INFO 1998: Introduction to Machine Learning

Pull up Lecture 5 Demo from website as well!

CDS Education

We explore, learn, and educate big minds.

Lecture 5: Fundamentals of Machine Learning Pt. 2

INFO 1998: Introduction to Machine Learning

Tuning Models

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Announcements

Mid-Semester Check-in

Where you should be right now:

- Have an idea of what your problem statement/hypothesis is
- Have your group chosen
- Have your data set chosen and some progress

Drop Deadline: **March 20th**

What We'll Cover

Last Time's Goal: identify what ML is and write ML code (to some extent)

This Time's Goal: how to tell if your ML model is *useful*

Agenda

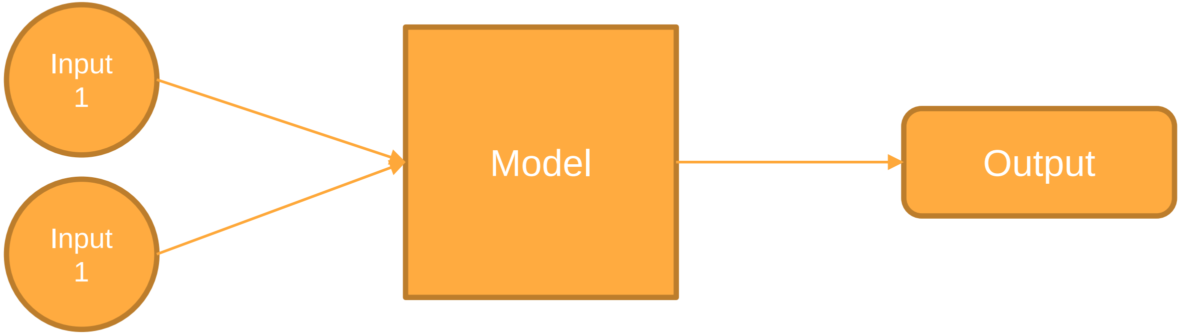
1. Review
2. Measuring Accuracy
3. Bias-Variance trade-off
4. Feature Selection
5. Other Types of machine learning

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

Review: Model



- Takes in input and output and learns the relationship
- Used to predict outputs

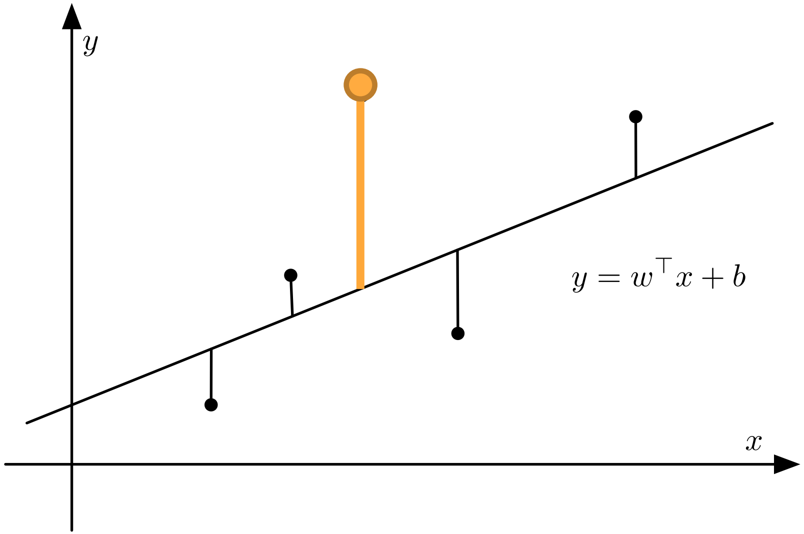
- “Model training” = learn a relationship/program
- “Model validation” = see if the learned relationship is accurate on other data
- “Model testing” = final model performance

Measuring Bias / Loss

(training accuracy)

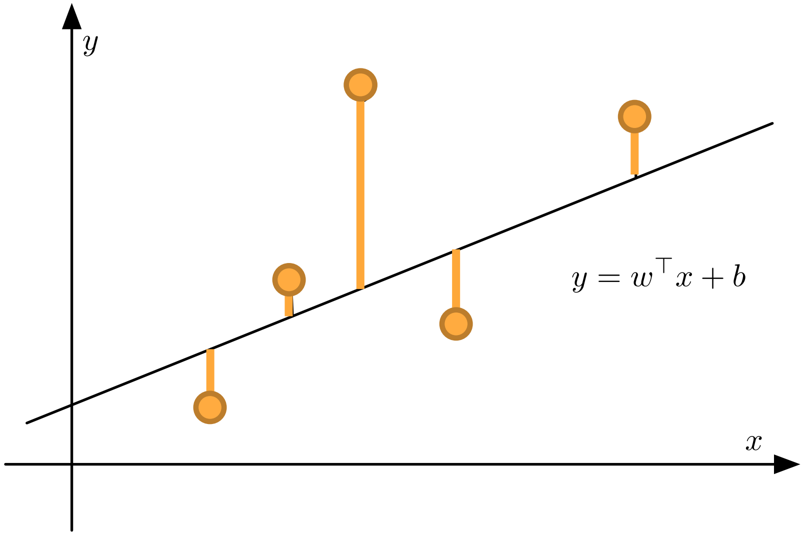
Loss, Cost, and Score Functions

Loss Function: Penalty for missing a single data point



Loss, Cost, and Score Functions

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)

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Loss, Cost, and Score Functions

Cost Function: Indicates how bad the whole model is

Cost =

- Applies loss function to each point, then combines that into a single number
  - Ex:, Total Loss, Average Loss

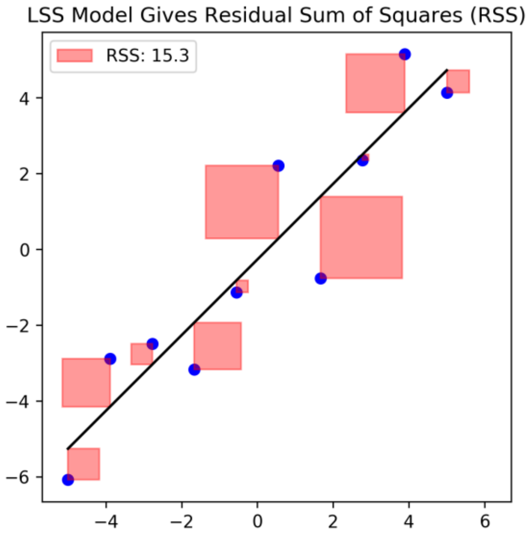
Loss, Cost, and Score Functions

- **Score Function**
  - A more interpretable version of the cost function (how well we did)
  - Loss/Cost used in training to help a model learn, Score is just what we use for interpretability

Cost = → Score = 50% Accuracy

Linear Regression Loss Formula: Euclidean Distance

$$\text{loss}\ (x, y^*) = (h(x) - y^*)^2$$



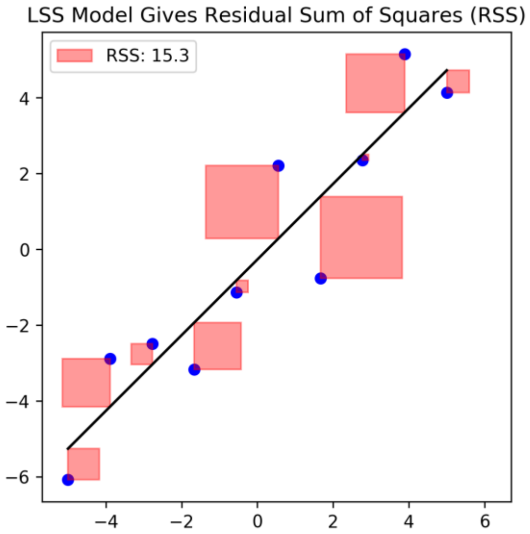
Two things to note about this loss function:

- Positives and negatives won't cancel
- Large errors are penalized to a power of 2 more

Cost Function - average of the loss function over all the points

Linear Regression Loss Formula: Euclidean Distance

$$\text{loss}(x, y^*) = (h(x) - y^*)^2$$



In what situations might you want a high penalty loss function as opposed to a lower penalty function?

- High stakes situations (Ex: Cancer Diagnosis)
- Data does not have many outliers

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 to Accuracy Score

- sklearn's score function is:

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

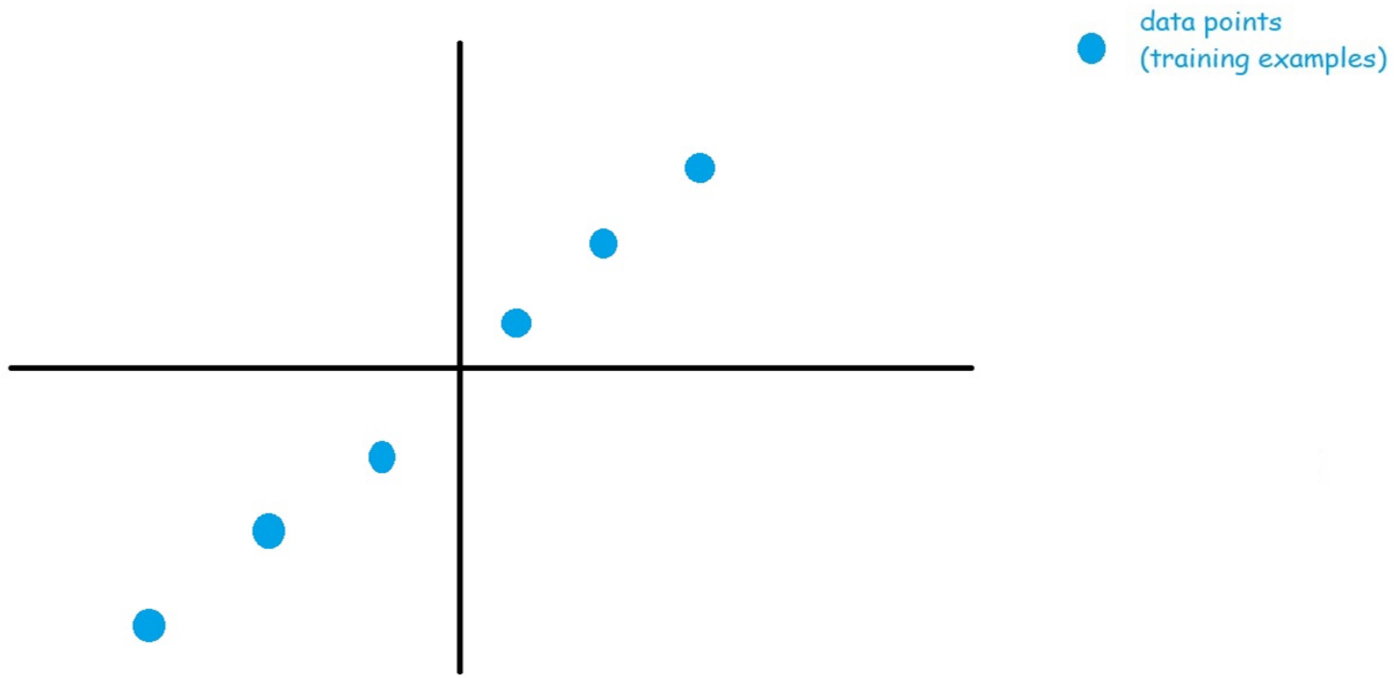
- **1** is very, very good
- **0** means you were as bad as the baseline
- **<0** means either your baseline predictions were accurate, or you really, really messed up

- **NOT USED IN TRAINING, For our interpretability**

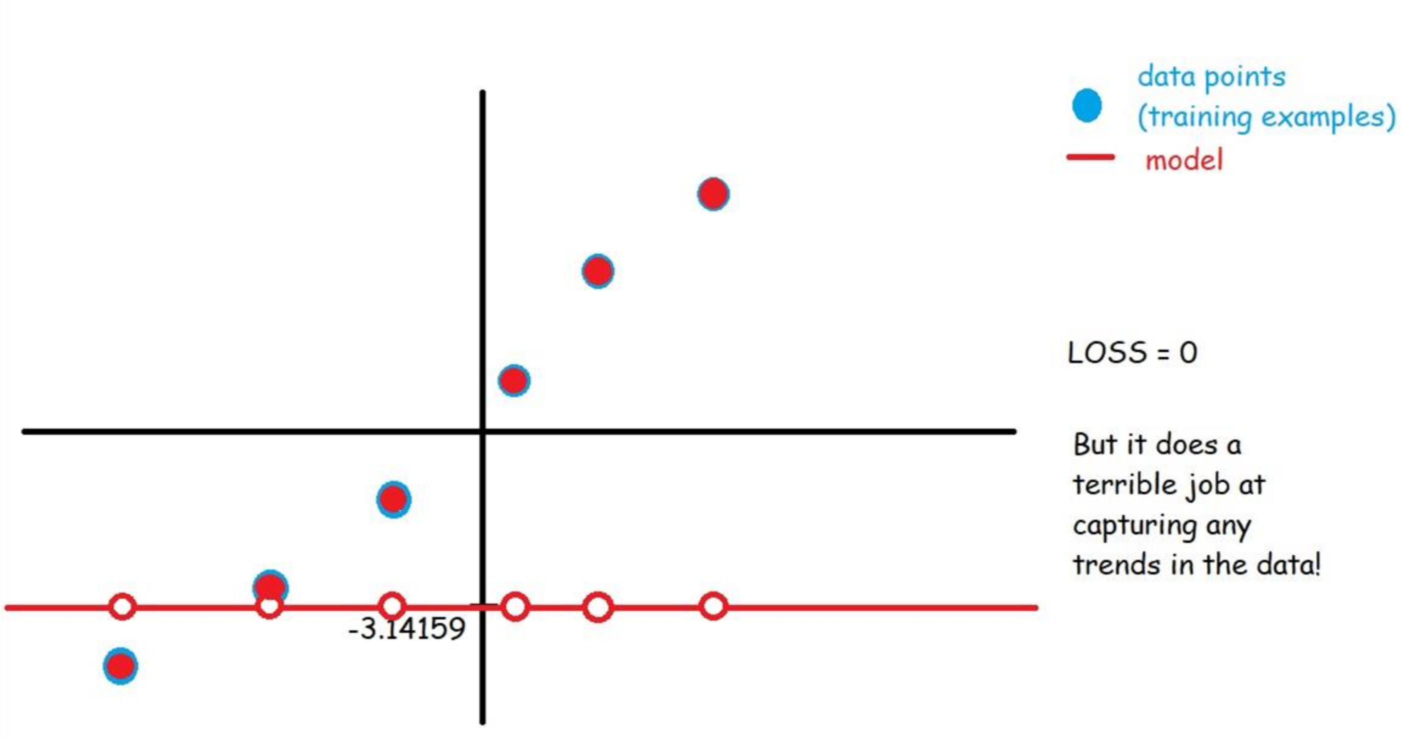
Question!

- Let's say we have a dataset $\{(x_1,y_1),(x_2,y_2),\ldots,(x_n,y_n)\}$.
- Suppose our model outputs the following:
  - y_i, if $x = x_i$ for some i in $\{1,2,\ldots,n\}$
  - -3.14159 otherwise
- What is the cost of this model (using Euclidean distance)? Hint: the answer is quite simple.
- Should we expect this algorithm to perform well in predicting outputs for new inputs?

Training Data



Cost = 0, but model is horrible…

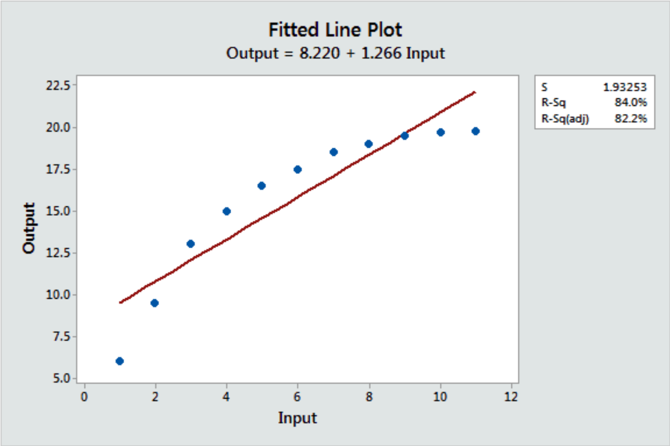


MORAL: Assumptions are important!

No Free Lunch Theorem

Every ML algorithm makes assumptions!

Ex: Linear regression assumes data has a linear relationship



MORAL: Assumptions are important!

Overfitting and Underfitting

(what makes a model good?)

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.

Model Goals

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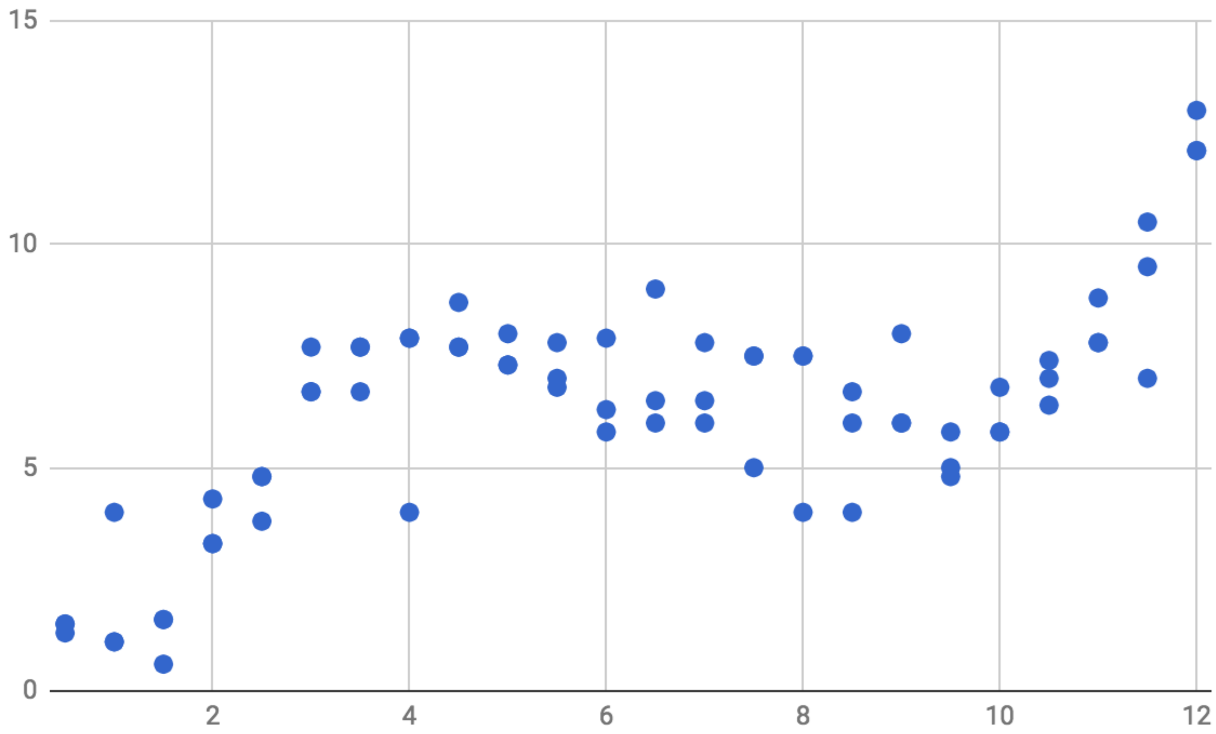
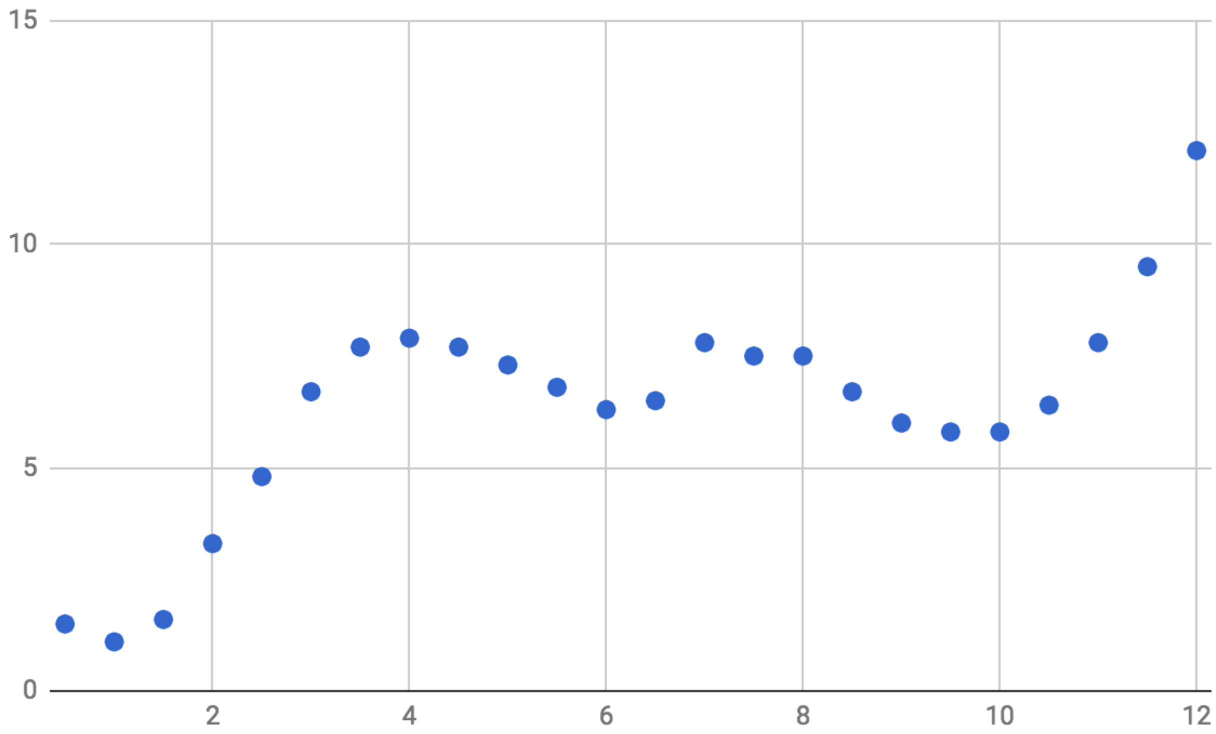
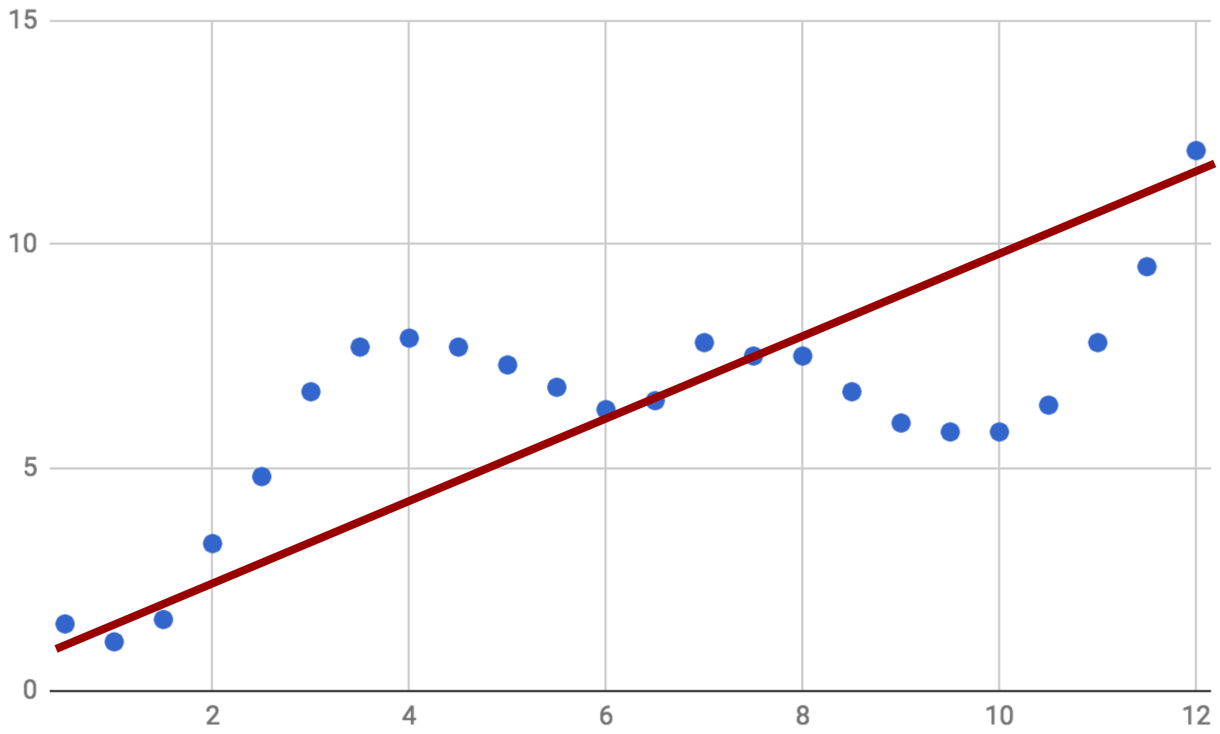
Underfitting: A situation when your model is **too simple** for your data.



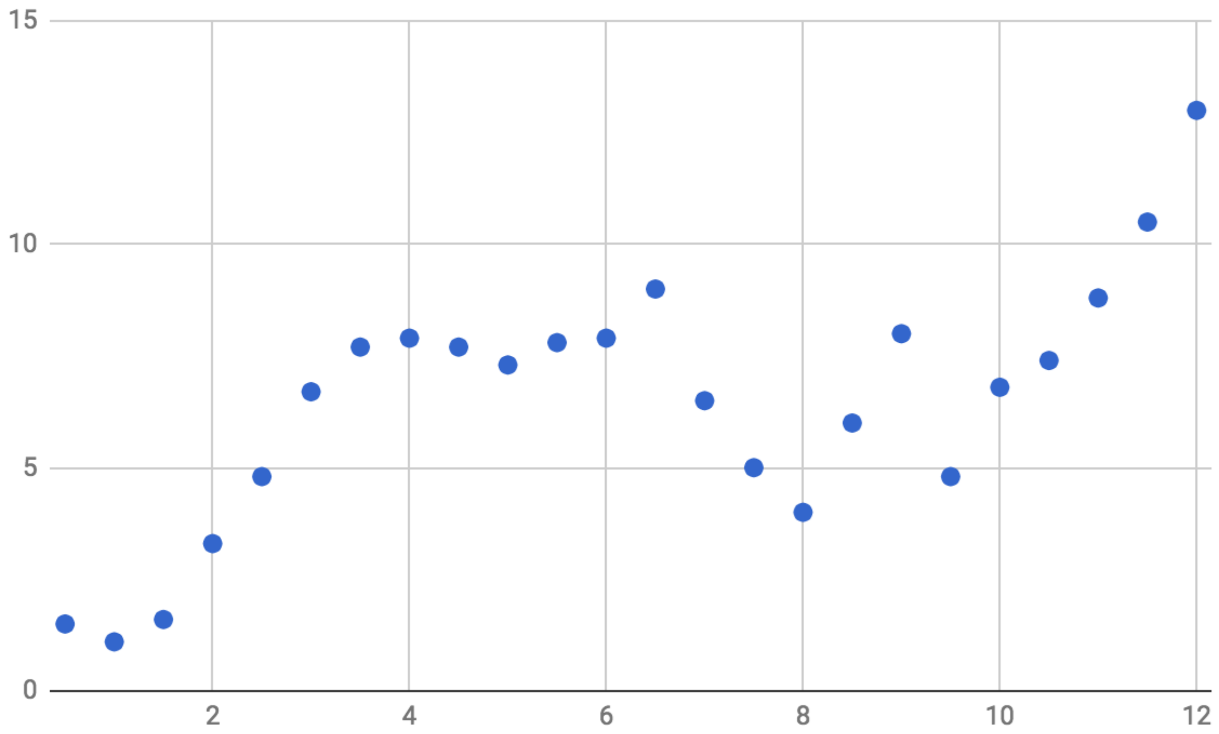
Underfitting



Underfitting



Underfitting



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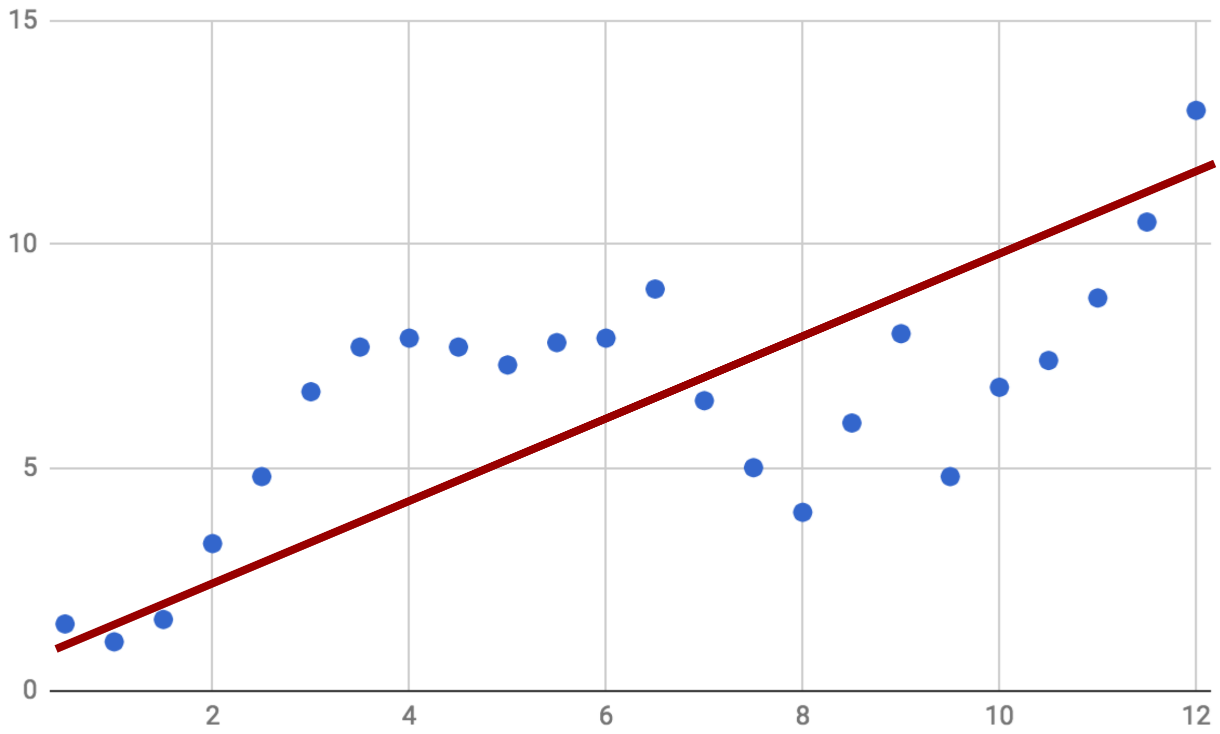
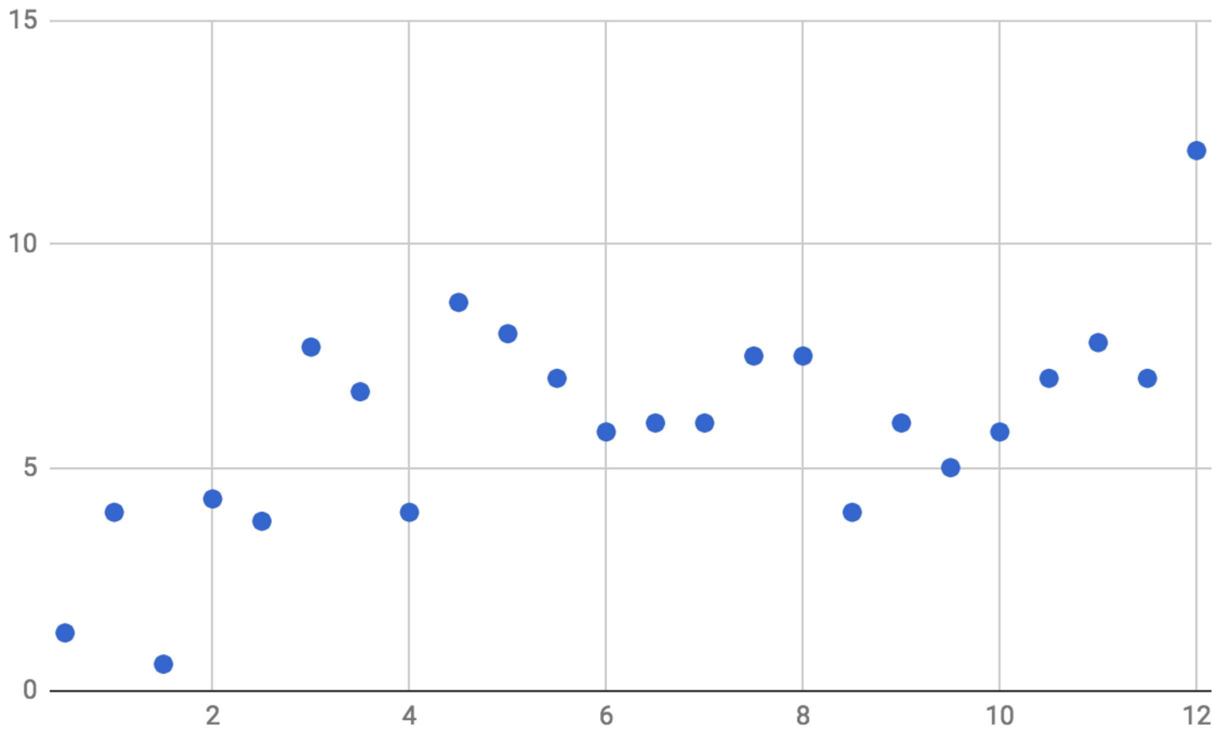


Underfitting



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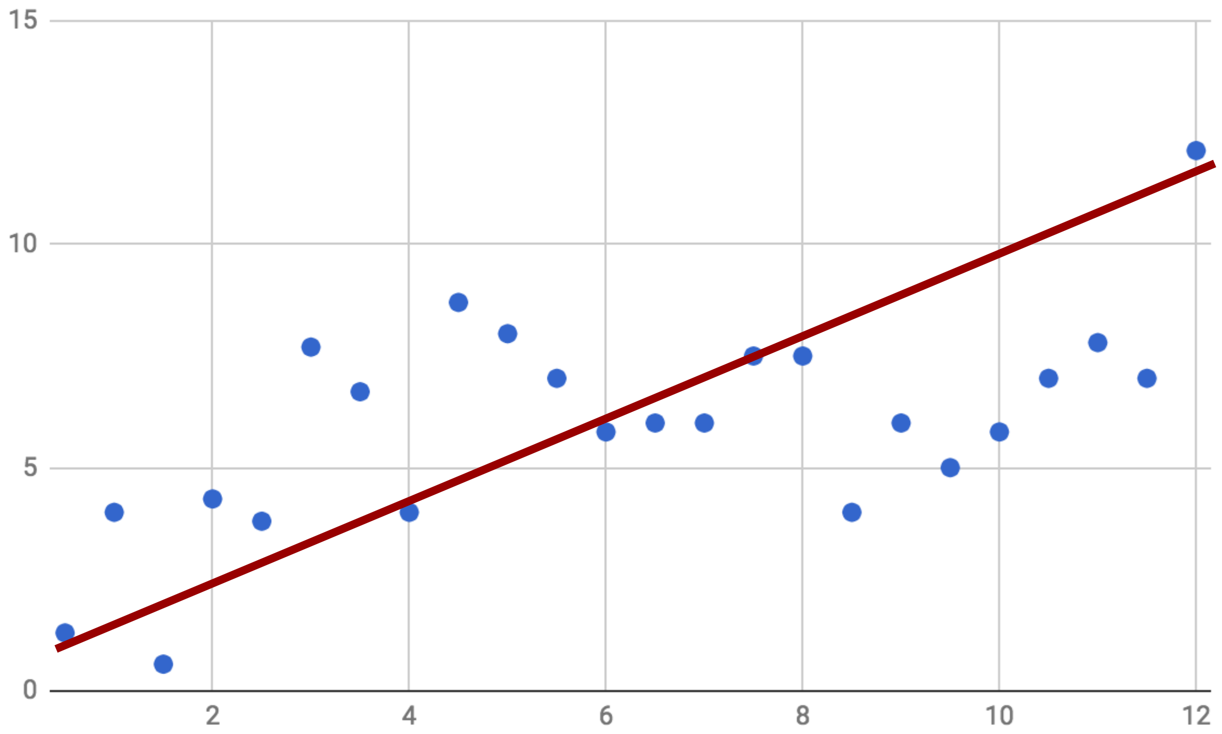
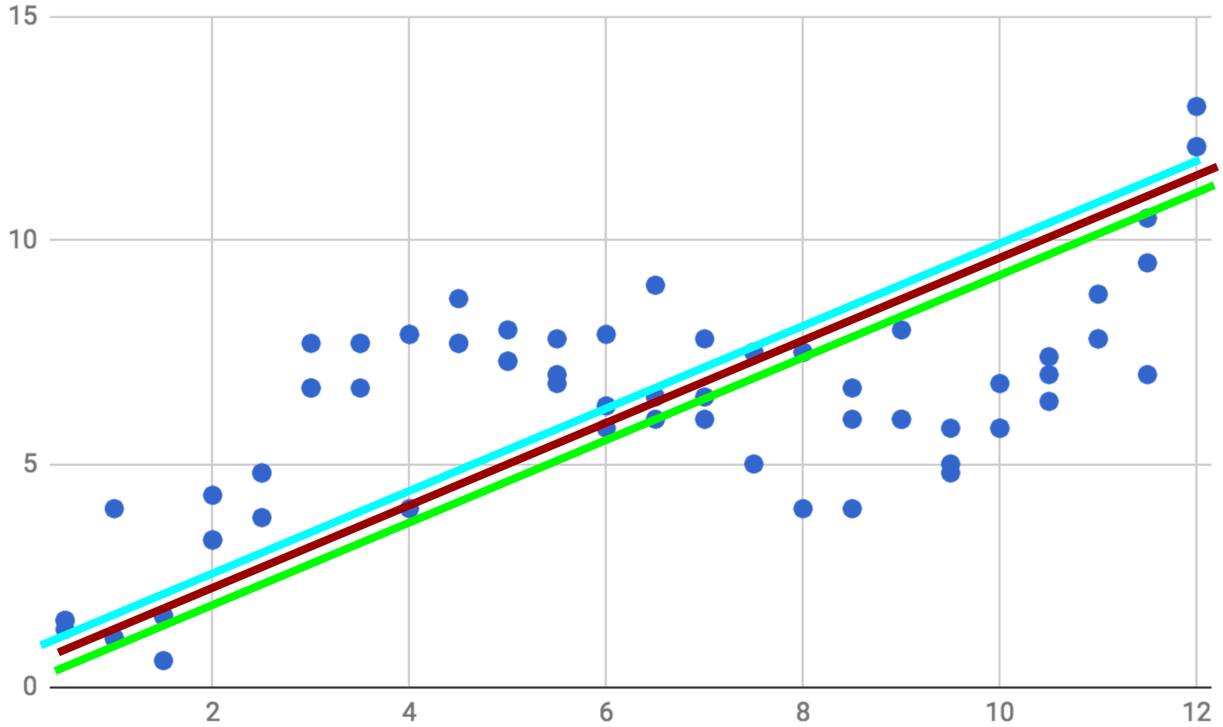


Underfitting: at least the models are consistent...



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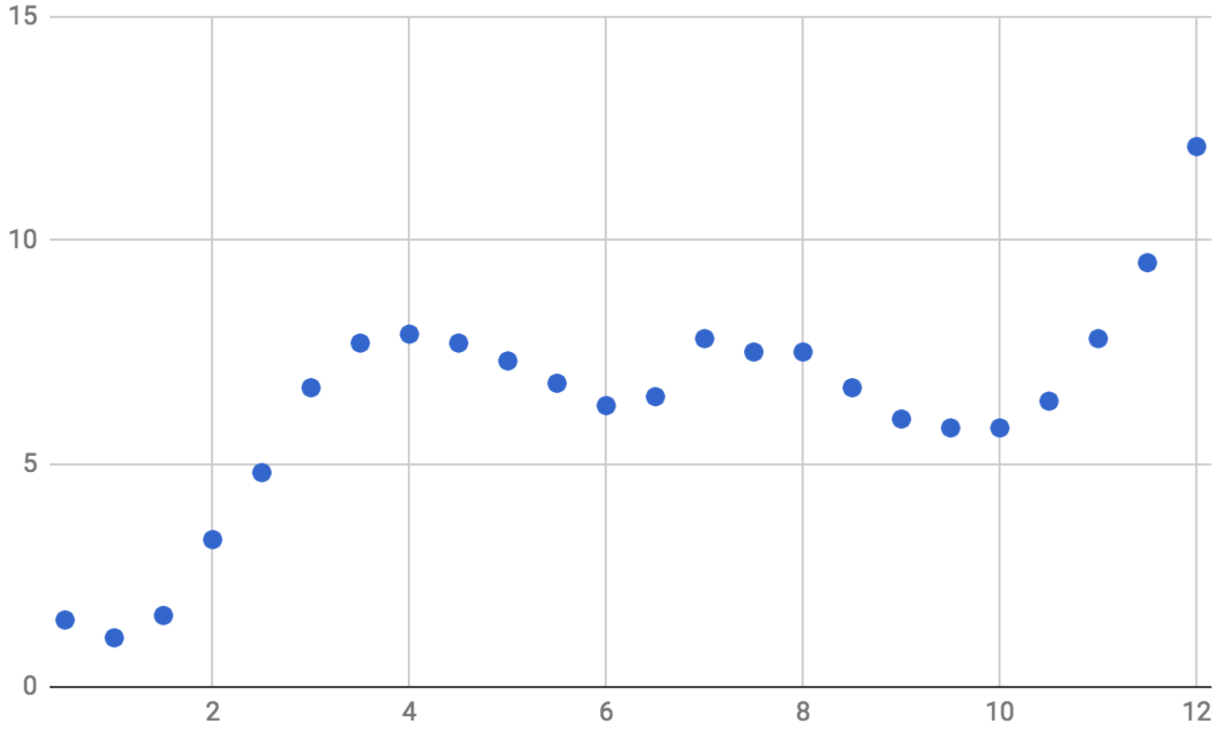
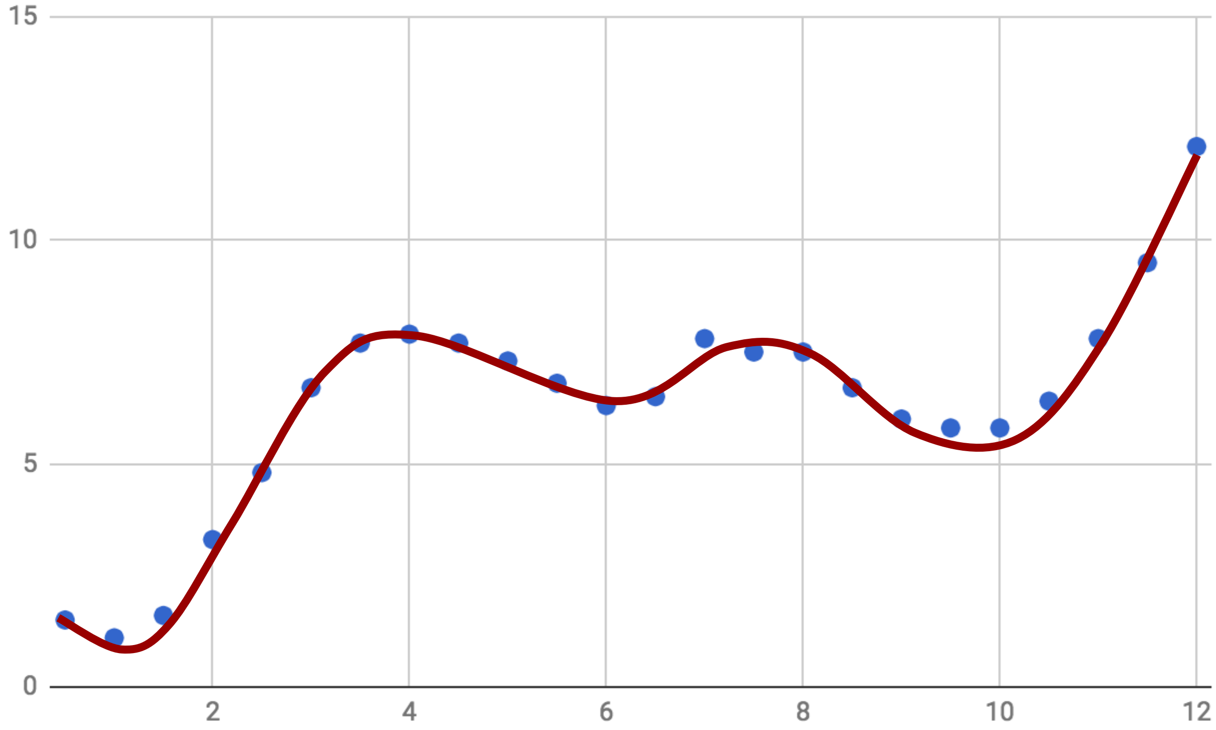
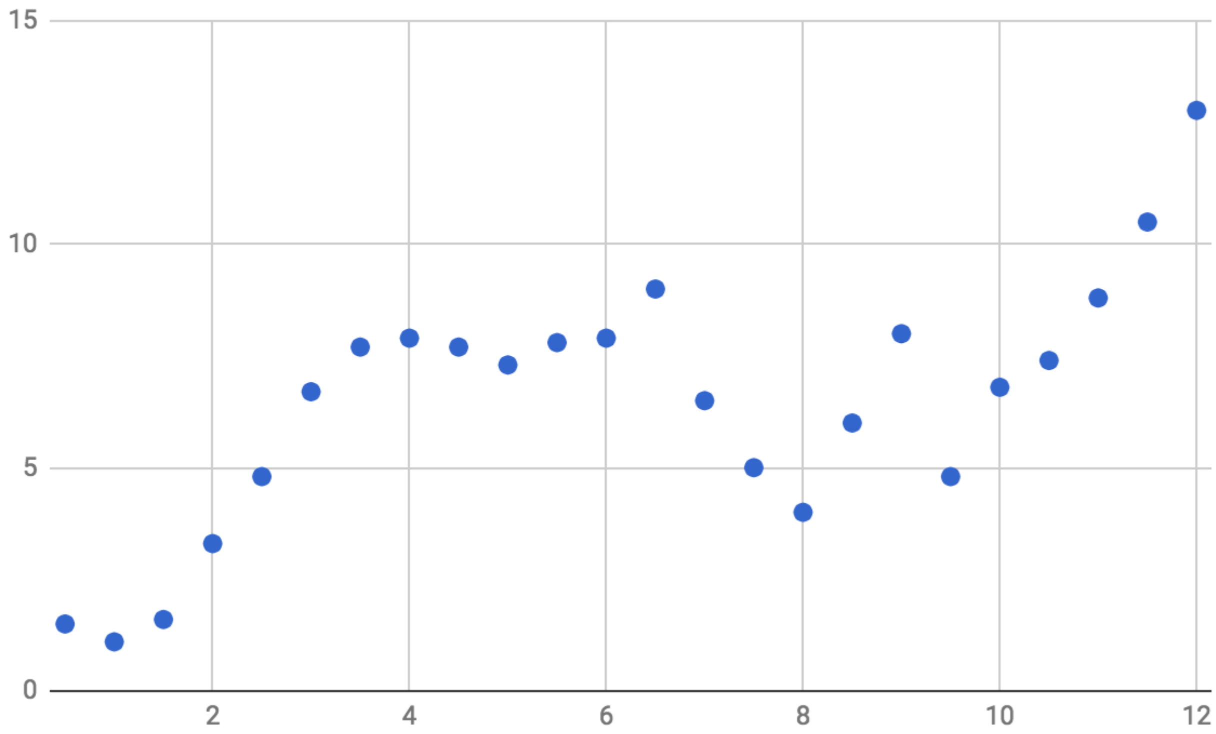


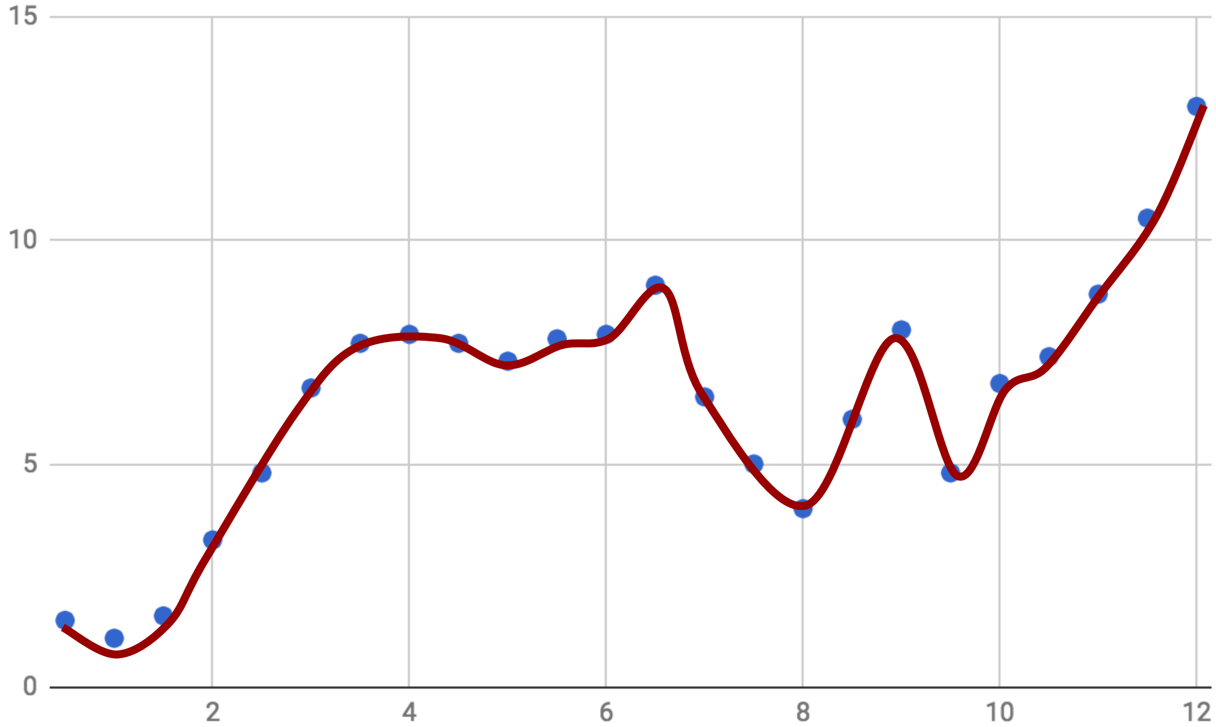
Overfitting



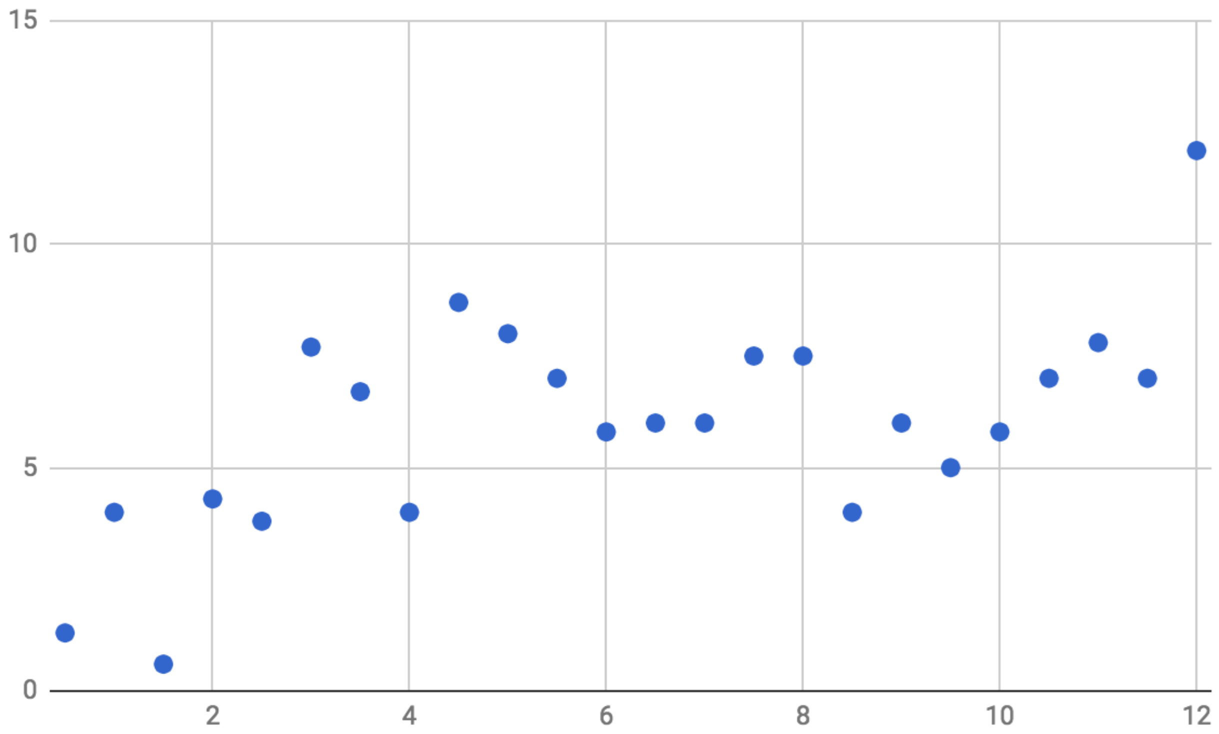
Overfitting



Overfitting



Overfitting



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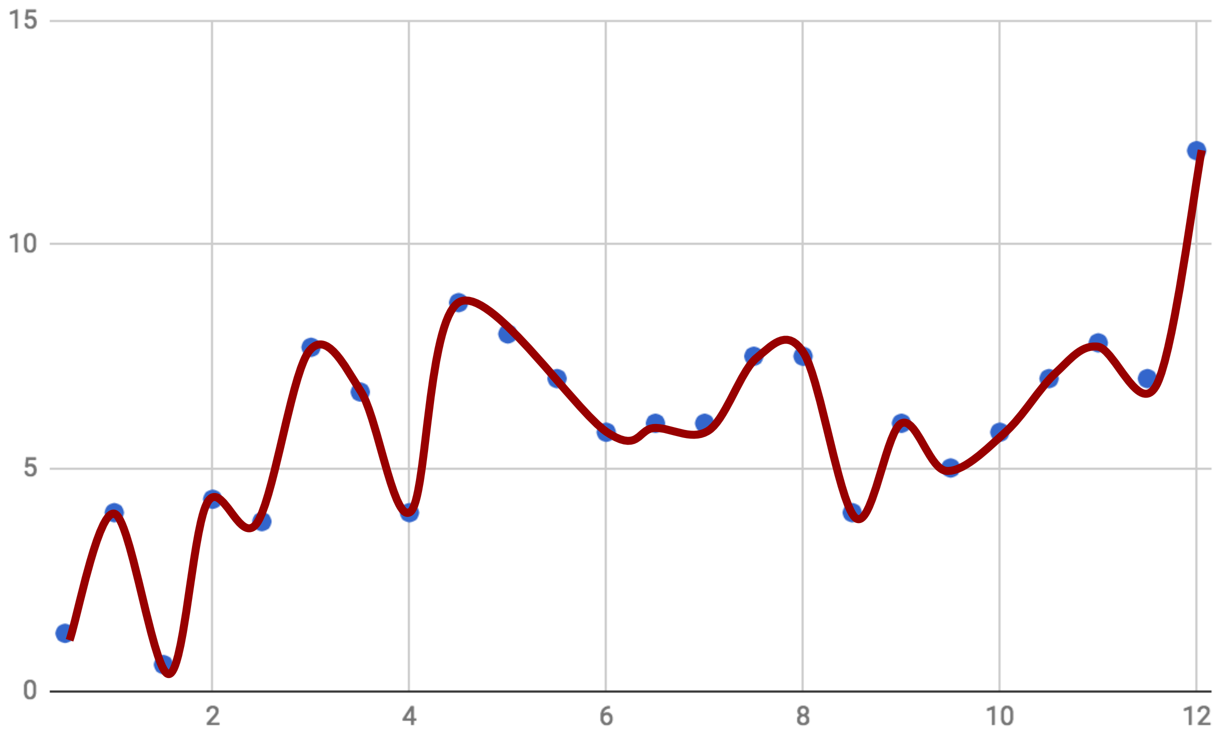
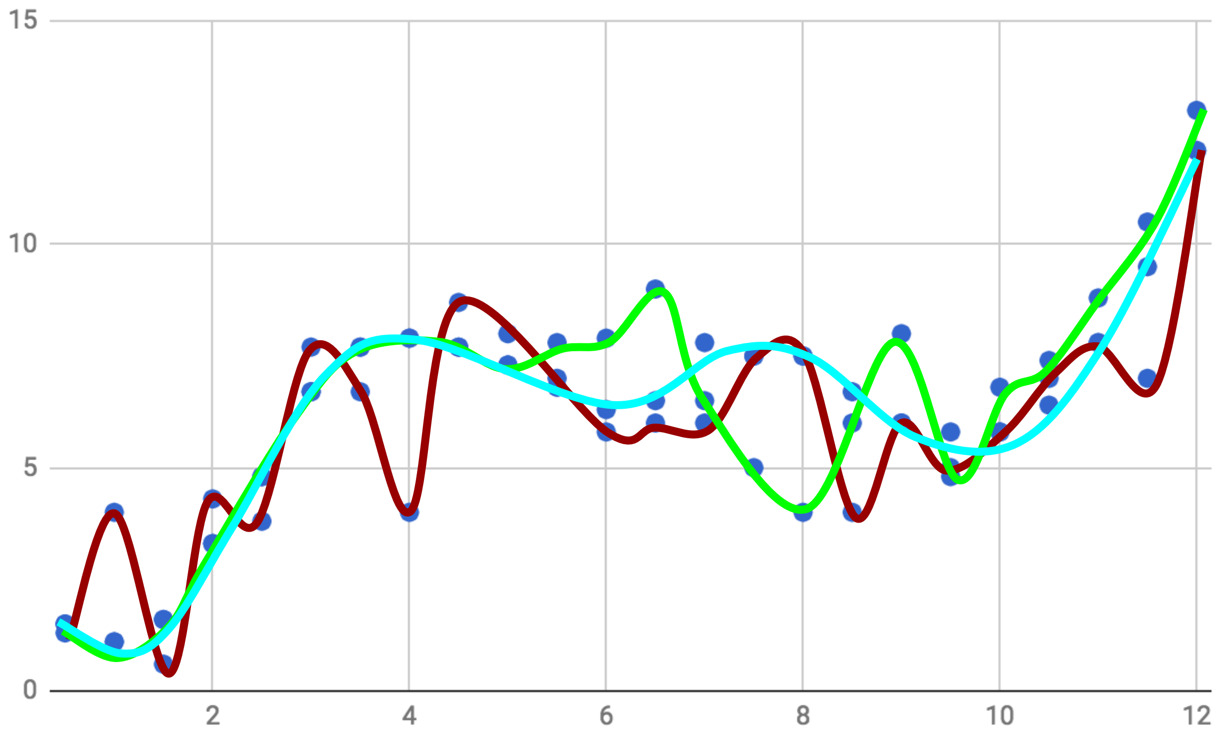
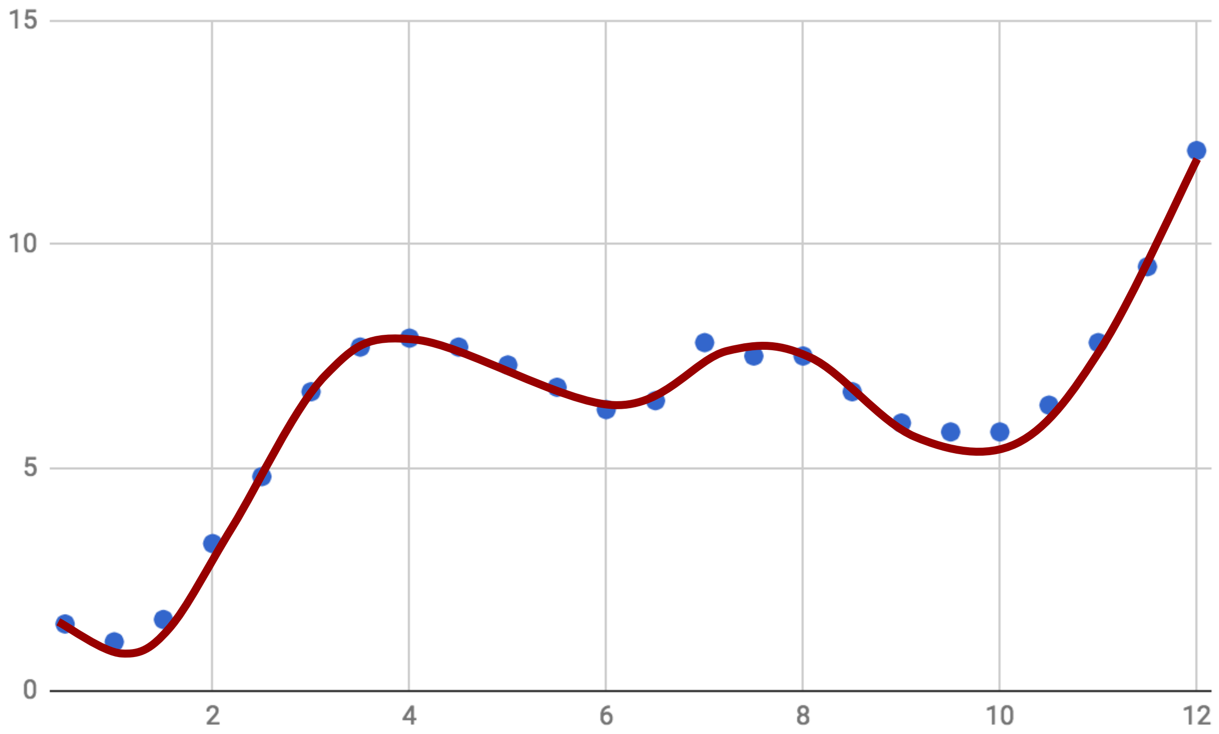


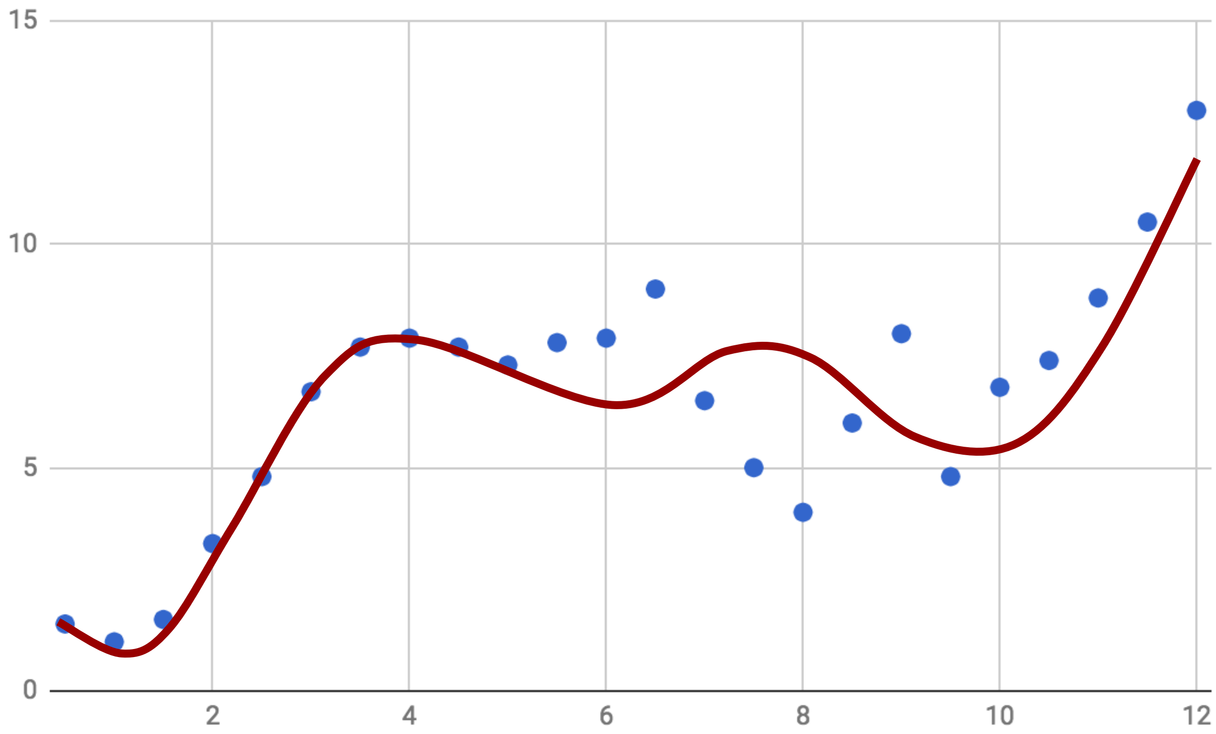
Overfitting: Inconsistent Models!



Overfitting: Results from training with high sensitivity



Overfitting: doesn't generalize well!



Bias and Variance

Definitions

Bias

- A measure of underfitting

Variance

- A measure of overfitting

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

http://www.r2d3.us/visual-intro-to-machine-learning-part-2/

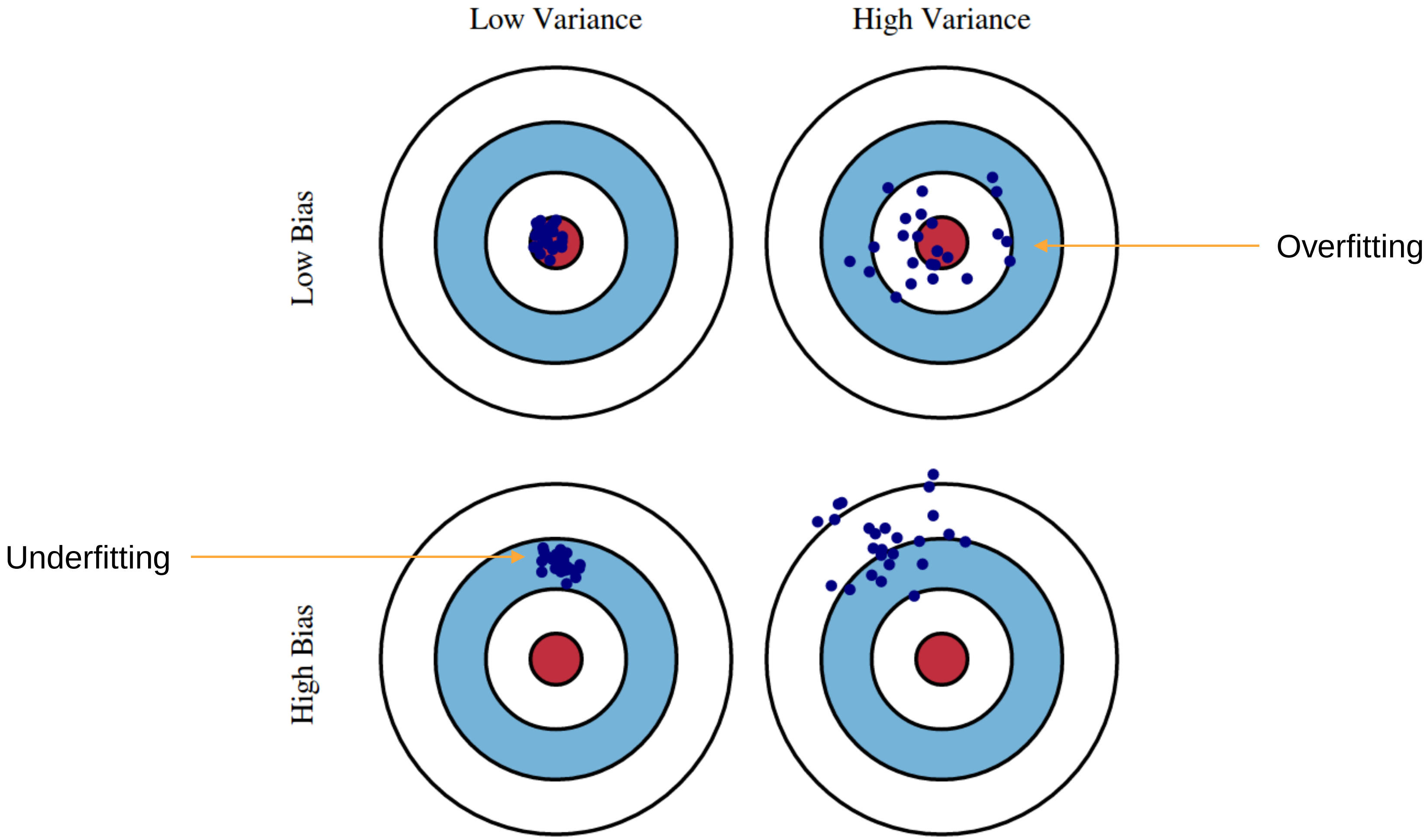
Balancing Bias and Variance

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

$$\mathrm{Bias}\left[\hat{f}(x)\right] = \mathrm{E}\left[\hat{f}(x) - f(x)\right]$$

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

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


Low Variance
High Variance
Low Bias
High Bias
Overfitting
Underfitting

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

What can you do to reduce Bias and Variance?

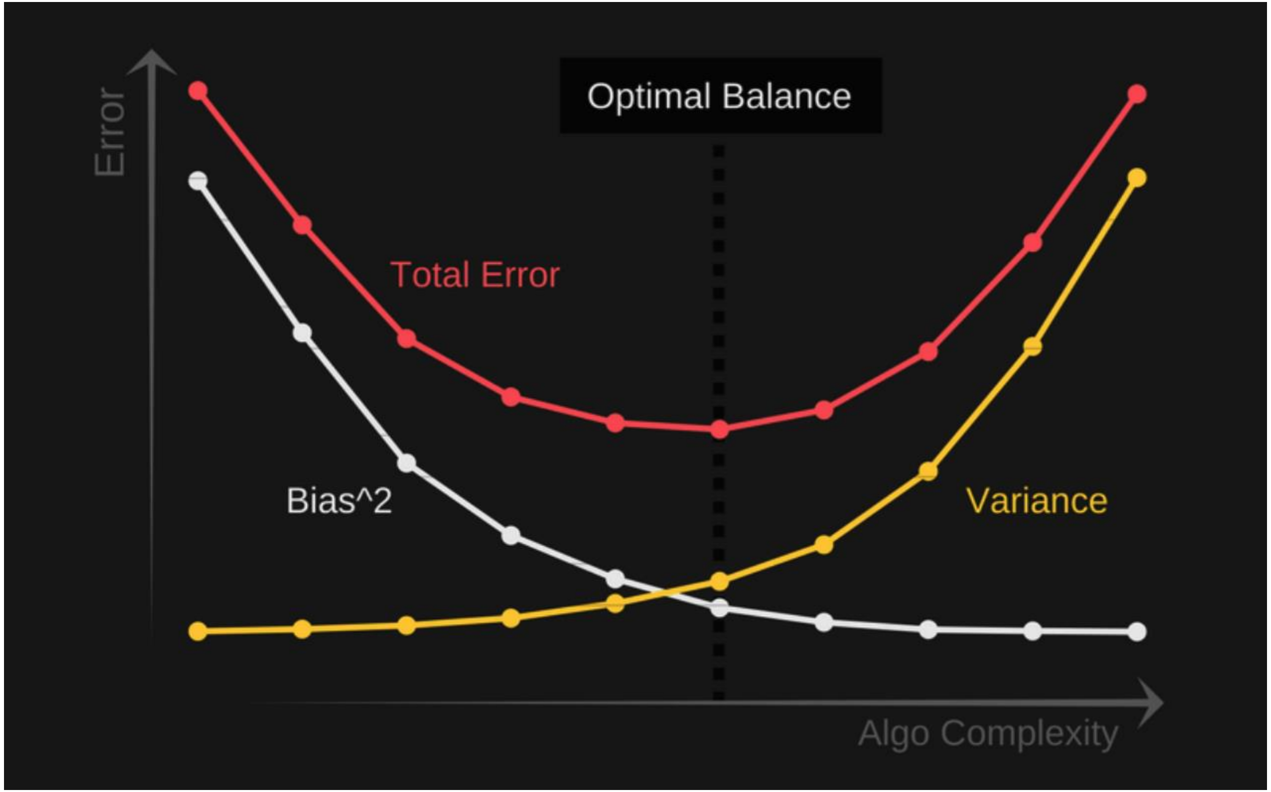
Bias

- Increase model size
- Change type of model
- Add new features

Variance

- Add more data
- Decrease model size
- Reduce features

Balancing Bias and Variance



Feature Selection

(adjusting models)

Methods

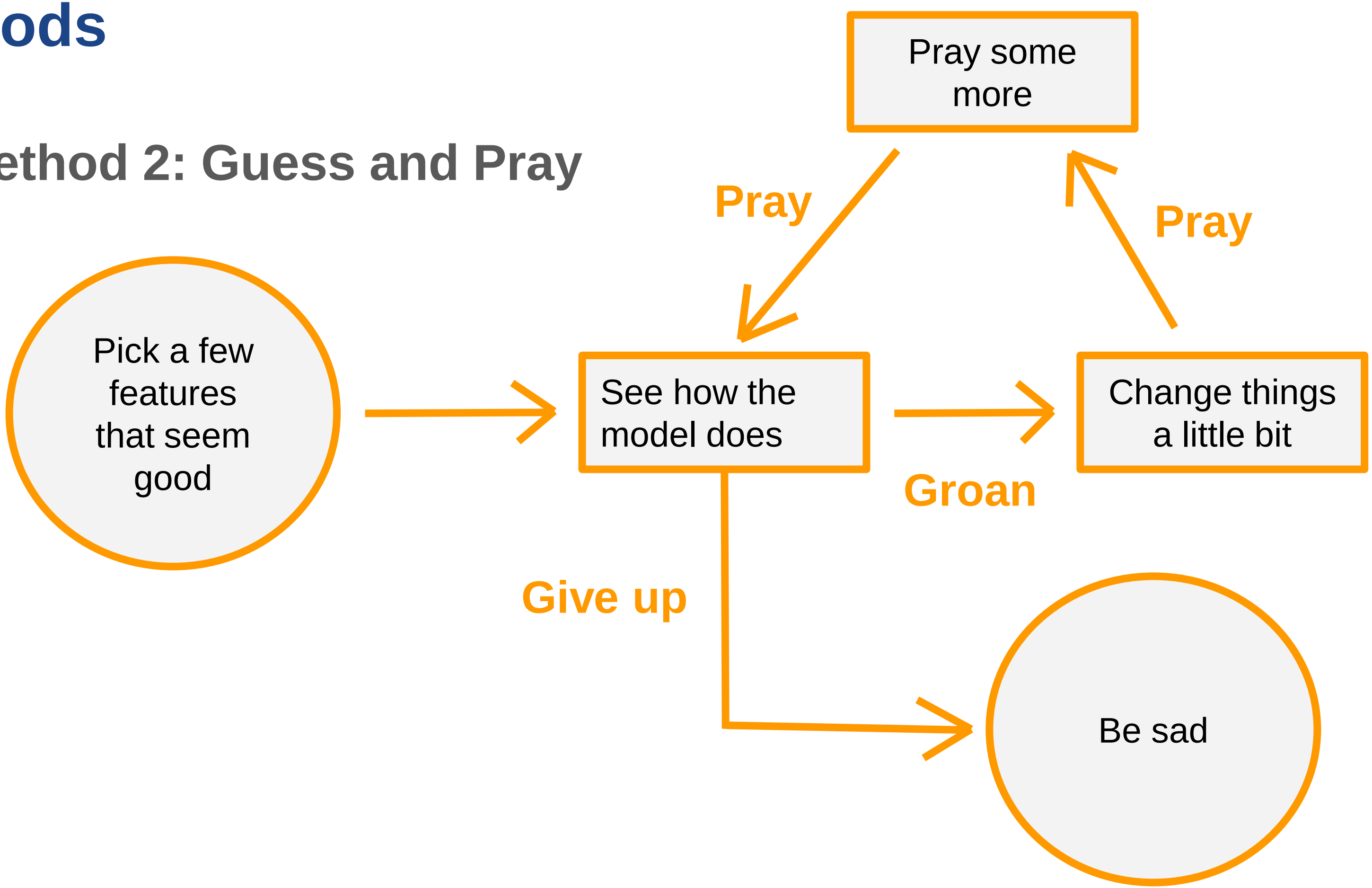
- **Goal:** Find subset of features that gives a good enough model, in a reasonable amount of time.

Methods

- **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

Methods

- **Method 2: Guess and Pray**



Methods

- **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

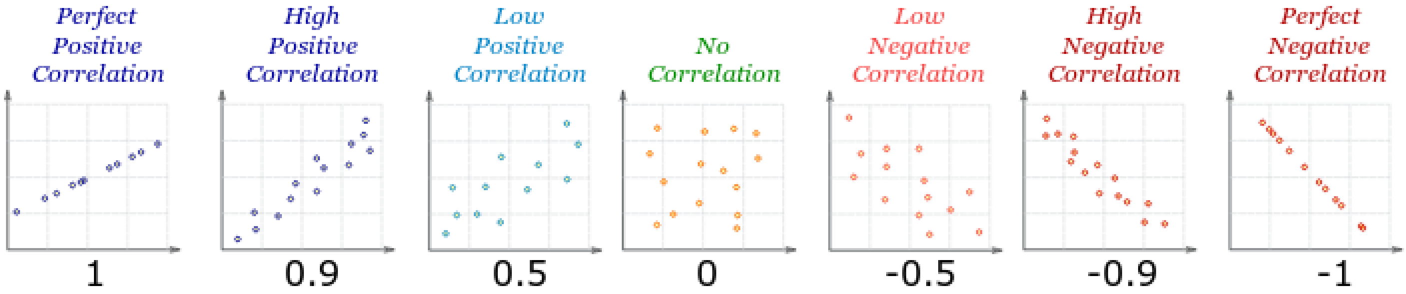
Methods

- **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* no collinear features
    - Takes more time, and doesn't add much information at the cost of *increased variance/sensitivity*

Side Note: Scaling and Normalizing

- Some models require data to be centered
- Some models need features to be on the same scale
    - Divide by max, minus min divide by max minus min, minus mean divide by standard deviation.

Side Note: Scaling and Normalizing

- Some models require data to be centered
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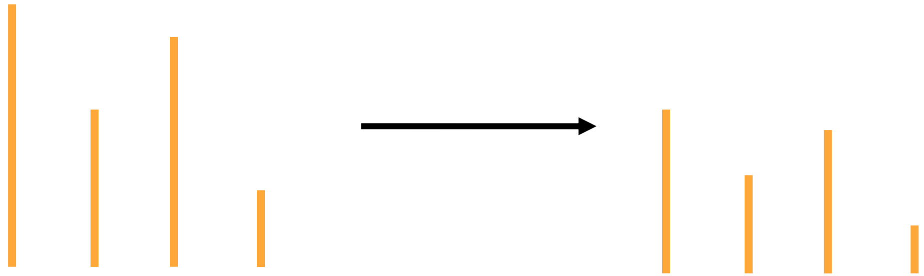
Divide by max: Bounds data <= 1



Side Note: Scaling and Normalizing

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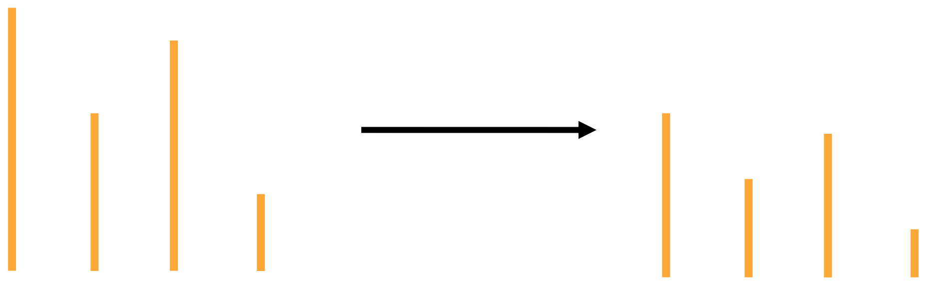
- min / (max – min) : Bounds data between [0,1]



Side Note: Scaling and Normalizing

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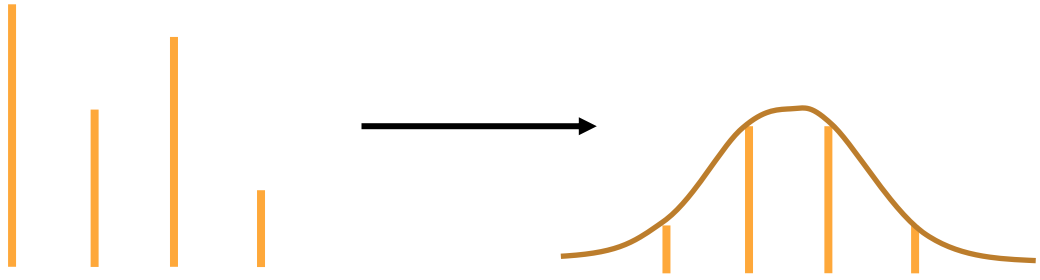
- **mean / standard deviation**: Z scores – Distance from mean



Other Ways to Adjust your Model

- Hyper Parameters – Ex: Learning rate, etc.

- Feature engineering – Ex: Manipulating dataset

- Just changing to a different algorithm

Demo

Different Types of ML

(supervised & unsupervised)
(classification & regression)

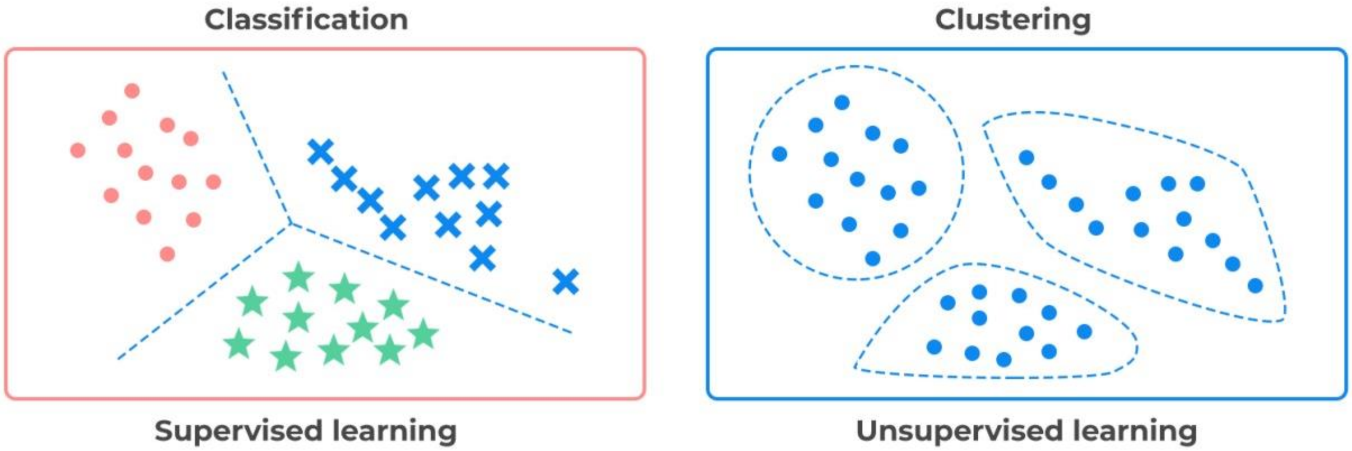
Supervised vs. Unsupervised

Supervised learning…

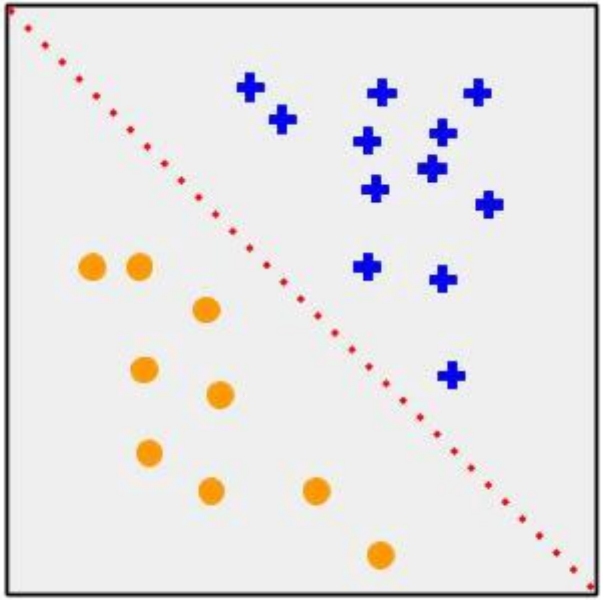
- Known target variable info
- Validation examples

Unsupervised learning…

- Unknown target variables
- Difficult to validate

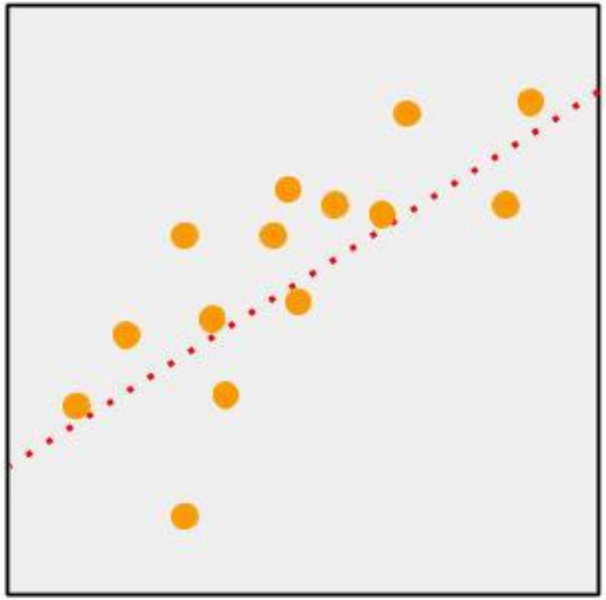


Classification vs. Regression



Classification

Discrete Class Labels



Regression

Continuous Quantity

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 midnight on March 22nd , 2023
- **Next Lecture**: Intro to Classification
- Last day to drop: March 20th (Next Monday)

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