

# Decision Trees and Random Forests

*Ivan Corneillet*

*Data Scientist*

# Learning Objectives

After this lesson, you should be able to:

- Understand and build decision tree models for classification and regression
- Understand the differences between linear and non-linear models
- Understand and build random forest models for classification and regression
- Know how to extract the most important predictors in a random forest model



DS

# Announcements and Exit Tickets

**DS**

Q & A



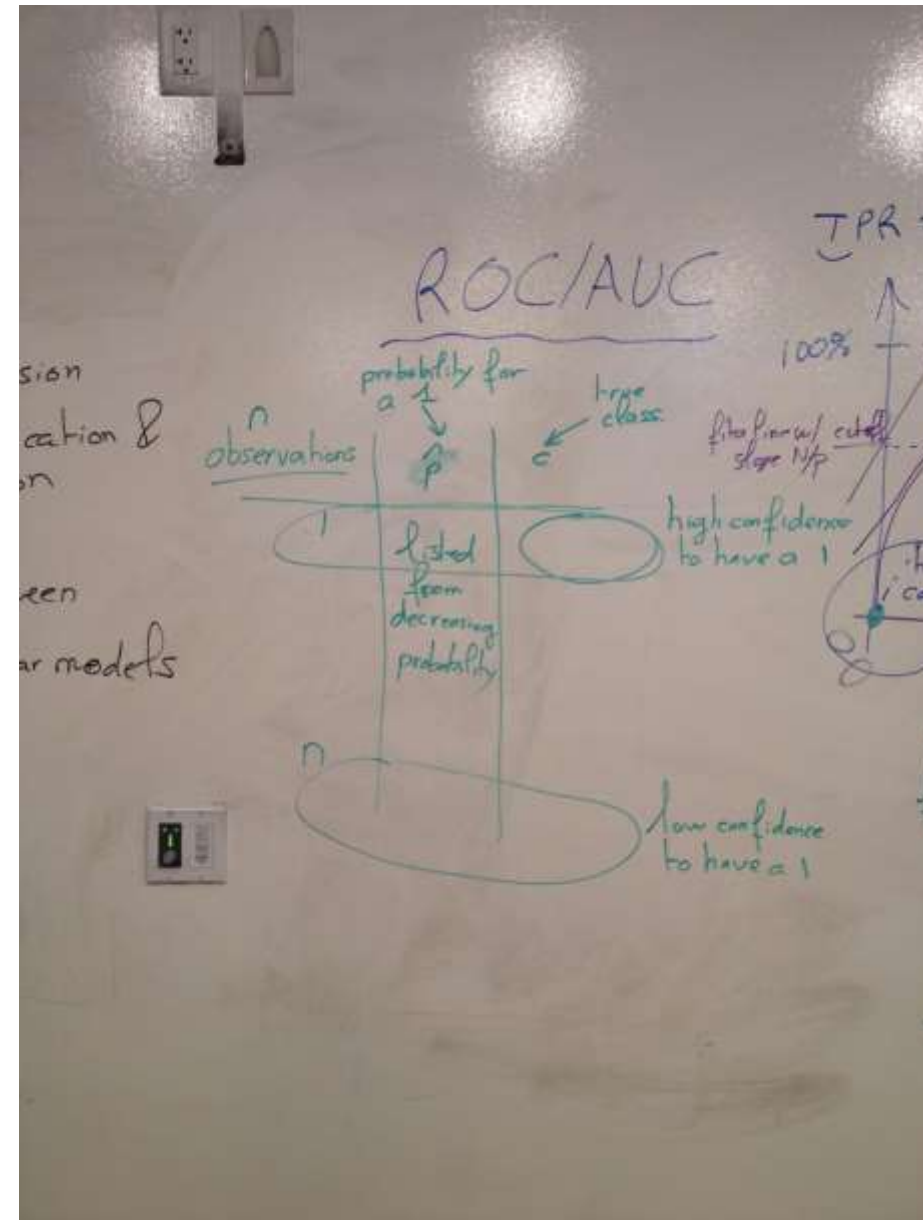
**DS**

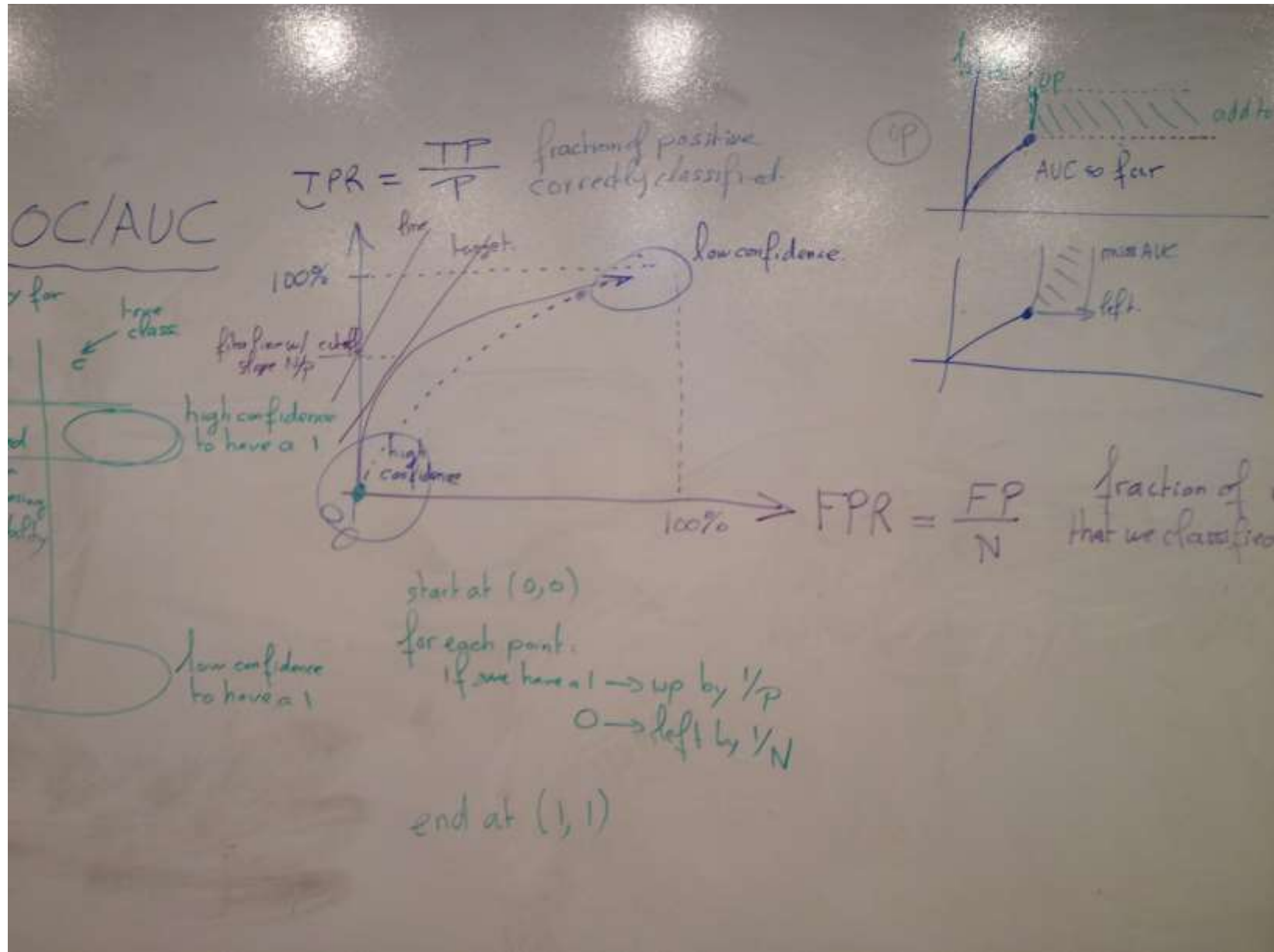
# Review

DS

# Review

*ROC/AUC*

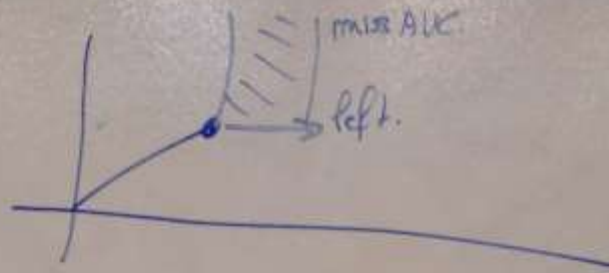
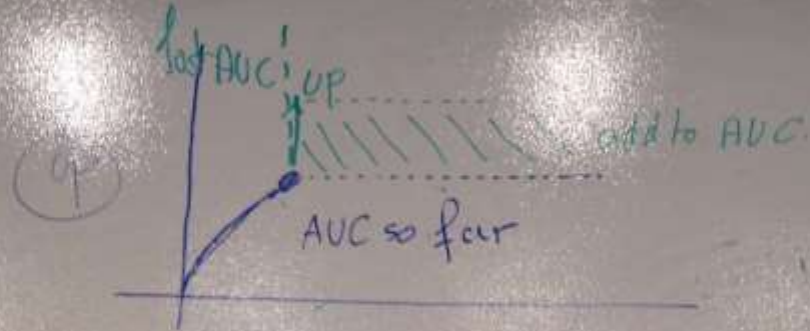






positive  
classification.

low confidence.



100%  $\Rightarrow$  
$$FPR = \frac{FP}{N}$$
 fraction of negative  
that we classified incorrectly.

A black circle containing the white text "DS".

DS

# Today

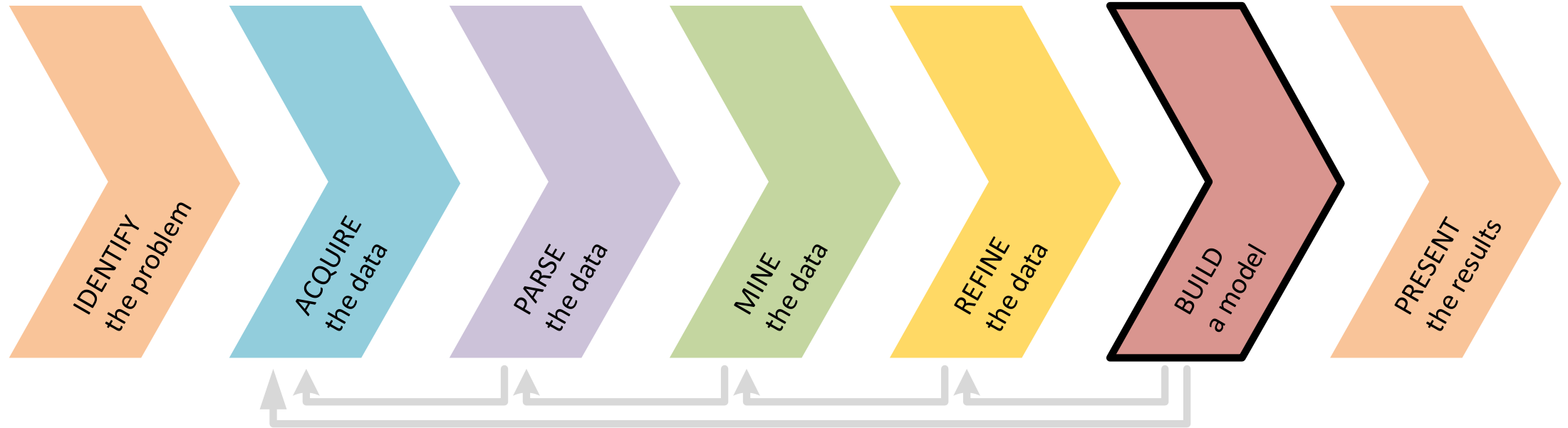
# Here's what's happening today:

- Final Project 3 (due today)
- Announcements and Exit Tickets
- Review
- **⑥ Build a Model | Decision Trees**
  - The 2008 Democratic Primaries
  - What is a decision tree?
  - Structure
  - Predicting
  - Entropy
  - Training
- Classification and Regression Decision Trees
- Pros and Cons
- Overfitting
- **⑥ Build a Model | Random Forests**
  - Pros and Cons
  - Training
  - Predicting
- Lab – Decision trees and random forests
- Review

Today, we are starting Unit 3 by introducing two new machine learning algorithms: first Decision Trees; then Random Forests (which will build upon decision trees)

Research Design and Data Analysis	Research Design	Data Visualization in <i>pandas</i>	Statistics	Exploratory Data Analysis in <i>pandas</i>
Foundations of Modeling	Linear Regression	Classification Models	Evaluating Model Fit	Presenting Insights from Data Models
Data Science in the Real World	Decision Trees and Random Forests	Time Series Data	Natural Language Processing	Databases

Therefore, today we are refocusing on **BUILD** a model step but with a focus on decision trees and random forests



**DS**

# Pre-Work

# Pre-Work

Before this lesson, you should already be able to:

- Explain the concepts of cross-validation, logistic regression, and overfitting
- Know how to build and evaluate some classification models in *sklearn* using cross-validation and AUC

DS

# Decision Trees



A black circle containing the white text "DS".

DS

# Decision Trees

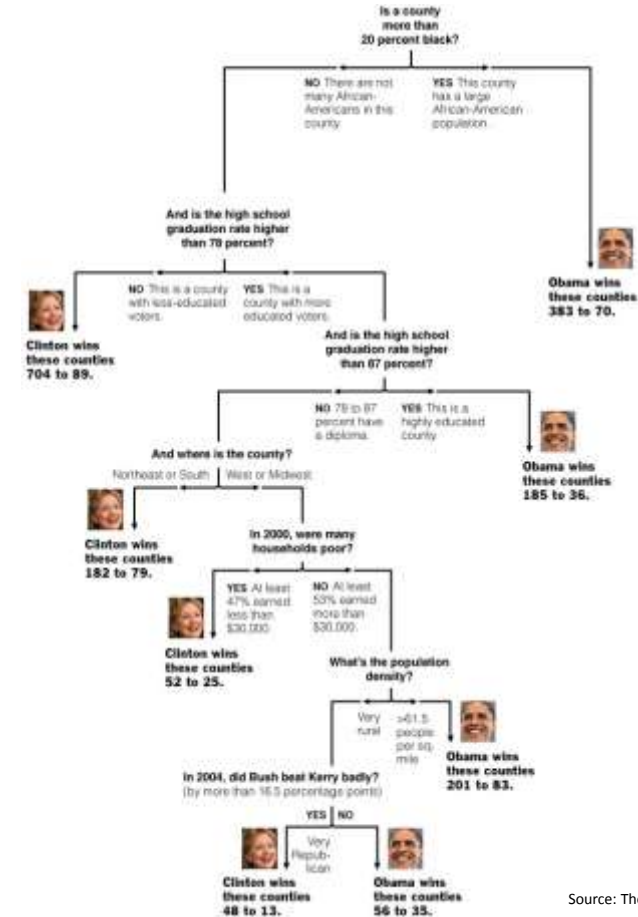
*Motivating Example and Activity | The 2008 Democratic Primaries*

# Motivating Example | The 2008 Democratic Primaries

## EXAMPLE

### ► Decision Tree: The Obama-Clinton Divide

- Published in The New York Times on April 16, 2008 while the Democratic Primaries were still running



Source: The New York Times

# Activity | The 2008 Democratic Primaries

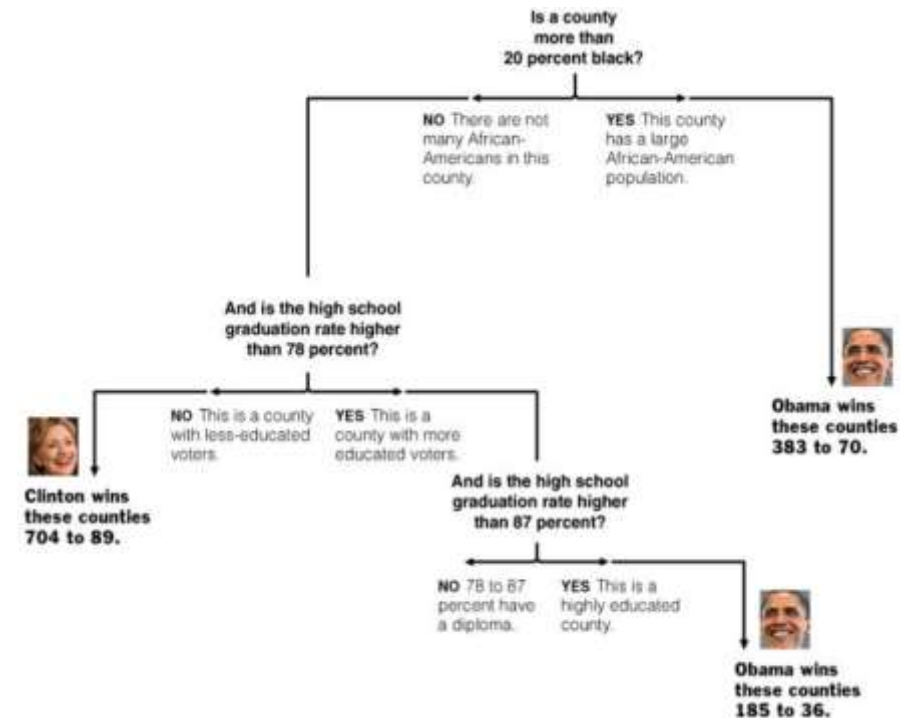
## EXERCISE

### DIRECTIONS (10 minutes)

1. In a couple of sentences, describe what counties senators Obama and Clinton have won so far in the nomination contest
2. Amanda Cox, a data scientist of The New York times created this excellent graphics. How do you think she proceeded to create it?
3. When finished, share your answers with your table

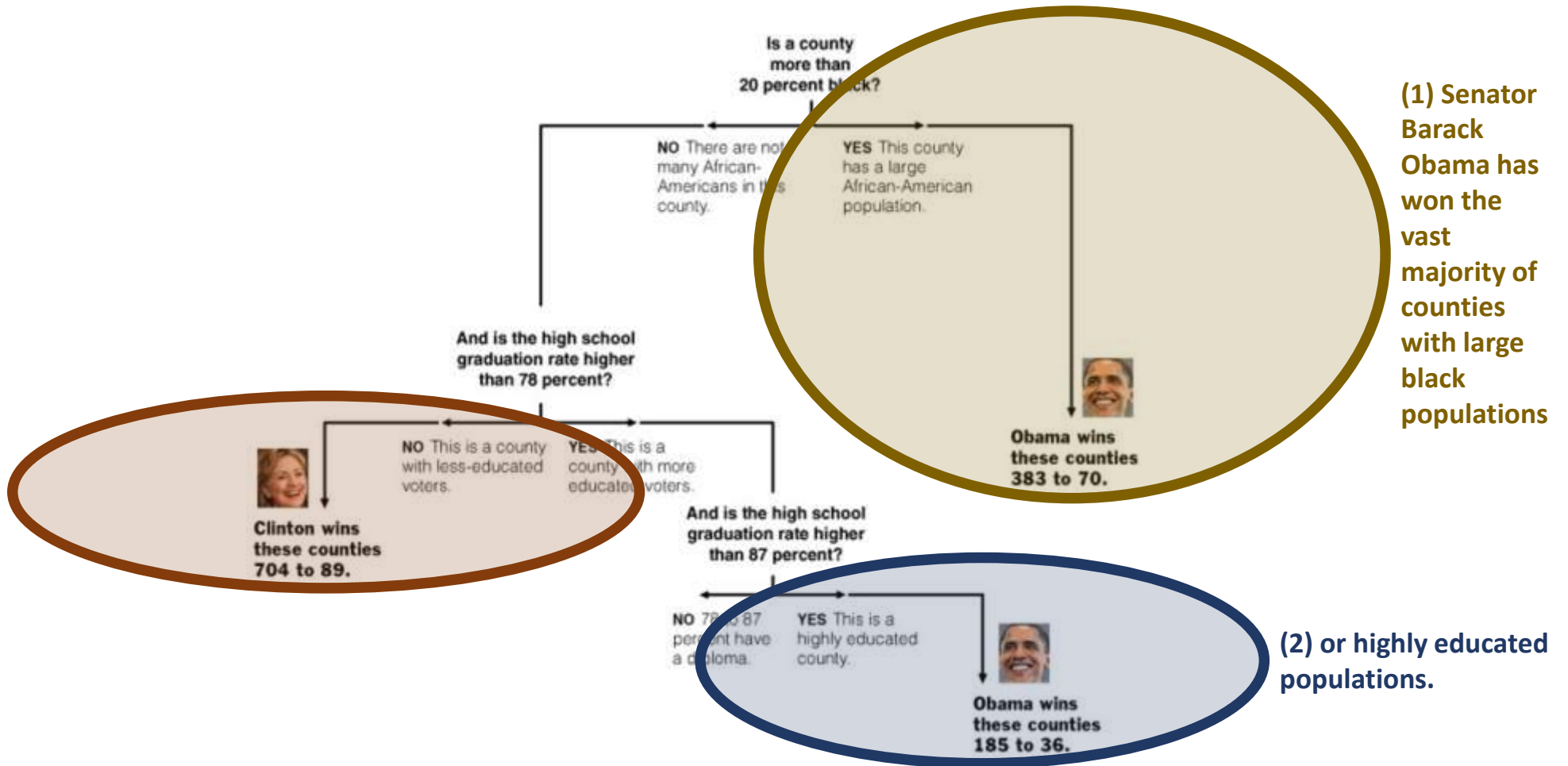
### DELIVERABLE

Answers to the above questions



# Activity | “In the nominating contests so far, ...

(3) Senator Hillary Rodham Clinton has a commanding lead in less-educated counties dominated by whites”



# Activity | The 2008 Democratic Primaries (cont.)

- “In the nominating contests so far, Senator Barack Obama has won the vast majority of counties with large black or highly educated populations. Senator Hillary Rodham Clinton has a commanding lead in less-educated counties dominated by whites”
- Surely an over-simplification but it is easy to display, interpret, and explain

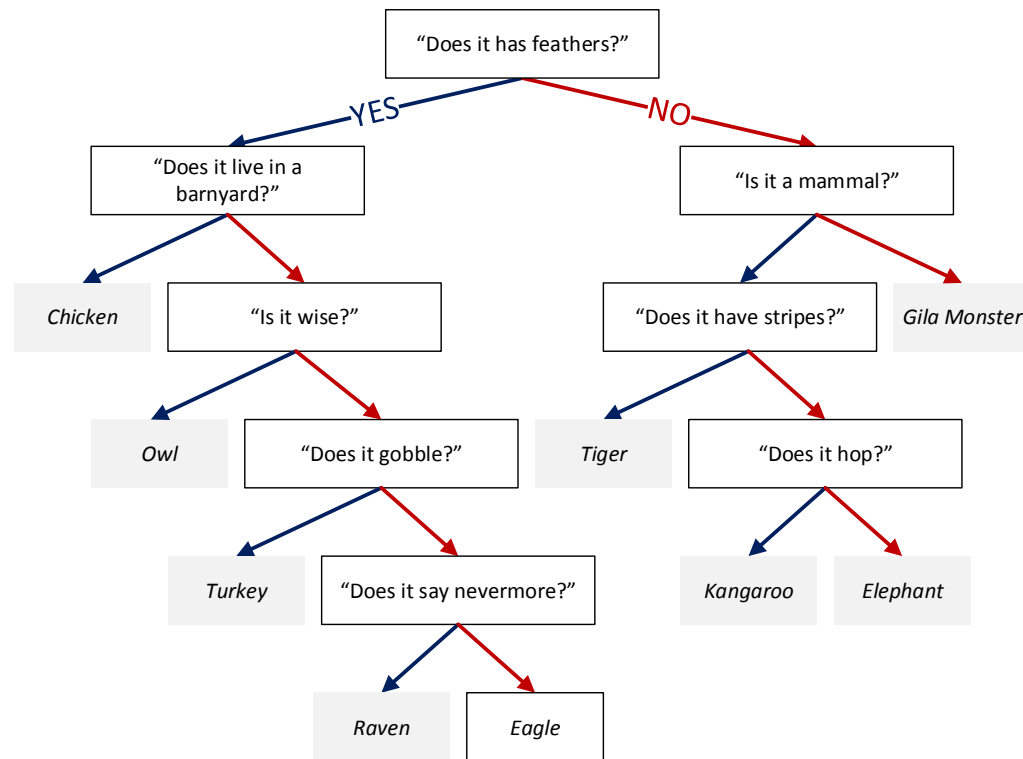
A black circle containing the white text "DS".

DS

# Decision Trees

*What is a decision tree?*

Decision trees are like the game “20 questions.” They make decision by answering a series of questions, most often binary questions. (yes or no) (cont.)



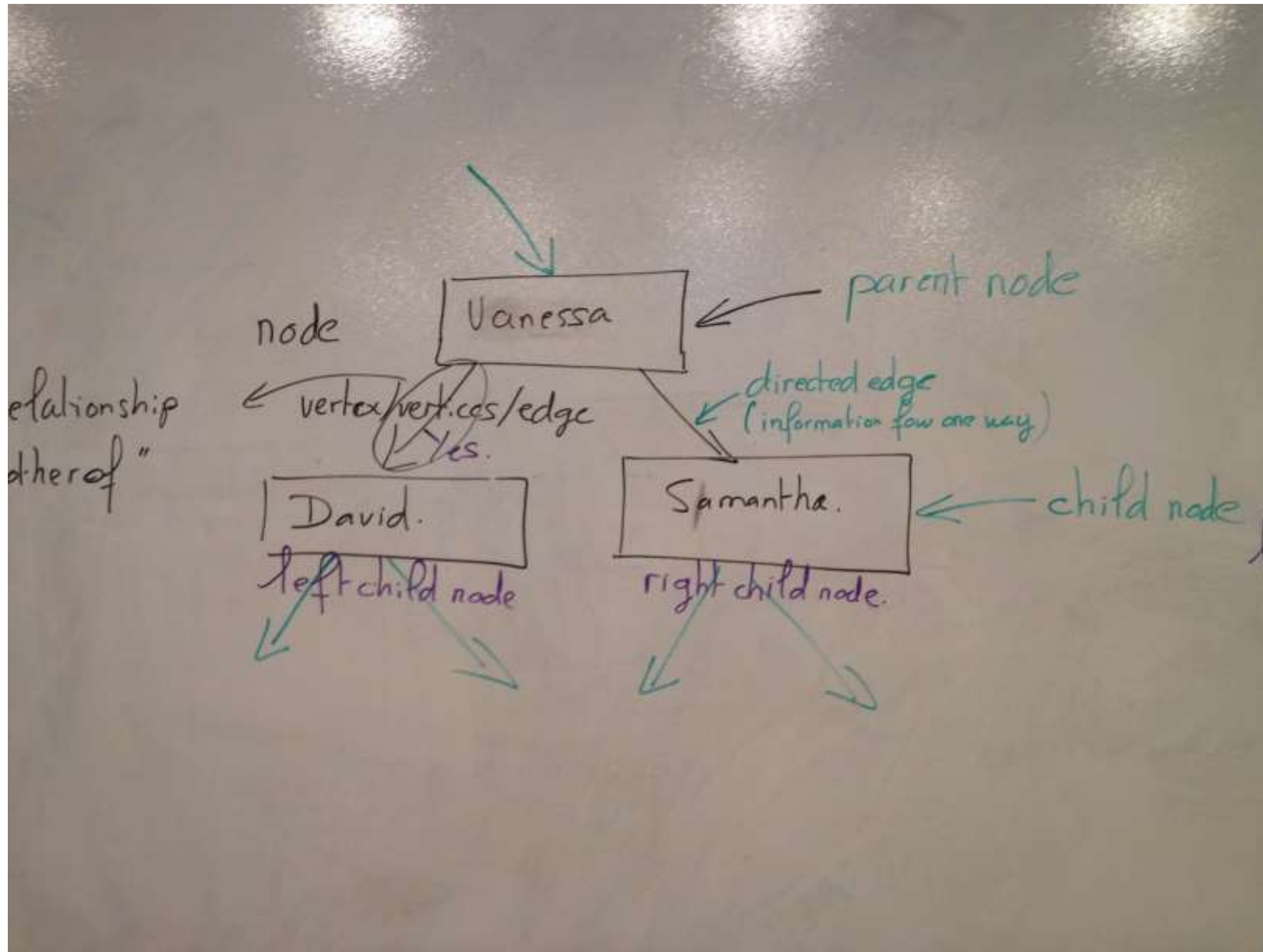
- ▶ We want the smallest set of questions to get to the right answer
- ▶ Each questions should reduce the search space as much as possible

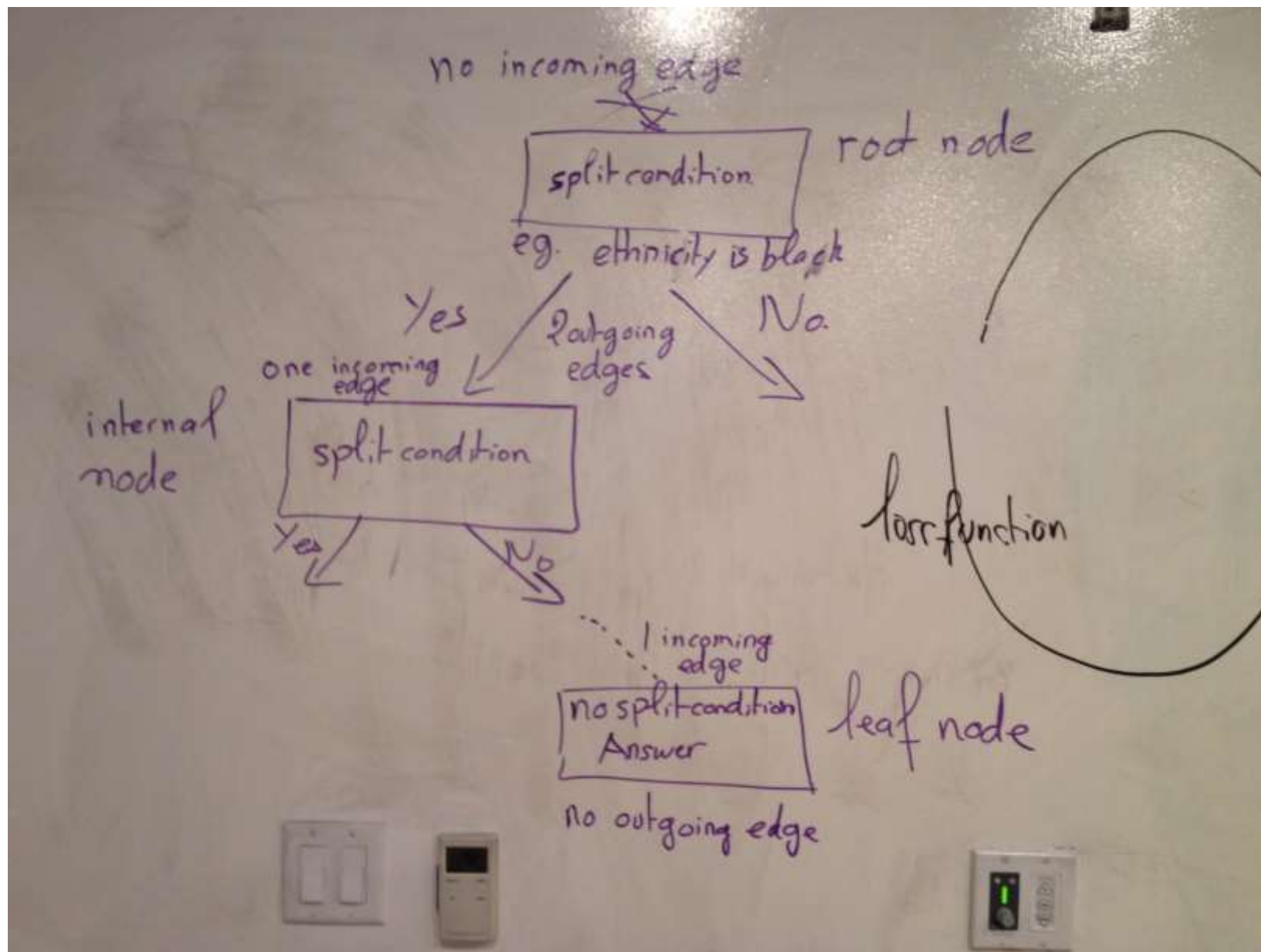
DS

# Decision Trees

*Structure*









DS

# Decision Trees

*Predicting*

predict ( features  
X matrix/vector ) :

set root node as current node.

$$x \leq a$$

evaluate split condition for current

while the current node using  $x$   
is not a leaf:

node

loop

if true:

set left child as current

else

set right child as current

return answer from leaf



DS

Using decision trees to make predictions is great but how do we build them in the first place?

# Open questions from the previous activity

- **❶** How to choose the split conditions? (variables and threshold values)
  - E.g., why is the threshold for African-American population set at 20%?
- **❷** How to choose the order of the conditions?
  - E.g., why is the first split on African-American population vs. the voters' education level?
- **❸** When to stop?
  - E.g., why didn't we include other factors such as voters' age?

Because it isn't computationally feasible to consider every possible partition of the feature space, we take a *top-down, greedy* approach known as recursive binary splitting

### **Top-Down**

- The approach begins at the top of the tree and then successively splits the predictor space; each split is indicated via two new branches further down on the tree

### **Greedy**

- At each step of the tree-building process, the *best* split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step

# Decision trees can be applied to both classification and regression problems

▸ We first consider classification problems to address ❷ (How to choose the order of the conditions?)

▸ We'll then move on to regression problems when addressing ❶ (How to choose the split conditions?)

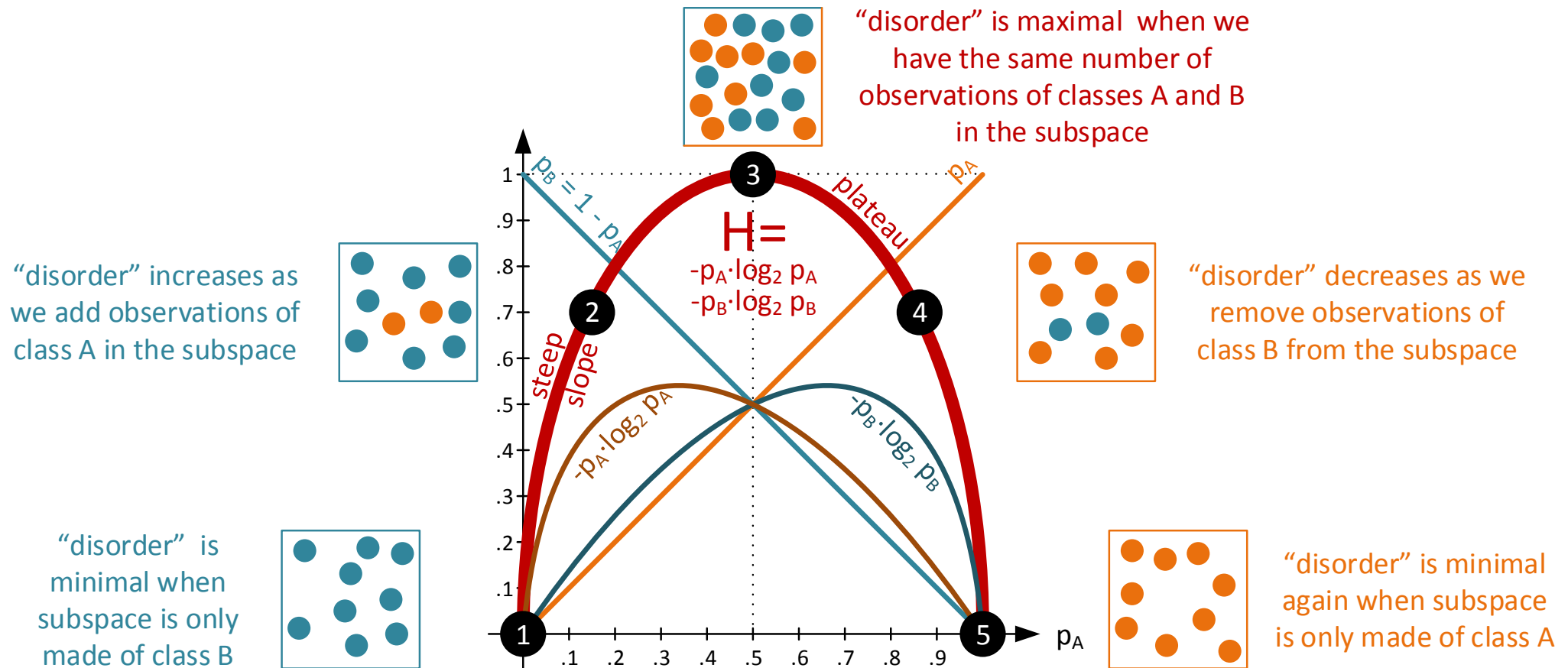


DS

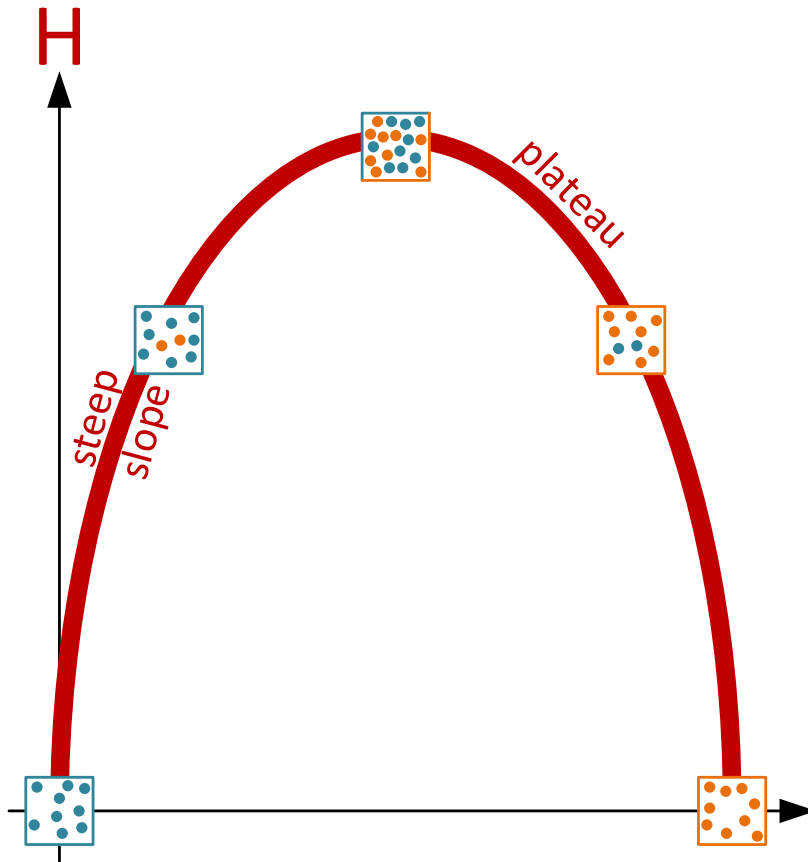
## ⑥ Build a Model

*Entropy*

# Entropy ( $H$ ) is a measure of disorder



# Entropy | What to remember



$$H = - \sum_{i=1}^k p_i \cdot \log_2(p_i)$$

( $p_i$  represents the proportion of observations in the region that are from the  $i^{\text{th}}$  class)

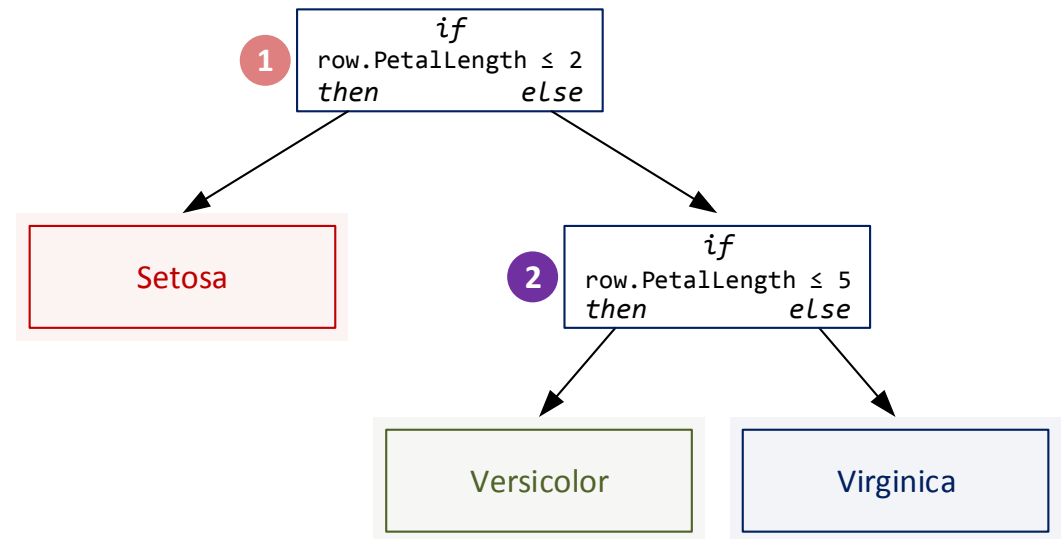
# Decision Trees

*Training a Classification Decision Tree*

② *How to choose the order of the conditions?*

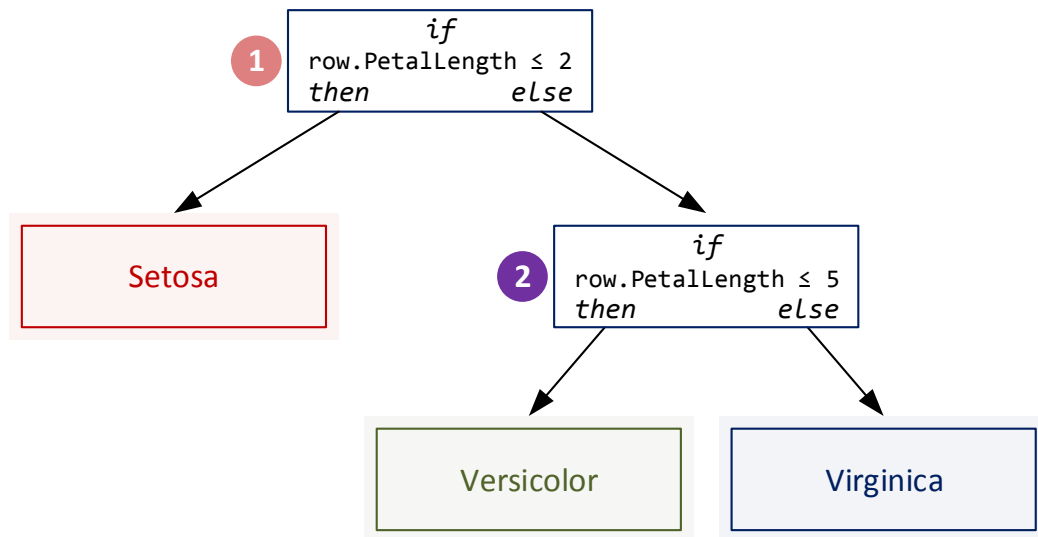
# Our first classifiers (session 8) are decision trees

```
def my_second_classifier(row):  
    if row.PetalLength <= 2:  
        return 'Setosa'  
    elif row.PetalLength <= 5:  
        return 'Versicolor'  
    else:  
        return 'Virginica'
```

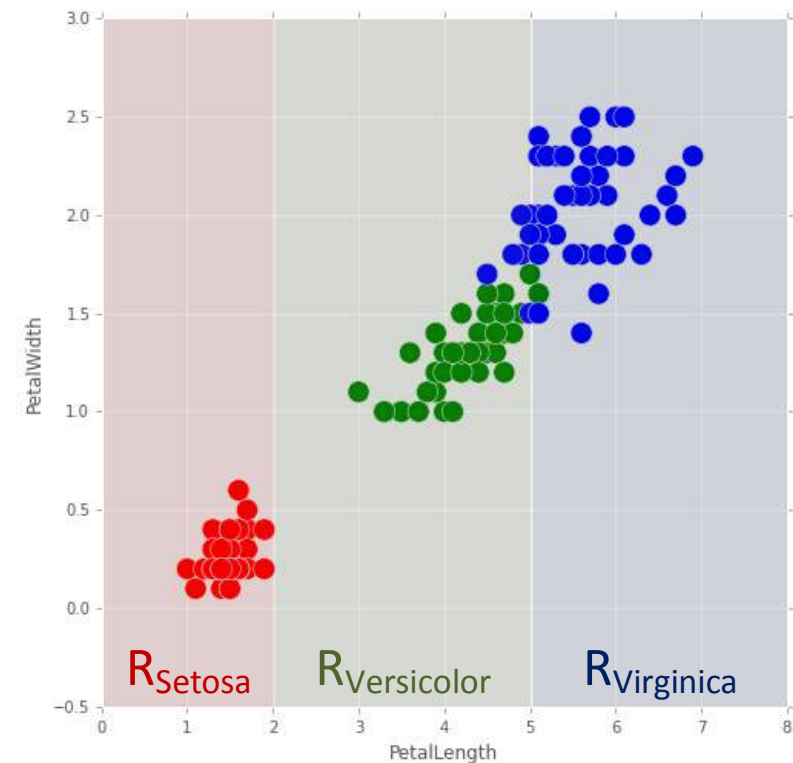


# Our first classifiers (session 8) are decision trees (cont.)

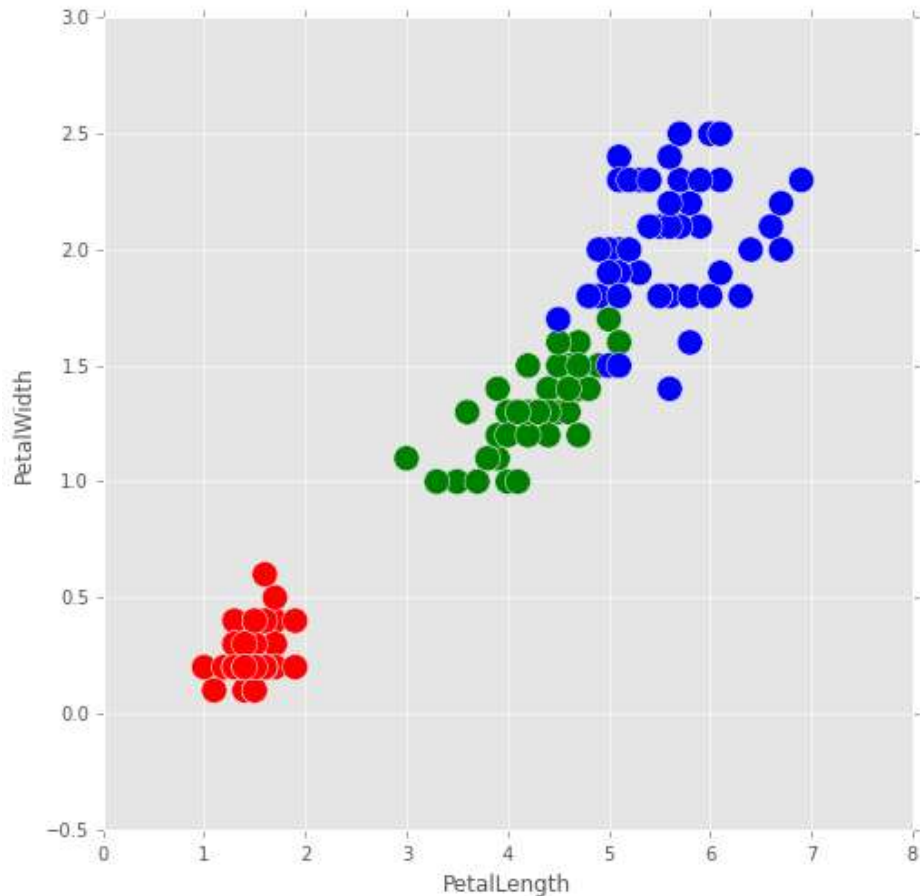
## Decision Tree



## Feature Space



❶ What's the entropy of the dataset/root node before the first split? What's your intuition of its level?



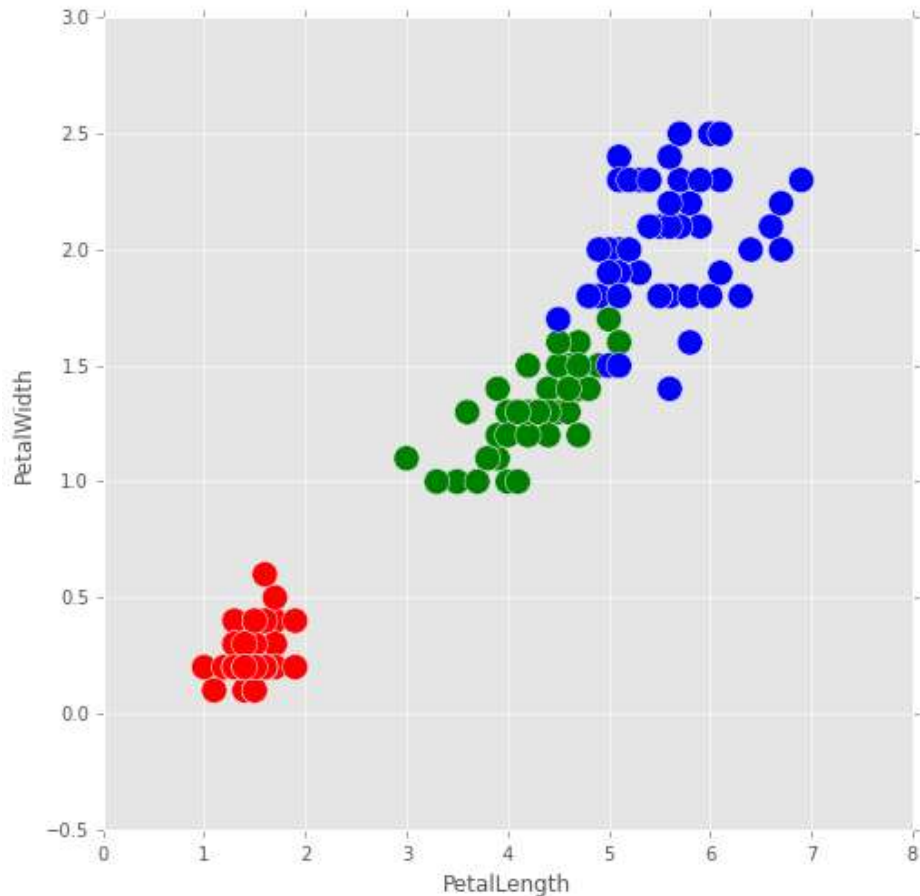
root node				
	red	green	blue	overall
$c_i$				
$p_i$				
$H$				

$$n = \sum_{i=1}^k c_i$$

$$p_i = \frac{c_i}{n}$$

$$H = - \sum_{i=1}^k p_i \cdot \log_2(p_i)$$

① The entropy of the dataset/root node is at the highest at 1.58; the intuition being that we have three classes in equal proportion



how much mess do we have in the root node

	root node			
	red	green	blue	total
$a_{\text{red, green, blue}}$	50	50	50	150 $n = \sum_i c_i$
$P_i$	$\frac{50}{150} = \frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	1 $P_i = \frac{c_i}{n}$

$H =$

- $P_{\text{red}} \times \log_2 P_{\text{red}}$
- $P_{\text{green}} \times \log_2 P_{\text{green}}$
- $P_{\text{blue}} \times \log_2 P_{\text{blue}}$

$$-\frac{1}{3} \log_2 \frac{1}{3} - \frac{1}{3} \log_2 \frac{1}{3} - \frac{1}{3} \log_2 \frac{1}{3}$$
$$-(3) \frac{1}{3} \log_2 \frac{1}{3} = -\log_2 \frac{1}{3} = \log_2 3 = 1.58$$

$H_{\text{before}}$

$\log_2 \frac{1}{a} = -\log_2 a$

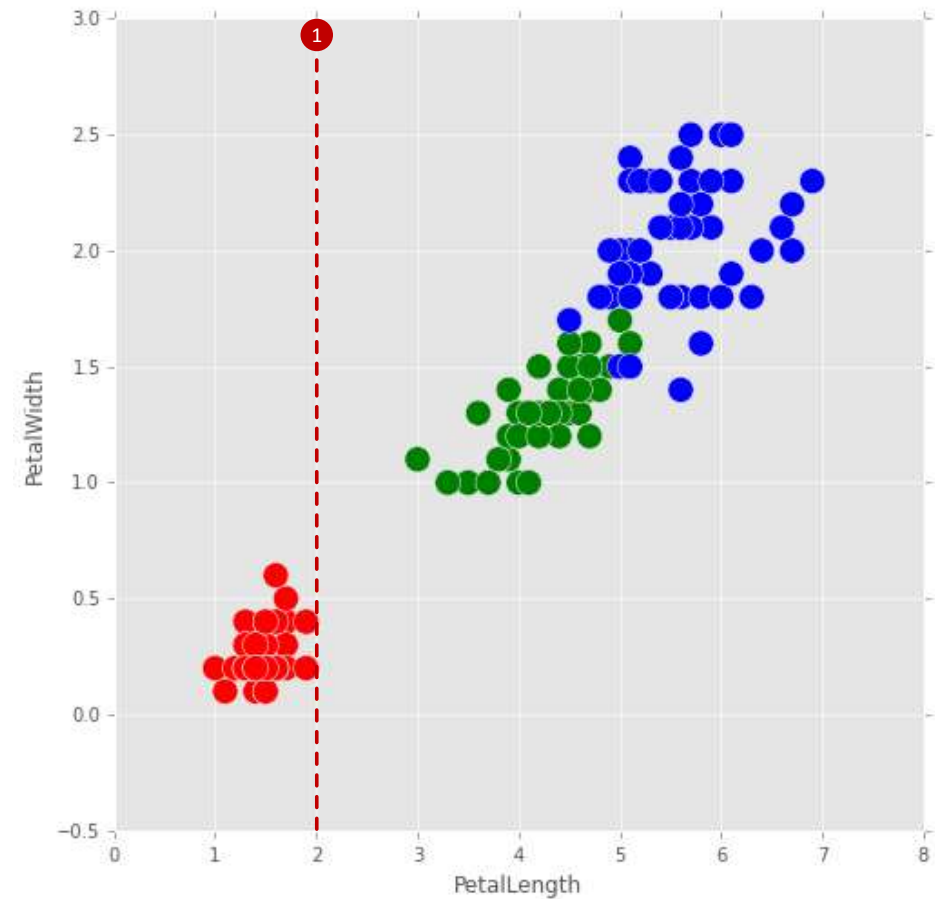


# ❶ What's the entropy after split 1? Intuition?

left node/lower subspace after split 1				
	red	green	blue	overall
$c_i$				
$p_i$				
$H_{left}$				

right node/higher subspace after split 1				
	red	green	blue	overall
$c_i$				
$p_i$				
$H_{right}$				

overall after split 1	
$H_{after}$	
$IG$	



The information gain is significant at .918. The subspace on the left is pure (0 entropy) bringing down significantly the weighted average entropy after the split

split 1

	R	G	B	total
left node	50	0	0	50
P <sub>i</sub>	1	0	0	1
H	$-1 \log_2 1 - 0 \log_2 0 - 0 \log_2 0 = 0$			

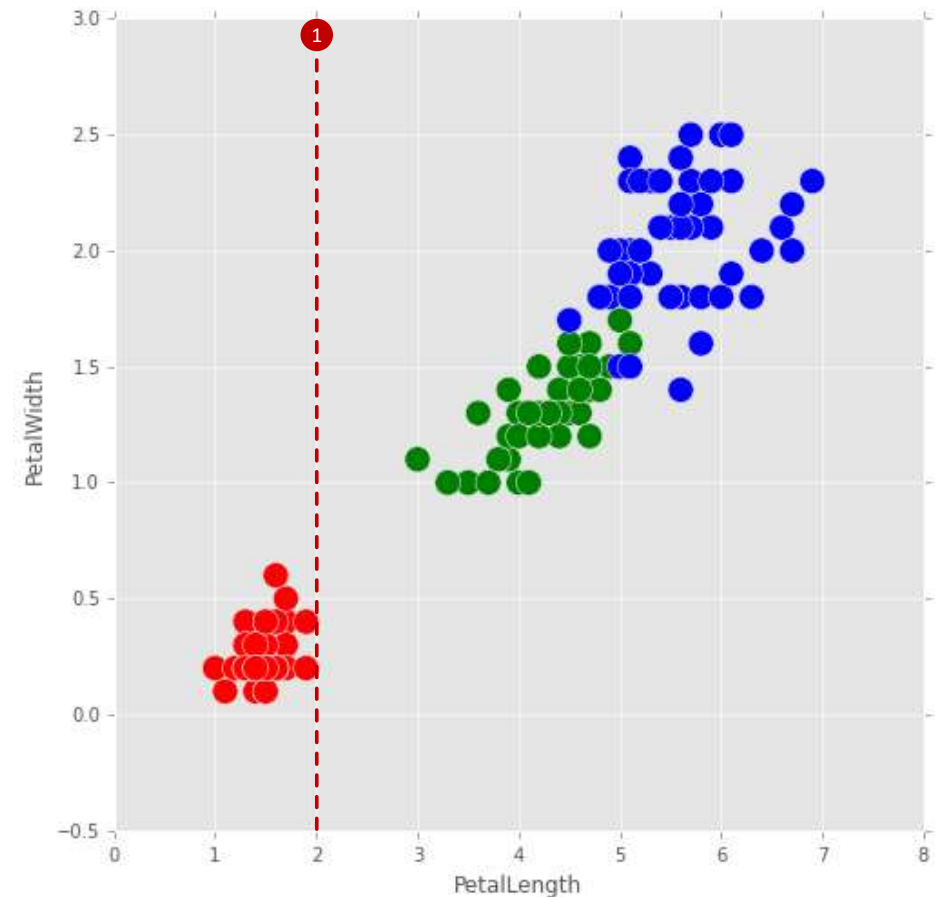
	R	G	B	total
right node	0	50	50	100
P <sub>i</sub>	0	1/2	1/2	1
H	$-0 \log_2 0 - \frac{1}{2} \log_2 \frac{1}{2} - \frac{1}{2} \log_2 \frac{1}{2}$ $= (1/2)(-\log_2 \frac{1}{2}) - \log_2 \frac{1}{2}$ $= \log_2 2 = 1$			

1.58

$$H_{after} = \frac{50}{150} \times 0 + \frac{100}{150} \times 1$$

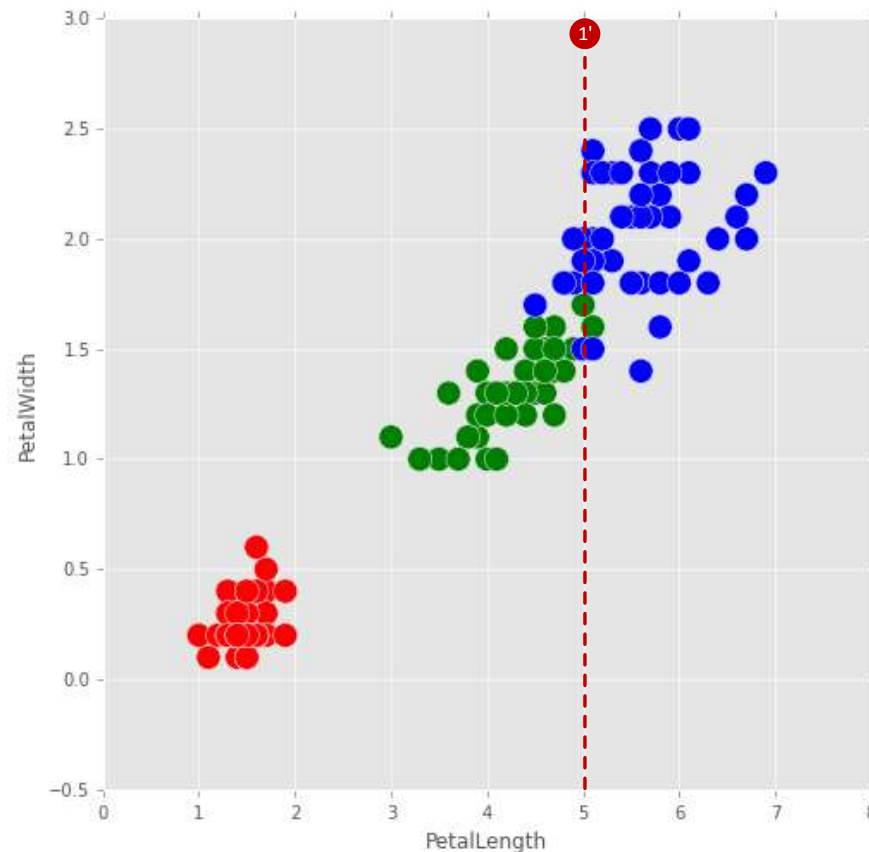
$$= \frac{2}{3} = 0.667$$

$$IG = H_{before} - H_{after}$$

$$= 1.58 - 0.667 = 0.918$$


Activity | ② What's the entropy after split 1'? Intuition? (Note: 9 "blues" on the left, 1 "green" on the right)

EXERCISE



left node after split 1'

	red	green	blue	overall
$c_i$				
$p_i$				
$H_{left}$				

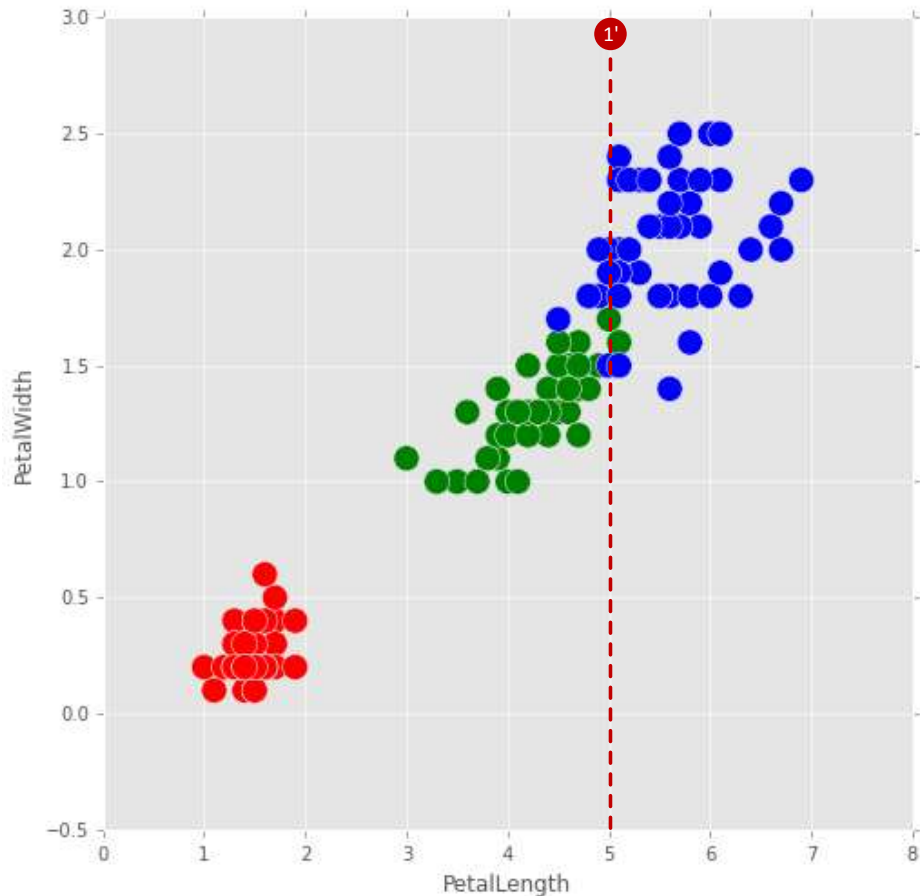
right node after split 1'

	red	green	blue	overall
$c_i$				
$p_i$				
$H_{right}$				

overall after split 1'

$H_{after}$				
$IG$				

The information gain for split 1' is modest at .582 and less than split 1's. Split 1 wins



split 1'

node	red	green	blue	total
left node	50	49	9	108
right node	0	1	41	42

$P: \frac{50}{108} = .463 \quad \frac{49}{108} = .454 \quad \frac{9}{108} = .0833$   
 $H = .463 \log_2 .463 + .454 \log_2 .454 + .0833 \log_2 .0833 = 1.33$

$H_{\text{right}} = \frac{0}{42} \log_2 \frac{0}{42} + \frac{1}{42} \log_2 \frac{1}{42} + \frac{41}{42} \log_2 \frac{41}{42} = .162$

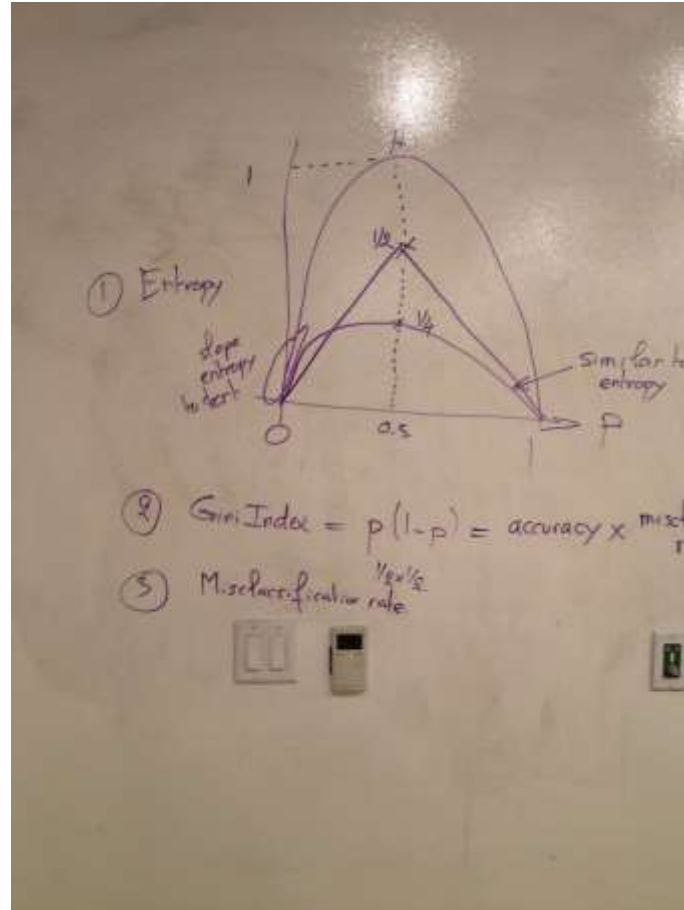
$H_{\text{after}} = \frac{108}{150} (1.33) + \frac{42}{150} (.162) = 1$

$IG = H_{\text{before}} - H_{\text{after}} = 1.58 - 1 = .0582$   
 $< .918 \text{ (split 1)}$

# Most common occurring class

- In practice, we don't expect each terminal region to hold a single class
- Instead, we predict that each observation belongs to the most commonly occurring class of training observations in the region to which it belongs

# Other measures | Gini index and misclassification rate



DS

## ⑥ Build a Model

*Classification and Regression Decision Trees*

# Commonalities and differences between classification and regression decision trees

- Just as in the classification setting, we use recursive binary splitting to grow a regression tree

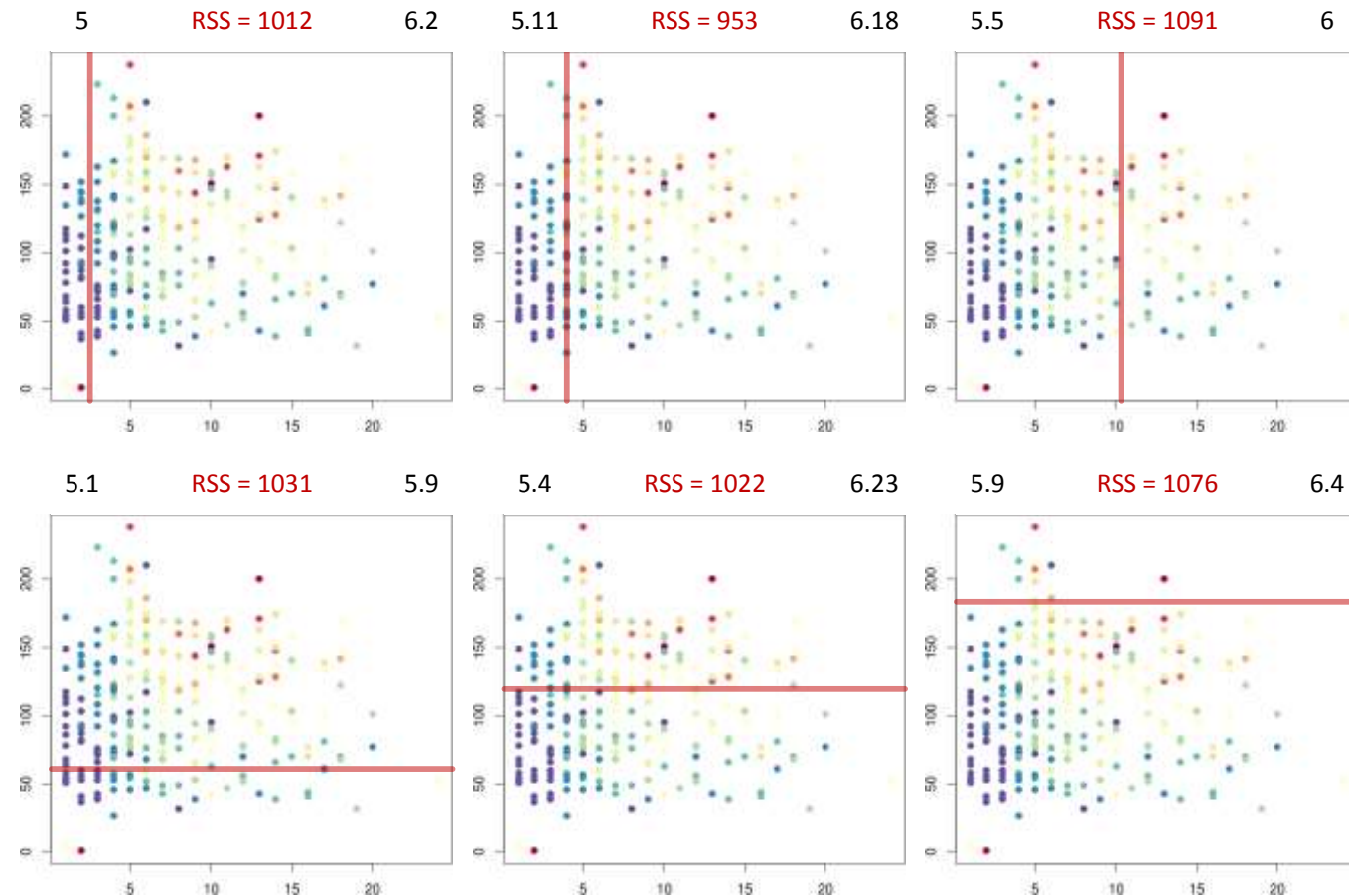
- For every observation that falls into the region  $R_j$ , we make the prediction  $\hat{y}_{R_j}$ , which is the mean of the response values for the training observations in  $R_j$

- In the regression setting, we cannot use entropy for making the binary splits. A natural alternative to  $H$  is RSS (residual sum of squares)

$$\sum_{j=1}^J \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$



We first select the feature and the cutpoint such that splitting the feature space into the regions  $\{x \mid \text{feature} \leq \text{cutpoint}\}$  and  $\{x \mid \text{feature} > \text{cutpoint}\}$  leads to the greatest possible reduction in RSS



Source: The Elements of Statistical Learning

# Top-down greedy approach (a.k.a., recursive binary splitting)

- Once the first cut is made, we recursively repeat the process in the two previously identified regions

- For *regression* trees, we would be looking for the best predictor and the *best cutpoint* in order to split the data further so as to minimize the *RSS* within each of the resulting regions

- For *classification* trees, we would be looking for the best predictor and the *highest* information gain in order to split the data further so as to minimize the *entropy* within each of the resulting regions

DS

# Decision Trees

*Pros and Cons*

# Decision Trees | Pros and cons

## ▸ Pros

- Trees are very easy to explain to people. They are even easier to explain than linear regression
- Decision trees more closely mirror human decision-making than do the regression and classification methods seen so far
- Trees can be displayed graphically and are easily interpreted even by non-experts
- Trees can easily handle qualitative predictors without the need to create binary variables

## ▸ Cons

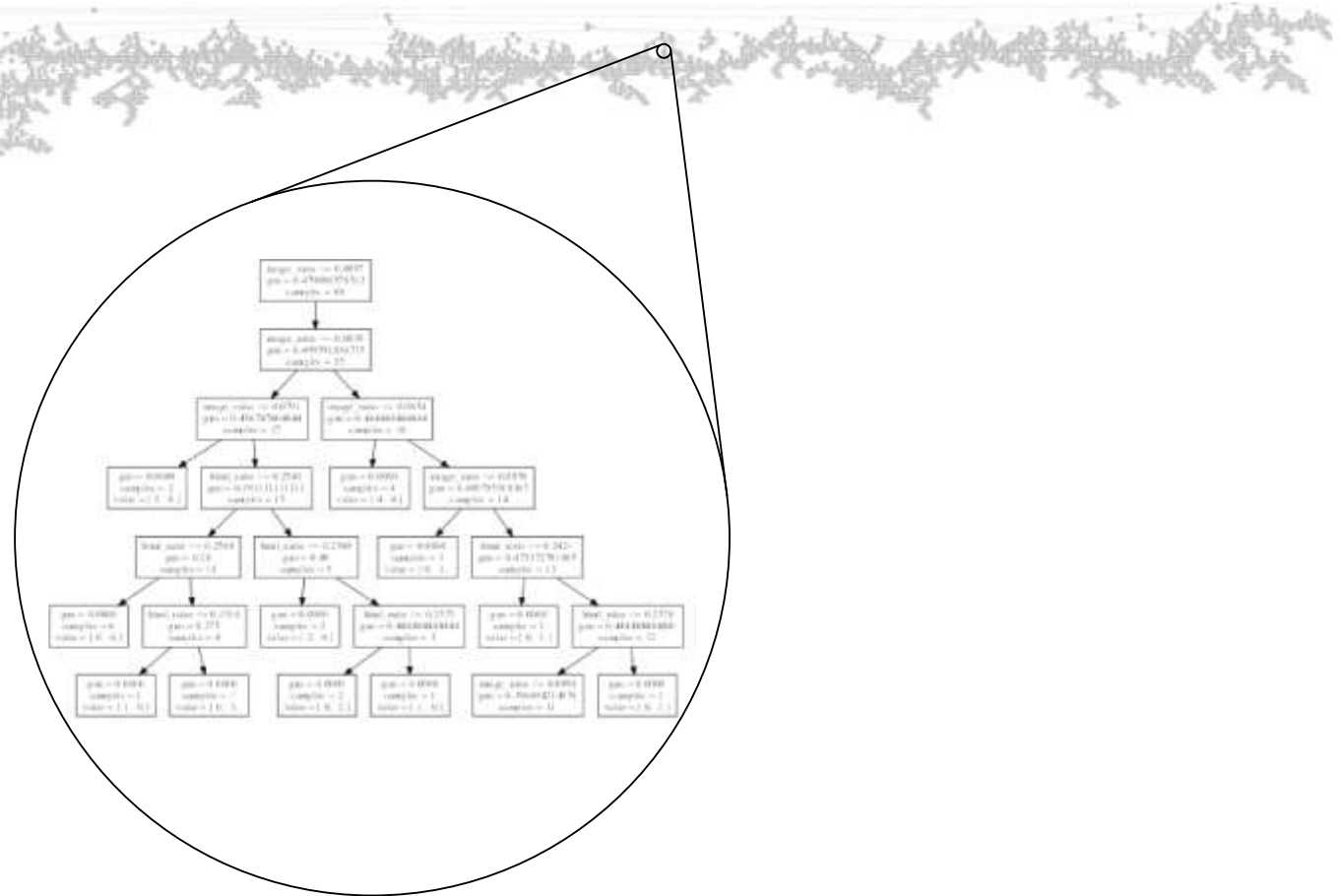
- Trees do not generally have the same level of predictive accuracy as some of the other regression and classification methods seen so far. However, by aggregating many decision trees, the predictive performance of trees can be substantially improved

DS

## ⑥ Build a Model

*Overfitting*

# An unconstrained decision tree can learn an extreme tree (e.g., below)



# Overfitting

- Decision trees tend to be weak models because they can easily memorize or overfit to a dataset
  - A model is overfit when it memorizes or bends to a few specific data points rather than picking up general trends in the data
- We can limit our decision trees using a few methods
  - Limit the number of questions (nodes) a tree can have
  - Limit the number of samples in the leaf nodes

A black circle containing the white text "DS".

DS

How can we avoid overfitting  
and increase predictability?

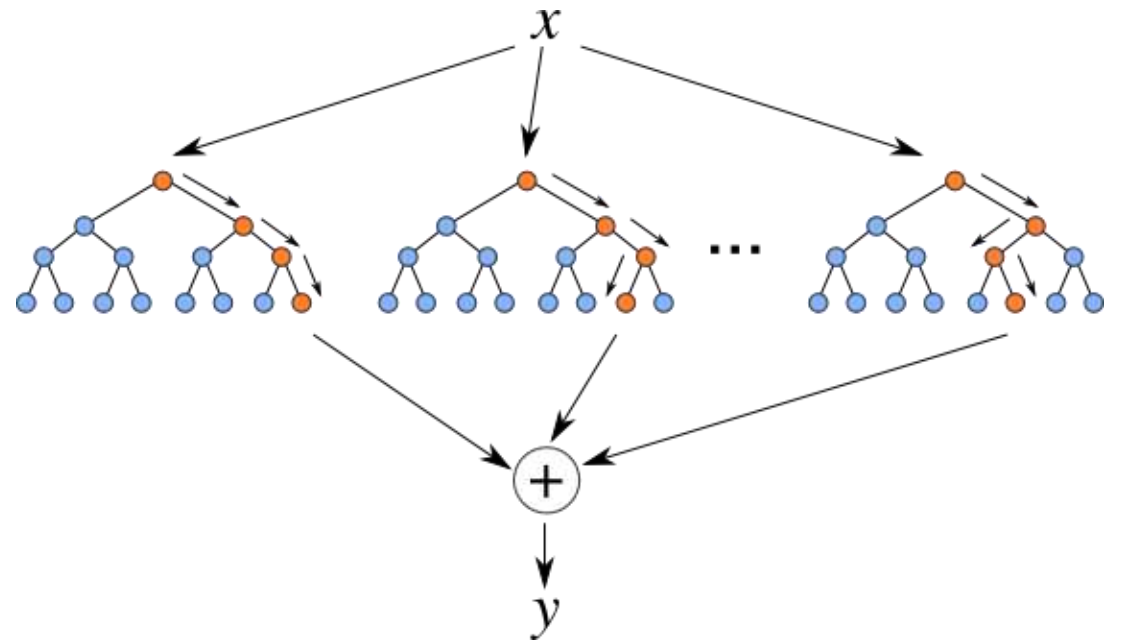


DS

# Random Forests

# Random forests are an *ensemble* or collection of individual decision trees

- ▶ Random forest models are one of the most widespread classifiers used
- ▶ They are relatively simple to use and help avoid overfitting



A black circle containing the white text "DS".

DS

# Random Forests

*Pros and Cons*

# Random Forests | Pros and cons

## ▸ Pros

- Easy to tune
- Built-in protection against overfitting
- Non-linear
- Built-in interaction effects

## ▸ Cons

- Slow
- No “coefficients”
- Black-box
- Harder to explain

A black circle containing the white text "DS".

DS

# Random Forests

*Training*

# Training a Random Forest

- Training a random forest model involves training many decision tree models
  - Since decision trees easily overfit, we use many decision trees together and randomize the way they are created
- Random Forest Training Algorithm
    - Take a bootstrap sample (random sample) of the dataset
    - Train a decision tree on the bootstrap sample
    - For each split/feature selection, only evaluate a *limited* number of features to find the best one
    - Repeat this for a number of trees

A black circle containing the white text "DS".

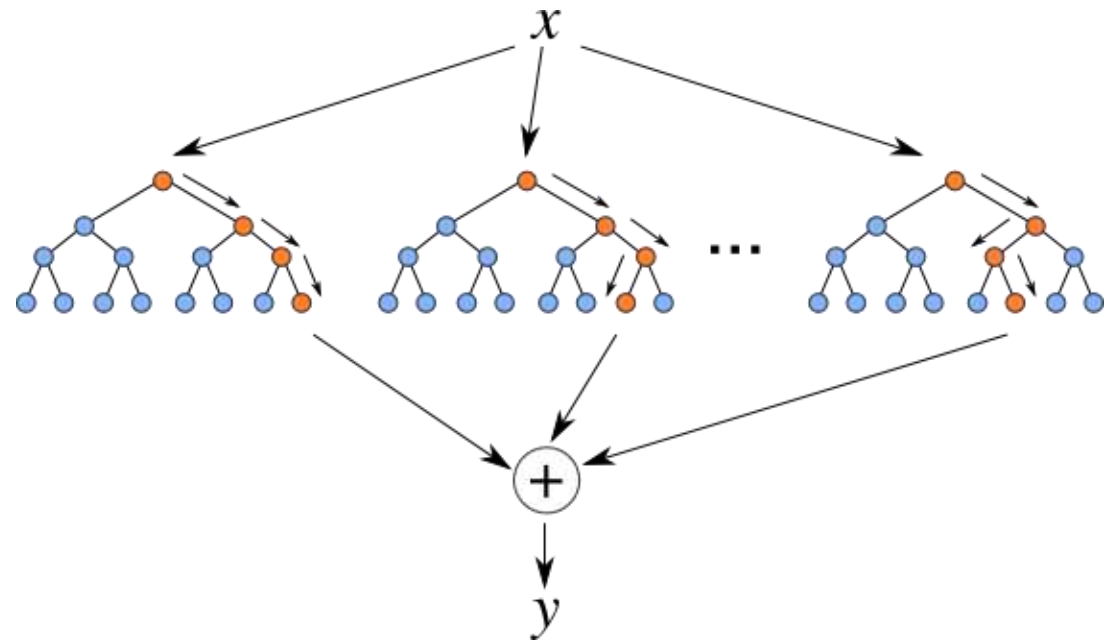
DS

# Random Forests

*Predicting*

# Predicting using a Random Forest

- Predictions for a random forest model come from each decision tree
- Make an individual prediction with each decision tree
- Combine the individual predictions and take the majority vote







# Lab

*Decision Trees and Random Forests*

A black circle containing the white text "DS".

DS

# Review

# Review

- What are decision trees?
- What does training involve?
- What are some common problems with decision trees?
- What are random forests?
- What are some common problems with random forests?

The logo consists of a solid black circle containing the white, bold, sans-serif letters "DS".

**DS**

Q & A



**DS**

# Before Next Class

# Before Next Class

Before the next lesson, you should already be able to:

- Experience with *sklearn* classifiers, specifically random forests and decision trees
- Install the Python package spacy with `conda install spacy`
- Run the spacy download data command with `python -m spacy.en.download --force all`

# Next Class

*Natural Language Processing and Text Classification*

# Learning Objectives

After the next lesson, you should be able to:

- Define natural language processing
- List common tasks associated with
  - Use-cases
  - Tokenization
  - Stemming and lemmatization
  - Tagging and parsing
- Demonstrate how to classify text or documents using scikit-learn





DS

# Exit Ticket

*Don't forget to fill out your exit ticket [here](#)*

Slides © 2016 Ivan Corneillet Where Applicable  
Do Not Reproduce Without Permission