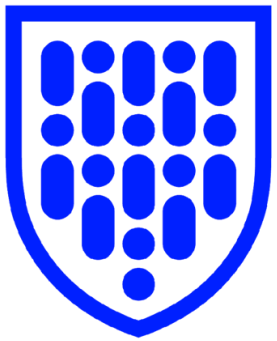

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2024

Data Science and AI

Module 7 Part 1

Decision Trees and Ensemble Methods

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Agenda: Module 7

- Overview
- Decision Trees
- Random Forests
- Ensemble Methods
    - Introduction – Bias vs Variance
    - Bagging
    - Boosting
    - Stacking

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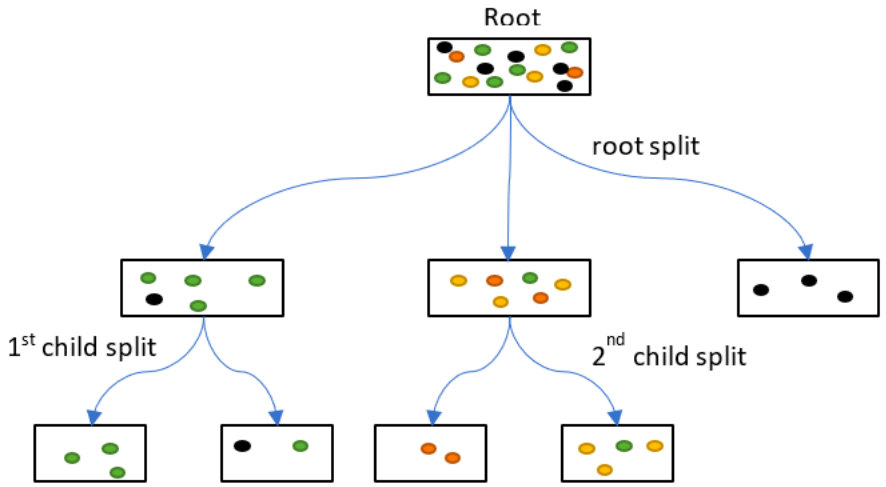
Decision Trees

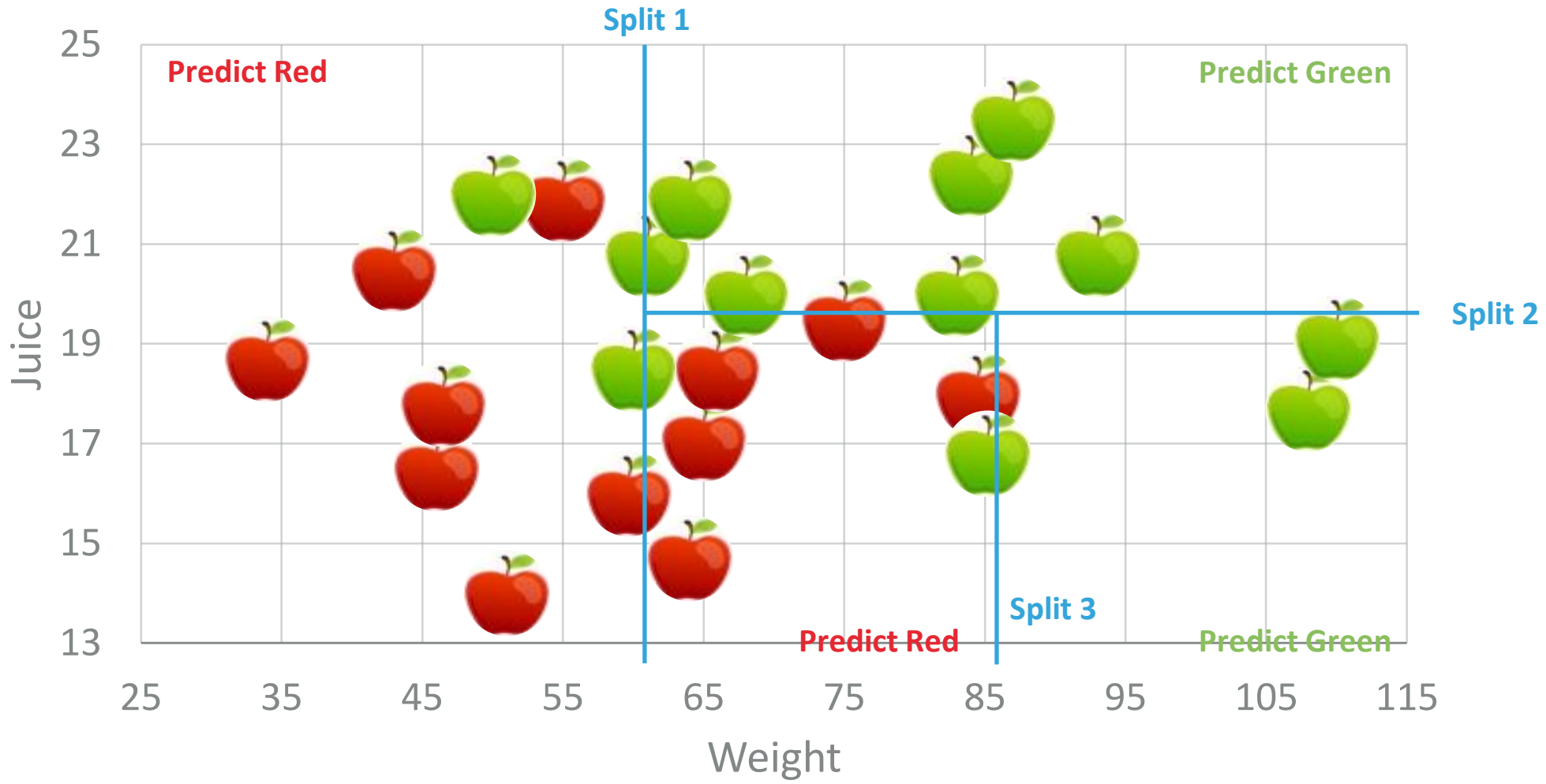
- A type of **supervised** Machine Learning algorithm.
- It is one of the **most widely used** and practical methods for classification. It is the **simplest** and yet the **most powerful** algorithm!
- A decision tree is a tree in which each branch node represents **a choice between a number of alternatives**, and each **leaf node** represents an **outcome**.
- The type of the **target variable** defines the type of Decision Tree
  - **Categorical** variable Decision Tree: Has categorical target variable
  - **Continuous** variable Decision Tree: Has continuous target variable

Constructing Decision Trees

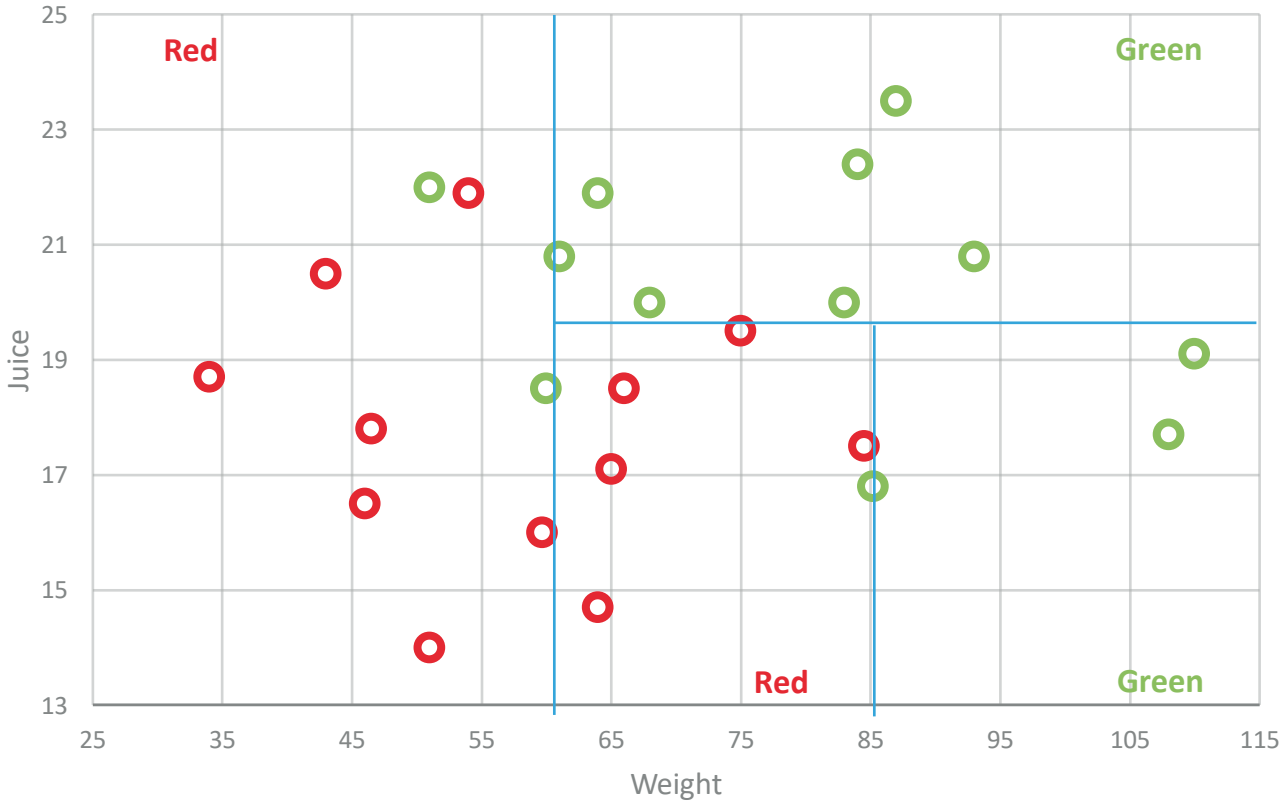
- The approach is to: **Iteratively** separate data into **homogeneous groups**
  - Split data by category or range, **one feature at a time**
  - Into groups as **pure** as possible
  - repeating the process until a certain stop condition is reached

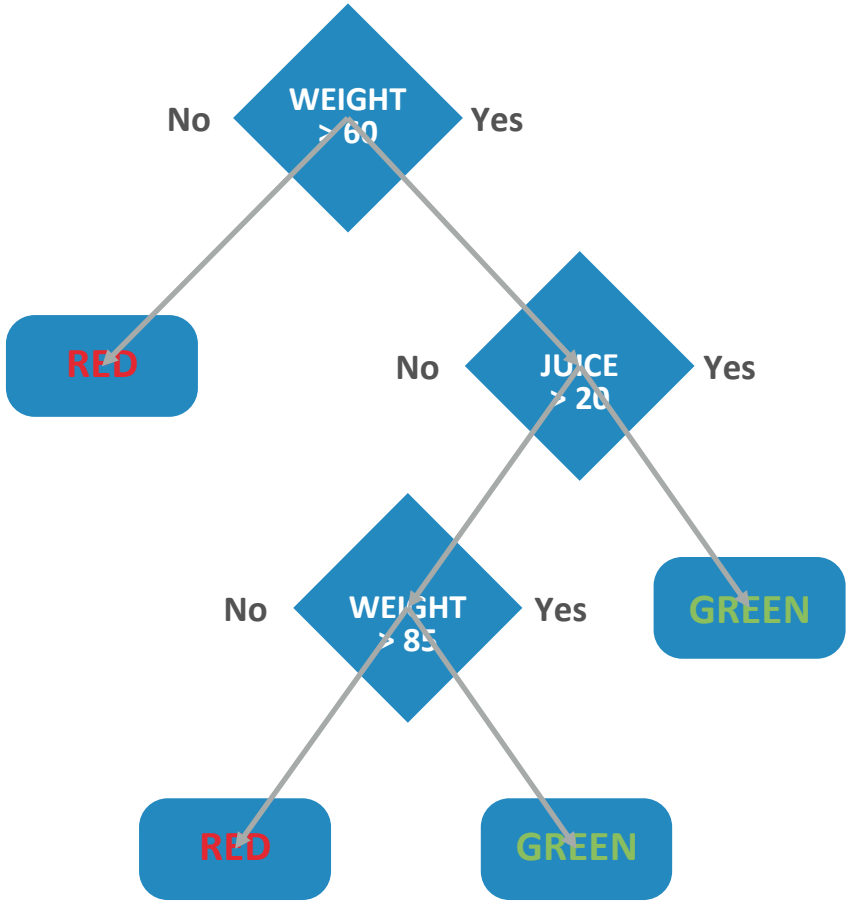


Iteratively separate data into homogeneous groups



Mapping the Decision Tree





Constructing Decision Trees - Example 2

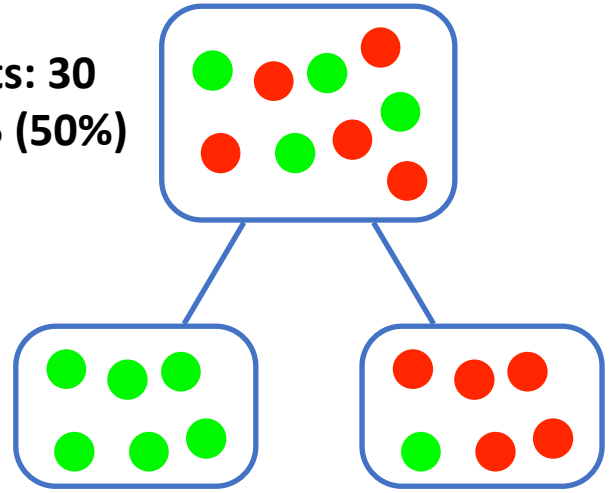
- Given 30 students with variables **Gender** (Boy, Girl), **Height** (5-6 ft) and **Class**(A, B). 15 out of these 30 play cricket in their leisure time. **Predict** who plays cricket during leisure period?
- Need to separate students who play cricket in their leisure time based on the most **highly significant** input variable among all three (gender, height, class).
- Decision Tree separates students based on all values of the three variables and identifies the variable, which creates **the most homogeneous** sets of students (heterogeneous to each other).
- Decision tree identifies the **most significant variable** and its value which gives the most homogeneous sets of population.

Constructing Decision Trees - Example 2

- The variable Gender can identify the **most homogeneous** sets compared to the other two variables

Split by Gender

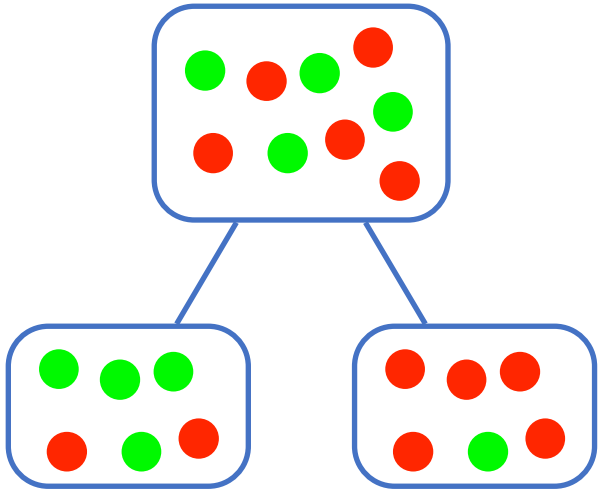
Students: 30
Play: 15 (50%)



Female
Students: 10
Play: 2 (20%)

Male
Students: 20
Play: 13 (65%)

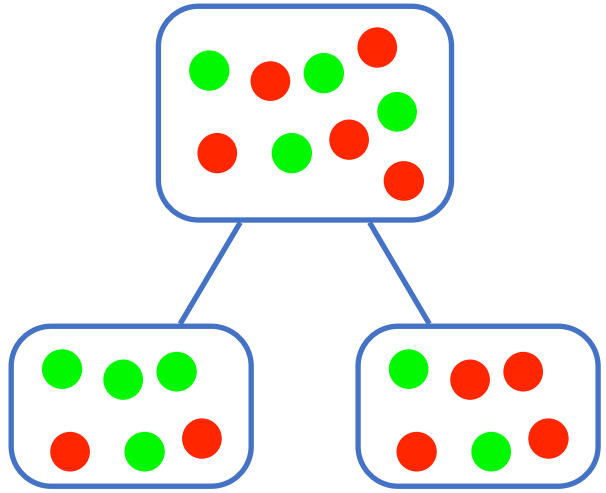
Split by Height



< 5.5 ft
Students: 12
Play: 5 (42%)

>= 5.5 ft
Students: 18
Play: 10 (56%)

Split by Class

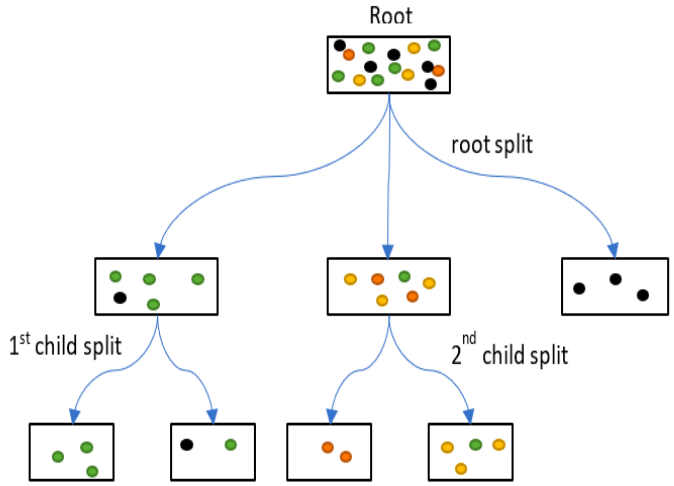


Class A
Students: 14
Play: 6 (43%)

Class B
Students: 16
Play: 9 (56%)

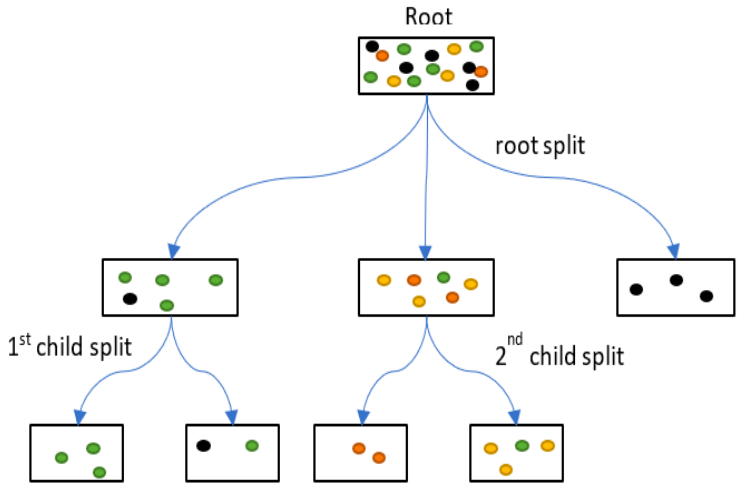
Terminology

- Root Node: Represents all the data and gets divided into two or more homogeneous sets
- Splitting: Process of dividing a node into two or more sub-nodes
- Decision Node: When a sub-node splits into further sub-nodes
- Leaf or Terminal Node: Nodes that do not split



Terminology

- Pruning: Remove of sub-nodes of a decision node
- Branch or Sub-Tree: A subsection of the entire tree
- Parent Node: A node divided into sub-nodes is the parent of those sub-nodes
- Child Node: Sub-nodes resulting of a node division are children of such node



Constructing Decision Trees - Greedy Decision Tree Learning

1. Start with an ***empty*** tree

2. Select a ***feature*** to split the data

    - (Look for the feature that gives the ***smallest classification error***)

3. For ***each split*** of the tree

    - If reached ***stop condition*** (purity, # elements, depth)
      then make predictions

    - Otherwise, go to 2. and continue recursively on this ***split***

Advantages of Decision Trees

- **Less data cleaning required**: it can deal with **categorical features** directly without encoding and is not confused too much by **outliers** and **missing values** to a fair degree.
- Non-Parametric Method: Have **no assumptions on space distribution** and classifier structure.
- **Easy to Understand**: It does not require any statistical knowledge to read and interpret.
- Its **graphical representation is very intuitive**, and users can easily relate their hypothesis.
- **Useful in Data Exploration**: Good way to identify the most significant variables and their relations;
- Can help to identify the most **significant variable** when working with hundreds of them.

Disadvantages of Decision Trees

- **Overfitting**: One of the most practical difficulty for decision tree models.Decision-tree can create **over-complex** trees that do not generalise the data well.
- Decision trees can be **unstable** as small variations in the data may result in a completely different tree being generated.
- Some concepts **are hard to learn** because decision trees do not express them easily, such as the XOR concept.
- Decision tree learners create **biased trees** if some classes dominate. Hence it is recommended to **balance** the dataset prior to fitting with the decision tree.

Decision Tree Algorithms (most common)

- CART (Classification And Regression Tree)
- **ID3** (Iterative Dichotomiser 3)
- **C4.5** (Successor of ID3)
- CHAID (CHi-squared Automatic Interaction Detector): Multi-level splits are performs for classification trees
- Conditional Inference Trees: This method results in unbiased feature selection and does not require pruning, being based on a statistical approach using non-parametric tests to split and to avoid overfitting
- MARS: Multivariate Adaptive Regression Splines

Splitting strategies

- The decision of how to **split nodes** affects a tree's accuracy heavily
- Decision Trees use different **algorithms** to decide to split a node into two or more sub-nodes
- The sub-nodes are required to be **more homogeneous**. i.e. The purity of the node increases in relation to the **target variable**
- Decision trees pick the split that results in the **most homogeneous** sub-nodes after calculating splits on **all available variables**.
- Common splitting strategies
  - **GINI**
    - The Gini index indicates the **degree of heterogeneity**. The higher the value of Gini, the higher the heterogeneity. (i.e. Gini = 0 means fully homogeneous)
  - **Information gain**
    - It chooses the split which has the lowest **entropy** (degree of disorder) compared to the parent node and other splits

Using decision trees in Scikit Learn

- Scikit-learn **DecisionTreeClassifier** is a class capable of performing multi-class classification on a dataset.
- Decision tree class works **the same as other classifiers** by taking a set of features and target variable.
- It does not require complex data preparation as it can deal with **categorical variables**, **missing data** and **outliers**. However, cleaning the data does not hurt and will help in improving results. Especially if you are going to use decision trees side by side with other models.
- Once trained, you can **plot the tree** with the plot_tree function.
- Note that the default values for the parameters controlling the size of the trees (e.g. max_depth, min_samples_leaf, etc.) lead to **fully grown and unpruned trees**. On some data sets these can be very large. The complexity and size of the trees should be controlled by setting those hyperparameter values.

Decision Trees hyperparameters

- **criterion** : string, optional (default=”gini”)
  - The function to measure the quality of a split. Supported criteria are “gini” for the Gini impurity and “entropy” for the information gain.
- **max_depth** : int or None, optional (default=None)
  - The maximum depth of the tree. If None, then nodes are expanded until all leaves are pure or until all leaves contain less than min_samples_split samples.
- **min_samples_split** : int, float, optional (default=2)
  - The minimum number of samples required to split an internal node
- **max_leaf_nodes** : int or None, optional (default=None)
  - Grow a tree with max_leaf_nodes in best-first fashion. Best nodes are defined as relative reduction in impurity. If None then unlimited number of leaf nodes.
- **class_weight** : dict, list of dicts, “balanced” or None, default=None
  - Weights associated with classes in the form {class_label: weight}. If not given, all classes are supposed to have weight one.

Decision trees - Summary

- Decision tree is one of the **most widely used** and **practical** supervised learning algorithm.
- Motivations for using decision trees include:
  - **Less data cleaning required**
  - **Easy to Understand and explain**
- However, decisions trees tend to **overfit** training data without the appropriate hyperparameters tuning

Lab 7.1.1: Decision Trees

- Purpose
  - Practice with Decision Tree Modelling
  - Practice coding in Python

- Resources
  - Your skills and resourcefulness

- Material
  - Jupyter Notebook (Lab-7_1_1)

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Random Forests

- Overview
- Algorithm
- Pros and Cons

Random Forest Overview

- Random Forest is a learning approach that uses an **ensemble** method for regression and classification.
- It uses "**Bagging**" (aka bootstrapping) where a set of relatively weak learners are combined to create a stronger learner. These techniques sample the training dataset with **replacement** and train a model of each subset then aggregate these models.
- Constructs a **large list of uncorrelated decision trees** at training time and chooses the **mean** prediction (regression) or the **mode** label of the classes (classification) of the individual trees.
- Random decision forests address the tendency of decision trees to **overfit** on the training data.

Random Forest Algorithm

- Let ***N*** be the number of cases in the training set
  - A random sample of ***N*** with replacement is the training set for growing the tree

- Let ***M*** be the number of input variables
  - Specify a number ***m < M*** such that at each node, ***m*** variables are randomly selected from ***M***
  - Use ***m*** to split the node. While the forest grows the value of ***m*** is held constant

- Trees grow to their terminal nodes without pruning

- Makes a prediction of data by aggregating the predictions of the n-tree trees (i.e., the majority votes for classification, the average for regression)

Random Forest Pros

- Can handle large datasets with **higher dimensionality**
  - Can identify most significant variables, so it is considered as one of the dimensionality reduction methods.
  - The model outputs the importance of variables
- Smaller prediction **variance** and therefore usually a **better general performance**.
- Keeps accuracy when a large fraction of the data are **missing**
- Has methods for balancing errors in datasets where classes are imbalanced
- Can solve both classification and regression problems

Random Forest Cons

- A **black box** approach for statistical modellers
  - Almost no visibility of what the model does

- Not as good for **regression** problems as it does not give precise, continuous nature predictions
  - In case of regression, it does not predict beyond the range in the training data, and that they may overfit datasets that are particularly noisy

Random Forest hyperparameters

- **n_estimators** : integer, optional (default=100)
  - The number of trees in the forest.
- **criterion** : string, optional (default="gini")
  - The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain.
- **max_depth** : int or None, optional (default=None)
  - The maximum depth of the tree. If None, then nodes are expanded until all leaves are pure or until all leaves contain less than min_samples_split samples.
- **min_samples_split** : int, float, optional (default=2)
  - The minimum number of samples required to split an internal node
- **max_leaf_nodes** : int or None, optional (default=None)
  - Grow a tree with max_leaf_nodes in best-first fashion. Best nodes are defined as relative reduction in impurity. If None then unlimited number of leaf nodes.
- **class_weight** : dict, list of dicts, "balanced" or None, default=None
  - Weights associated with classes in the form {class_label: weight}. If not given, all classes are supposed to have weight one.

Lab 7.1.2: Random Forests

- Purpose
  - Practice with Decision Random Forests
  - Practice coding in Python

- Resources
  - Your skills and resourcefulness

- Material
  - Jupyter Notebook (Lab-7_1_2)

Questions?

Appendices

Common splitting algorithms: Gini Index

- The Gini index indicates the **degree of homogeneity**. The higher the value of Gini, the higher the homogeneity.
- Gini is used only for Binary splits
- Steps to calculate Gini for a split
  - Calculate Gini for sub-nodes, using the **Sum of Square of probability for success and failure**

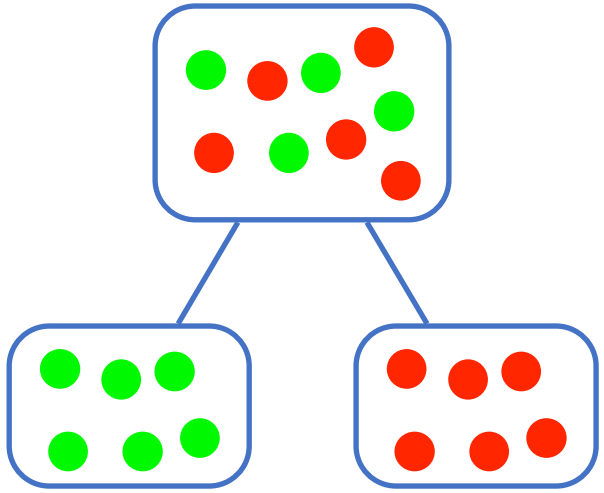
$$p^2 + q^2$$

  - Calculate Gini for split using weighted Gini score of each node of that split

Common splitting algorithms: Gini Index

Students: 30
Play: 15 (50%)

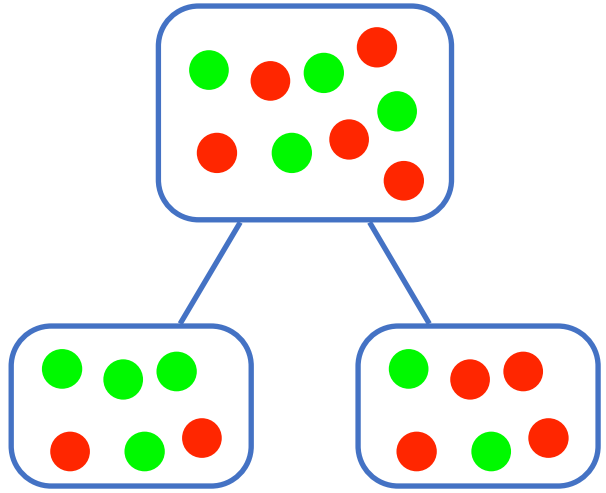
Split by Gender



Female
Students: 10
Play: 2 (20%)

Male
Students: 20
Play: 13 (65%)

Split by Class



Class A
Students: 14
Play: 6 (43%)

Class B
Students: 16
Play: 9 (56%)

Common splitting algorithms: Gini Index

- Split on Gender
  - Gini for sub-node Female = $0.2^2 + 0.8^2 = 0.68$
  - Gini for sub-node Male = $0.65^2 + 0.35^2 = 0.55$

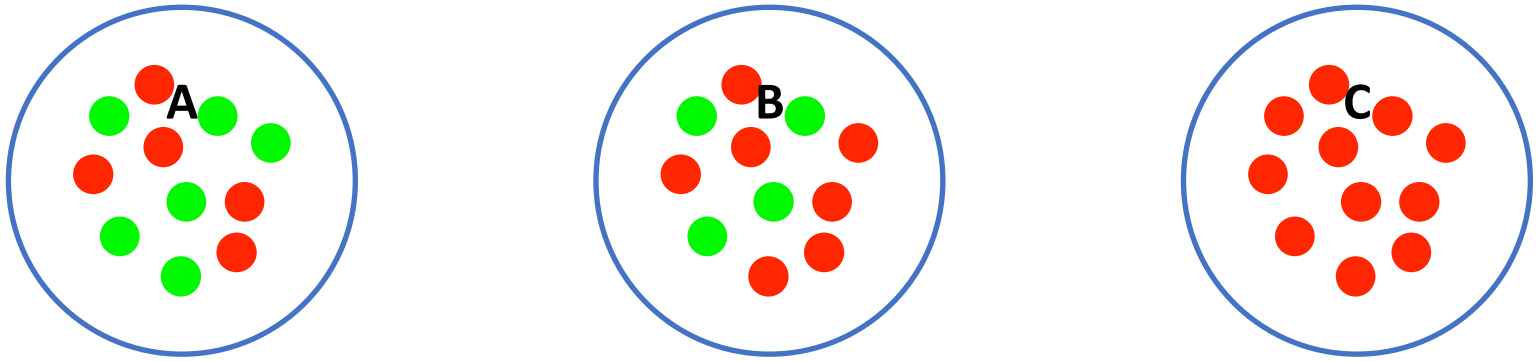
- Split on Class
  - Gini for sub-node A = $0.43^2 + 0.57^2 = 0.51$
  - Gini for sub-node B = $0.56^2 + 0.44^2 = 0.51$

Common splitting algorithms: Gini Index

- Split on Gender
  - Gini Weight on Split Gender = ***(10/30*0.68) + (20/30*0.55) = 0.59***
- Split on Class
  - Gini Weight on Split Class = ***(14/30*0.51) + (16/30*0.51) = 0.51***
- The Gini score for on Gender (***0.59***) is higher than on Class (***0.51***) so it splits on Gender

Common splitting algorithms: Information Gain

- Which image is easier to describe?
  - A requires the maximum information (A is more impure)
  - B requires more information to describe it (B is less Pure than C)
  - C requires less information as all values are similar or the same (C is a Pure node)



Common splitting algorithms: Information Gain

- Used with splitting the data using entropy
- Calculated as the entropy reduction after the dataset is branched on some attribute

$$Gain(T, X) = Entropy(T) - Entropy(T, X)$$

$$where:$$

$$T: Target\ \ variable$$

$$X: Feature\ to\ be\ split\ on$$

$$Entropy(T, X): The\ entropy\ calculated\ after\ the\ data\ is\ split\ on\ feature\ X$$

Common splitting algorithms: Information Gain

- So less impure node requires less information to describe it
- A more impure node requires more information
- Information theory is a measure to define this degree of **disorganisation** in a system known as Entropy

Common splitting algorithms: Information Gain

- Categorical target variables also use entropy
  - It chooses the split which has the lowest entropy compared to the parent node and other splits
- Entropy can be calculated using the formula:

$$Entropy = -p\,log_2\,p - q\,log_2\,q$$

Common splitting algorithms: Information Gain

- If the sample is entirely homogeneous, then the entropy is zero
- If the sample is an equally divided (50% / 50%), it has an entropy of one
- Where ***p*** and ***q*** are the probability of success and failure respectively in that node
- The lesser the entropy, the better it is

Common splitting algorithms: Information Gain

- Steps to calculate Entropy for a split

    1. Calculate entropy of the parent node

    2. Calculate entropy of each node of split and calculate the weighted average of all sub-nodes available in split

Common splitting algorithms: Information Gain

1. Parent node's entropy = ***-(15/30) log_2 (15/30) -(15/30) log_2 (15/30) = 1***
   - The result of 1 shows an impure node

2. Gender's entropy
   - Female = ***-(2/10) log_2 (2/10) -(8/10) log_2 (8/10) = 0.72***
   - Male = ***-(13/20) log_2 (13/20) -(7/20) log_2 (7/30) = 0.93***

3. Entropy for split Gender(Weighted entropy) =
   (10/30) * 0.72 + (20/30) * 0.93 = 0.86

Common splitting algorithms: Information Gain

1. Entropy for Class
    1. A = ***-(6/14) log_2 (6/14) -(8/14) log_2 (8/14) = 0.99***
    2. B = ***-(9/16) log_2 (9/16) -(7/16) log_2 (7/16) = 0.99***

2. Entropy for split Class = ***(14/30) * 0.99 + (16/30) * 0.99 = <u>0.99</u>***

- The tree splits on Gender as the Entropy for Split on Gender is the lowest among all

End of Presentation