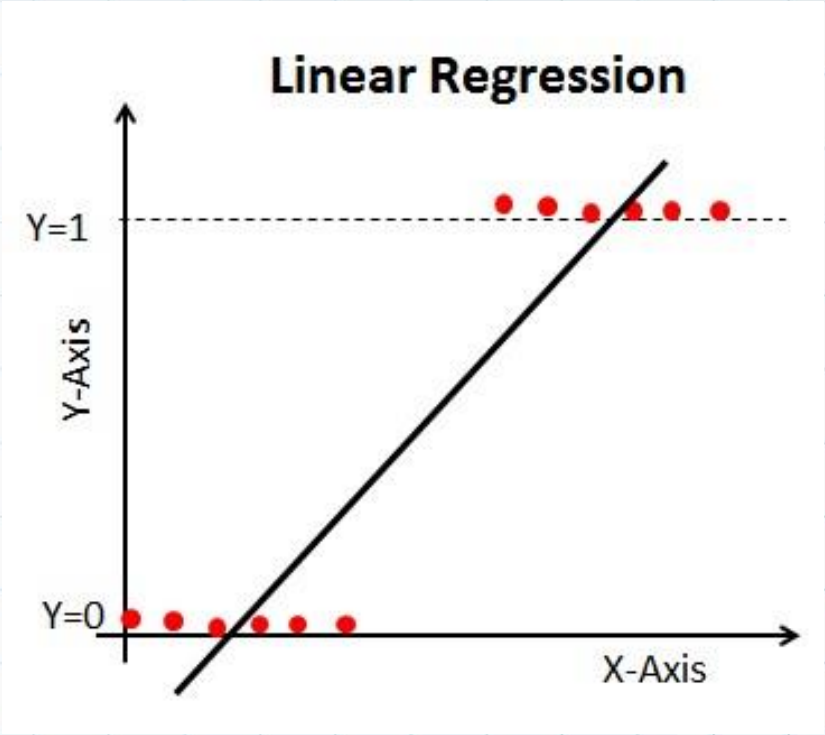
- Residual Analysis
  - Normal Q-Q
  - Leverage
  - Cook's Distance
- Nonlinear Regression
  - Regression Splines
- Model/Variable Selection
  - AIC, BIC, $C_p$
  - Subsetting
- Dimensionality Reduction
  - Principal Components Analysis



# What about qualitative responses?

I want to perform a linear regression to predict if I'll get accepted into a college or not. Y=1 if YES and Y=0 if NO.

Dummy Variables

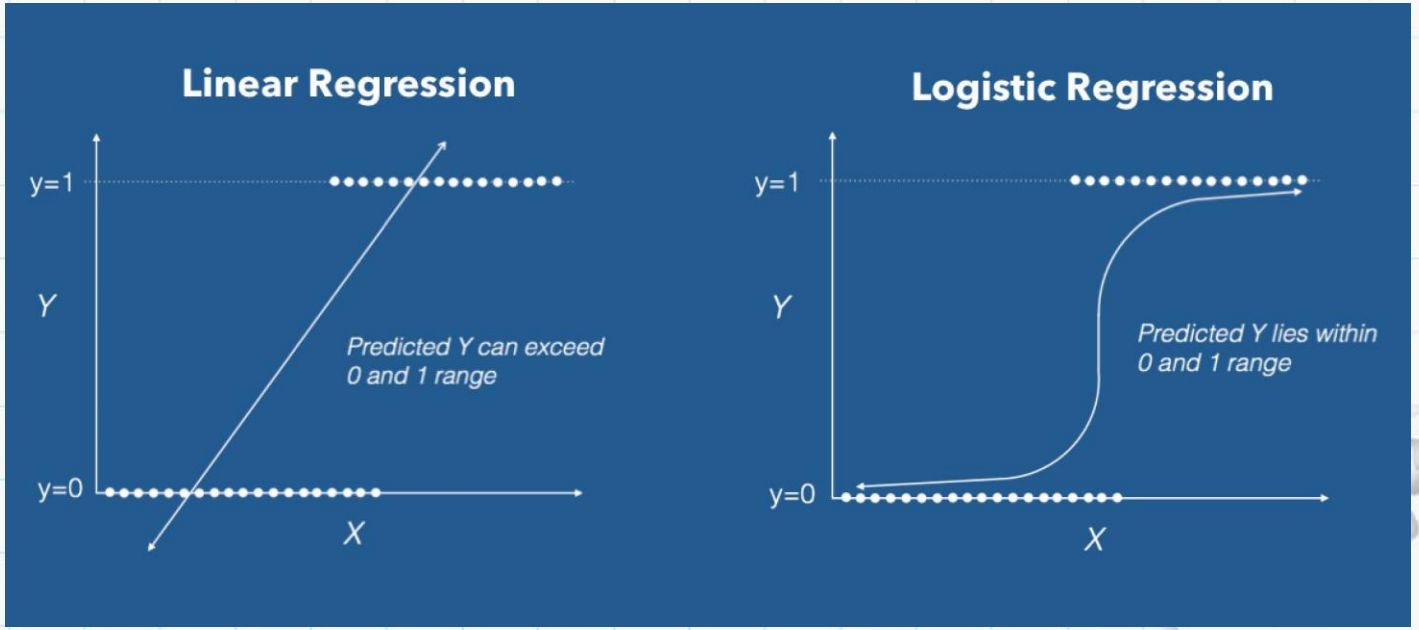



What could be wrong with this approach?

# LOGISTIC REGRESSION

## Classification

- A simple classification method for binary categorical responses
- Predicts the probability of an outcome that can only have two values
- Linear regression is unbounded; logistic regression only falls within [0,1]
- Typically for predicting a TRUE/FALSE or YES/NO problem
  - An email is spam (1) or not spam (0)
  - Will I get accepted into a college (1) or not (0)?



# LOGISTIC REGRESSION

## Odds and Log-Odds

- I will derive the logistic regression equations on the board

- The Odds
  - Value of odds close to 0 = very low probabilities
    $\infty$ = very high probabilities

- The Log-Odds / Logit
  - Coefficients are estimated by the maximum likelihood estimation
  - Essentially, $\beta_0$, $\beta_1$ are determined such that p(x) = 1 when an observation belongs to a class
    p(x) = 0 when it does NOT belong to a class

- Not all values of p(x) = 0 or 1; we need to define a threshold. Usually, it's 0.5
  - If p(x) < 0.5, we round down to p(x) = 0 and state that the observation does NOT belong to a class

# RESAMPLING METHODS

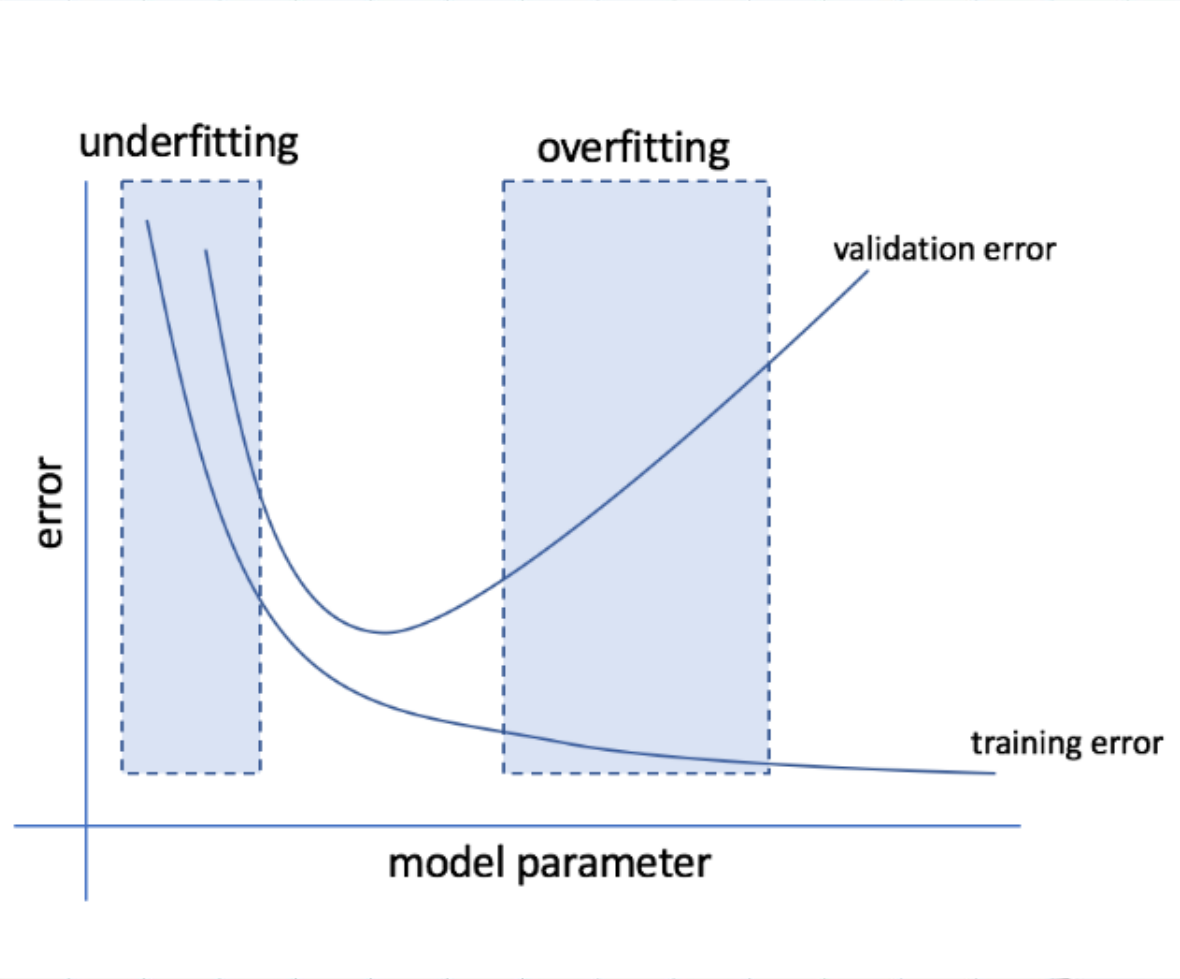
- Involves repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model

- Can our model generalize to new data?

- Two ways: cross-validation and bootstrap

Cross-validation is used to assess model performance

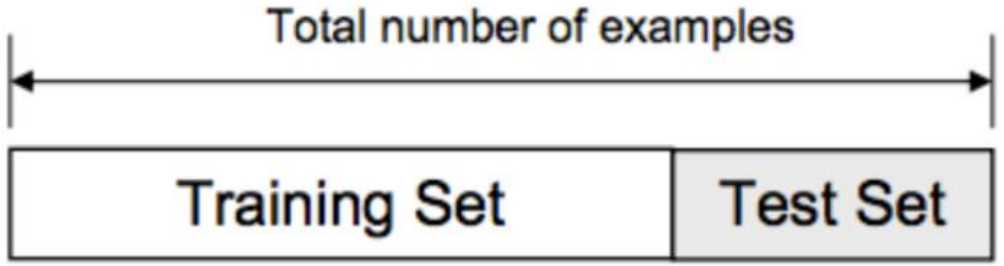
Bootstrap can estimate confidence intervals, accuracy of parameter estimate, etc.



# TRAIN / TEST SPLIT

- The simplest resampling method
- You just need to make sure the sets are not overlapping
- NOT THE BEST
  Subsets may not be completely randomized
  Training set could have people with same age, people who live in the same state, etc.
  OVERFITTING!

  Also, it causes a reduction in training data size
  UNDERFITTING!



# K-FOLD CROSS VALIDATION

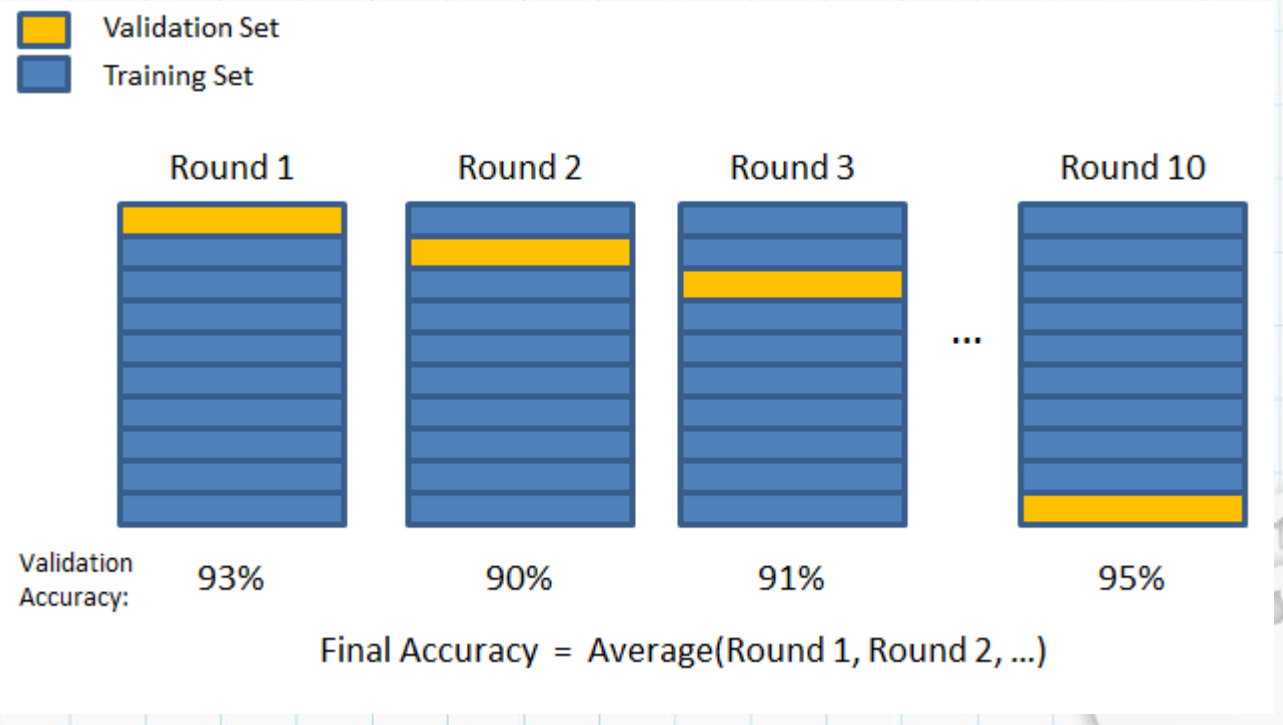
- Train/test split → 2 groups
  k-fold cross validation → k # of groups

- Essentially an iterative / repeated train/test split

- Average the resulting accuracies after repeating k times

- Reduces OVERFITTING
  Most data is being used in the test set

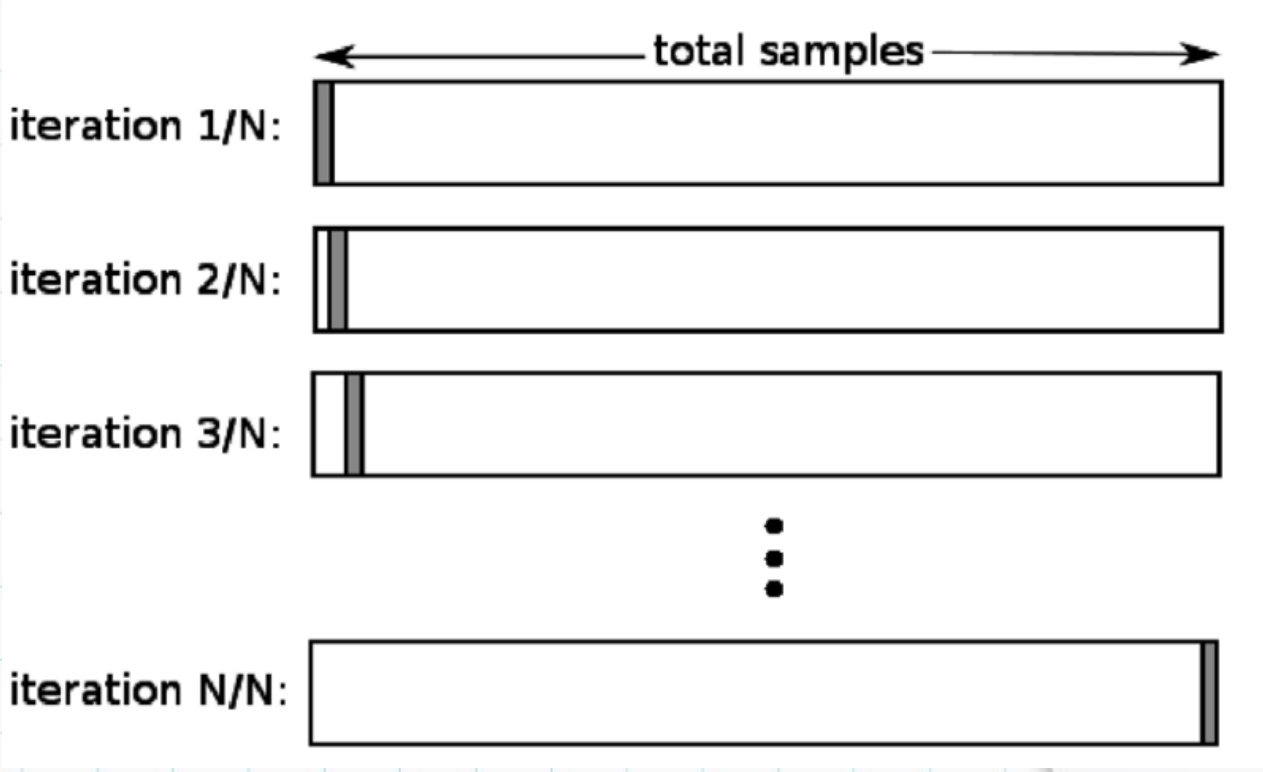
- Reduces UNDERFITTING
  Most data is being used in the training set




General guideline is k=5 or k=10

# LEAVE ONE OUT

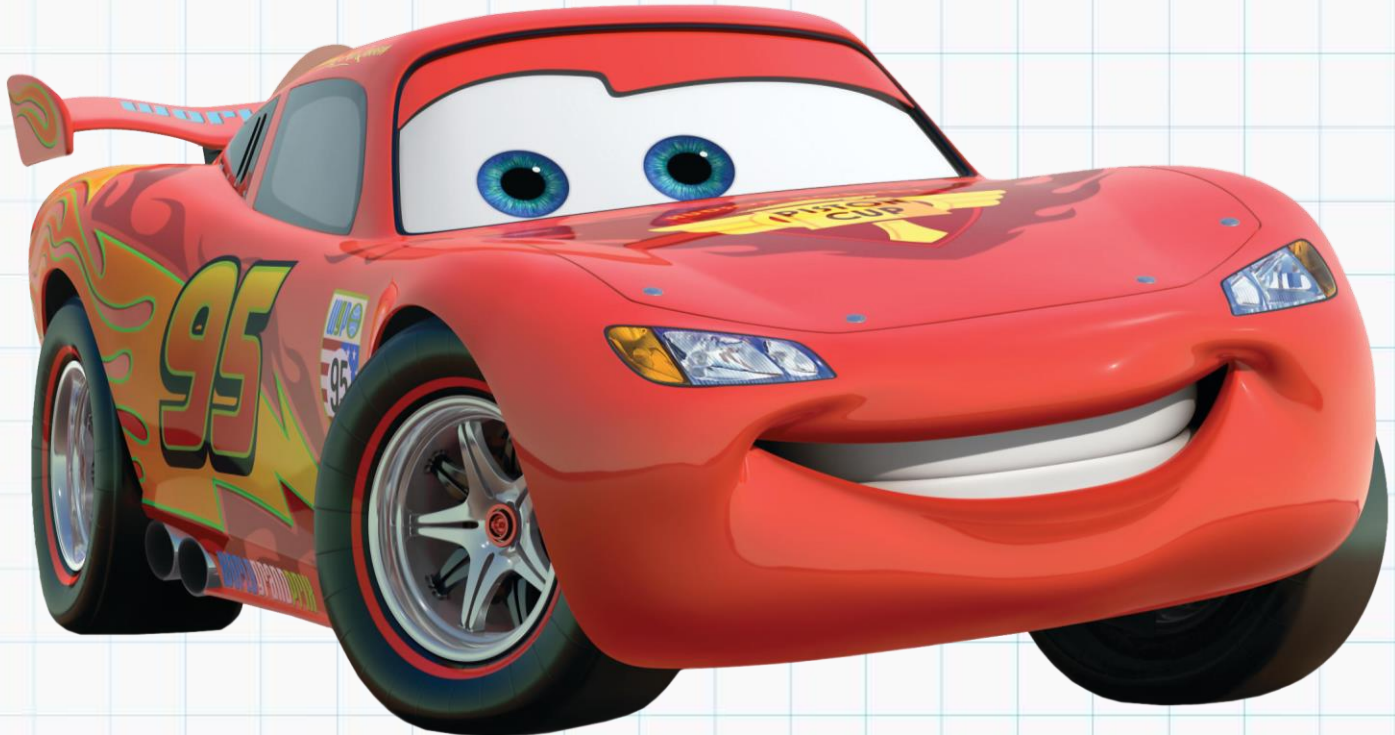
- A special case of k-fold cross validation
- We have n # of observations
  Repeat train/test split n times
  Only one element in the test set
- Great if you have small data sets
- Computationally eXpEnSiVe



# CASE STUDY

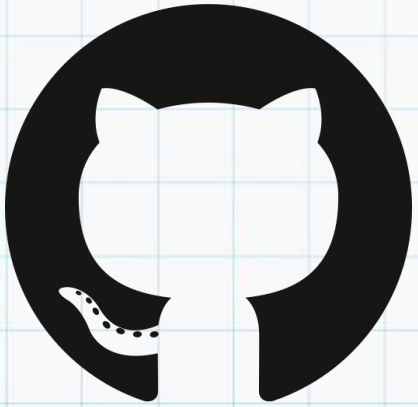
## From Simulated to Real-Life Data

Let's fit some regression models to predict MPG for different cars



# CONNECT WITH ME

www.linkedin.com/in/andira-putri/



@diramputri

diramputri@gmail.com

# THAT'S ALL FOLKS!

Thank You



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# QUESTIONS?