Lecture 7: Classification Models and Cross Validation

INFO 1998: Introduction to Machine Learning

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Agenda

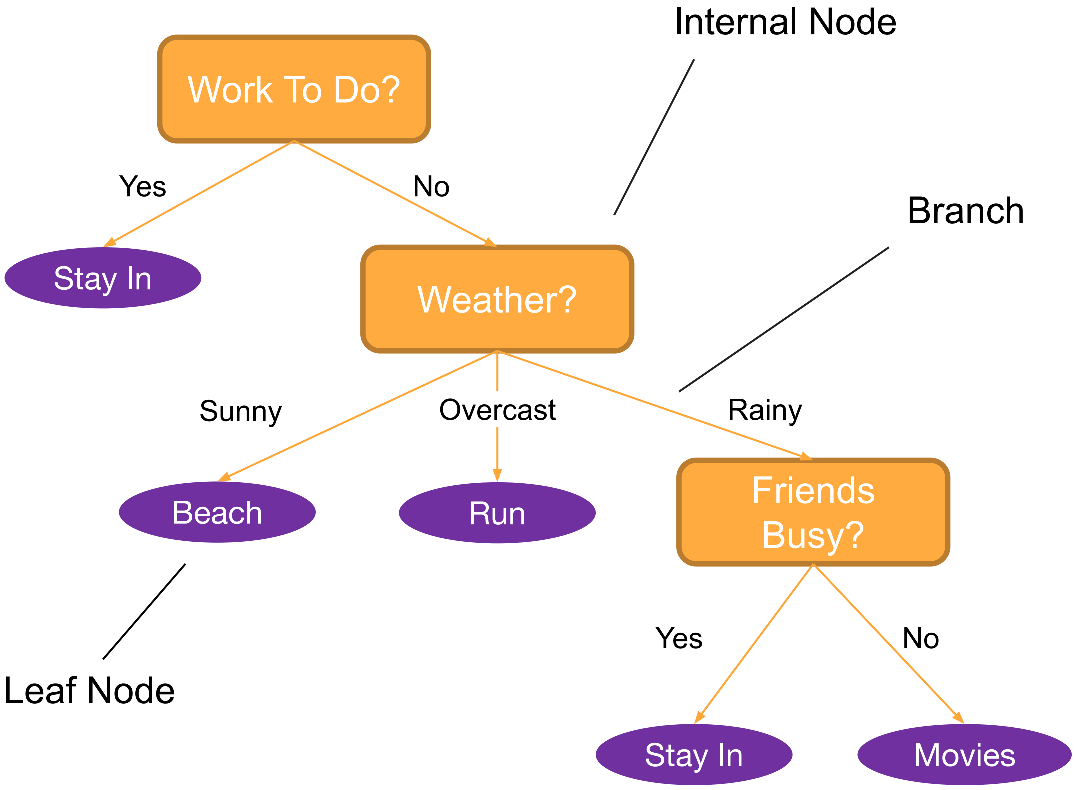
1. Decision Trees
2. Logistic Regression and Its Applications
3. Cross Validation

Decision Trees

Source

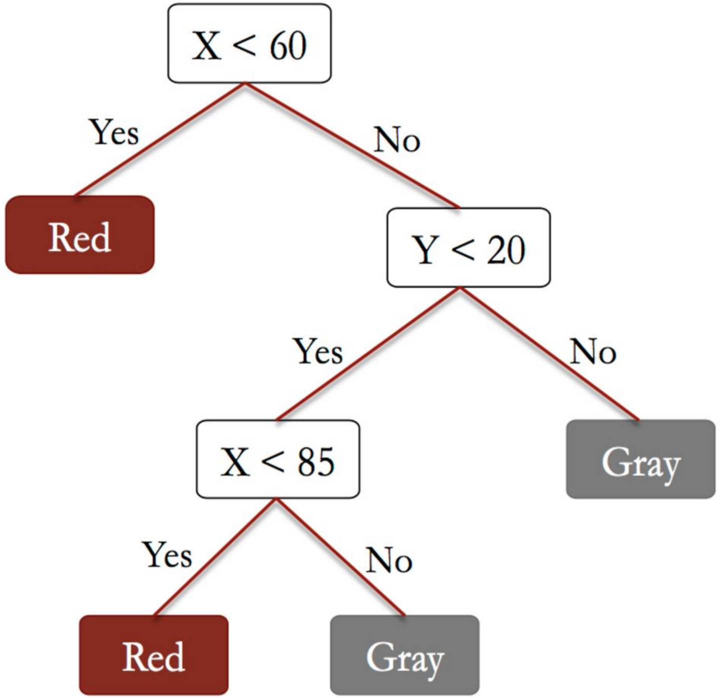
How Should I Spend My Weekends

A **decision tree** is a supervised machine learning model used to predict a target by learning decision rules from features. As the name suggests, we can think of this model as **breaking down** our data by **making a decision** based on **asking a series of questions.**



CART (Classification and Regression Trees)

- Used for Classification and Regression
- At each node, split on variables
- Each split minimizes error function
- Very interpretable
- <u>Models a non-linear relationship!</u>

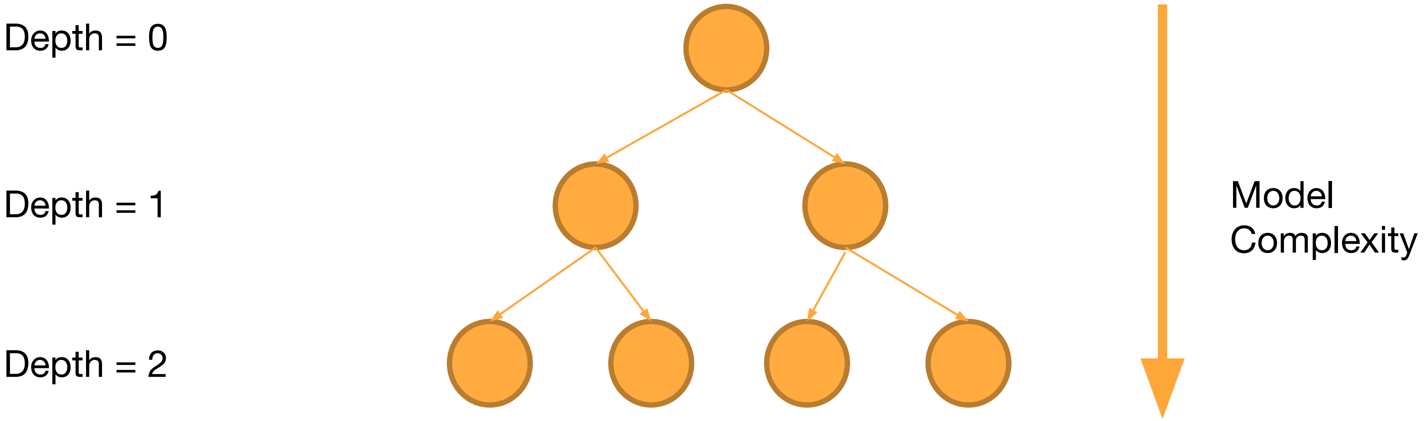


Pros and Cons of Using Decision Trees

Pros	Cons
Easy to interpret	Overfitting ☹️
Requires little data preparation (robust to missing data)	Requires parameter tuning (max depth)
Can use a lot of features	
Can capture non-linear relationships	

How to Reduce Overfitting

1. Limit the max depth of the tree

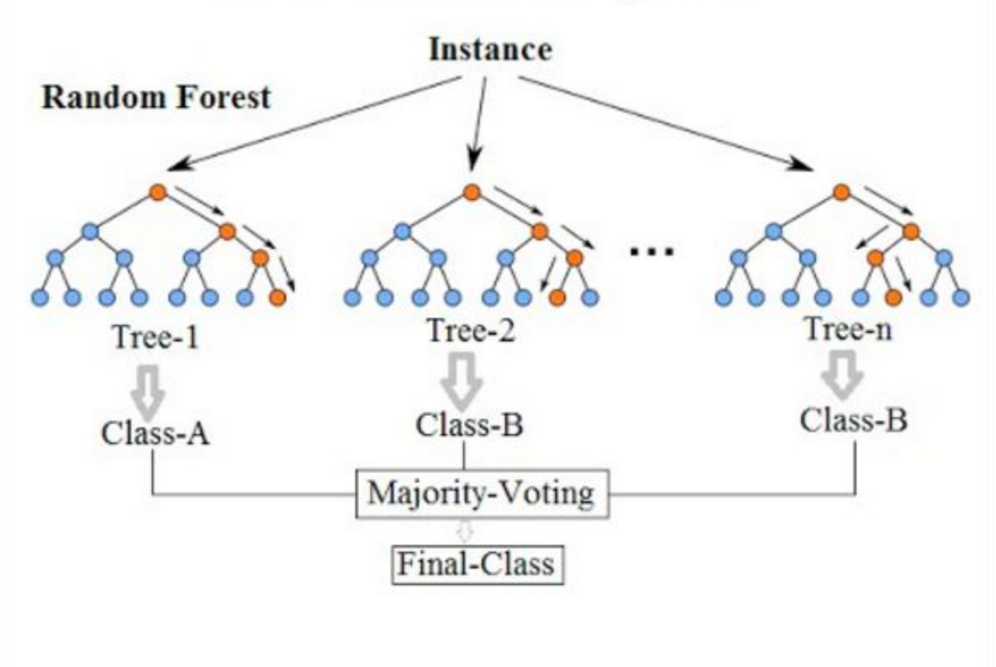


When training a decision tree, we have to specify the maximum depth a constructed tree can have

Source

How to Reduce Overfitting

2) Train multiple decision trees and determine final output based on output of each decision tree



This is called a **Random Forest Classifier**

Demo

Logistic Regression

Logistic Regression

- Used for Binary Classification:

$$Y = \begin{cases} 1 \\ 0 \end{cases}$$

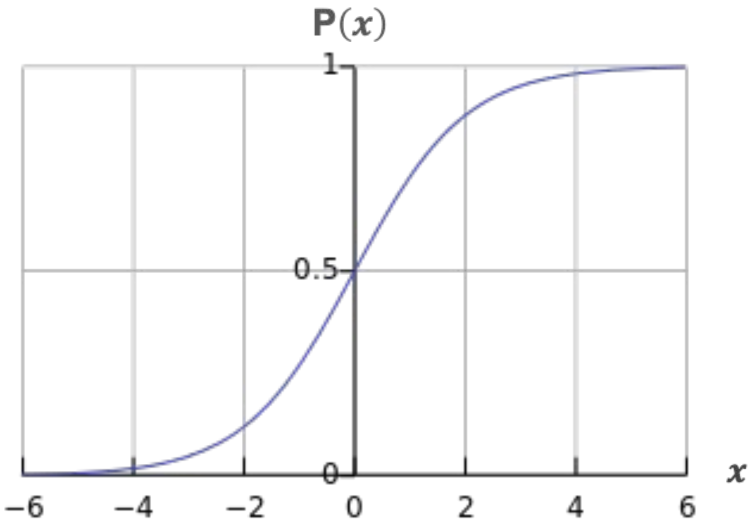
- Fits a linear relationship between the variables
- Transforms the linear relationship of probability that the outcome is 1 by using the **sigmoid function**

Formula:

$$P(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k)}} \longrightarrow \ln\left(\frac{P}{1-P}\right) = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k$$

Logistic Function

- $$P(x) = \frac{1}{1+e^{-x}}$$



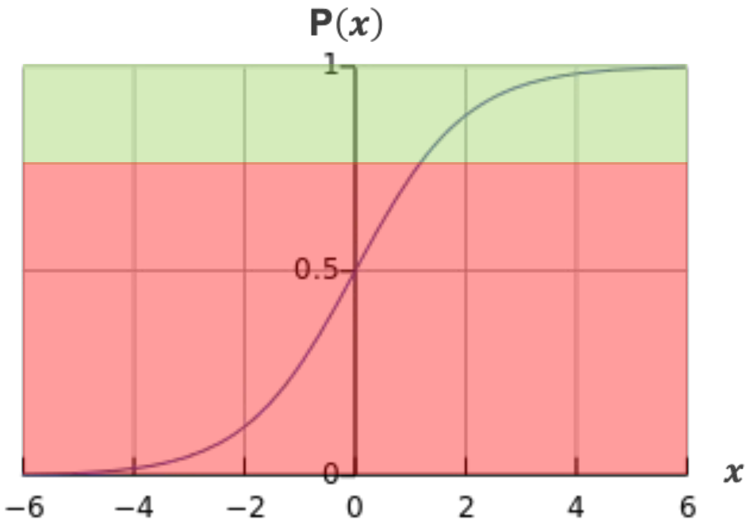
The Logistic Function "**squeezes**" numbers to be between 0 and 1

→ Allows us to interpret our prediction as a "**probability**" that something is true

Threshold

At what point point do we differentiate between our classifications?

- f(x) below threshold: predict 0
- f(x) above threshold: predict 1



Pros and Cons of Using Logistic Regression

Pros	Cons
Easy to interpret (probability)	Only Capable of Binary Classification
Computationally efficient to compute	
Does not require parameter tuning	

Logistic Regression is a simple model, therefore, oftentimes it is used as a good “baseline” to compare more complex models to

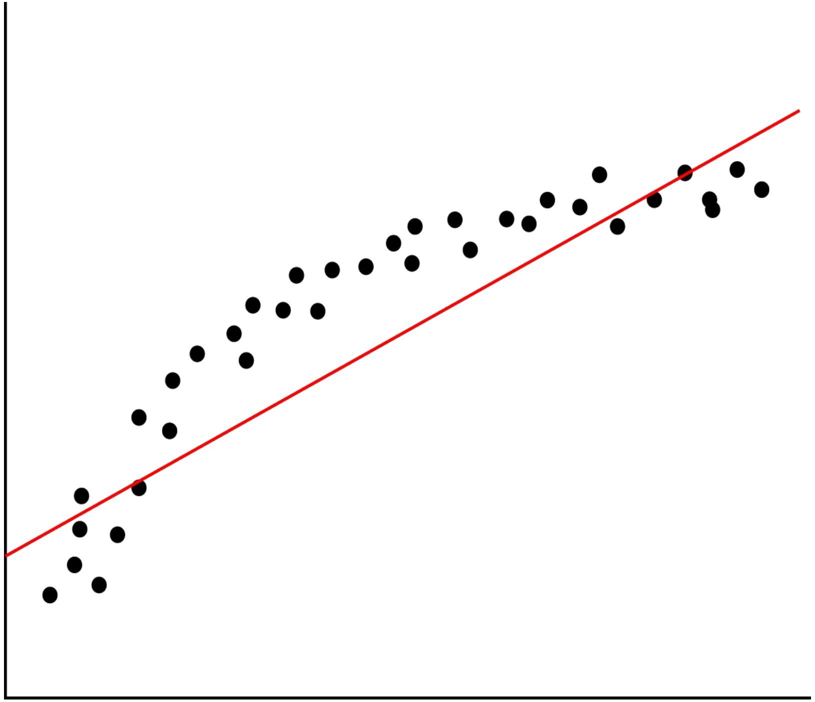
Demo

Cross Validation

Underfitting

Underfitting means we have high bias and low variance.

- Lack of relevant variables/factor
- Imposing limiting assumptions
  - Linearity
  - Assumptions on distribution
  - Wrong values for parameters



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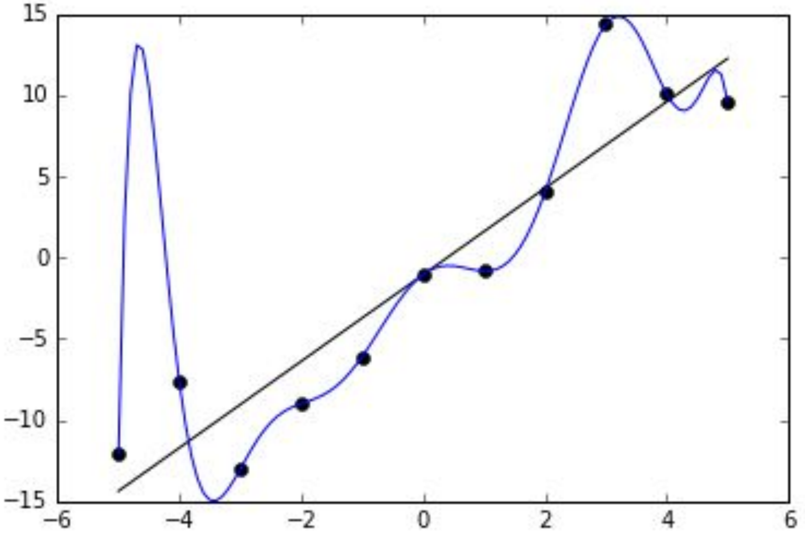
Overfitting

Overfitting means we have low bias and high variance.

- Model fits too well to specific cases
- Model is over-sensitive to sample-specific noise
- Model introduces too many variables/complexities than needed



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K-fold Cross Validation

Often used in practice with *k*=5 or *k*=10.

Create equally sized *k* partitions, or **folds**, of training data

For each fold:

- Treat the *k-1* other folds as training data.
- Test on the chosen fold.

The average of these errors is the validation error

K-fold Cross Validation

Dataset

Suppose K = 5,

5-Fold CV

K-fold Cross Validation

Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5

K-fold Cross Validation

Test Sample	Training Sample	Training Sample	Training Sample	Training Sample

Calculate MSE = mse1

K-fold Cross Validation

Training Sample	Test Sample	Training Sample	Training Sample	Training Sample

Calculate MSE = mse2

K-fold Cross Validation

Training Sample	Training Sample	Test Sample	Training Sample	Training Sample

Calculate MSE = mse3

K-fold Cross Validation

And so on

K-fold Cross Validation

Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

MSE = Avg(mse1…5)

K-fold Cross Validation

Matters less how we divide up

Selection bias not present

Leave-1-Out Cross Validation

For each sample:

- Treat all other data as training data.
- Test on that one sample

The average of these errors is the validation error

Pro: Better on small datasets

Pro: More realistic (trained on most of the data)

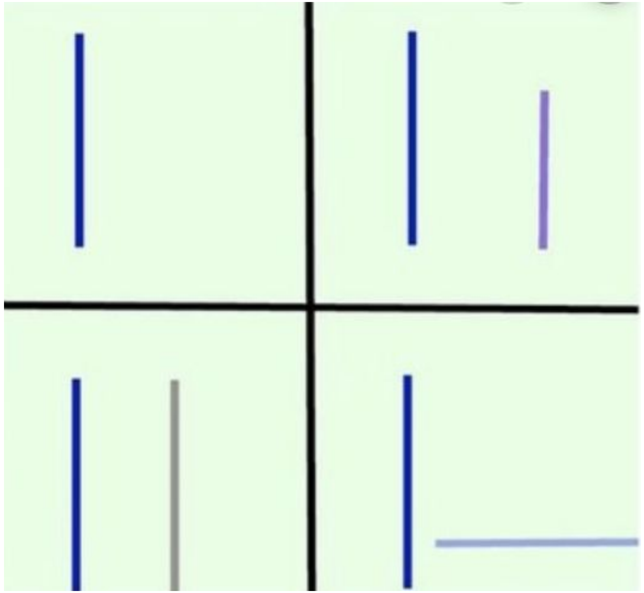
Con: Takes longer to run

Demo

Review

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



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 very good, or you really, really messed up

Balancing Bias and Variance

$$\text{Error} = (\text{Bias})^2 + (\text{Variance}) + (\varepsilon)$$

Bias = expected loss of accuracy

Variance = inconsistency of model

ε = irreducible error

Linear Regression

$$y = B_0 + B_1 x_1 + \ldots + B_p x_p + \varepsilon$$

- x is an input; $x_1, x_2, \ldots, x_p$ are the features of x
- y is an output (usually a single value)
- B's are "weights"
  - A linear regression equation is defined by its B's
  - This linear regression equation is the "program" produced by ML
- Given a set of x's and y's, the program finds a set of B's that (almost) satisfies the equation above for all x's and y's
  - **Minimizes bias, but not variance**
  - Then, you can plug in the feature values of a new x and to predict its y

Coming Up

- **Assignment 7**: Due 4:30pm on Nov. 10
- **Next Lecture**: Linear Classifiers and Model Validation
- **Final Project Check in:** Due 4:30pm on Nov. 10

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