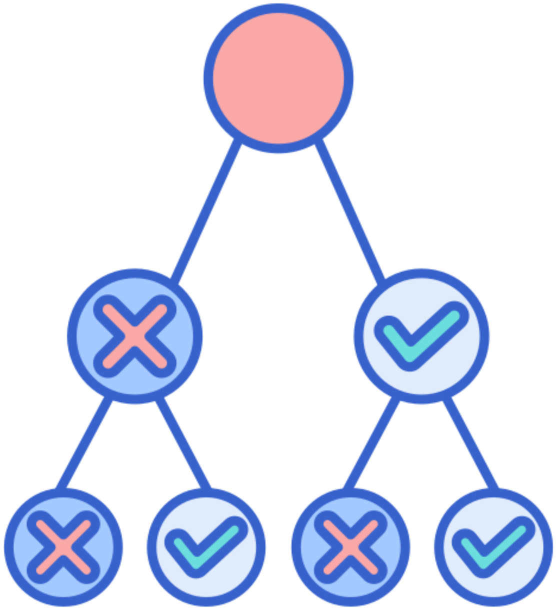
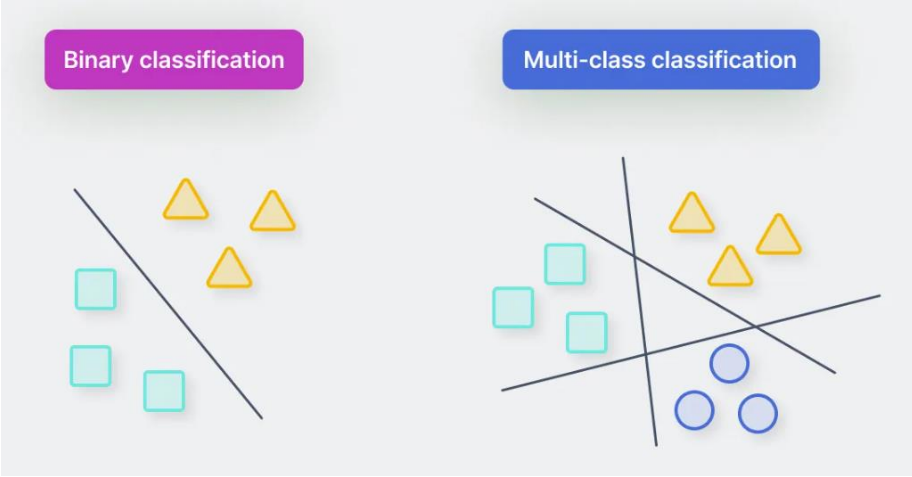
Classification using Decision Trees



Outline

- Classification
- Decision Tree (based on Classification Error)
- Gini Impurity Index
- Entropy
- Decision Boundaries

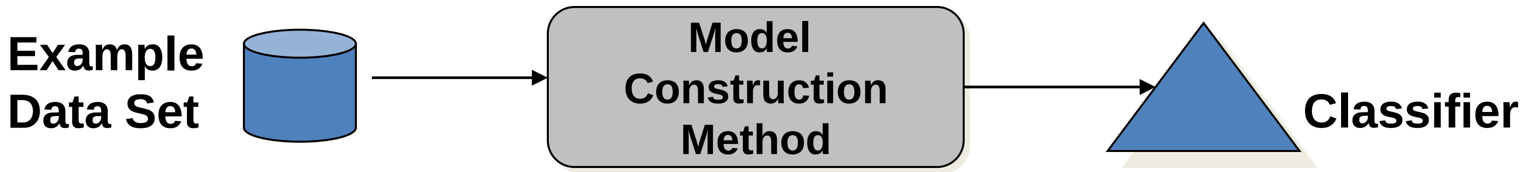
Classification



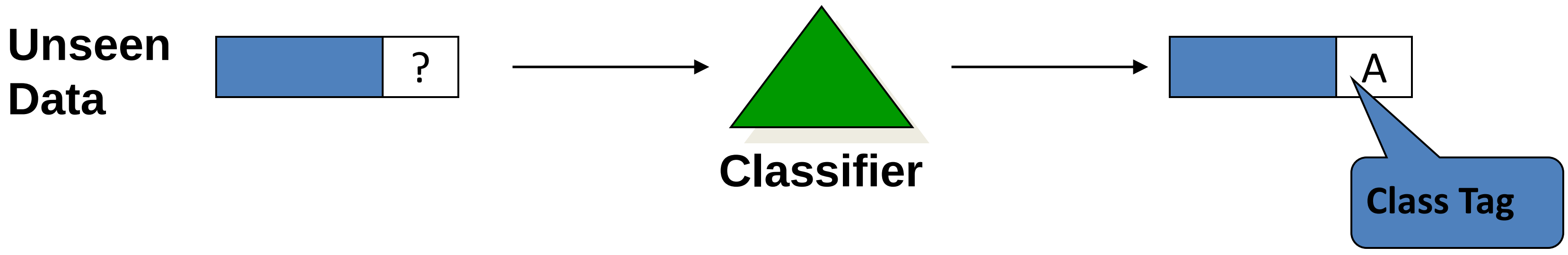
Classification Models

- Assign labels to objects (predicting classes)
- Two-Stage Process

  - Given a data set of **labeled** examples, use a classification method to train a classification model, known as **classifier**



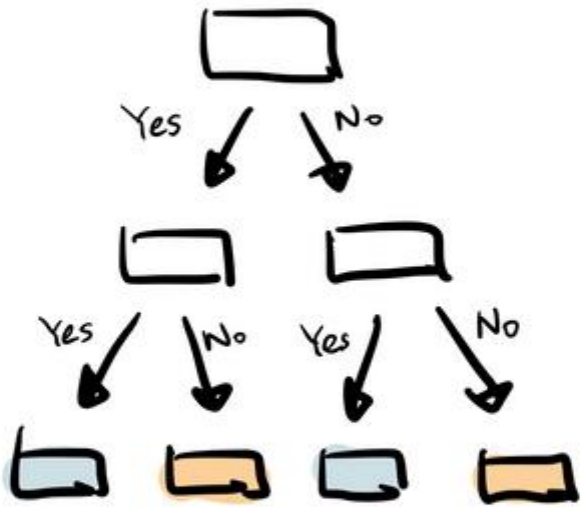
  - Given a trained classifier, classify a data record with unknown class to one of the pre-defined classes

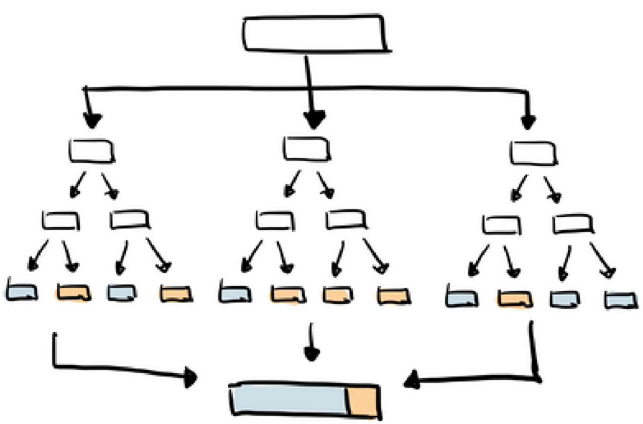


Classification Examples

- **Spam Email Filter (binary classifier)**: classify emails labeled as spam or not spam by learning patterns in the content, sender information, and other features
- **Sentiment Analysis (multi-class classifier)**: classify media posts or product reviews as positive, negative, or neutral sentiments expressed by the author
- **Medical Diagnosis (binary)**: a model trained on patient symptoms and medical history can classify whether a patient is likely to have a certain disease
- **Credit Risk Assessment (multi-class)**: classify loan applicants as low, medium, or high risk based on factors such as credit score, income, and debt-to-income ratio
- **Image Recognition (multi-class)**: a model can classify images of animals into different categories such as cats, dogs, or birds

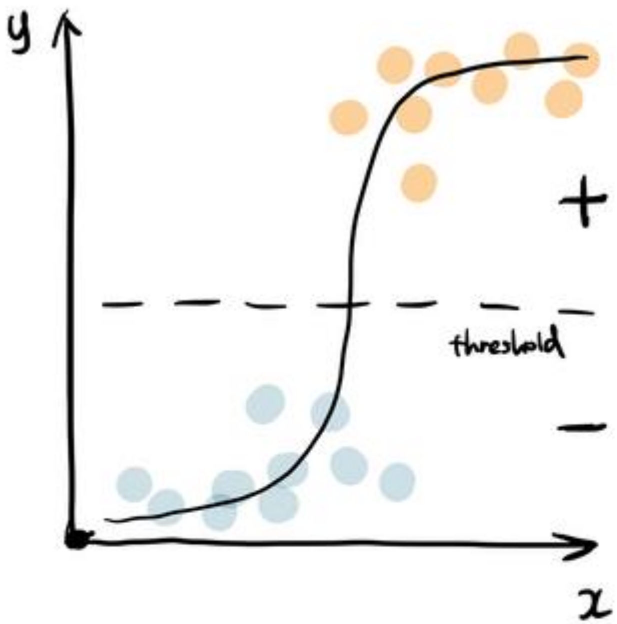
Decision Trees & Random Forest





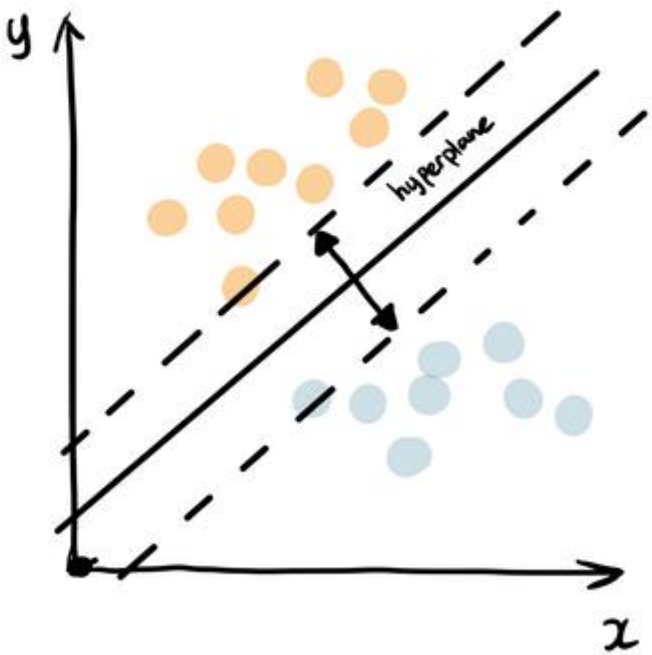
- **Decision Trees**:
  - A tree-like model where each internal node represents a "test" on an attribute
  - It splits the data into different branches based on the attribute values
  - Decision trees are interpretable and can handle both numerical and categorical data
- **Random Forest**:
  - A collection of decision trees where each tree is built using a random subset of features and a random subset of the training data
  - It reduces overfitting and improves generalization compared to individual decision trees
  - Random forests are robust and perform well on a variety of datasets

Logistic Regression



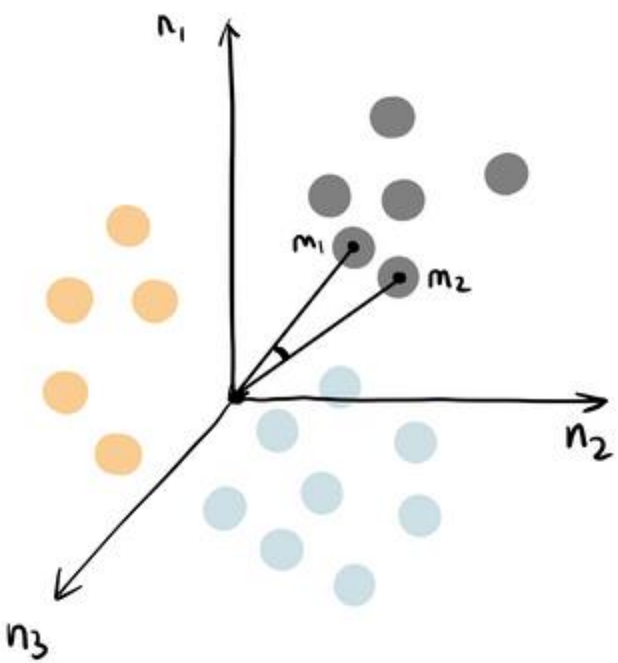
- A linear model used for **binary** classification problems
- It models the probability that a given input belongs to a certain class using the logistic function
- It's simple, interpretable, and efficient for linearly separable data

Support Vector Machine (SVM)



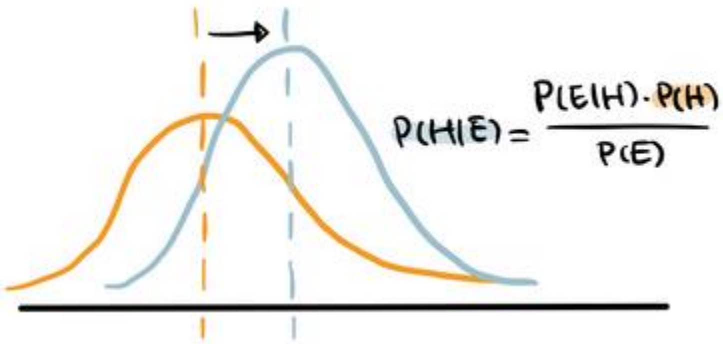
- A model that finds the optimal hyperplane separating different classes in the feature space
  - Classify the data based on the position in relation to the hyperplane between positive class and negative class
- SVM aims to maximize the margin between classes, thus enhancing generalization
- It can handle both linear and non-linear classification tasks using different kernel functions

K-Nearest Neighbors (KNN)



- Each data point is represented in a n dimensional space, which is defined by n features
  - And it calculates the distance between one point to another, then assign the label of unobserved data based on the labels of nearest observed data points
  - The classification of a data point is determined by the majority class among its k nearest neighbors in the feature space
- KNN is simple to understand and implement, especially for small datasets
- It does not learn explicit models and can be sensitive to the choice of k

Naive Bayes



- A probabilistic classifier based on Bayes' theorem with an assumption of independence between features
- It calculates the probability of each class given a set of features and selects the class with the highest probability
- Naive Bayes is efficient, especially for text classification and other high-dimensional datasets

ML Metrics: Influential Factors for a Good Model

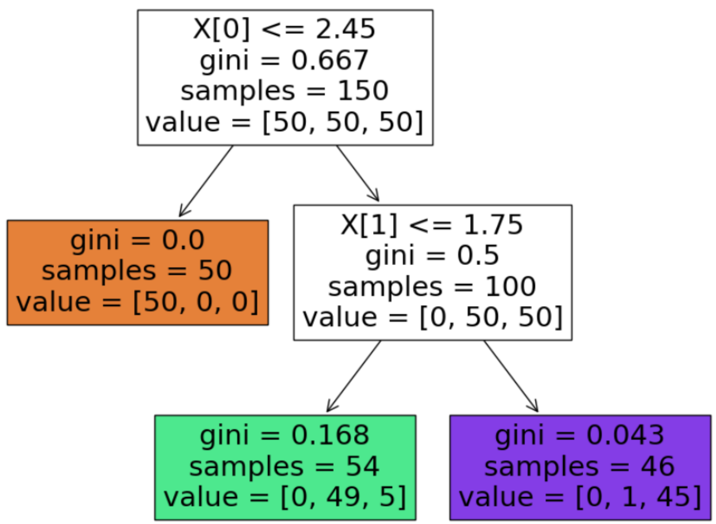
- Accuracy
  - Estimated accuracy during development stage vs. actual accuracy during practical use
- Performance
  - Time taken for model construction (training time)
  - Time taken for the model to infer
- Interpretability
  - Ease of interpreting decisions by the model
  - Understanding and insight provided by the model
- Robustness:
  - Handling noise and missing values
- Scalability:
  - Ability to handle large datasets
- Other measures, e.g., decision tree size or compactness of rules

Decision Tree for the Iris dataset: using two attributes

In [15]:
```
iris = load_iris(as_frame=True)
columns_to_use = ["petal length (cm)", "petal width (cm)"]
X_iris = iris.data[columns_to_use].values
y_iris = iris.target
tree_clf = DecisionTreeClassifier(max_depth=2, random_state=42)
tree_clf = tree_clf.fit(X_iris, y_iris)
```

In [18]:
```
plt.figure(figsize=(10,8))
plot_tree(tree_clf, filled=True)
plt.title("Decision tree trained on two attributes")
plt.show()
```

Decision tree trained on two attributes



In [19]:
```
tree_clf.predict([[3, 2.5]])
```
Out[19]:
```
array([2])
```

In [16]:
```
tree_clf.predict([[5, 1.5]])
```
Out[16]:
```
array([1])
```

In [17]:
```
tree_clf.predict([[.5, 1.5]])
```
Out[17]:
```
array([0])
```

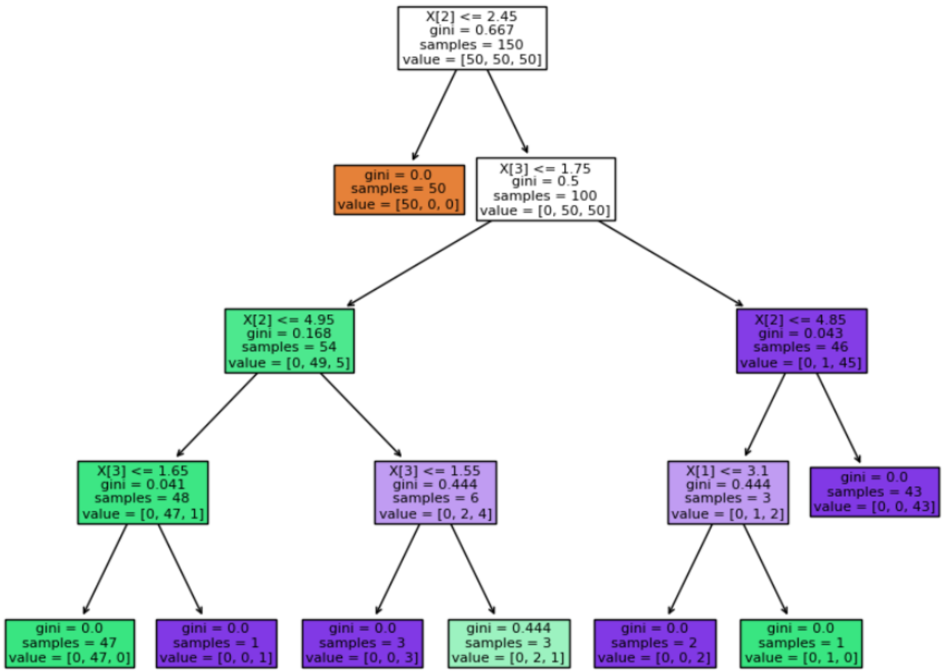
In [20]:
```
r = export_text(tree_clf, feature_names=columns_to_use)
print(r)
```
```
|--- petal length (cm) <= 2.45
|   |--- class: 0
|--- petal length (cm) >  2.45
|   |--- petal width (cm) <= 1.75
|   |   |--- class: 1
|   |--- petal width (cm) >  1.75
|   |   |--- class: 2
```

Decision Tree for the Iris dataset: using all the four attributes

```
X_iris = iris.data.values
y_iris = iris.target
tree_clf = DecisionTreeClassifier(max_depth=4, random_state=42)
tree_clf = tree_clf.fit(X_iris, y_iris)
```

```
tree_clf.fit(X_iris, y_iris)
plt.figure(figsize=(10,8))
plot_tree(tree_clf, filled=True)
plt.title("Decision tree trained on all attributes")
plt.show()
```

Decision tree trained on all attributes



In [31]:
```
print(tree_clf.predict([[.5, 1.5,5,7.5]]))
print(tree_clf.predict([[.5, 1.5,2.5,1.2]]))
print(tree_clf.predict([[5, 1.5,2,3]]))
```

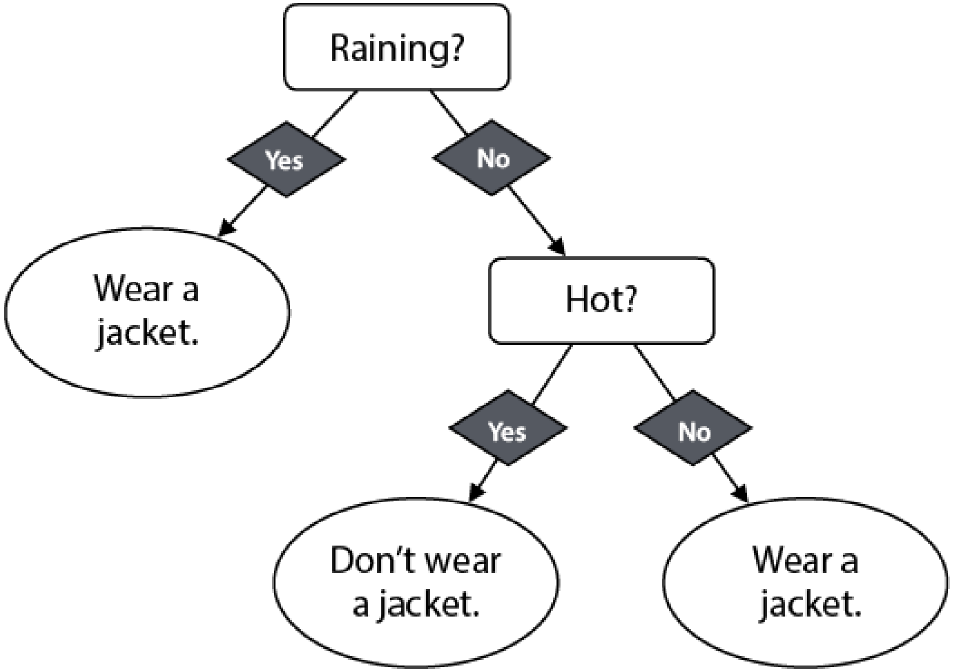
In [31]:
```
print(tree_clf.predict([[.5, 1.5,5,7.5]]))
print(tree_clf.predict([[.5, 1.5,2.5,1.2]]))
print(tree_clf.predict([[5, 1.5,2,3]]))
```

```
[2]
[1]
[0]
```

Decision Trees

Should I ware jacket today?

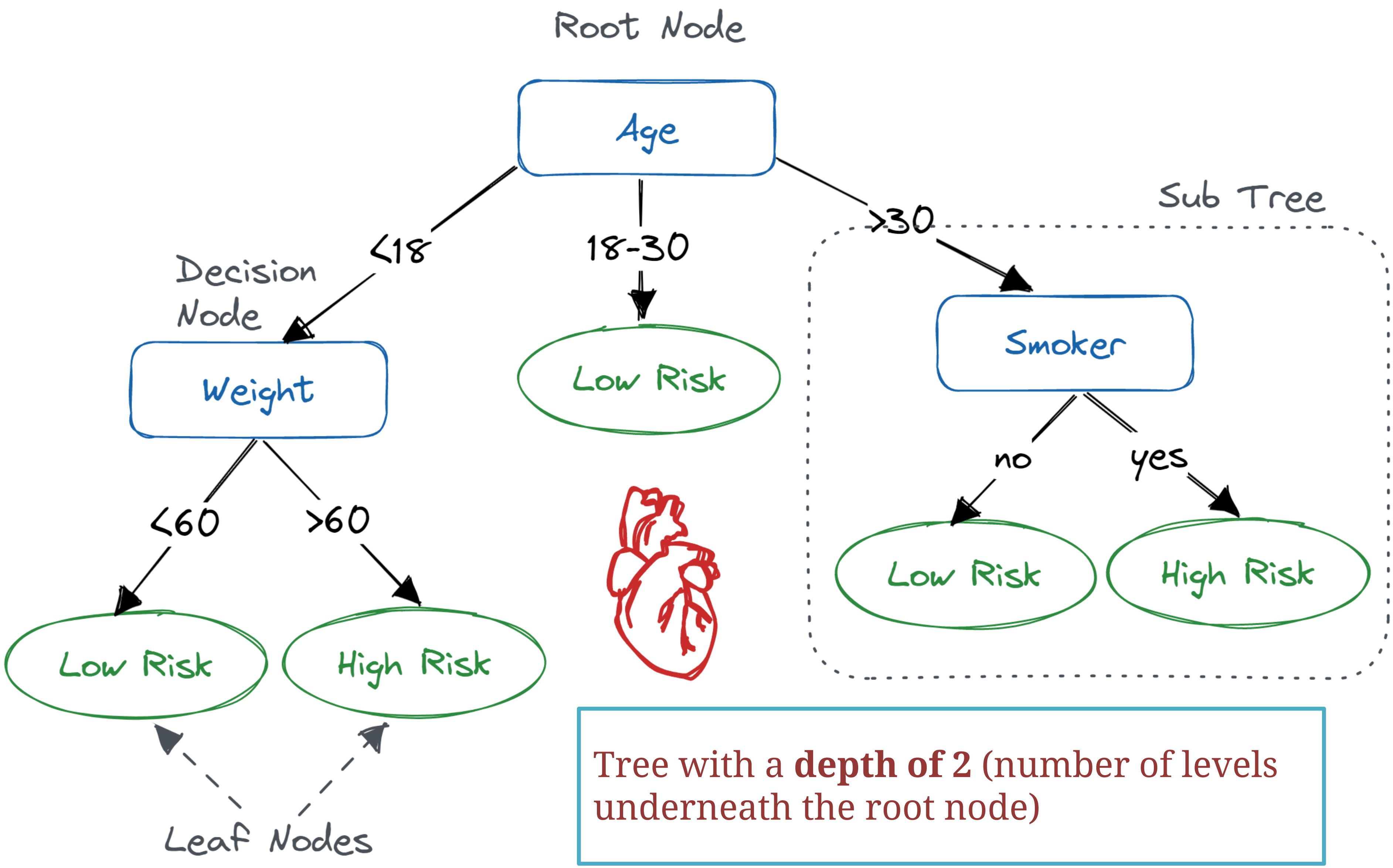
- If it’s raining, then wear a jacket
- If it’s not, then we check the temperature:
  - If it is hot, then don’t wear a jacket
  - But if it is cold, then wear a jacket
- The decision tree depicts the decision process, where the **decisions are made by traversing the tree from top to bottom**



We arrive to a decision (i.e., a class) by asking a series of questions

Image source

Decision Tree – Risk of heart attack



Class Label

Tree with a **depth of 2** (number of levels underneath the root node)

Image source

16

Decision Tree

- **Decision Tree (DT)**: ML model based on yes-or-no questions and represented by a binary tree that describes the decision flow
  - The tree has a **root node**, **decision nodes**, **leaf nodes**, and **branches**
- Can be used:
  - When a series of questions (yes/no) are answered to arrive at a classification decision
    - E.g., Checklist of symptoms during a doctor's evaluation of a patient
  - When **interpretable** "if-then" conditions are preferred to mathematical models
    - E.g.: Financial decisions such as loan approval or fraud detection

App Recommendation System using a DT

What to recommend for?

Gender	Age	App
Female	15	
Female	25	
Male	32	
Female	35	
Male	12	
Male	14	

Female, 16 years old

Female, 30 years old

Male, 35 years old

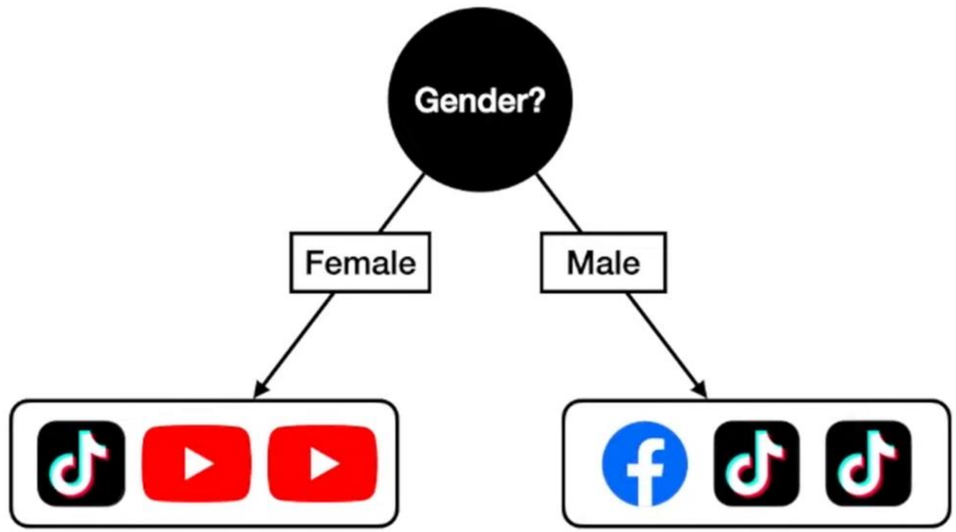
Adopted from source

Which feature is more important?

- Which one of the two features (gender or age) **is more important** in determining the app to recommend?
  - This is the most important step in building a decision tree!
- Let's **split** the data to compare them

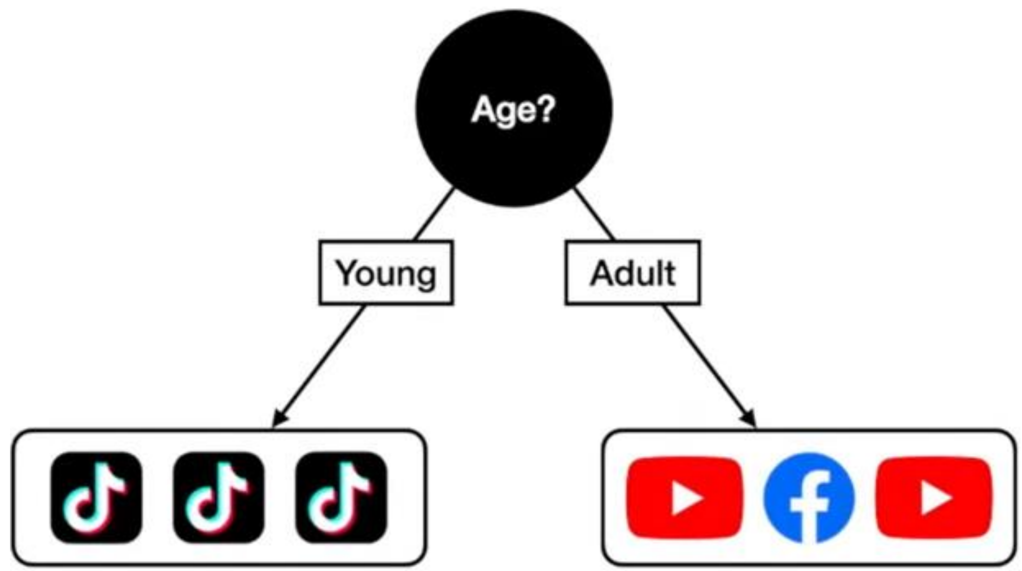
Splitting by Gender => Gender decision stump

Gender	App
Female	
Female	
Female	
Male	
Male	
Male	



Splitting by Age => Age decision stump

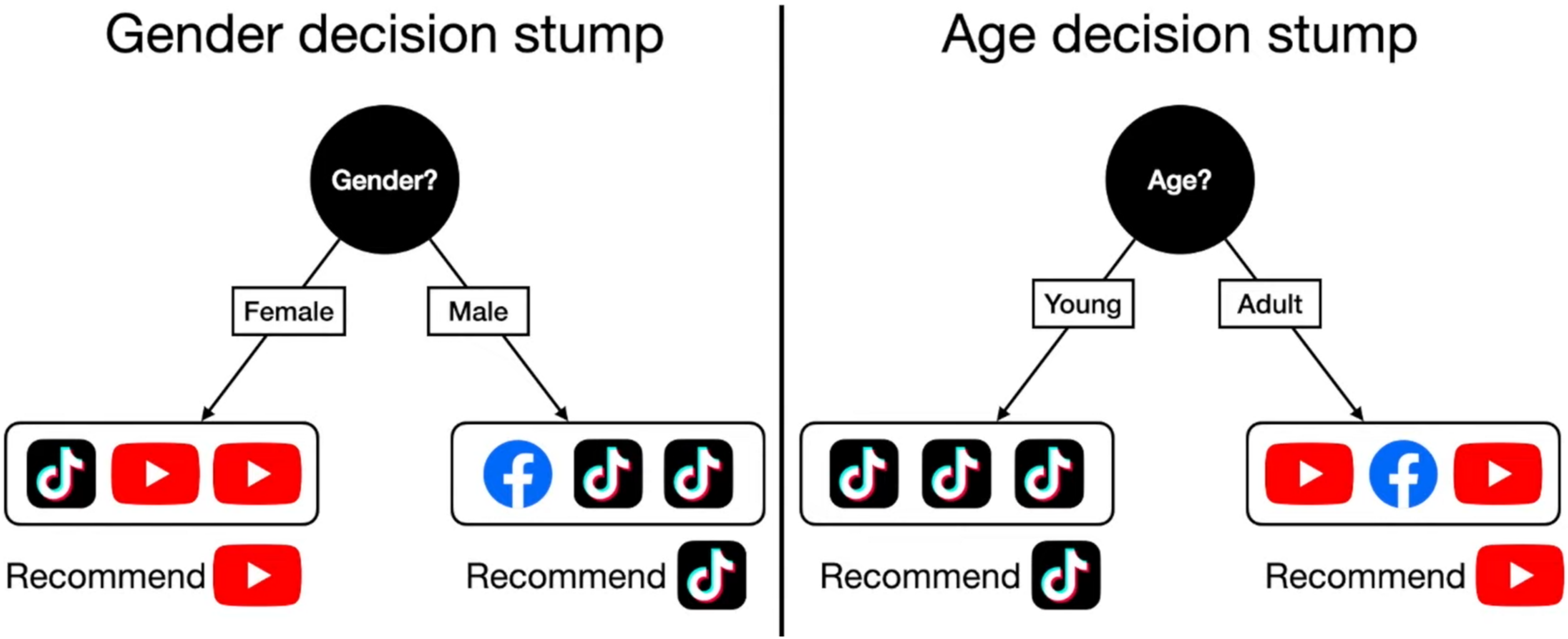
Age	App
Young	
Young	
Young	
Adult	
Adult	
Adult	



Young = Age <= 18

Adult : Age > 18

Which one is better?

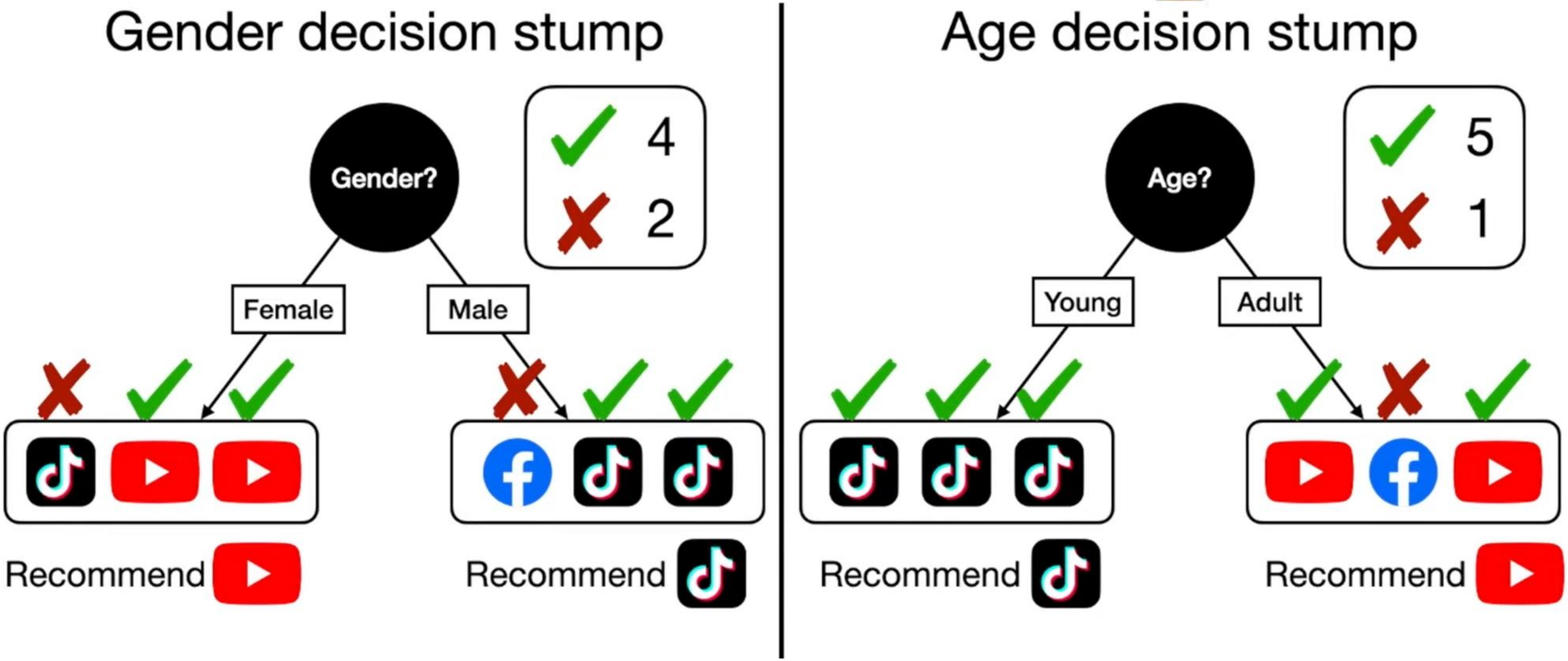


Each feature splits the data into two smaller datasets

Which one is better?

Accuracy: 66.7% & Error Rate: 33.3%

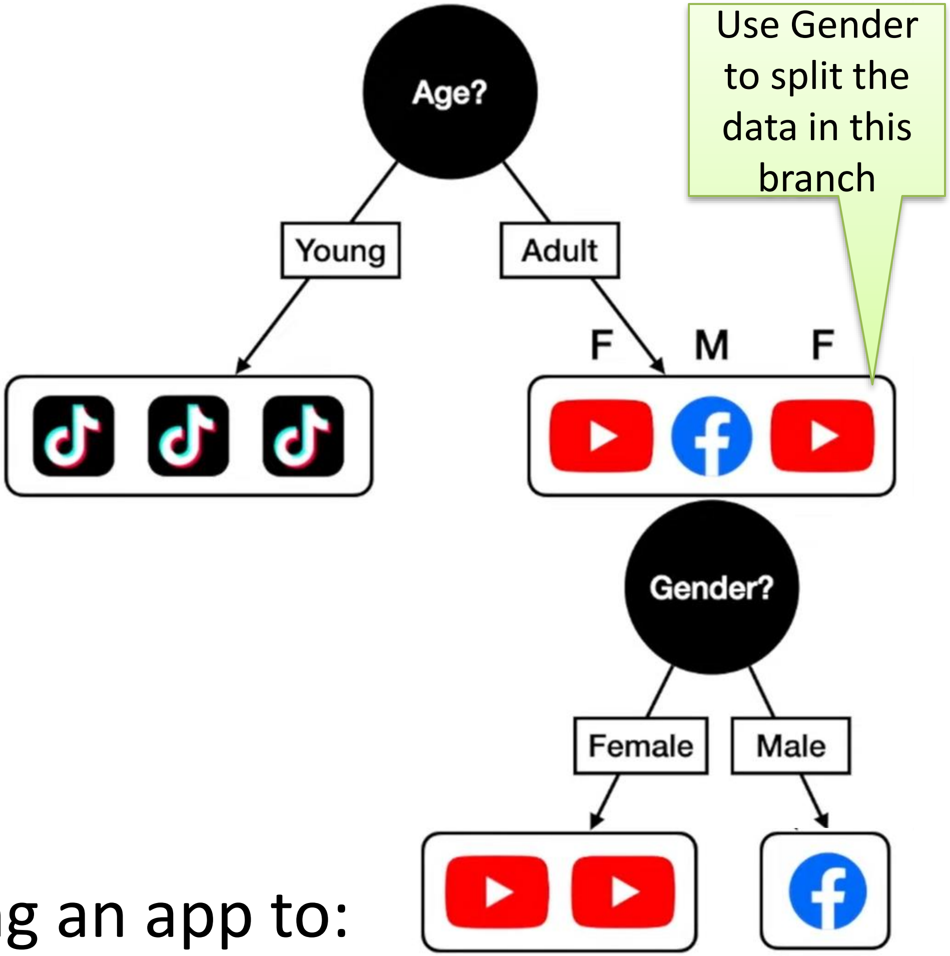
Accuracy: 83.3% & Error Rate: 16.7%



- Based on **accuracy**, the **Age** feature is the winner => It is **determinant** in the prediction and deserve to be the **root of the tree** 🏆 (it has the highest accuracy and the lowest misclassification rate)
  - It is more successful at determining which app to recommend

Building the Tree

Gender	Age	App
Female	Young	
Female	Adult	
Male	Adult	
Female	Adult	
Male	Young	
Male	Young	



- Let's test it for recommending an app to:
  - Female, 16 years old
  - Female, 30 years old
  - Male, 35 years old

Classification Error Rate

- The Classification Error Rate, also known as the **Misclassification Rate**, is the ratio of the number of incorrectly classified instances to the total number of instances in the node

$$Classification\ Error\ Rate = \frac{Number\ of\ Misclassified\ Instances}{Total\ Number\ of\ Instances}$$

$$Error(t) = 1 - \max P(i|t)$$

Where $P(i|t)$ is the probability of class i at node t

- $Error(t)$ measures the classification error made by a node
  - **Fraction of the observations in the region that do not belong to the most common class**
  - Minimum **0** for pure node (containing one class label)
  - Maximum $(\mathbf{1 - \frac{1}{n_c}})$ when the node has equally distributed $\mathbf{n_c}$ classes
- The DT algorithms selects the feature that minimizes impurity the Misclassification Rate

Examples for Computing Classification Error Rate

$$\boxed{Error(t) = 1 - \max_i P(i \mid t)}$$

Female (Left)		
	T	1
	Y	2

$P(T) = \frac{1}{3}$ $P(Y) = \frac{2}{3}$

$\text{Error(L)} = 1 - \max\left(\frac{1}{3}, \frac{2}{3}\right) = 1 - \frac{2}{3} = \frac{1}{3}$

Male (Right)		
	F	1
	T	2

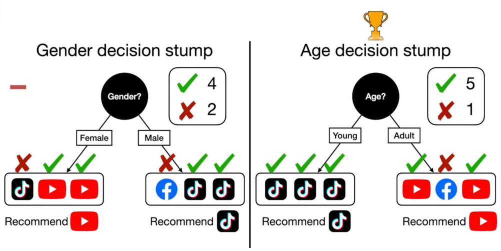
$P(F) = \frac{1}{3}$ $P(T) = \frac{2}{3}$

$\text{Error(R)} = 1 - \max\left(\frac{1}{3}, \frac{2}{3}\right) = 1 - \frac{2}{3} = \frac{1}{3}$

Weighted Average

$$\overline{x}_{weighted} = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}$$

Error(Gender) = $\frac{1}{3}$ = 33.3%



Young (Left)		
	T	3

$P(T) = \frac{3}{3}$

$\text{Error(L)} = 1 - \max(1) = 1 - 1 = 0$

Adult (Right)		
	Y	2
	F	1

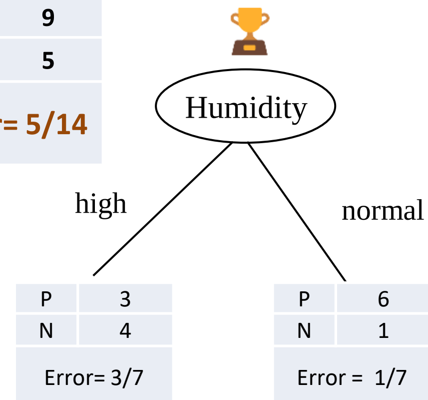
$P(Y) = \frac{2}{3}$ $P(F) = \frac{1}{3}$

$\text{Error(R)} = 1 - \max\left(\frac{2}{3}, \frac{1}{3}\right) = 1 - \frac{2}{3} = \frac{1}{3}$

Error(Age) = $\frac{1}{6}$ = 16.7%

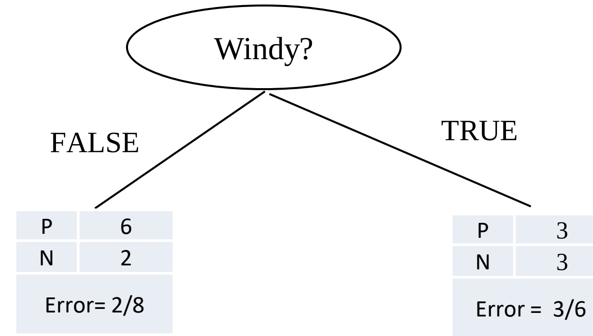
Outlook	Temperature	Humidity	Windy	Class
sunny	Hot	high	FALSE	N
sunny	Hot	High	TRUE	N
Overcast	Hot	high	FALSE	P
Rain	Mild	high	FALSE	P
Rain	Cool	Normal	FALSE	P
Rain	Cool	Normal	TRUE	N
Overcast	Cool	Normal	TRUE	P
Sunny	Mild	High	FALSE	N
Sunny	Cool	normal	FALSE	P
Rain	Mild	Normal	FALSE	P
Sunny	Mild	Normal	TRUE	P
Overcast	Mild	High	TRUE	P
Overcast	Hot	Normal	FALSE	P
Rain	mild	high	TRUE	N

	Parent
P	**9**
N	**5**
Error= 5/14	



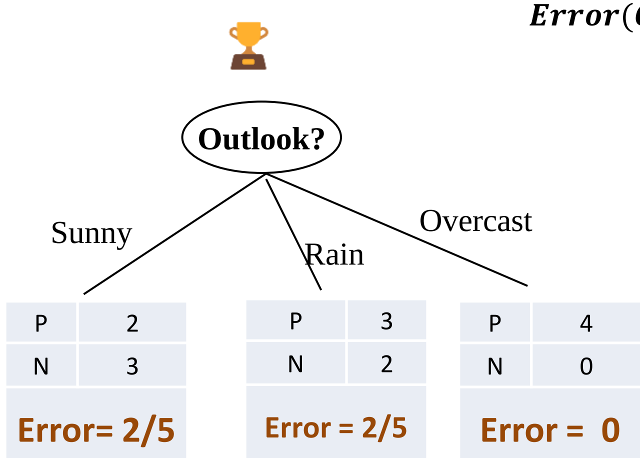
Weighted Average Error for the Humidity Split

$$\boldsymbol{Error(Outlook)} = \frac{7}{14}\times\frac{3}{7}+\frac{7}{14}\times\frac{1}{7}=\frac{3}{14}+\frac{1}{14}=\frac{4}{14}$$



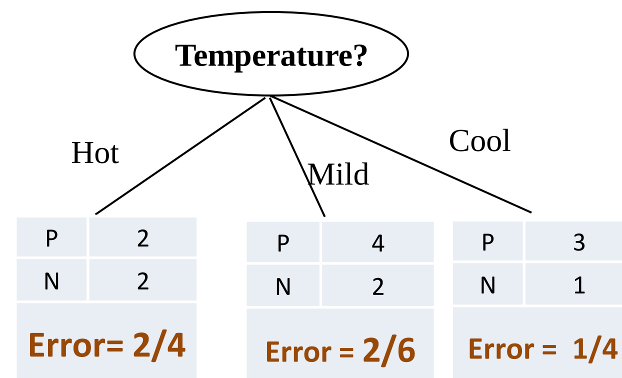
Weighted Average Error for the Windy Split

$$\boldsymbol{Error(Temperature)} = \frac{8}{14}\times\frac{2}{8}+\frac{6}{14}\times\frac{3}{6}=\frac{5}{14}$$



Weighted Average Error for the Outlook Split

$$\boldsymbol{Error(Outlook)} = \frac{5}{14}\times\frac{2}{5}+\frac{5}{14}\times\frac{2}{5}+\frac{4}{14}\times 0=\frac{2}{14}+\frac{2}{14}=\frac{4}{14}$$



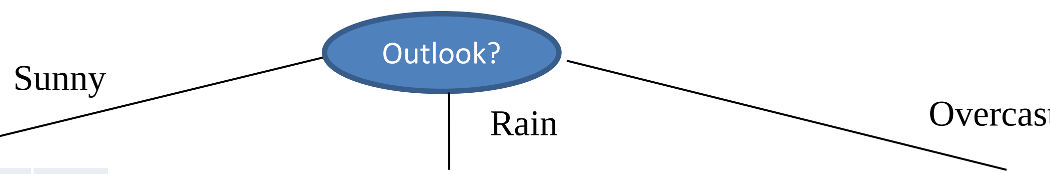
Weighted Average Error for the Temperature Split

$$\boldsymbol{Error(Temperature)} = \frac{4}{14}\times\frac{2}{4}+\frac{6}{14}\times\frac{2}{6}+\frac{4}{14}\times\frac{1}{4}=\frac{2}{14}+\frac{2}{14}+\frac{1}{14}=\frac{5}{14}$$

The best two splits are Outlook and Humidity

We can use Outlook or Humidity since both have the same error

Outlook	Temperature	Humidity	Windy	Class
sunny	Hot	high	FALSE	N
sunny	Hot	high	TRUE	N
Overcast	Hot	high	FALSE	P
Rain	Mild	high	FALSE	P
Rain	Cool	normal	FALSE	P
Rain	Cool	normal	TRUE	N
Overcast	Cool	normal	TRUE	P
Sunny	Mild	high	FALSE	N
Sunny	Cool	normal	FALSE	P
Rain	Mild	normal	FALSE	P
Sunny	Mild	normal	TRUE	P
Overcast	Mild	high	TRUE	P
Overcast	Hot	normal	FALSE	P
Rain	mild	high	TRUE	N



Outlook	Temperature	Humidity	Windy	Class
sunny	Hot	high	FALSE	N
sunny	Hot	high	TRUE	N
Sunny	Mild	high	FALSE	N
Sunny	Cool	normal	FALSE	P
Sunny	Mild	normal	TRUE	P

Outlook	Temperature	Humidity	Windy	Class
Rain	Mild	high	FALSE	P
Rain	Cool	normal	FALSE	P
Rain	Cool	normal	TRUE	N
Rain	Mild	normal	FALSE	P
Rain	mild	high	TRUE	N

Outlook	Temperature	Humidity	Windy	Class
Overcast	Hot	high	FALSE	P
Overcast	Cool	normal	TRUE	P
Overcast	Mild	high	TRUE	P
Overcast	Hot	normal	FALSE	P

Next: Repeat selecting the best feature to split on

Building the Tree – Key Decisions

1. **Choosing the Best Feature to Split On (i.e., asking the best question):**
   - At each node, the algorithm **selects the feature that best separates the data** into distinct classes or reduces **impurity** (uncertainty) the most
   - Use **Attribute Selection Measure (ASM)** like **Classification error, Gini impurity**, **Information gain**
2. **Determining the Split Point:**
   - Once a feature is selected, the algorithm needs to find the **optimal Split Point** (i.e., **splitting condition/threshold)** that minimizes the impurity (i.e., maximizes the information gain)
3. **Recursive Partitioning stop condition:**

   - Recursively partition the dataset based on the selected best feature and its split point. Continues **until a stopping condition is met**
     - Common stopping criteria include limiting the maximum depth of the tree

Decision Tree Construction Algorithms

- **CART Algorithm** (Classification and Regression Trees)
  - Produce binary decision tree
  - Use Gini Index of Impurity as attribute selection measure

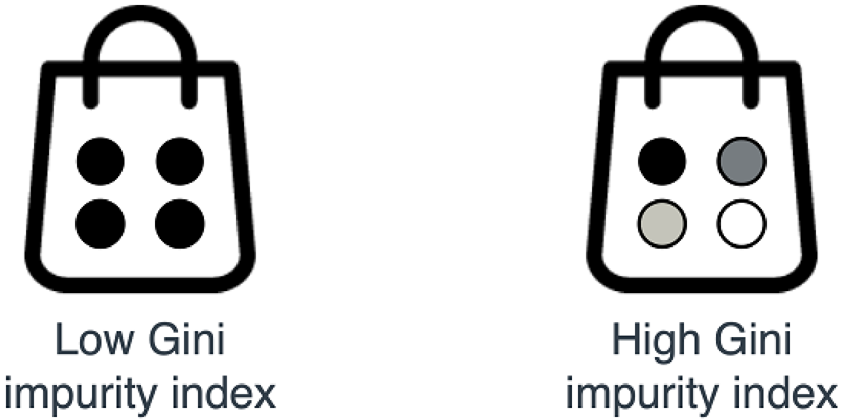
- **ID3** (Iterative Dichotomiser 3)
  - Uses entropy and information gain for attribute selection
  - C4.5: An extension of ID3 that handles both continuous and discrete attributes, and can handle missing values.

- **CHAID Algorithm** (Chi-squared Automatic Interaction Detection)
  - Use Chi-square test (χ^2) as attribute selection measure

- The algorithms mainly differ in adopted **attribute selection measures**

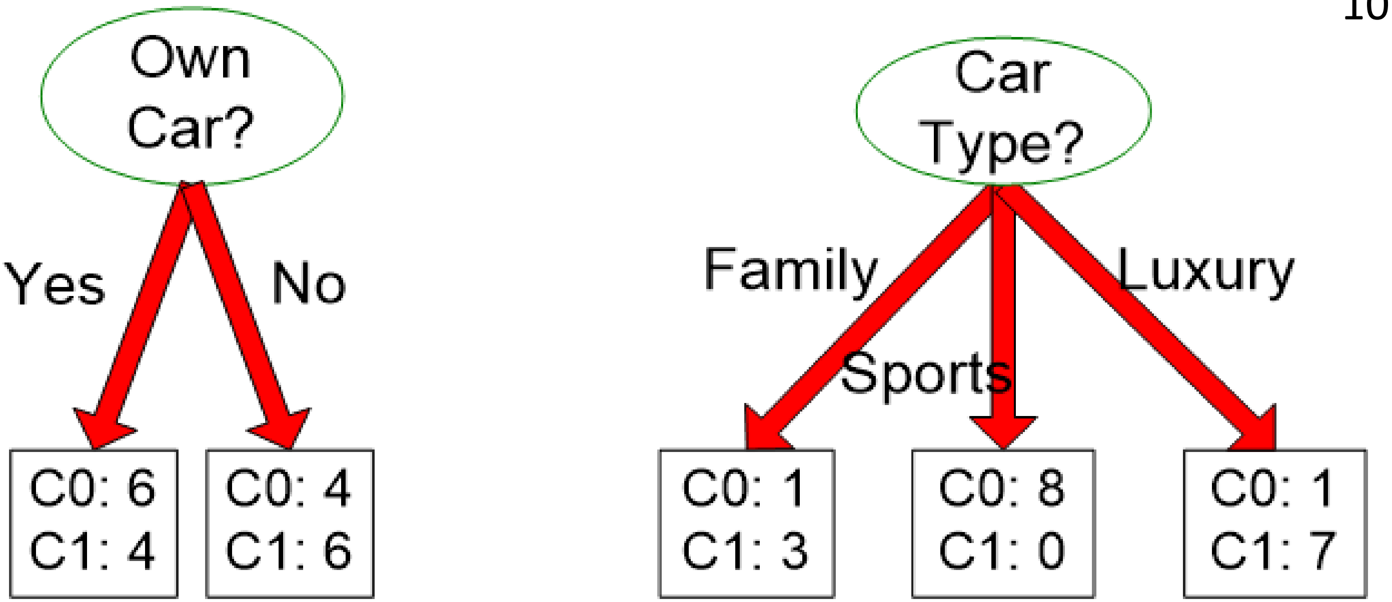
- Studies show that there are only marginal differences among the attribute selection measures w.r.t. model accuracy

Gini Impurity Index



How to choose the best Feature to Split On?

Before Splitting: 10 records of Class 0
10 records of class 1



Which best feature to split on?

=> We need an **Attribute Selection Measure (ASM)**

For choosing the best feature to split that **maximizes the separation of classes** (i.e., **minimizes impurity within each subset**)

How to choose the best Feature to Split On?

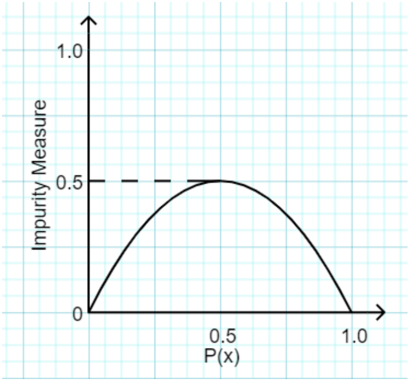
- Nodes with **homogeneous** class distribution (having low impurity) are preferred

C0: 5 C1: 5	C0: 9 C1: 1
Non-homogeneous, **High impurity**	**Homogeneous,** **Low impurity**

- Need an **Attribute Selection Measure (ASM)** to measure **the node impurity** and compare features to choose the best Feature to Split On
  – Classification Error Rate
  – **Gini Impurity Index** (or Gini index), and **Entropy** are measures of node impurity
- Then choose the feature that **minimizes impurity** within each subset (i.e., maximizes the separation of classes)

Gini Index

- The Gini Index is a **measure of impurity** or randomness in a dataset
  - The Gini Index ranges from 0 to 0.5, where:
    - 0: indicates perfect purity, meaning all node elements belong to a single class
    - 0.5: indicates maximally impure node, having elements evenly distributed across all classes



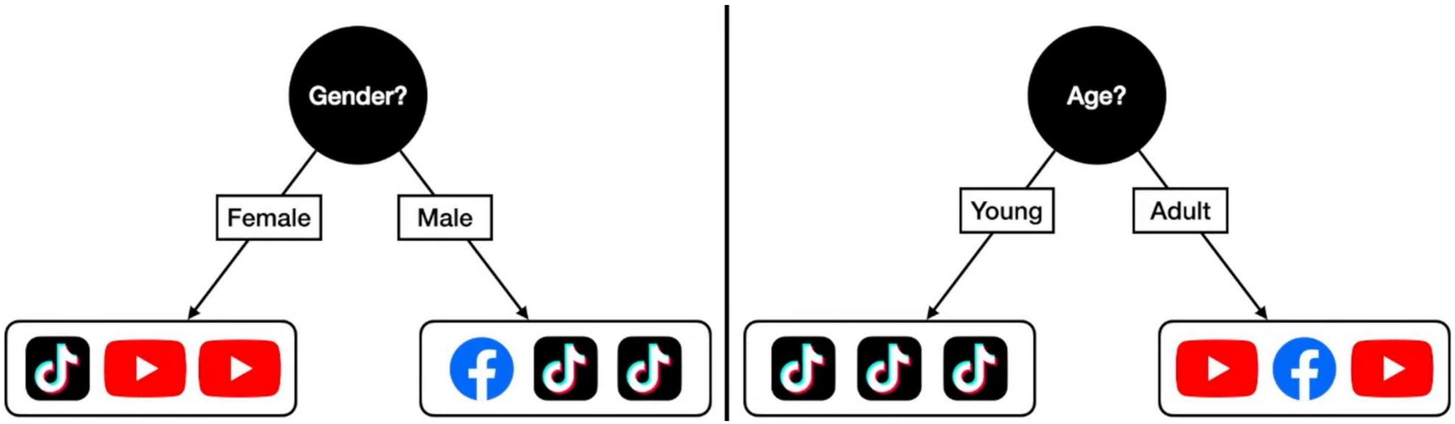
- The formula to calculate the Gini Index for a node t with K classes is:

$$Gini(t) = 1 - \sum_{i=1}^{K} p(i|t)^2$$

Where $p(i|t)$ is the probability of class i at node t

- DT algorithm selects the feature and split point that **minimizes** the weighted sum of the Gini indices for the resulting child nodes

Which one is better? => Compute Gini Index



Classifier 1 (by Gender): **Avg Gini = (0.44 + 0.44) / 2 = 0.44**

- Left leaf (Female): {T, Y, Y}

$$\textbf{Gini} = 1 - (\mathbf{P}(\mathrm{T})2 - \mathbf{P}(\mathrm{Y})2) = 1 - \left(\frac{1}{3}\right)^2 - \left(\frac{2}{3}\right)^2 = \mathbf{0.44}$$

- Right leaf (Male): {F, T, T}

$$\textbf{Gini} = 1 - (\mathbf{P}(\mathrm{F})2 - \mathbf{P}(\mathrm{T})2) = 1 - \left(\frac{1}{3}\right)^2 - \left(\frac{2}{3}\right)^2 = \mathbf{0.44}$$

Measures the **impurity** of the split

Classifier 2 (by age): **Avg Gini = (0 + 0.44) / 2 = 0.22**

- Left leaf (young): {T, T, T}. **Gini** $= 1 - (\mathbf{P}(\mathrm{T})2) = 1 - \left(\frac{3}{3}\right)^2 = \mathbf{0}$

- Right leaf (adult): {Y, F, Y}. **Gini** $= 1 - (\mathbf{P}(\mathrm{Y})2 - \mathbf{P}(\mathrm{F})2) = 1 - \left(\frac{2}{3}\right)^2 - \left(\frac{1}{3}\right)^2 = \boldsymbol{0.44}$

Attribute Selection Measures

Measure of Impurity: Gini (used by CART Algorithm)

- Gini Index for a given node *t* :

$$GINI(t) = 1 - \sum_{j} [p(j \mid t)]^2$$

(NOTE: $p(j \mid t)$ is the relative frequency of class *j* at node *t*).

  - Maximum ($1 - 1/n_c$) when records are equally distributed among all classes, implying most impure set

  - Minimum (0.0) when all records belong to one class, implying least impure set

C1	**0**
C2	**6**
Gini=0.000	

C1	**1**
C2	**5**
Gini=0.278	

C1	**2**
C2	**4**
Gini=0.444	

C1	**3**
C2	**3**
Gini=0.500	

Examples for computing Gini

$$Gini(t) = 1 - \sum_{i=1}^{K} p(i|t)^2$$

Where $p(i|t)$ is the probability of class i at node t

C1	**0**
C2	**6**

P(C1) = 0/6 = 0   P(C2) = 6/6 = 1

Gini = 1 – $P(C1)^2$ – $P(C2)^2$ = 1 – 0 – 1 = 0

C1	**1**
C2	**5**

P(C1) = 1/6   P(C2) = 5/6

Gini = 1 – $(1/6)^2$ – $(5/6)^2$ = 0.278

C1	**2**
C2	**4**

P(C1) = 2/6   P(C2) = 4/6

Gini = 1 – $(2/6)^2$ – $(4/6)^2$ = 0.444

Splitting Based on Gini

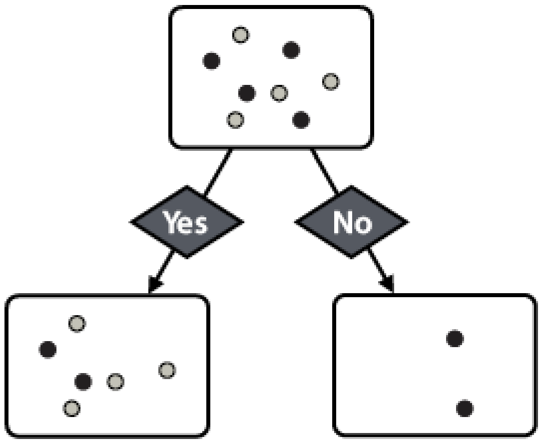
- When a node p is split into k partitions (children), the **quality of split** is computed as

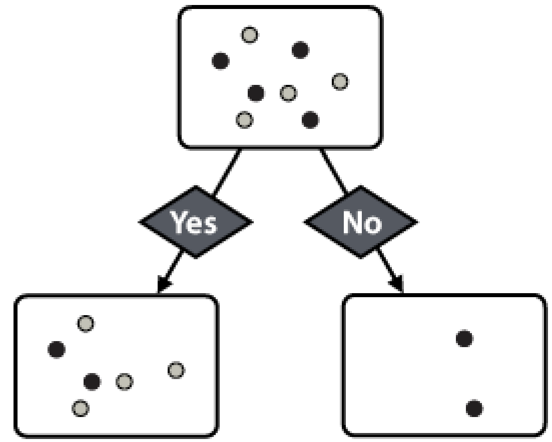
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

Where: **n_i** = number of instances at child i

n = number of instances at node p

Splits of different sizes? => take weighted averages





Gini = 0.444 Gini = 0

Entropy = 0.918 Entropy = 0

$$\text{Weighted average Gini} = 0.444 \cdot \frac{6}{8} + 0 \cdot \frac{2}{8} = 0.333$$

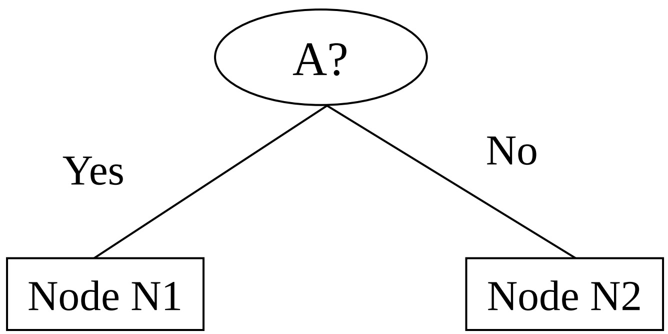
$$\text{Weighted average entropy} = 0.918 \cdot \frac{6}{8} + 0 \cdot \frac{2}{8} = 0.689$$

- A split of a dataset of size eight into two datasets of sizes six and two.
- To calculate the avg Gini index and the avg entropy, we weight the index of the left dataset by 6/8 and that of the right dataset by 2/8

Computing Gini Index of a Split

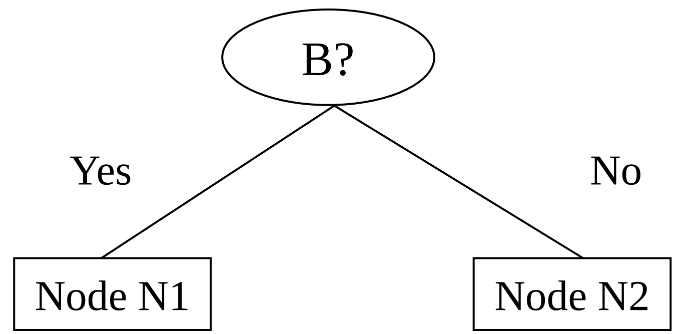
- Split into two partitions
- Compute the Gini Index per split
- Choose the split with the lowest Gini Index

	Parent
C1	**6**
C2	**6**
Gini = 0.500	



	N1
C1	6
C2	1

	N2
C1	0
C2	5



	N1
C1	4
C2	2

	N2
C1	2
C2	4

Gini(N1) = $1 - (6/7)^2 - (1/7)^2 = 0.245$

Gini(N2) = $1 - (0/5)^2 - (5/5)^2 = 0$

Gini(Left-Node) = 7/12 * 0.245 + 5/12 * 0 = **0.1429**

Gini(N1) = $1 - (4/6)^2 - (2/6)^2 = 0.2222$

Gini(N2) = $1 - (2/6)^2 - (4/6)^2 = 0.2222$

Gini(Right-Node) = 6/12 * 0.2222 + 6/12 * 0.2222 = **0.2222**

Choose split A as it has less Gini Index than split B

Computing Gini Index – Example (1/2)

$$Gini(t) = 1 - \sum_{i=1}^{K} p(i|t)^2$$

Where $p(i|t)$ is the probability of class i at node t

Outlook	Temperature	Humidity	Windy	Class
sunny	Hot	high	FALSE	N
sunny	Hot	high	TRUE	N
Overcast	Hot	high	FALSE	P
Rain	Mild	high	FALSE	P
Rain	Cool	normal	FALSE	P
Rain	Cool	normal	TRUE	N
Overcast	Cool	normal	TRUE	P
Sunny	Mild	high	FALSE	N
Sunny	Cool	normal	FALSE	P
Rain	Mild	normal	FALSE	P
Sunny	Mild	normal	TRUE	P
Overcast	Mild	high	TRUE	P
Overcast	Hot	normal	FALSE	P
Rain	mild	high	TRUE	N

	Parent
P	9
N	5
Gini Index = 1 –(25/196 + 81/196) = 90/196 = 0.4592	

Outlook?

Sunny

P	2
N	3
Gini Index = 1-(9/25+4/25) =1-(13/25) = 12/25	

Rain

P	3
N	2
Gini Index = 1-(13/25) = 12/25	

Overcast

P	4
N	0
Gini Index = 0	

Temperature?

hot

P	2
N	2
Gini Index = 1-(8/16) = 8/16	

mild

P	4
N	2
Gini Index = 1-(20/36) = 16/36	

cool

P	3
N	1
Gini Index = 1-(10/16) = 6/16	

Weighted Average Gini Index for the Outlook Split

$$Gini(Outlook) = \frac{5}{14} \times \frac{12}{25} + \frac{5}{14} \times \frac{12}{25} + \frac{4}{14} \times 0 = \frac{6}{35} + \frac{6}{35} = \frac{12}{35} = 0.3429$$

Weighted Average Gini Index for the Temperature Split

$$Gini(Temperature) = \frac{4}{14} \times \frac{8}{16} + \frac{6}{14} \times \frac{16}{36} + \frac{4}{14} \times \frac{6}{16}$$

$$Gini(Temperature) = \frac{2}{14} + \frac{4}{21} + \frac{3}{28} = \frac{4}{21} + \frac{7}{28} = 0.4405$$

Computing Gini Index – Example (2/2)

$Gini(t) = 1 - \sum_{i=1}^{K} p(i|t)^2$

Where $p(i|t)$ is the probability of class i at node t

Outlook	Temperature	Humidity	Windy	Class
sunny	Hot	high	FALSE	N
sunny	Hot	high	TRUE	N
Overcast	Hot	high	FALSE	P
Rain	Mild	high	FALSE	P
Rain	Cool	normal	FALSE	P
Rain	Cool	normal	TRUE	N
Overcast	Cool	normal	TRUE	P
Sunny	Mild	high	FALSE	N
Sunny	Cool	normal	FALSE	P
Rain	Mild	normal	FALSE	P
Sunny	Mild	normal	TRUE	P
Overcast	Mild	high	TRUE	P
Overcast	Hot	normal	FALSE	P
Rain	mild	high	TRUE	N

	Parent
P	9
N	5

Gini Index = 1 –(25/196 + 81/196)
= 90/196 = 0.4592

Humidity

high

P	3
N	4

Gini Index = 1-(25/49)
= 24/49

normal

P	6
N	1

Gini Index = 1-(37/49)
= 12/49

Weighted Average Gini Index for the Humidity Split

$$Error(Outlook) = \frac{7}{14} \times \frac{24}{49} + \frac{7}{14} \times \frac{12}{49} = \frac{12}{49} + \frac{6}{49} = \frac{18}{49} = 0.3673$$

Windy?

FALSE

P	6
N	2

Gini Index = 1-(40/64)
= 24/64

TRUE

P	3
N	3

Gini Index = 1-(18/36)
= 18/36

Weighted Average Gini Index for the Windy Split

$$Error(Temperature) = \frac{8}{14} \times \frac{24}{64} + \frac{6}{14} \times \frac{18}{36} = \frac{3}{14} + \frac{3}{14} = \frac{6}{14} = 0.4286$$

The best split is Outlook (0.3429)

Decide optimal Split Point using Gini Index
Categorical Attributes

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make **Split Point** decisions

Multi-way split

	CarType		
	Family	Sports	Luxury
C1	1	2	1
C2	4	1	1
Gini	0.393		

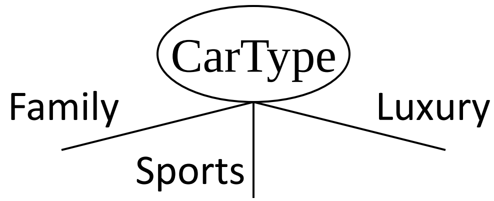
Two-way split
(find best partition of values)

	CarType	
	{Sports, Luxury}	{Family}
C1	3	1
C2	2	4
Gini	0.400	

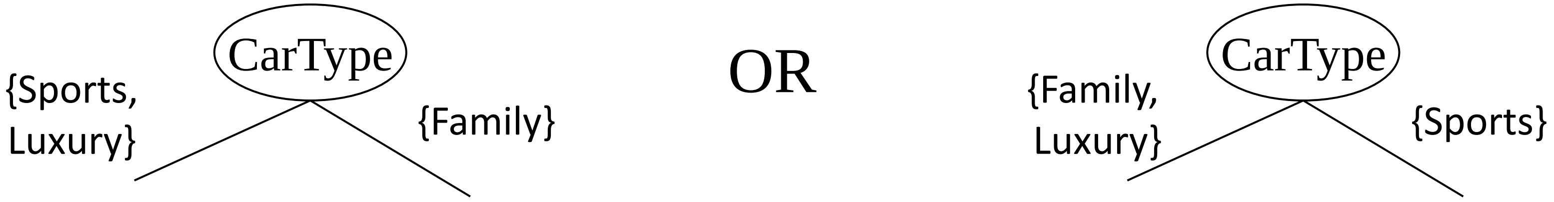
	CarType	
	{Sports}	{Family, Luxury}
C1	2	2
C2	1	5
Gini	0.419	

Splitting Based on Nominal Attributes

- Multi-way split: Use as many partitions as distinct values.

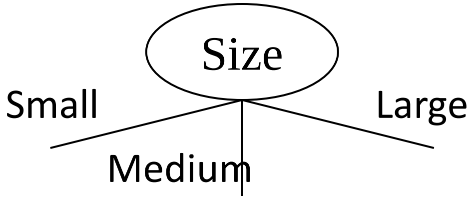


- Binary split: Divides values into two subsets.
  Need to find optimal partitioning.

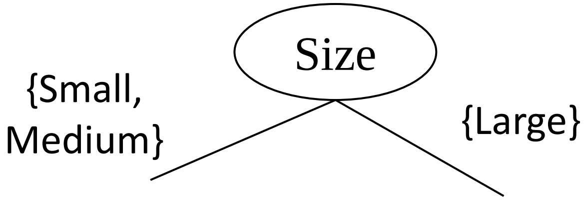


Splitting Based on Ordinal Attributes

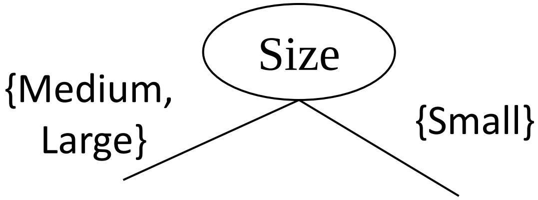
- Multi-way split: Use as many partitions as distinct values.



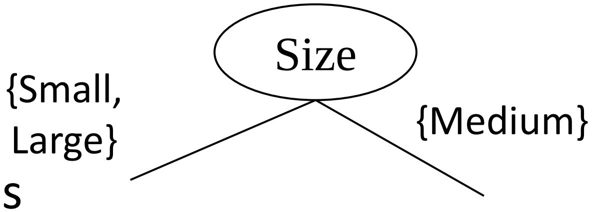
- Binary split: Divides values into two subsets. Need to find optimal partitioning.



OR



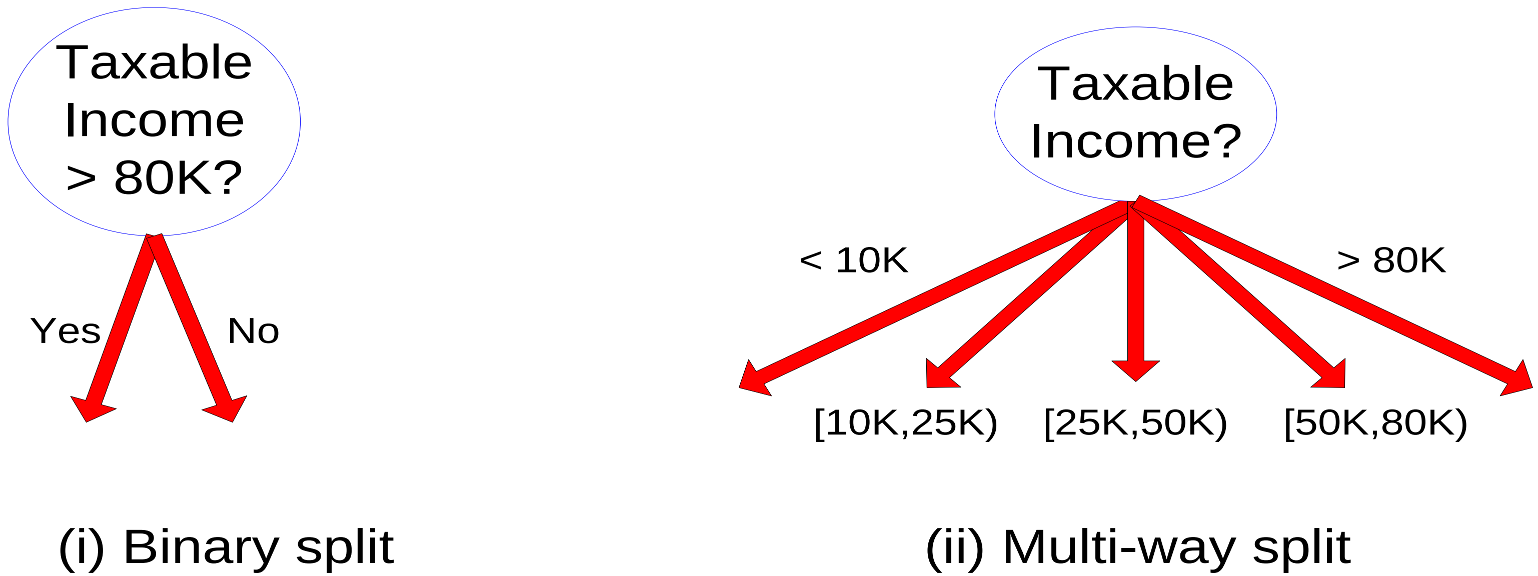
- What about this split?
  - No! the grouping should not violate the order property of the attribute values



Splitting Based on Continuous Attributes

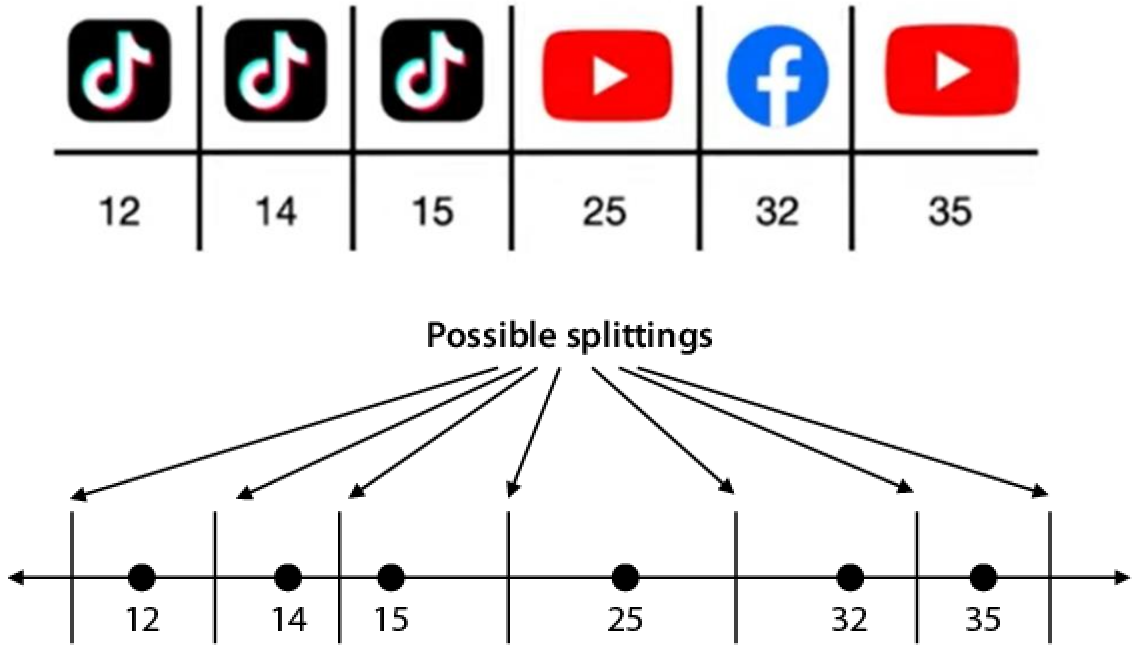
- Different ways of handling continuous attributes
  - Let attribute *A* be a continuous attribute
  - Discretization to form an ordinal categorical attribute
    - ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering
  - Sort the value *A* in increasing order
    - Typically, the midpoint between each pair of adjacent values is considered as a possible *split point*
      - $(a_i+a_{i+1})/2$ is the midpoint between the values of a_i and a_{i+1}
  - Binary split: ($A < v$) or ($A \geq v$), OR A in a range
    - Consider all possible splits and finds the best cut
  - Multi-way split: A in one of the ranges
- Can be compute intensive

Splitting Based on Continuous Attributes



Decide optimal Split Point using Gini Index
Continuous Attributes

Gender	Age	App
Female	15	
Female	25	
Male	32	
Female	35	
Male	12	
Male	14	



- Sort the entries by **age**
- We pick the **midpoints** between consecutive ages to be the age for splitting
  - For the endpoints, we can pick any random value that is out of the interval
- Then calculate the Gini impurity index of each of the splits
- Choose the **Split Point** that has the lowest Gini index

Decide optimal **Split Point** using Gini Index - Example

	Age													
	12		14		15		25		32		35			
	7		**13**		**14.5**		**20**		**28.5**		**33.5**		**100**	
App	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
T	0	3	1	2	2	1	3	0	3	0	3	0	3	0
Y	0	2	0	2	0	2	0	2	1	1	2	1	2	0
F	0	1	0	1	0	1	0	1	2	0	1	0	1	0
Gini	**0.611**		**0.533**		**0.417**		**0.22**		**0.416**		**0.467**		**0.611**	

Best **Split Point** is age <= 20

Entropy

$$E(S)=\sum_{i=1}^{c}-p_i \log_2 p_i$$

Play Golf	
Yes	No
9	5

Entropy(PlayGolf) = Entropy (5,9)
= Entropy (0.36, 0.64)
= - (0.36 $\log_2$ 0.36) - (0.64 $\log_2$ 0.64)
= 0.94

Entropy

- Entropy is a **measure of impurity** or randomness in a dataset. It quantifies the **amount of uncertainty** associated with the distribution of class labels in the dataset
- The formula to calculate entropy for a set ***S*** with ***K*** classes is:

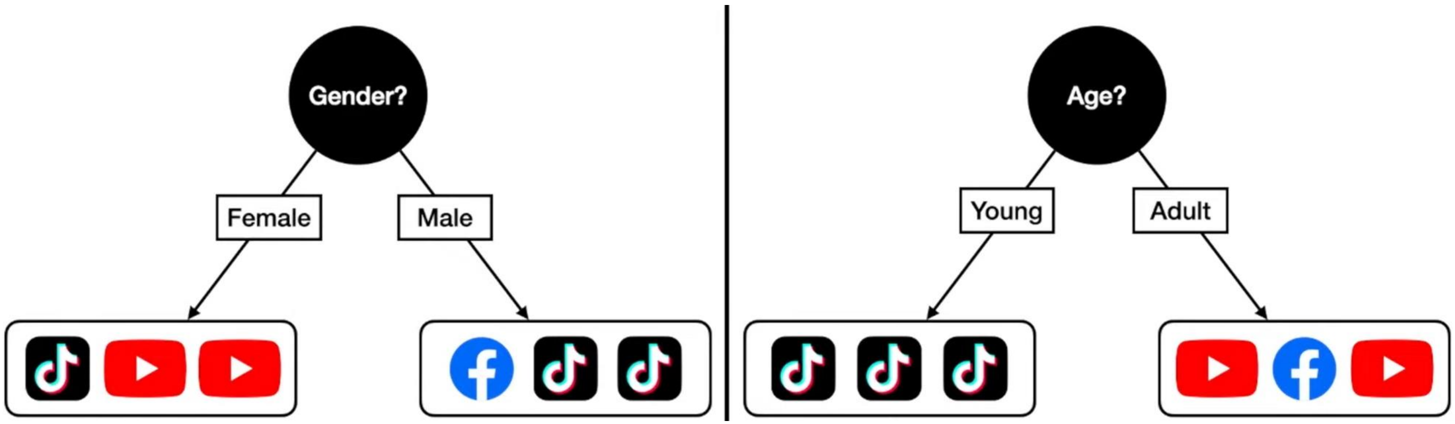
$$\text{Entropy}(S) = -\sum_{i=1}^{K} p_i \log_2(p_i)$$

Where p_i is the probability of class i in set S.

Fraction of instances of a given class....

- Entropy ranges from 0 to $\log_2(K)$, where:
  - 0 indicates that the set *S* is pure (all instances belong to the same class)
  - **log2(*K*)** indicates maximum entropy (the instances are evenly distributed across all classes)
- DT algorithm selects the feature and split point that **result in subsets with lower entropy**

Which one is better? => Compute Entropy



Classifier 1 (by Gender): **Avg Entropy = (0.918 + 0.918)/2 = 0.918**

- Left leaf (Female): {T, Y, Y}

$\textbf{Gini} = -\mathbf{P}(\mathrm{T})\log_2 \mathbf{P}(\mathrm{T}) - \mathbf{P}(\mathrm{Y})\log_2 \mathbf{P}(\mathrm{Y}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} = \mathbf{0.918}$

- Right leaf (Male): {F, T, T}

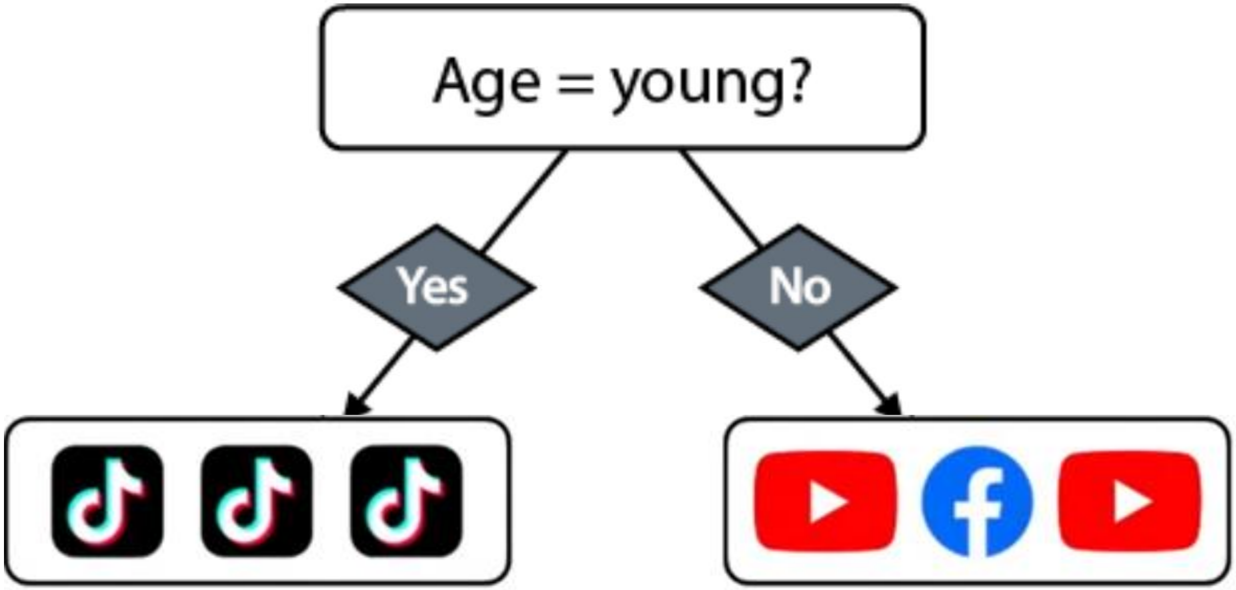
$\textbf{Gini} = -\mathbf{P}(\mathrm{F})\log_2 \mathbf{P}(\mathrm{F}) - \mathbf{P}(\mathrm{T})\log_2 \mathbf{P}(\mathrm{T}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} = 0.918$

Classifier 2 (by age): **Avg Gini = (0 + 0.918)/2 = 0.459**

- Left leaf (young): {T, T, T}. $\textbf{Gini} = -\mathbf{P}(\mathrm{T})\log_2 \mathbf{P}(\mathrm{T}) = -\frac{3}{3}\log_2\frac{3}{3} = \mathbf{0}$

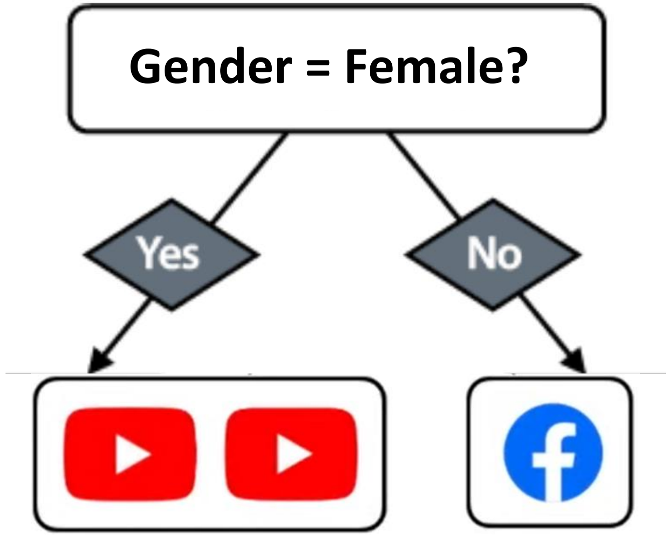
- Right leaf (adult): {Y, F, Y}. $\textbf{Gini} = -\mathbf{P}(\mathrm{Y})\log_2 \mathbf{P}(\mathrm{Y}) - \mathbf{P}(\mathrm{F})\log_2 \mathbf{P}(\mathrm{F})$

$= -\frac{2}{3}\log_2\frac{2}{3} - \frac{1}{3}\log_2\frac{1}{3} = 0.918$



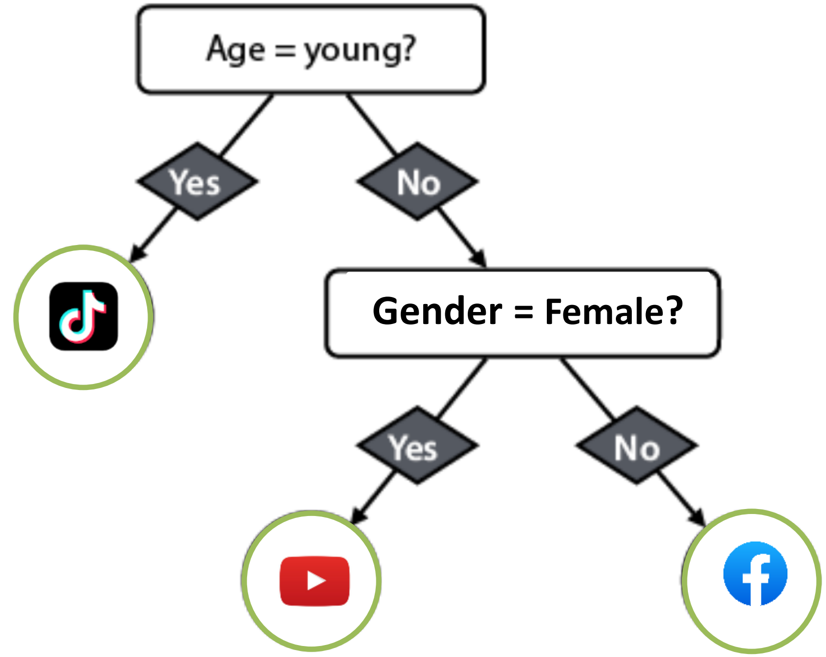
Accuracy: 100%	Accuracy: 66.67%
Gini: 0	Gini: 0.444
Entropy: 0	Entropy: 0.918

- When we split our dataset by age, we get two datasets
- The one on the left **is pure** (all the labels are the same), its accuracy is 100%, and its Gini index and entropy are both 0
  - Thus, this node becomes **a leaf node**, and when we get to that leaf, we return the prediction **TikTok**
- The split on the right is **impure** and can still be divided using the Gender feature



Accuracy: 100%
Gini: 0
Entropy: 0

Accuracy: 66.67%
Gini: 0.444
Entropy: 0.918



- We can split the right leaf of the tree in the previous slide using Gender and we obtain two pure datasets. Each having an accuracy of 100% and a Gini index and entropy of 0
- After this split, we are done, because we can't improve our splits any further
- The resulting decision tree (shown on the right) has two nodes and three leaves. This tree predicts every point in the original dataset correctly

Entropy Calculation - Example

- **Algorithm Illustration**

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	FALSE	N
sunny	hot	high	TRUE	N
overcast	hot	high	FALSE	P
rain	mild	high	FALSE	P
rain	cool	normal	FALSE	P
rain	cool	normal	TRUE	N
overcast	cool	normal	TRUE	P
sunny	mild	high	FALSE	N
sunny	cool	normal	FALSE	P
rain	mild	normal	FALSE	P
sunny	mild	normal	TRUE	P
overcast	mild	high	TRUE	P
overcast	hot	normal	FALSE	P
rain	mild	high	TRUE	N

$$\text{Entropy}(S) = -\sum_{i=1}^{K} p_i \log_2(p_i)$$

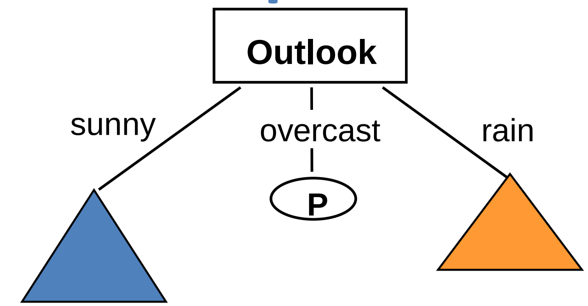
Where p_i is the probability of class i in set S.

$$E(S) = -\frac{9}{9+5} \cdot \log_2 \frac{9}{9+5} - \frac{5}{9+5} \cdot \log_2 \frac{5}{9+5} \approx 0.94$$

Entropy Calculation & ID3 Algorithm - Example

$$E(S) = -\frac{9}{9+5}\cdot\log_2\frac{9}{9+5} - \frac{5}{9+5}\cdot\log_2\frac{5}{9+5} \approx 0.94$$

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	FALSE	N
sunny	hot	high	TRUE	N
overcast	hot	high	FALSE	P
rain	mild	high	FALSE	P
rain	cool	normal	FALSE	P
rain	cool	normal	TRUE	N
overcast	cool	normal	TRUE	P
sunny	mild	high	FALSE	N
sunny	cool	normal	FALSE	P
rain	mild	normal	FALSE	P
sunny	mild	normal	TRUE	P
overcast	mild	high	TRUE	P
overcast	hot	normal	FALSE	P
rain	mild	high	TRUE	N



Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	FALSE	N
sunny	hot	high	TRUE	N
sunny	mild	high	FALSE	N
sunny	cool	normal	FALSE	P
sunny	mild	normal	TRUE	P

$$E(Sunny) = -\frac{2}{5}\cdot\log_2\frac{2}{5} - \frac{3}{5}\cdot\log_2\frac{3}{5} \approx 0.971$$

Outlook	Temperature	Humidity	Windy	Class
overcast	hot	high	FALSE	P
overcast	cool	normal	TRUE	P
overcast	mild	high	TRUE	P
overcast	hot	normal	FALSE	P

$$E(Overcast) = -\frac{4}{4}\cdot\log_2\frac{4}{4} = 0$$

Outlook	Temperature	Humidity	Windy	Class
rain	mild	high	FALSE	P
rain	cool	normal	FALSE	P
rain	cool	normal	TRUE	N
rain	mild	normal	FALSE	P
rain	mild	high	TRUE	N

$$E(Rain) = -\frac{3}{5}\cdot\log_2\frac{3}{5} - \frac{3}{5}\cdot\log_2\frac{3}{5} \approx 0.971$$

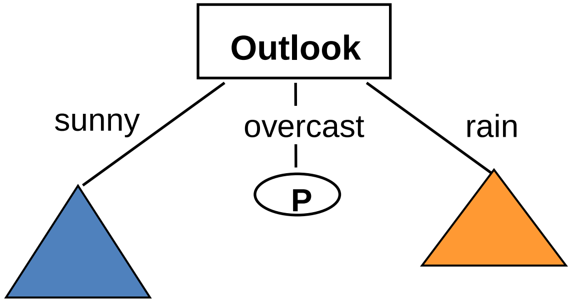
$$\boldsymbol{E(Outlook) = \frac{5}{15}\cdot E(Sunny) + \frac{5}{15}\cdot E(Overcast) + \frac{5}{15}\cdot E(Rain) = 0.694}$$

$$\boldsymbol{Gain(Outlook) = E(S) - E(Outlook) = 0.94 - 0.694 = 0.246}$$

ID3 Algorithm - Example

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	FALSE	N
sunny	hot	high	TRUE	N
overcast	hot	high	FALSE	P
rain	mild	high	FALSE	P
rain	cool	normal	FALSE	P
rain	cool	normal	TRUE	N
overcast	cool	normal	TRUE	P
sunny	mild	high	FALSE	N
sunny	cool	normal	FALSE	P
rain	mild	normal	FALSE	P
sunny	mild	normal	TRUE	P
overcast	mild	high	TRUE	P
overcast	hot	normal	FALSE	P
rain	mild	high	TRUE	N

Gain(Outlook) = 0.246
Gain(Temperature) = 0.029
Gain(Humidity) = 0.151
Gain(Windy) = 0.048
=> Outlook is chosen as the root



ID3 Algorithm - Example

Training Set(outlook=Sunny)

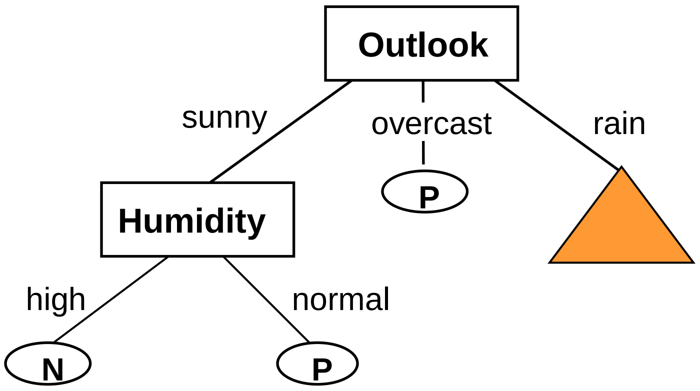
Temperature	Humidity	Windy	Class
hot	high	FALSE	N
hot	high	TRUE	N
mild	high	FALSE	N
cool	normal	FALSE	P
mild	normal	TRUE	P

Gain(Temperature) = 0.571 bits

Gain(Humidity) = 0.971 bits

Gain(Windy) = 0.020 bits

∴ Humidity is chosen as the root.



ID3 Algorithm - Example

Training Set(outlook=Rain)

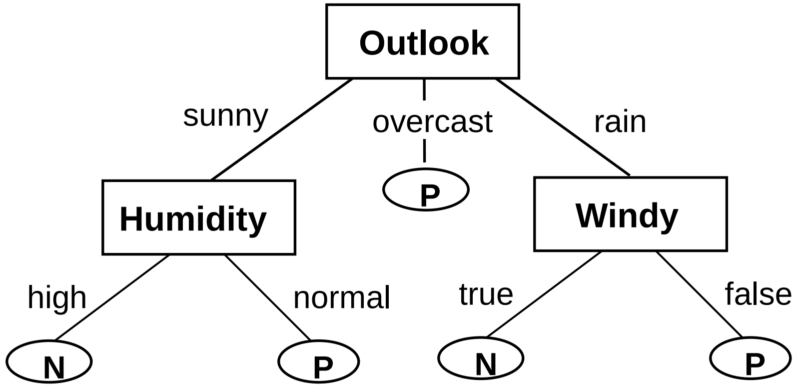
Temperature	Humidity	Windy	Class
mild	high	FALSE	P
cool	normal	FALSE	P
cool	normal	TRUE	N
mild	normal	FALSE	P
mild	high	TRUE	N

Gain(Temperature) = 0.020 bits

Gain(Humidity) = 0.020 bits

Gain(Windy) = 0.971 bits

∴ Windy is chosen as the root.



When to stop building the tree

- We built a decision tree by **recursively splitting our dataset**
  - Each split was performed by choosing the best feature to split (using accuracy, Gini index, or entropy)
  - We stop when the leaf nodes is pure (i.e., all the samples on it have the same label)
- To avoid overfitting the stop condition can be any of the following:
  - Don’t split a node if it has less than a certain number of samples
  - Split a node only if both of the resulting leaves contain at least a certain number of samples
  - Stop building the tree after you reach a certain depth
  - Don’t split a node if the change in accuracy, Gini index, or entropy is below some threshold

Decision tree algorithm

- **Feature Selection:**
  - Selects the best feature to split the dataset based on an **Attribute Selection Measure (ASM)** such as Gini impurity, or Entropy
  - Make the selected feature **a decision node** and split the dataset into smaller subsets. The algorithm needs to find the optimal **split point** that minimizes impurity (i.e., maximizes the homogeneity of subsets created after the split)
- **Splitting:**
  - At each node, the dataset is split into subsets based on the selected feature and split point
  - The process continues recursively for each spit until a stopping condition is met, such as a maximum depth, minimum number of samples per leaf, or no further improvement in impurity reduction

Decision tree algorithm

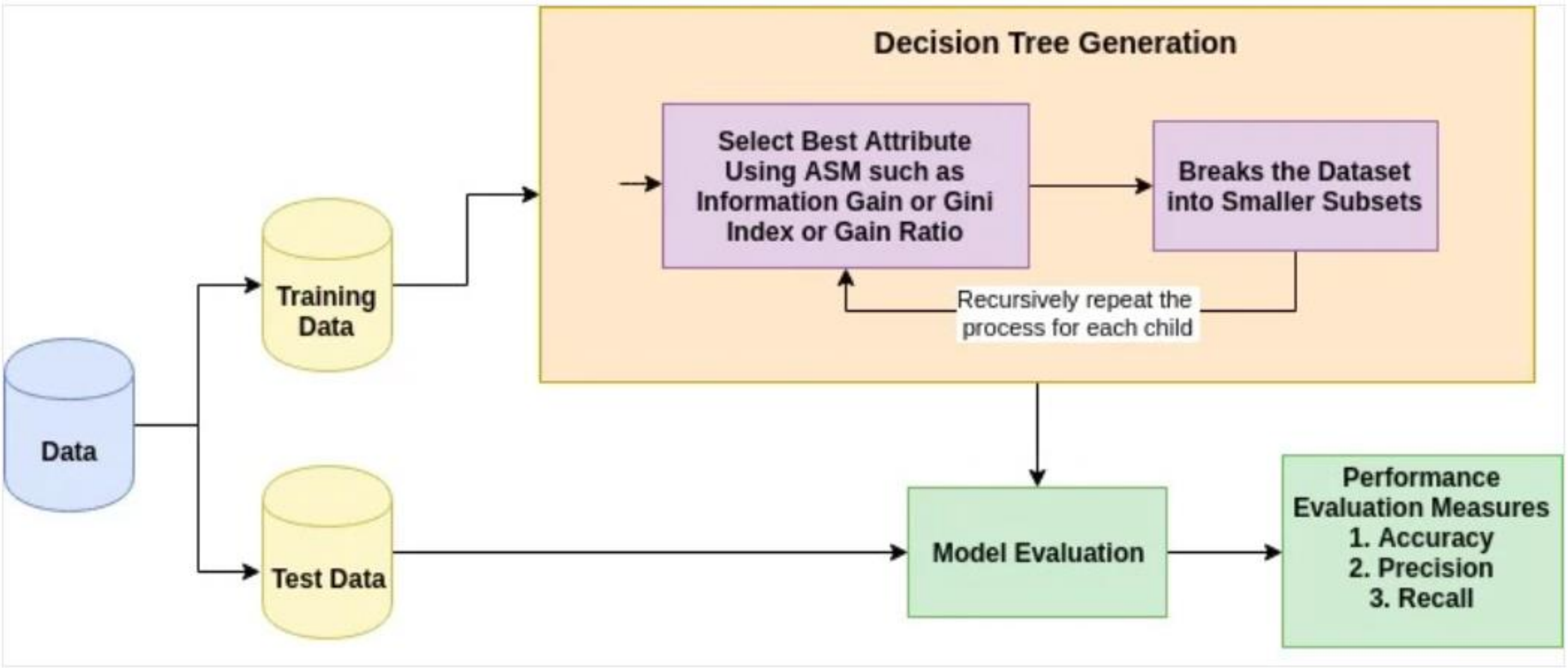
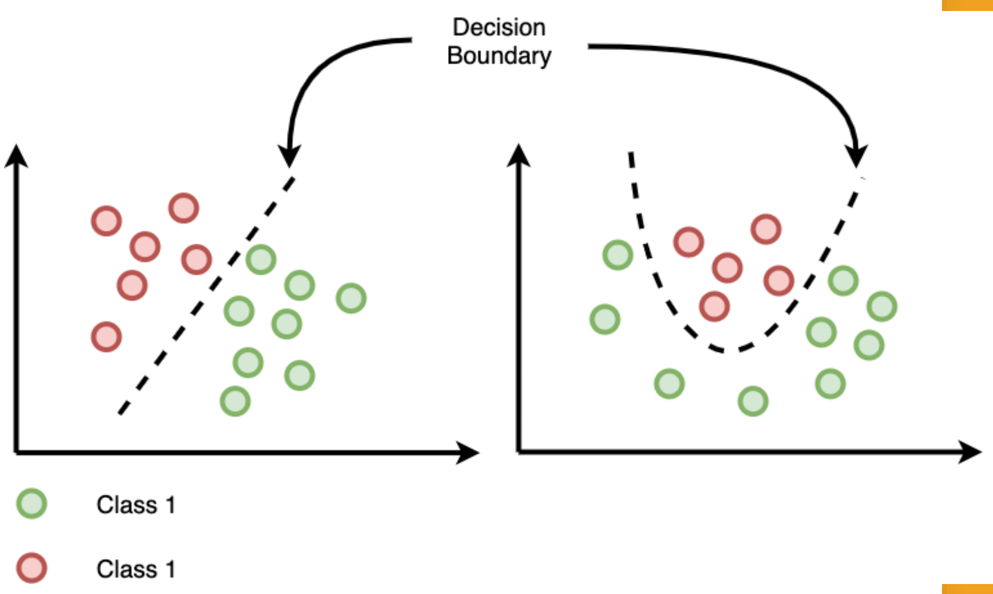


Image [source]

Decision Boundaries

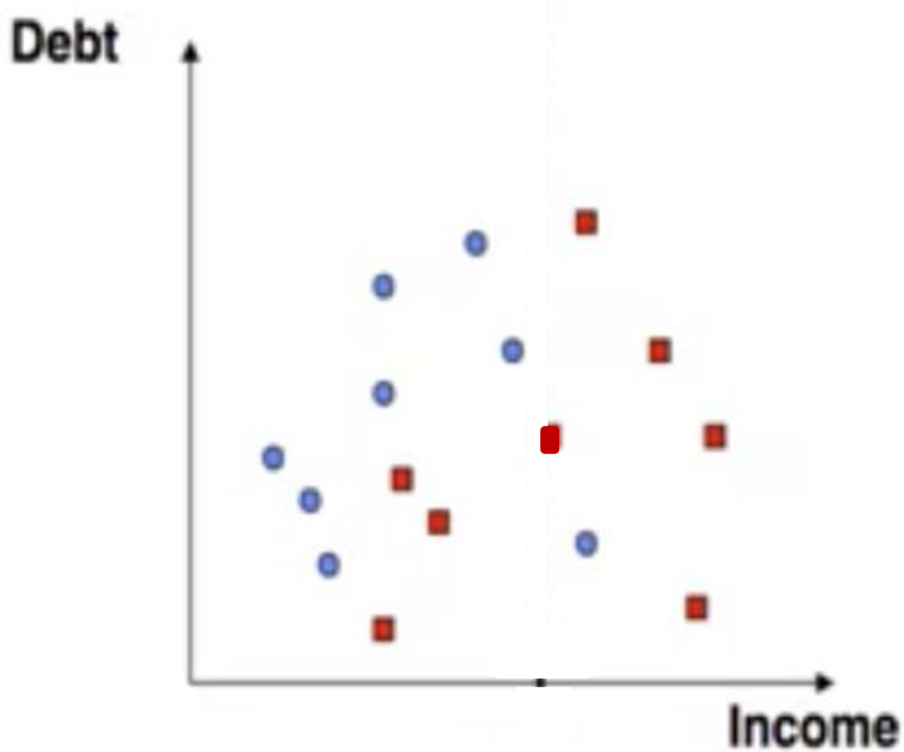


Decision Boundries (Univeriate)

- In the Decision Tree, each internal node represents a decision based on a feature (e.g., income > 100k), and each leaf node represents a class (e.g., Likely to repay)
  - The decision boundaries determined by the Decision Tree **divide the feature space into regions** corresponding to different classes

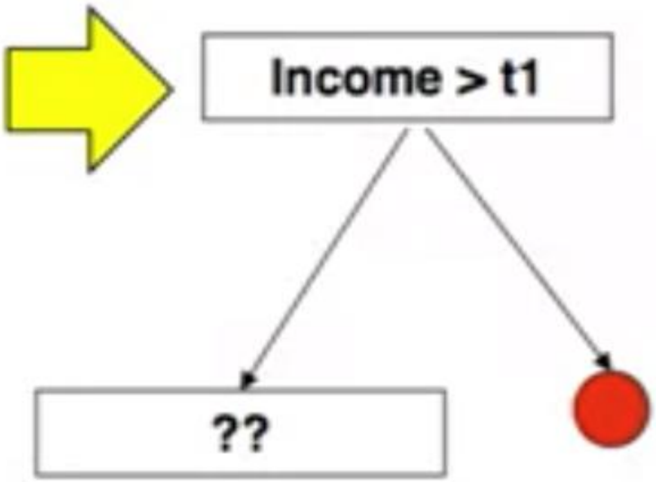
E.g., classify loan applicants to:

→ Not-/likely to repay, based on income and existing debt



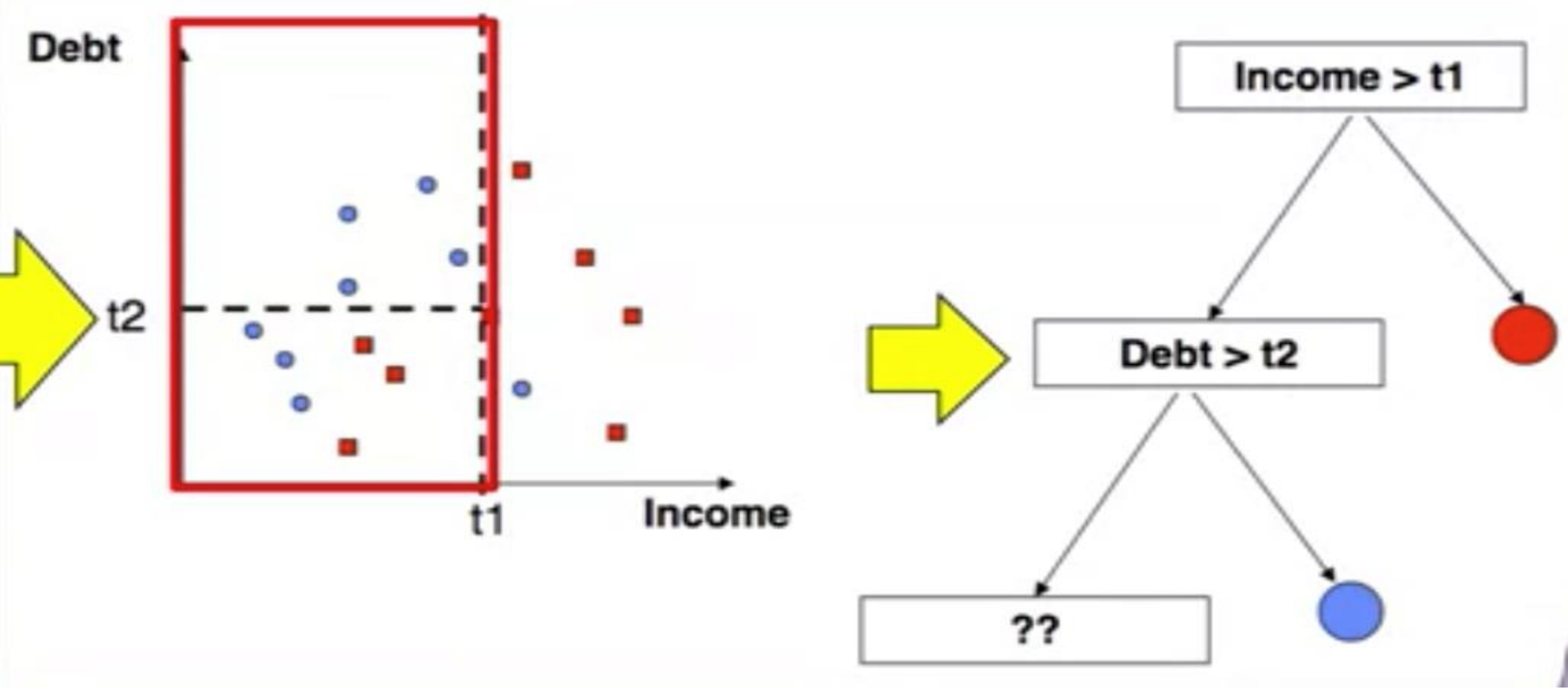
Decision Boundries (Univeriate)

- Split 1



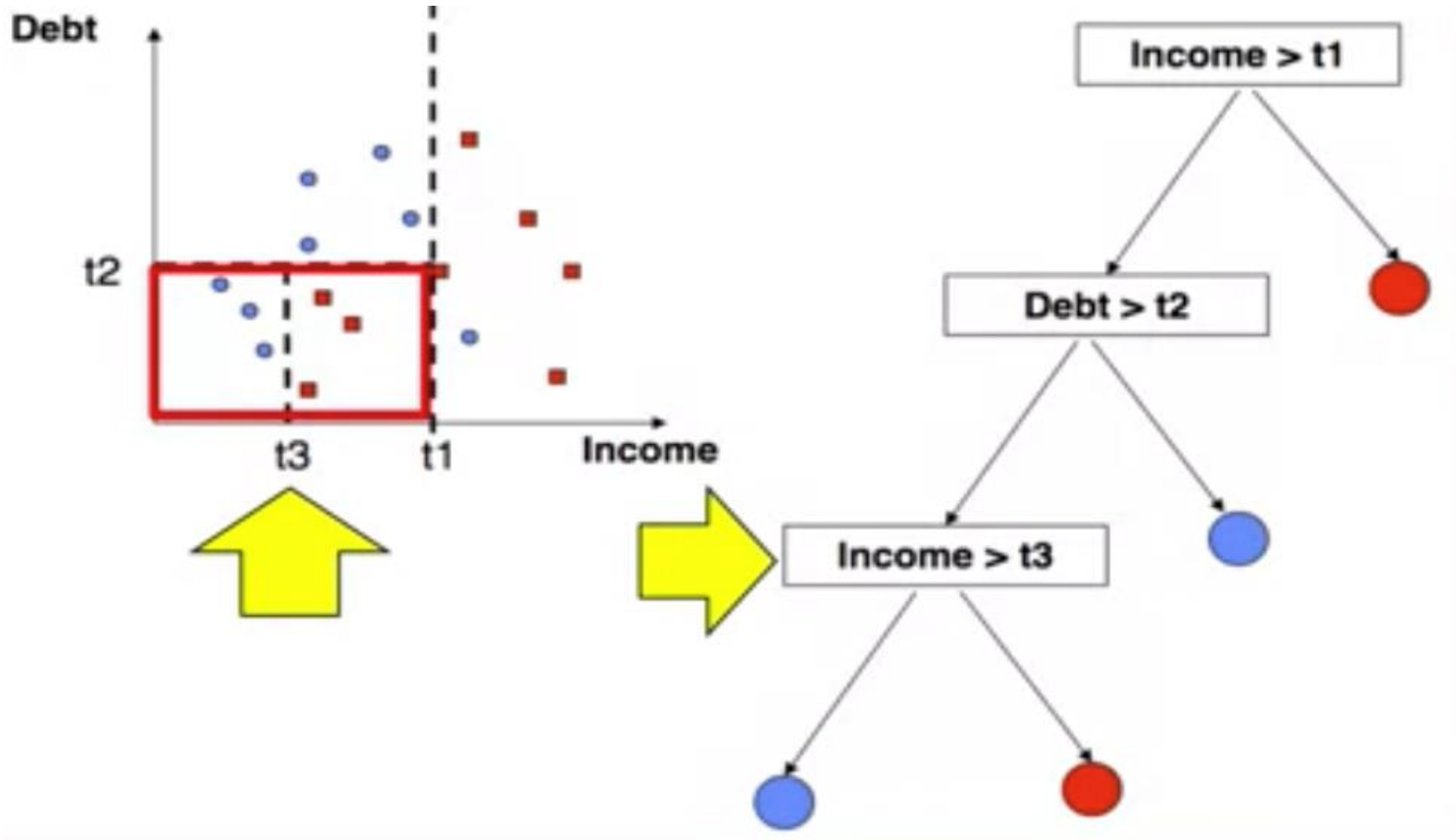
Decision Boundries (Univeriate)

- Split 2



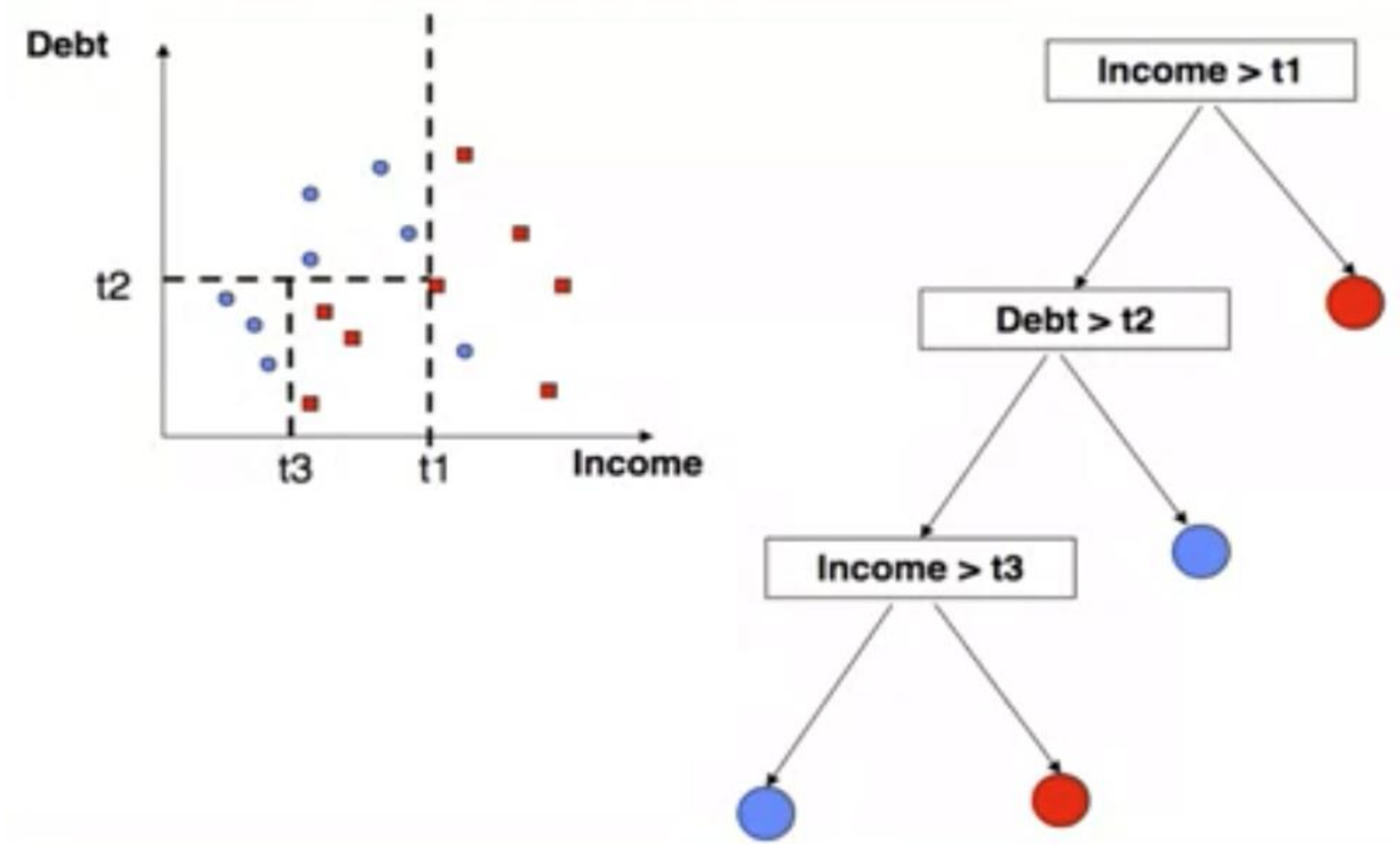
Decision Boundries (Univeriate)

- Split 3



Decision Boundries (Univeriate)

- Resulting model
  - Boundaries are “Rectilinear” = Parallel to the axes

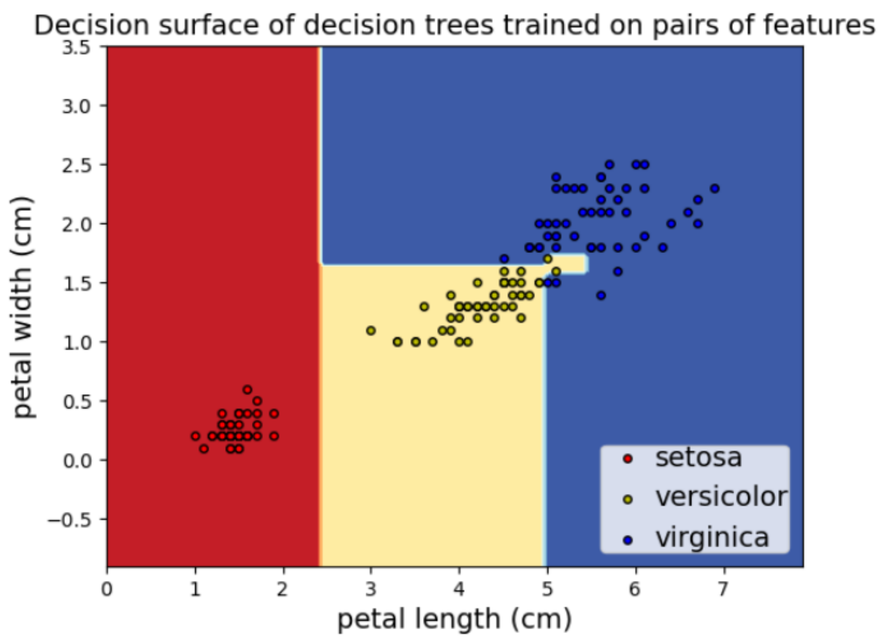


Decision Boundries (Univeriate)

In [27]:

```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from sklearn.inspection import DecisionBoundaryDisplay

# Parameters
n_classes = 3
plot_colors = "ryb"
plot_step = 0.02

pair_of_columns = [2, 3]

# We only take the two corresponding features
X = iris.data.values[:, pair]
y = iris.target
# Train
tree_clf = DecisionTreeClassifier().fit(X, y)

plt.figure(figsize=(10,8))
plot_tree(tree_clf, filled=True)
plt.title("Decision tree trained on two attributes")
plt.show()
```


```python
ax = plt.subplot(1, 1, 1)
# Plot the decision boundary
DecisionBoundaryDisplay.from_estimator(tree_clf, X, cmap=plt.cm.RdYlBu, response_method="predict",
        ax=ax,
        xlabel=iris.feature_names[pair[0]],
        ylabel=iris.feature_names[pair[1]],
    )

# Plot the training points
for i, color in zip(range(n_classes), plot_colors):
    idx = np.where(y == i)
    plt.scatter(X[idx, 0], X[idx, 1], c=color, label=iris.target_names[i],
            cmap=plt.cm.RdYlBu, edgecolor="black", s=15,)

plt.title("Decision surface of decision trees trained on pairs of features")
plt.legend(loc="lower right", borderpad=0, handletextpad=0)
plt.show()
```



Decision Boundries (Univeriate)