Intro to Machine Learning - Week 3



## Classification (Part 2)

Decision Trees Overfitting, Underfitting Ensembles Learning



# What will we focus on?

#### Concepts, Problems

1 hour

#### Google Colab Project

1 hour

#### Schedule



#### **Supervised Learning**

Classification & Regression, Hypothesis Testing

#### **Classification 2**

Information Gain, Decision Trees, Random Forest, Ensembles

#### **Regression 2**

Logistic Regression, Support Vector Machine, Model Tuning

#### **Classification 1**

Conditional Probability, Naive Bayes, Bayesian Learning

#### **Regression 1**

Linear Regression, Loss Function, Gradient Descent, Back Propagation

#### **Model Evaluation**

Accuracy Metrics, Over-& Underfitting, Cross Validation



## Classification

- ◆ Target responses are categorical in nature
- We are going to see decision tree based classification in this session





- Class of algorithms that learn decision rules from a dataset.
- ◆ It generates a tree-like model of decisions and their possible consequences.
- Represented using a flow-chart like structure.
- Since it maps all possible consequences observed in your data, this would represent the hypothesis space.



- ♦ 14 rows
- Class variable play
- Features outlook, temperature, humidity, windy

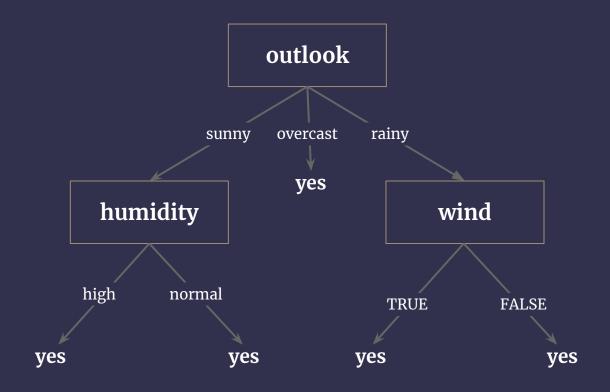


outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	FALSE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	FALSE	yes
rainy	mild	high	TRUE	no
rainy	mild	normal	FALSE	yes
sunny	cool	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	mild	normal	TRUE	yes

#### Decision Tree Example

How can we represent categorical values?

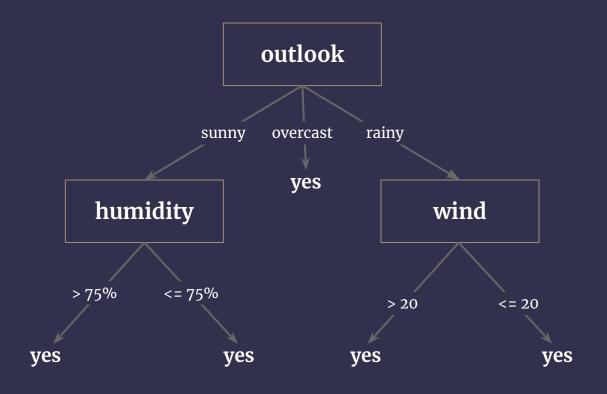
Let us ignore temperature for this.



#### Decision Tree Example

How can we represent continuous values?

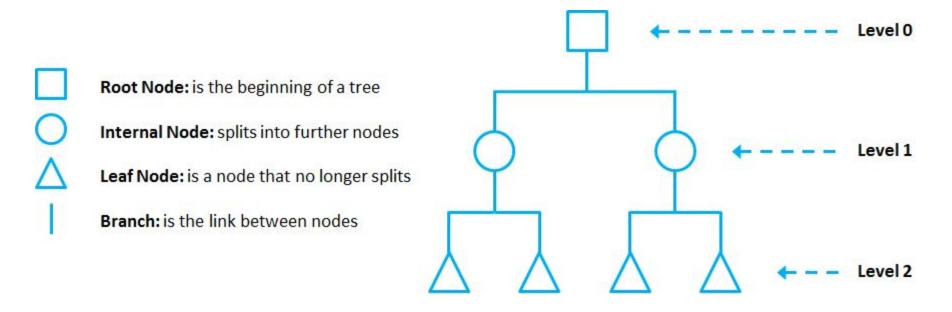
Let us assume humidity and wind are continuous for this.



#### How does it work?



#### **Elements in a Decision Tree**





# How to build a Decision Tree

Decision tree is built top-down from a root node and involves partitioning the data into subsets that contain instances with similar values (homogenous)

How do we decide which feature is the root of the tree?



## Entropy

How do we decide which feature is the root of the tree?

- Entropy is used to calculate homogeneity of a data sample.
- Average rate at which information is produced by a stochastic data source
- Entropy value ranges from 0 1
  - 0 = completely homogeneous
  - ► 1 = more uncertainity



- **♦ 14 rows**
- Features
  - $\mathbf{x}_1 = \text{outlook}$
  - $x_2$  = temperature
  - $\mathbf{x}_3$  = humidity
  - $\mathbf{x}_{4} = \mathbf{windy}$
- ◆ Target
  - $\rightarrow$  y = play
    - ho  $c_1 = yes$
    - $\rightarrow$   $C_2 = no$



outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	FALSE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	FALSE	yes
rainy	mild	high	TRUE	no
rainy	mild	normal	FALSE	yes
sunny	cool	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	mild	normal	TRUE	yes

#### **Entropy Formula**



$$\mathbf{E}(\mathbf{y}) = \sum_{i=(1,C)} -\mathbf{P}(\mathbf{c}_i) \times \mathbf{log}_2 \mathbf{P}(\mathbf{c}_i)$$

1----

Entropy of **Target Response**  Probability of class c.

~----/

$$\mathbf{E}(\mathbf{y},\mathbf{X}) = \sum_{\mathbf{c} \in \mathbf{X}} \mathbf{P}(\mathbf{c}_{\mathbf{i}}) \times \mathbf{E}(\mathbf{c}_{\mathbf{i}})$$

Entropy of target class for input feature  $x \in X$ 

1\_----

Probability of class c of x, class c of x,

~-----

Entropy of



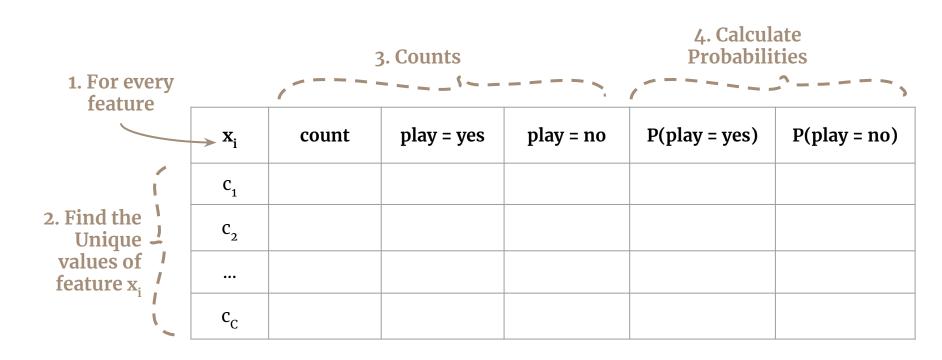
**Entropy of the target response** 

Unique values of target y

у	count	probability
<b>y</b> <sub>1</sub>		
<b>y</b> <sub>2</sub>		
y <sub>Y</sub>		
total		



Entropy of the feature class with respect to target response



## E(play)



play	count	probability
yes	9	0.64
no	5	0.36
total	14	1

$$E(y) = \sum_{i=(1,C)} -P(c_i) \times log_2 P(c_i)$$
Entropy of Target Response

Probability of class  $c_i$ 

$$E(play) = -0.64\log_2(0.64) - 0.34\log_2(0.34)$$
$$= 0.94$$

## E(play,outlook)



$E(y,X) = \sum_{i=1}^{N} E(y_i,X_i)$	$\mathbf{E}_{c \in \mathbf{X}} \mathbf{P}(\mathbf{c}_i) \times \mathbf{E}(\mathbf{c}_i)$	)
Entropy of target class for input feature x <sub>i</sub> ∈ X	$\begin{array}{ccc} \text{Probability of} & \text{Entropy of} \\ \text{class c of } x_i & \text{class c of } x_i \end{array}$	,

TRUE

ves

					LICOIT VA
outlook	count	yes	no	P(yes)	P(no)
sunny	5	3	2	0.6	0.4
overcast	4	4	0	1	0
rainy	5	2	3	0.4	0.6
			•		

	input feature x <sub>i</sub> e		class c of x <sub>i</sub>	class c of x
outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	FALSE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	FALSE	yes
rainy	mild	high	TRUE	no
rainy	mild	normal	FALSE	yes
sunny	cool	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no

normal

mild

sunny

sunny
 5
 3
 2
 0.6
 0.4

 overcast
 4
 4
 0
 1
 0

 rainy
 5
 2
 3
 0.4
 0.6

$$E(\text{play,outlook}) = \frac{P(\text{sunny}) \times E(\text{sunny})}{F(\text{sunny})} + \frac{P(\text{overcast}) \times E(\text{overcast})}{F(\text{sunny})} \times \frac{F(\text{sunny})}{F(\text{sunny})} = \frac{5}{14} \times \frac{F(\text{sunny})}{F(\text{sunny})} + \frac{5}{14} \times \frac{F(\text{sunny})}{F(\text{sunny})} = \frac{5}{14} \times \frac{F(\text{sunny})}{F(\text{sunny})} + \frac{F(\text{sunny})}{F(\text{sunny})} = \frac{5}{14} \times \frac{F(\text{sunny})}{F(\text{sunny})} = \frac{F(\text{sunny})}{F(\text{sunny}$$

 $E(4,0) = -1\log_2 1 - 0\log_2 0 = 0$ 

E(2,3) = E(3,2) = 0.971

= 
$$\frac{0.357 \times 0.971}{0.286 \times 0} + \frac{0.357 \times 0.971}{0.357 \times 0.971}$$
  
= 0.693  
E(play, outlook) = 0.693

 $E(3,2) = -\frac{1}{9}\log_{2}\% - \frac{1}{9}\log\% = -(0.6 \times 0.737) - (0.4 \times 0.529) = 0.971$ 

## E(play,temperature)



$E(y,X) = \sum_{i=1}^{N} E(y,X_i)$	$\sum_{c \in X} P(c_i) >$	E(c <sub>i</sub> )
Entropy of target class for input feature x₁∈ X	Probability of class c of x <sub>1</sub>	Entropy of class c of x <sub>i</sub>

temperature	count	yes	no	P(yes)	P(no)
hot	4	2	2	0.5	0.5
mild	6	4	2	0.67	0.33
cool	4	3	1	0.75	0.25

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	FALSE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	FALSE	yes
rainy	mild	high	TRUE	no
rainy	mild	normal	FALSE	yes
sunny	cool	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	mild	normal	TRUE	yes

$$E(\text{play,temp}) = \frac{P(\text{hot}) \times E(\text{hot}) + P(\text{mild}) \times E(\text{mild})}{P(\text{cool}) \times E(\text{cool})}$$

$$= \frac{4}{14} \times E(2,2) + \frac{6}{14} \times E(4,2) + \frac{4}{14} \times E(3,1)$$

$$E(2,2) = -\frac{2}{4} \log_2 \frac{2}{4} - \frac{2}{4} \log_2 \frac{2}{4} = 1.0$$

$$E(4,2) = -\frac{4}{6} \log_2 \frac{4}{6} - \frac{2}{6} \log_2 \frac{2}{6} = 1.811$$

$$E(3,1) = -\frac{3}{4} \log_2 \frac{3}{4} - \frac{1}{4} \log_2 \frac{1}{4} = 0.918$$

$$= \frac{0.286 \times 1.0}{0.429 \times 1.811} + \frac{0.286 \times 0.918}{0.286 \times 0.911}$$

$$= \frac{0.911}{0.911}$$

## E(play, humidity)

outlook

overcast

overcast

overcast

overcast

rainy

rainy

rainy

rainy

rainy

sunny

sunny

sunny

sunny

sunny

mild

mild



$E(y,X) = \sum_{i=1}^{N} E(y,X_i)$	$\mathbf{C}_{\mathbf{c}\in\mathbf{X}}\mathbf{P(c_i)}\times$	$E(c_{i})$
1		
Entropy of target class for input feature x <sub>i</sub> ∈ X	Probability of class c of x <sub>i</sub>	Entropy of class c of x

humidity	count	yes	no	P(yes)	P(no)
normal	7	6	1	0.86	0.14
high	7	3	4	0.43	0.57

high 7 3 4 0.43 0.57

$$E(\text{play,humidity}) = P(\text{normal}) \times E(\text{normal}) + P(\text{high}) \times E(\text{high})$$

$$= 7/14 \times E(6,1) + 7/14 \times E(3,4)$$

$$E(3,2) = -6/7\log_{10}6/7 - 1/7\log_{1/7} = 0.985$$

**FALSE** 

TRUE

no

yes

high

normal

$$= 7/14 \times E(6,1) + 7/14 \times E(3,4)$$

$$E(3,2) = -6/7\log_{2}6/7 - 1/7\log_{1/7} = 0.985$$

$$E(3,4) = -3/7\log_{2}3/7 - 4/7\log_{4/7} = 0.592$$

$$= 0.5 \times 0.985 + 0.5 \times 0.592$$

$$= 0.788$$

E(play, humidity) = 0.788

## E(play,windy)

cool

hot

hot

mild

mild

outlook

overcast overcast overcast overcast rainy rainy rainy rainy rainy

sunny

sunny

sunny

sunny

sunny



E(y,X) = 2	$\sum_{c \in X} P(c_i) \times$	$E(c_{i})$
1		
Entropy of target class for input feature x ∈ X	Probability of class c of $x_i$	Entropy of class c of x

windy	count	yes	no	P(yes)	P(no)
TRUE	6	3	3	0.5	0.5
FALSE	8	6	2	0.75	0.25

Entropy of target class for input feature x <sub>i</sub> ∈ X		$\begin{array}{ll} \text{Probability of} & \text{Entropy of} \\ \text{class c of } x_i & \text{class c of } x_i \end{array}$		
temperature	humidity	windy	play	
cool	normal	TRUE	yes	
hot	high	FALSE	yes	
hot	normal	FALSE	yes	
mild	high	TRUE	yes	
cool	normal	FALSE	yes	
cool	normal	TRUE	no	
mild	high	FALSE	yes	
mild	high	TRUE	no	
mild	normal	FALSE	yes	

FALSE

**FALSE** 

TRUE

**FALSE** 

TRUE

ves

no

no

no

yes

normal

high

high

high

normal

E(play,windy)	$= P(TRUE) \times E(TRUE) + P(I$	FALSE) × E(FALSE)
	= $6/14 \times E(3,3) + 8/14 \times E(6)$	5,2)
	$og_{23}/6 - 3/6log_{3}/6 = 1.0$ $og_{26}/8 - 2/8log_{2}/8 = 0.811$	
	= 0.428 × 1.0 + 0.571 × 0	0.811
	= 0.892	

E(play, windy) = 0.892

#### What do we have till now?





Calculate the information gain of each input feature



Information gain of input feature x,∈ X

Entropy of **Target Response** 

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Entropy of target class for input feature  $x_i \in X$ 

\\_\_\_\_/



#### Calculate the information gain of each input feature

```
y = play

x<sub>1</sub> = outlook

x<sub>2</sub> = temperature

x<sub>3</sub> = humidity

x<sub>4</sub> = windy
```

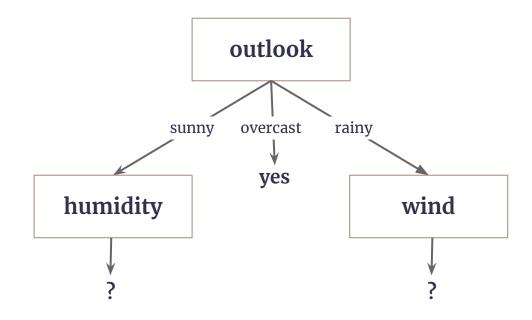
Gain(play, windy) = E(play) - E(play, windy)

= 0.94 - 0.892 = 0.048



Pick the feature with highest information gain for first split

Gain(play, outlook) = 0.247 Gain(play, temp) = 0.029 Gain(play, humidity) = 0.152 Gain(play, windy) = 0.048

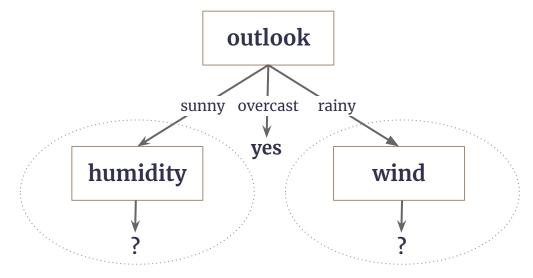


#### **Decision Tree - Next Steps**



 Filter the data samples based on previous decision.

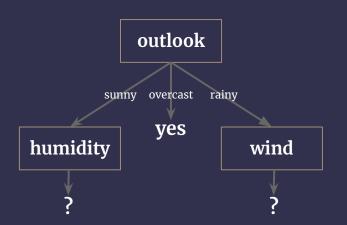
Recursively conduct
 Step 1 - 3 for every
 decision required.



- ◆ Filter on outlook=sunny
- ◆ Conduct Step 1 3 on this data sample

- ◆ Filter on outlook=rainy
- ◆ Conduct Step 1 3 on this data sample

## Homework #1





Complete the decision tree from the previous slide. Data sample listed below:

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	FALSE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	FALSE	yes
rainy	mild	high	TRUE	no
rainy	mild	normal	FALSE	yes
sunny	cool	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	mild	normal	TRUE	yes



Assumption



- Feature values are required to be categorical to calculate information gain
  - Continuous data can be discretized easily.
    - Eg. Bucketing ages, splitting based on quantile, etc



Advantages



- Easy to understand/explain
  - Intuitive way to make decisions
- Features are not assumed to be equally important to the target response (hint: Naive Bayes)



#### **Variations**



- Iterative Dichotomiser 3 (ID3)
- **◆** C4.5
- Chi-squared Automatic Interaction Detection (CHAID)
- ◆ CART



## ID3

- Mainly used to produce Classification Trees
- Uses the Information Gain metric to select the most useful attributes for classification
  - ► The example we solved is ID3!



## C4.5

- Can be used for both classification and regression trees
- Uses the Gain Ratio metric to select the most useful attributes for classification
  - Information gain that takes into account the number and size of the branches when choosing an attribute (IG shows unfair favoritism towards attributes with many outcomes)
  - Basically "normalizes" the Information Gain by using a split information value.



#### **CHAID**

- Chi-square tests check if there is a relationship between two variables
- Applied at each stage of the DT to ensure that each branch is significantly associated with a statistically significant predictor of the response variable.
- For classification trees, it uses the Chi squared test. For regression trees, it uses f-test
  - If the test fails, the nodes are merged into one



#### CART

- Produces binary classification/regression trees.
- Uses a metric called **Gini Impurity** to create decision points for classification tasks.
  - Classification Measure of how mixed the classes are in groups created by the split.
     This has to be minimized.
  - Regression minimizes the sum of the squared distances (or deviations) between the observed values and the predicted values (Least Square Deviation)



#### Disadvantages



- Calculations become complicated if there are many class labels
- Cannot estimate missing data
- Overfitting
  - Biased towards class value with more data samples (bias vs. variance)
  - Biased on data samples in the training data (pruning)



Overcoming Disadvantages



- Understanding your data
  - Bias vs. Variance Trade-Off
- Understanding the algorithm
  - Overfitting and underfitting
- Understanding the Decision Tree
  - Pruning
  - Ensemble Learning

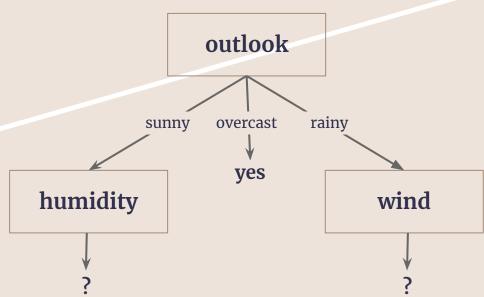


#### **Terminology**

#### **Overfitting**

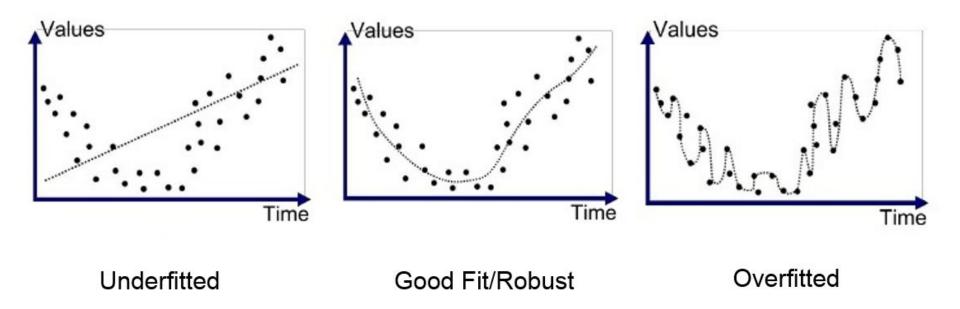
When the model isn't generalizable and contain biases from the dataset it was built on.

- eg. The relationship between play and outlook - there are no examples in the dataset of outlook=overcast and play=no.
  - A model is as good as its data





### What is a good fit?





#### **Terminology**

#### **Bias**

- Bias is the tendency of a statistic to overestimate or underestimate a parameter.
- Assumptions made to make the target function easier to learn.
  - Low Bias: Suggests less assumptions about the form of the target function.
  - High-Bias: Suggests more assumptions about the form of the target function.



### **Terminology**

#### **Variance**

- Variance measures how far a set of numbers are spread out from their average value.
- Variance error is the amount that the estimate of the target function will change if different training data was used.
  - High Variance: Machine learning algorithms that have a high variance are strongly influenced by the specifics of the training data.
  - Low Variance: Suggests small changes to the estimate of the target function with changes to the training dataset.



Bias and variance are 2 sources of errors in supervised learning problems.

A models goal is to minimize the error



- Bias is an erroneous assumption made by the algorithm
  - High bias can lead to missing relevant relations between features and targets (underfitting).
- Variance is an error from sensitivity to small fluctuations in the training set.
  - High variance can lead to modeling the random noise in the training data, rather than the intended outputs (overfitting).



# Bias vs. Variance Trade-off

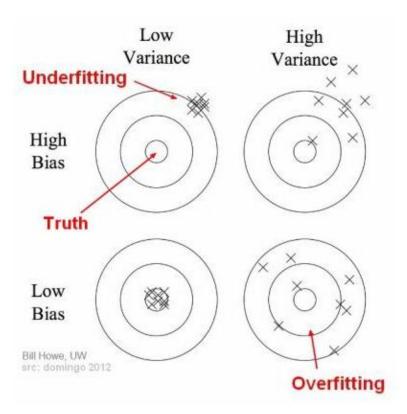
- Models with a lower bias have a higher variance across samples
- Models with a higher bias have a lower variance across samples



Low Bias = High Variance

High Bias = Low Variance







Low Bias = High Variance

High Bias = Low Variance



- If our model is too simple and has very few parameters then it may have high bias and low variance.
- On the other hand if our model has large number of parameters then it's going to have high variance and low bias.
- This tradeoff in complexity is why there is a tradeoff between bias and variance. An algorithm can't be more complex and less complex at the same time.
- So we need to find the right/good balance without overfitting and underfitting the data.



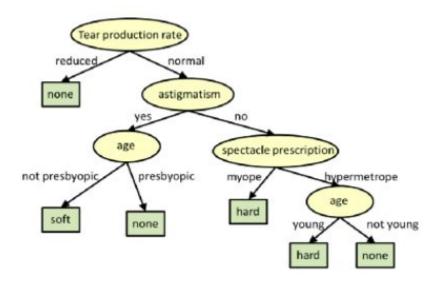


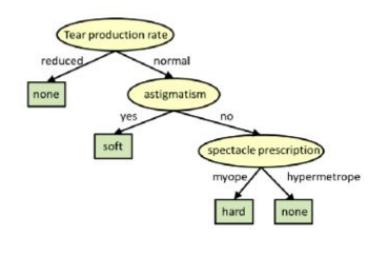


- Pruning is a technique used to deal with overfitting, that reduces the size of DTs by removing sections of the Tree that provide little predictive or classification power.
  - Reduces complexity of final classifier
  - Overcome overfitting → improve accuracy



#### **Pruning Example**





**Original Tree** 

Pruned Tree



## Pruning Strategies

#### Pre-pruning

 When you stop growing DT branches when information becomes unreliable.

#### Post-pruning

In a fully grown DT, removing leaf nodes only if it results in a better model performance.



## Ensemble Learning

- Ensemble learning is a machine learning paradigm where multiple models (or "weak learners") are trained to solve the same problem and combined to get better results.
- The main hypothesis is that when weak models are correctly combined we can obtain more accurate and/or robust models.



How to combine models?



- ◆ Bagging considers homogeneous weak learners, learns them independently from each other and combines them following some kind of deterministic averaging process.
- Boosting considers homogeneous weak learners, learns them sequentially in a very adaptative way (a base model depends on the previous ones) and combines them following a deterministic strategy
- ▶ Stacking considers heterogeneous weak learners, learns them in parallel and combines them by training a meta-model to output a prediction based on the different weak models predictions



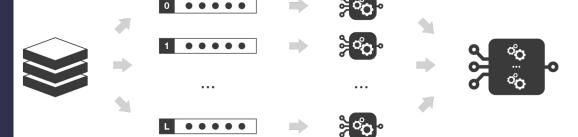
Bagging

**Bootstrap** generates samples of size B from an dataset of size N by randomly drawing with replacement B observations.



ensemble model (kind of average

of the weak learners)



weak learners fitted on

each bootstrap sample

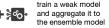
L bootstrap samples

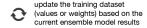
initial dataset

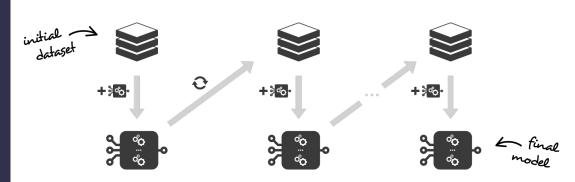
## Ensemble Learning

Boosting









- Adaboost updates weights of the observations at each iteration.
  - Weights of well classified observations decrease relatively to weights of misclassified observations.
  - Models that perform better have higher weights in the final ensemble model.



## Ensemble Learning

Stacking

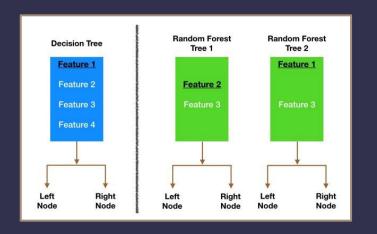


initial dataset

L weak learners (that can be non-homogeneous)

meta-model (trained to output predictions based on weak learners predictions)

## Random Forest

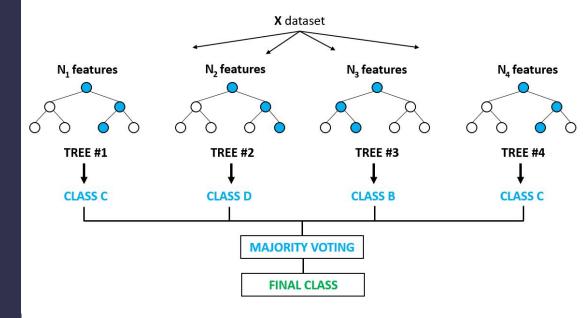




- Random Forest is an extension over bagging.
- It builds models on random subsets of data (bootstrapping)
  - Additionally, it also takes a random selection of features rather than using all to grow DTs.
- Each individual tree in the random forest outputs a class prediction and the class with the most votes becomes our model's prediction.



## Random Forest





Advantages



- This model can estimate missing data
  - maintains accuracy when large proportion of the data is missing
- Bagging balances errors in data sets where classes are imbalanced.
- Powerful due to the number of combinations it considers



Disadvantages



#### No interpretability

- Feels like a "black box" approach since we have very little control on what the model does
- ▶ Time consuming due to the number of combinations considers and computations it does.

## Theory Recap



#### Decision Trees

- Entropy, Information Gain
- Example
- Advantages
- Variations
- Disadvantages

#### Overcoming Disadvantages

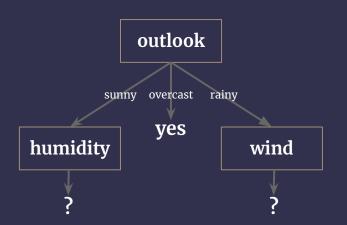
- Overfitting
- Bias vs. Variance
- Pruning
- Ensemble Learning

#### Random Forest



# Google Colab Project

# Homework #1





Complete the decision tree from the previous slide. Data sample listed below:

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	FALSE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	FALSE	yes
rainy	mild	high	TRUE	no
rainy	mild	normal	FALSE	yes
sunny	cool	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	mild	normal	TRUE	yes



# Homework #2

Try to solve an end-to-end project on the <u>Titanic</u> <u>dataset</u>. This table has multiple columns which can be used to predict if a passenger survived or not.

For your ease, we have uploaded the titanic dataset to our github and you can use the below URL as the parameter to read\_csv to load the dataset in Google Colab

https://github.com/WomenWhoCode/WWCodeDa taScience/tree/master/Intro\_to\_MachineLearning /data/titanic

Note: The dataset has already been split into train and test

https://www.machinelearningplus.com/predictive-modeling/how-naive-bayes-algorithm-works-with-example-and-full-code/



Note: You have to download these datasets from links and host it on your Google Drive. This video will help you get set up!



Our leaders have curated 2 other datasets you can try out your classification skills on.

Dataset	Link	Task Description
Wids 2020 hospital Dataset	https://www.kaggle.com/c/widsdatathon2020/data	This dataset has patient details such as heart rate, temperature and few other essential measurements from 1st 24 hours in a Intensive care unit. The task is to build a model to predict patient survival
Credit card fraud Dataset	https://www.kaggle.com/mlg-ulb/creditcardfraud	This dataset has credit card transaction details which have been anonymized using PCA. The task is to identify fraudulent transactions from others



## See you next week!

#### **Questions?**

Join us on slack (<a href="mailto:bit.ly/wwcodedatascience-slack">bit.ly/wwcodedatascience-slack</a>) and post it on our #help-me channel.

#### Register?

Register for all sessions at <a href="linktr.ee/wwcodedatascience">linktr.ee/wwcodedatascience</a> <a href="registration">registration</a>