INFO 1998: Introduction to Machine Learning

Download Lecture5Homework.ipynb, lecture5dataA.csv, and lecture5dataB.csv

(also pull up Lecture4Homework.ipynb — you'll find it helpful)



Lecture 5: Fundamentals of Machine Learning Pt. 2

INFO 1998: Introduction to Machine Learning

Tuning Models



What We'll Cover

Last Time's Goal: be able to write code to do some kind of ML (to some extent)

This Time's Goal: create useful ML models



Agenda

- 1. Review
- 2. Measuring Accuracy
- 3. Bias-Variance trade-off
- 4. Feature Selection
- 5. Other Types of machine learning



Review (placeholder text for aesthetic)



Review: Defining ML

We want to predict the future

- Take some known input and output
- Learn the data's pattern and come up with a way to, given a future input, predict the corresponding output

Now: *how* do we learn the data's pattern?





Review: Model

- Something you use to predict outputs
- The Linear Regression Algorithm produces Linear Regression Models
- "Model training" = learn a relationship/program
- "Model validation" = see if the learned relationship is accurate on other data

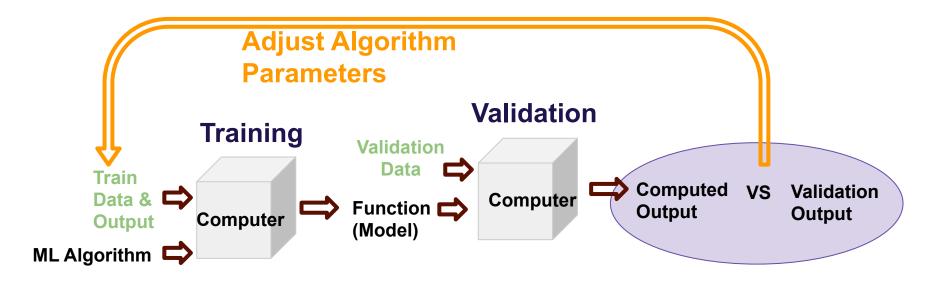




Measuring Bias / Loss (training accuracy)







- 1. Split data (lecture 7)
- 2. Assess model accuracy (today)
- 3. Adjust Model (a bit today)





Loss, Cost, and Score Functions

Loss Function

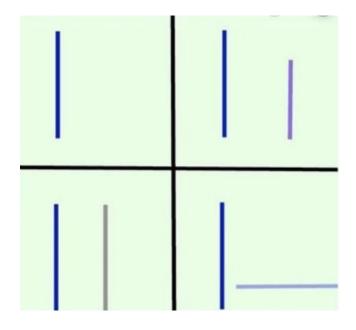
Penalty for missing a single data point

Cost Function

- Indicates how bad the whole model is
- Applies loss function to each point, then combines that into a single number
 - ex: average of (loss from each point)

Score Function

A more interpretable version of the cost function







Linear Regression Loss Formula: Euclidean Distance

loss
$$(x, y^*) = (h(x) - y^*)^2$$

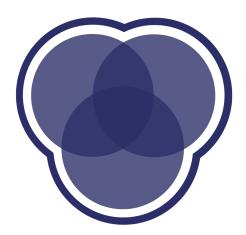
Two things to note about this loss function:

- Positives and negatives won't cancel
- Large errors are penalized exponentially more
- Cost Function average of the loss function over all the points





Demo







Solution: Compare to Baseline

- When determining accuracy, usually want to compare our model to a baseline
 - For regression, one baseline model is the model that predicts the average of the target value for every point
 - For our purposes: don't worry about the baseline model, just have a set of baseline predictions





Cost -> Accuracy Score

sklearn's score function is:

1 - ([Cost of model] / [Cost of baseline])

- 1 is very, very good
- 0 means you were as bad as the baseline
- <0 means either your baseline predictions were accurate, or you really, really messed up





Overfitting and Underfitting (what's a good model?)





Model Goals

When training a model, we want our model to:

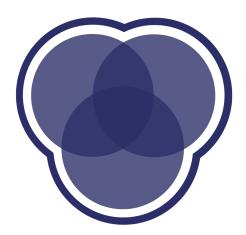
- Capture the trends of the training data
- Generalize well to other samples of the population
- Be moderately interpretable

The first two are especially difficult to do simultaneously!
The more sensitive the model, the less generalizable and vice versa.



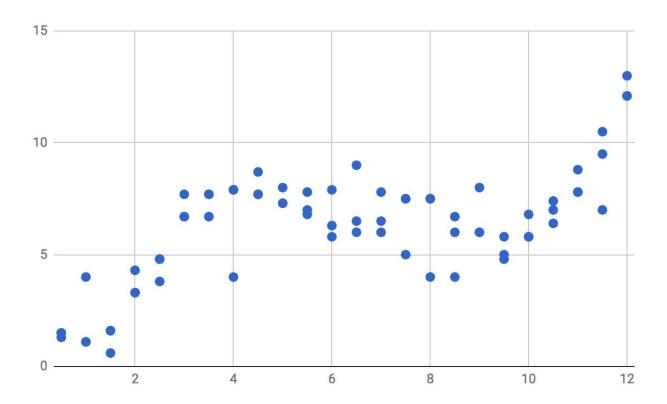


Demo



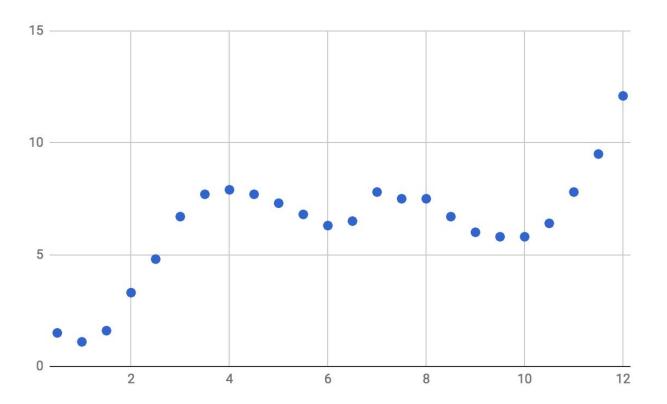






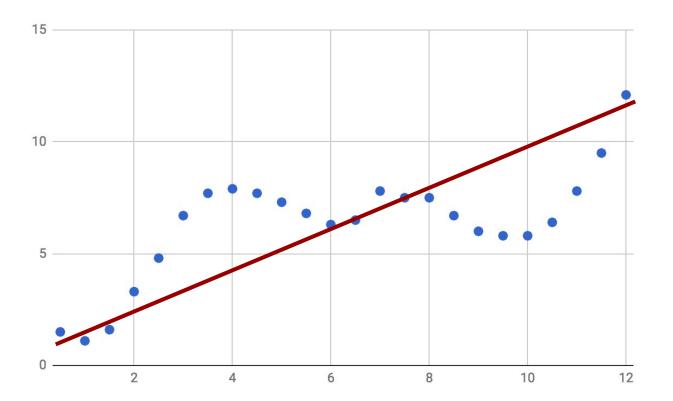






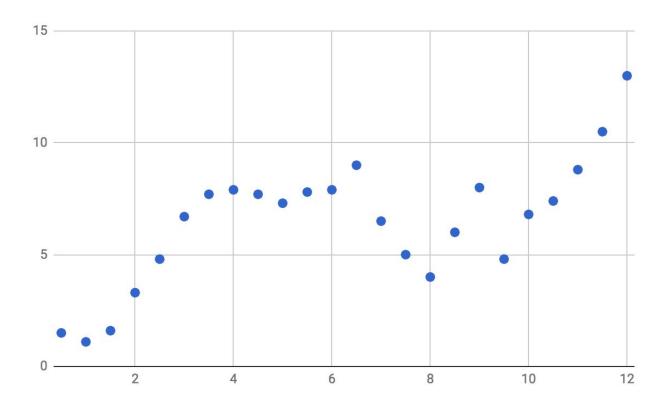




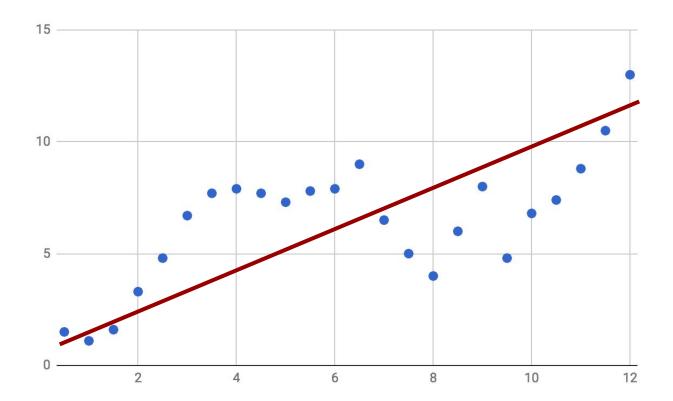






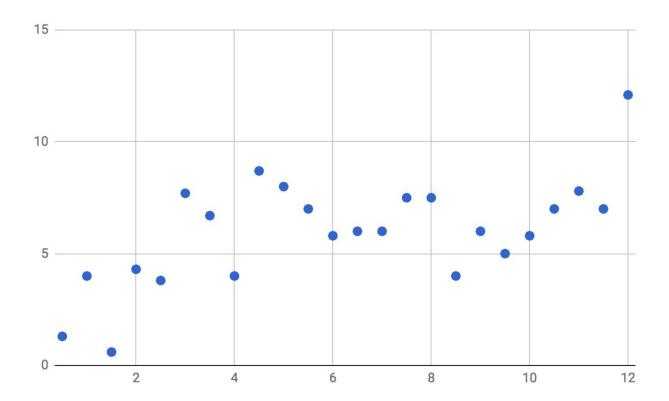






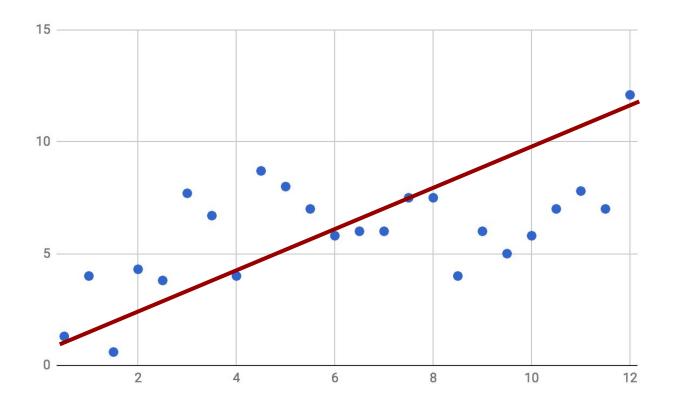








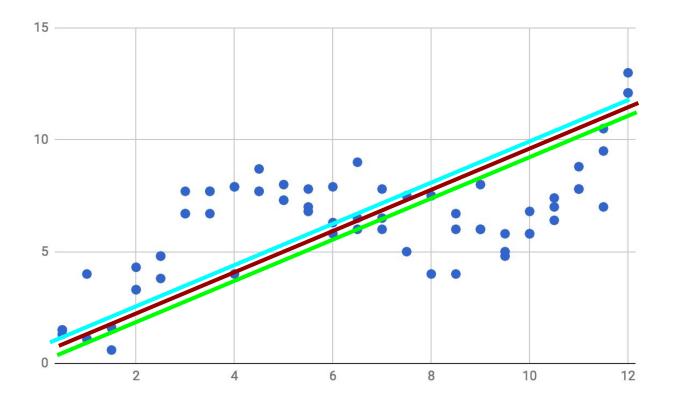






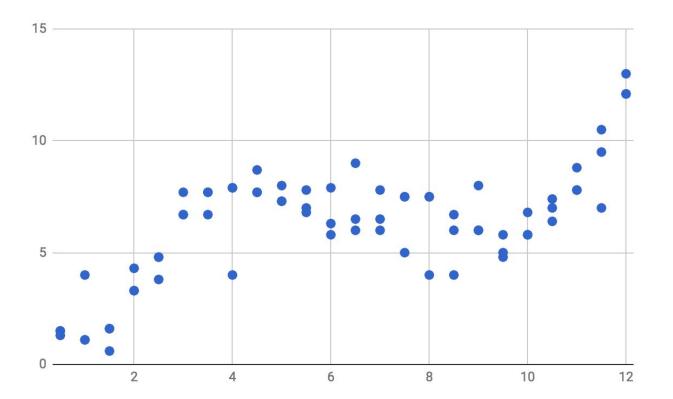


Underfitting: at least the models are consistent...



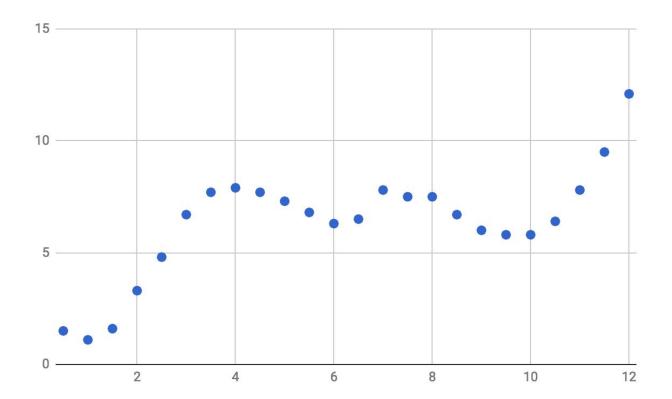






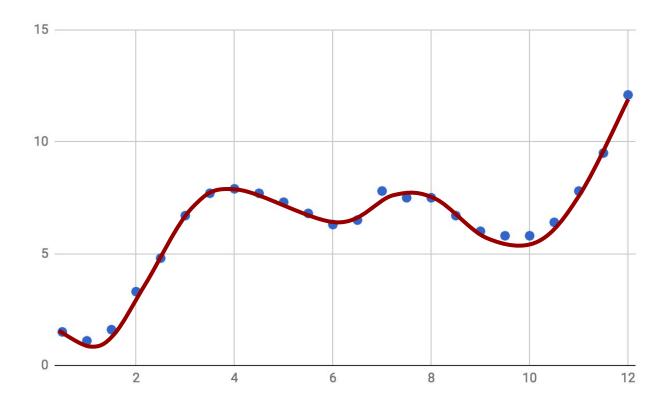






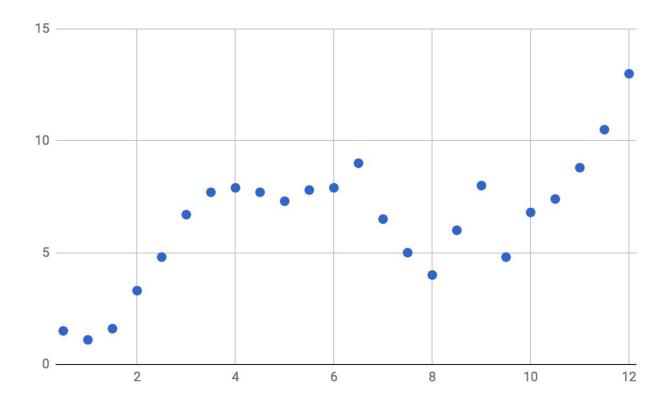






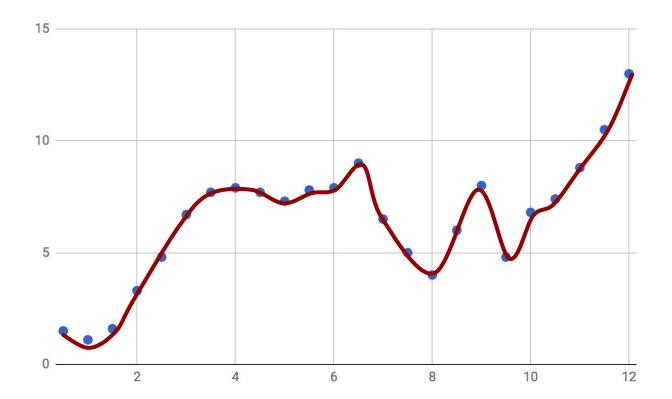






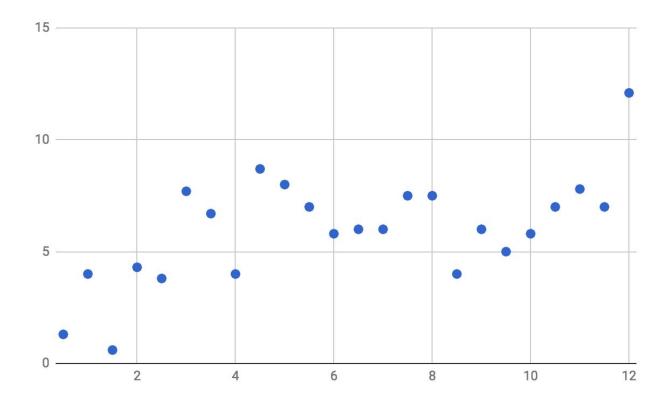






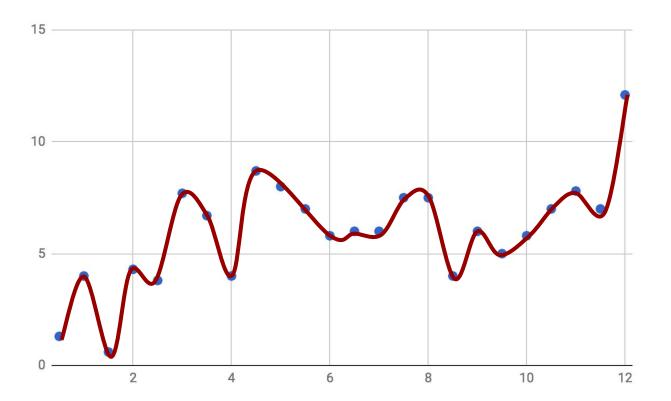








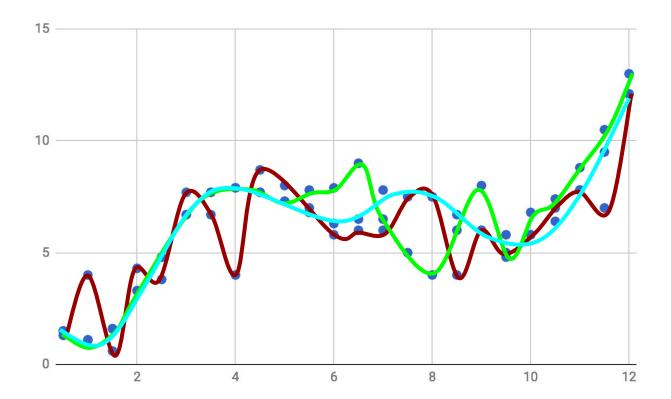








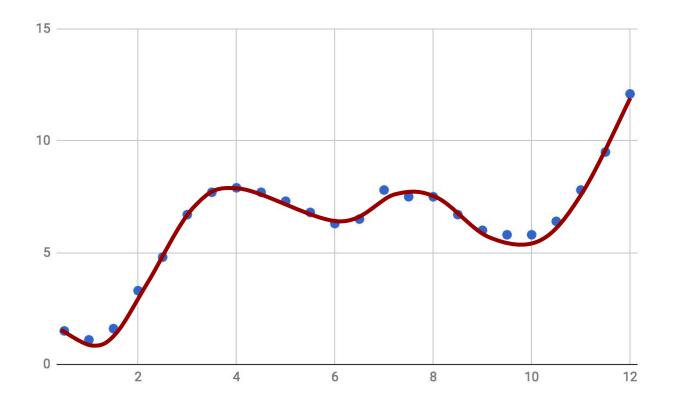
Overfitting: Inconsistent Models!







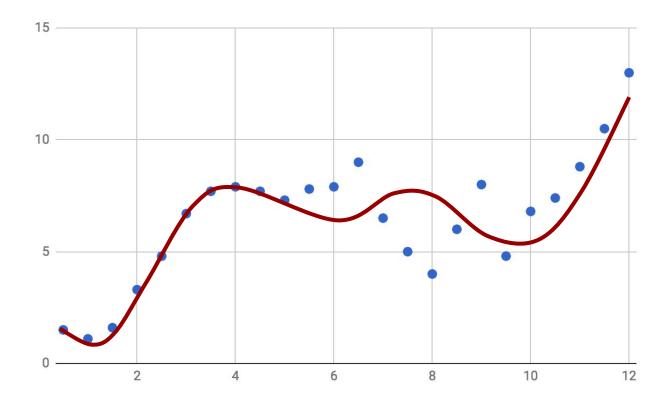
Overfitting: Results from training with high sensitivity







Overfitting: doesn't generalize well!







Definitions

Bias

- A measure of underfitting

Variance

- A measure of overfitting

Either alone is hard to interpret, but together they are helpful





Balancing Bias and Variance

$$\mathrm{E}\!\left[\left(y-\hat{f}\left(x
ight)
ight)^{2}
ight]=\mathrm{Bias}\!\left[\hat{f}\left(x
ight)
ight]^{2}+\mathrm{Var}\!\left[\hat{f}\left(x
ight)
ight]+\sigma^{2}$$

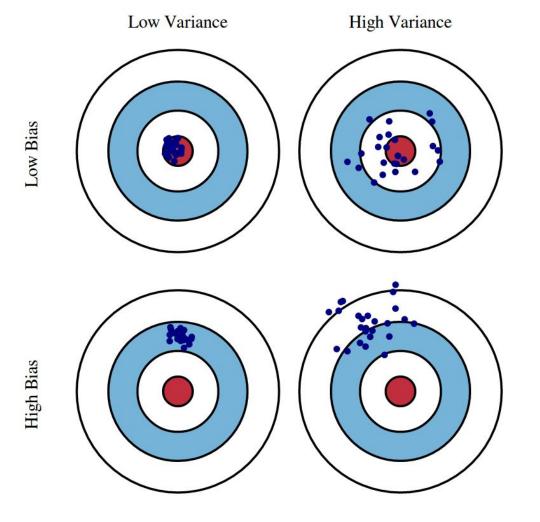
$$\operatorname{Bias}igl[\hat{f}\left(x
ight)igr] = \operatorname{E}igl[\hat{f}\left(x
ight) - f(x)igr]$$

$$\operatorname{Var} \left[\hat{f} \left(x
ight)
ight] = \operatorname{E} \left[\hat{f} \left(x
ight)^2
ight] - \operatorname{E} \left[\hat{f} \left(x
ight)
ight]^2$$

Error = $(expected loss of accuracy)^2 + inconsistency of model + irreducible error$











What does this mean intuitively?

Bias

- Bad
- Results from incorrect assumptions in the learning algorithm

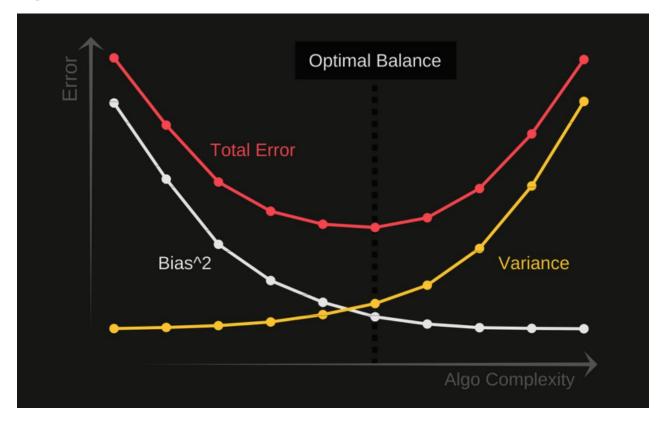
Variance

- Bad
- Results from sensitivity to fluctuations in the data





Balancing Bias and Variance







Feature Selection (adjusting models)





 Goal: Find subset of features that gives a good enough model, in a reasonable amount of time.

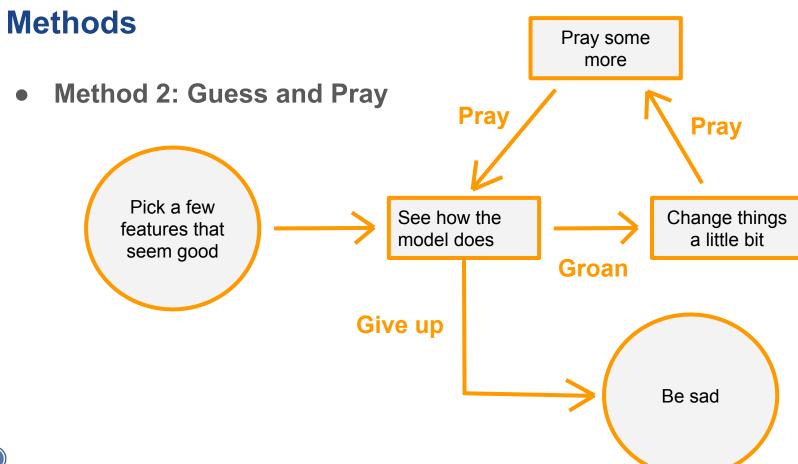




- Goal: Find subset of features that gives a good enough model, in a reasonable amount of time.
- Method 1: Best Subset
 - Test all subsets for best one
 - Benefits:
 - **Best** subset out of current features
 - Drawbacks:
 - Slow
 - Even slower with feature engineering











- Goal: Find subset of features that gives a good enough model, in a reasonable amount of time.
- Method 2: Guess and Pray
 - Guess
 - Benefits:
 - **?**?
 - Drawbacks:
 - Time consuming for data scientist
 - Unreliable





- Goal: Find subset of features that gives a good enough model, in a reasonable amount of time.
- Method 3: Stepwise
 - Pick a few features, then programmatically add/remove features using statistics
 - Benefits:
 - Complexity and runtime are adjustable
 - Drawbacks:
 - Can do very badly if you're not careful
 - Requires more thinking

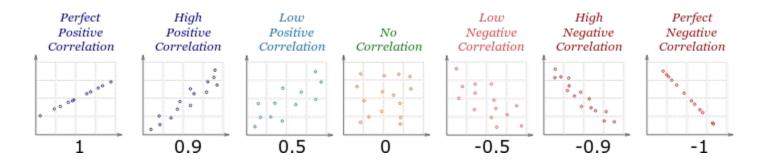




Correlation, r

The correlation between two variables describes to what extent changing one would change the other.

- Real-valued in [-1,1]
- A variable is always perfectly correlated with itself (correlation=1)







Important Case: Collinearity

Collinear: when two features have a correlation near -1 or 1

- If a feature is collinear with the target, then it's a good choice for linear regression
- If two features are collinear, they're *redundant*
 - Might as well not use one of them
 - Some models require/assume that no features used are collinear





Side Note: Scaling and Normalizing

- Some models require data to be centered
 - Some models need features to be on the same scale





Other Ways to Adjust your Model

- HyperParameters

- Feature engineering

- Just changing to a different algorithm





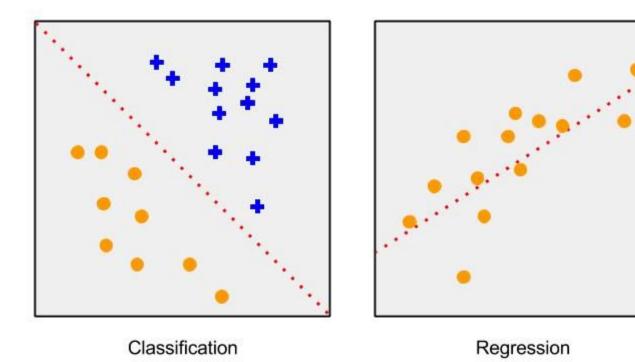
Different Types of ML

(classification & unsupervised)





Classification vs. Regression







Supervised vs. Unsupervised

Supervised learning...

- Known target variable info
- Validation examples

Unsupervised learning...

- Unknown target variables
- Difficult to validate





Other Classes of ML Algorithms (which we won't cover)

- What if you can't / don't want to see all your data at once?
- Maybe you only want to use a few pieces of your data (but don't have the time to manually select each piece of data...)

- A different approach, Trial & Error: The algorithm tries one thing, sees how that works, makes adjustments, tries again, etc.





Final Notes

Always remember both bias and variance!



Coming Up

- Assignment 5: Due at 5:30pm on March 18, 2020
- Midsemester Project
- Next Lecture: Intro to Classification

