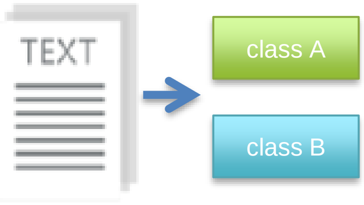
DATA SCIENCE COURSE

MACHINE LEARNING DAY 03

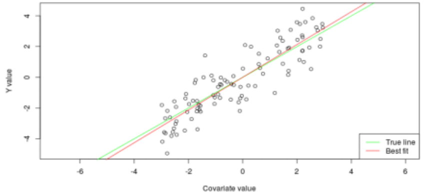
Machine Learning Types

Machine Learning Basics

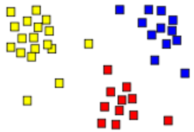
- ***Supervised***: learning with labeled data
  - Example: email classification, image classification
  - Example: regression for predicting real-valued outputs
- ***Unsupervised***: discover patterns in unlabeled data
  - Example: cluster similar data points
- ***Reinforcement learning***: learn to act based on feedback/reward
  - Example: learn to play Go



Classification



Regression



Clustering

Slide credit: Ismini Lourentzou – Introduction to Deep Learning

Decision Tree and Random Forest

Let’s play a Game!

Decision Trees

Gender	Age	App
F	15	
F	25	
M	32	
F	40	
M	12	
M	14	

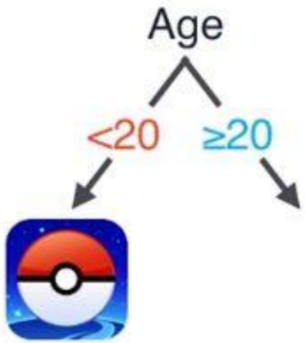
Quiz 1

Answer

Gender	Age	App
F	15	
F	25	
M	32	
F	40	
M	12	
M	14	

Gender	Age	App
F	15	
F	25	
M	32	
F	40	
M	12	
M	14	

Gender	Age	App
F	15	
F	25	
M	32	
F	40	
M	12	
M	14	



Gender	Age	App
F	25	
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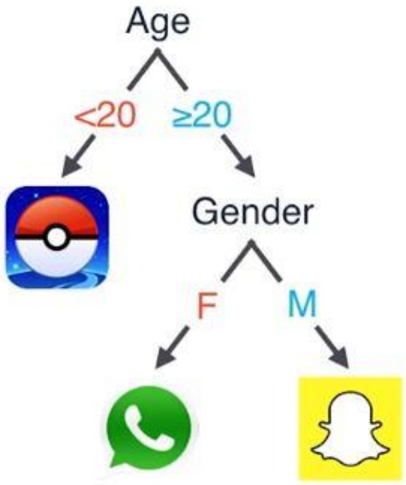
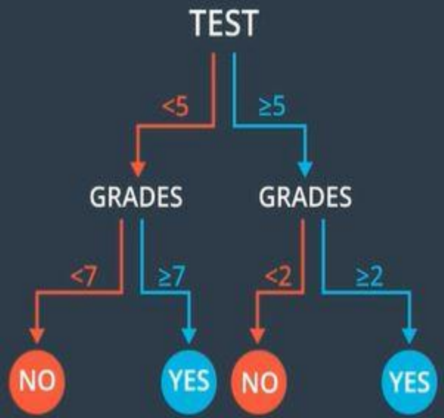
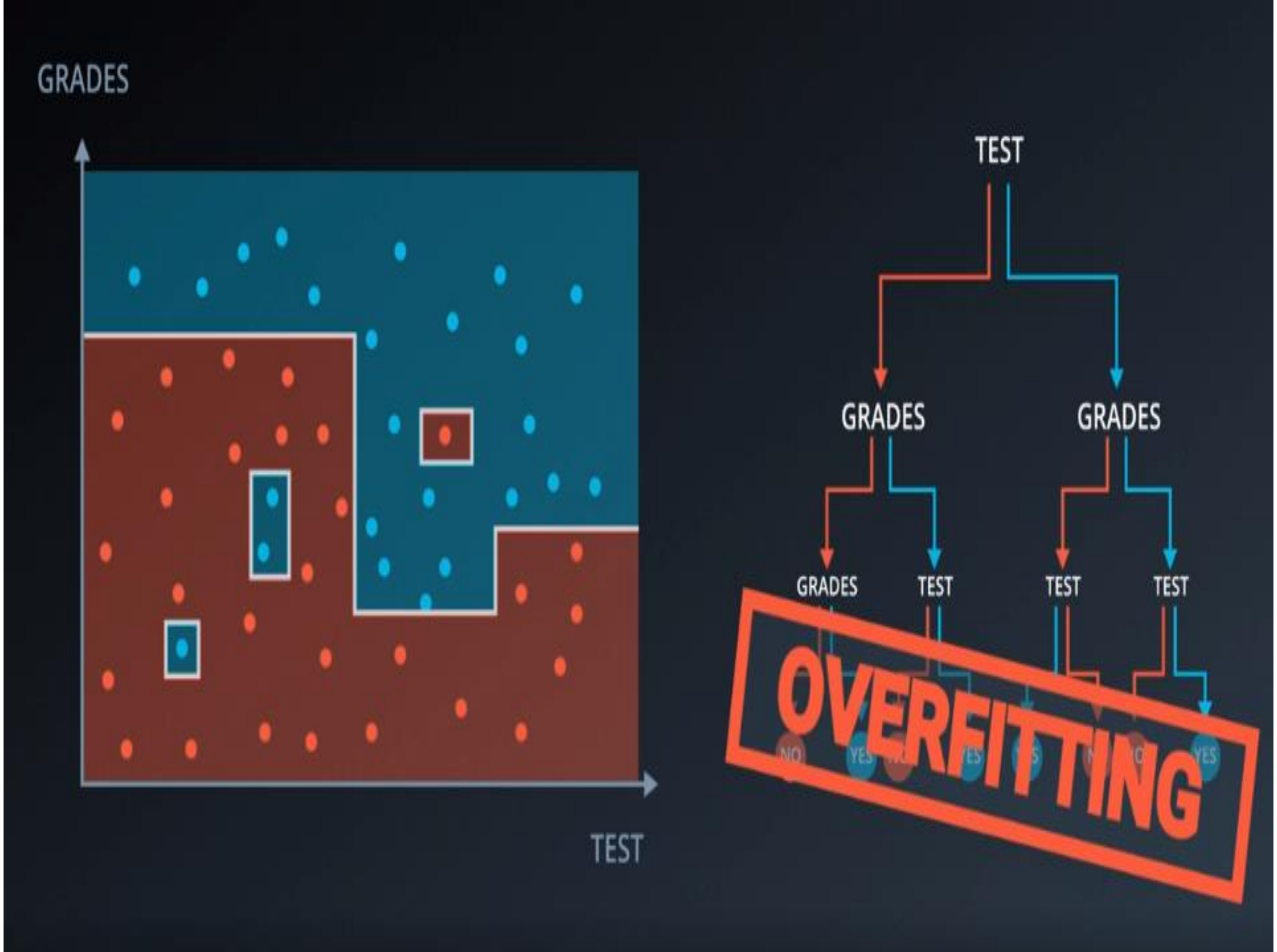


Student Admissions

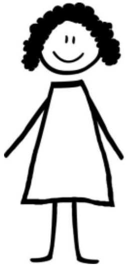



GRADES
TEST
TEST
GRADES
GRADES
GRADES
TEST
TEST
TEST
OVERFITTING

Definition

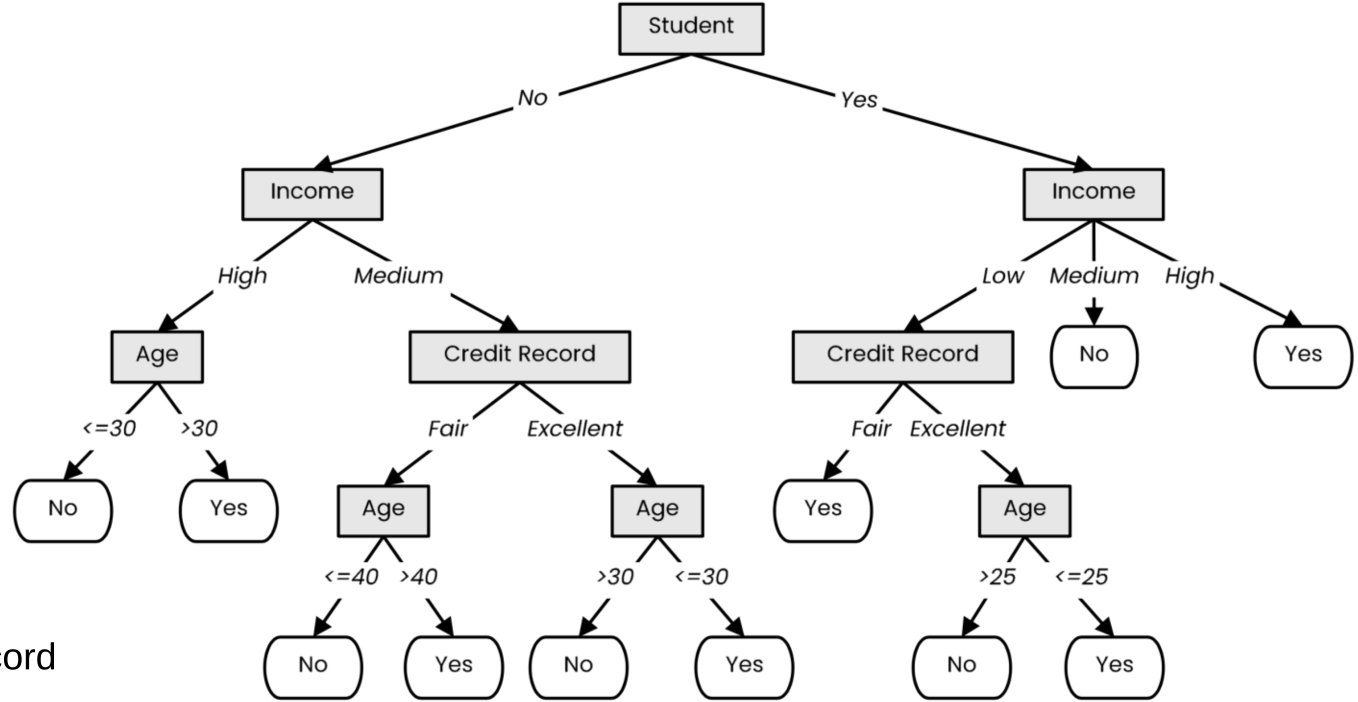
- A tree-like model that illustrates series of events leading to certain decisions
- Each node represents a test on an attribute and each branch is an outcome of that test

Who to loan?



- Not a student
- 45 years old
- Medium income
- Fair credit record

- Student
- 27 years old
- Low income
- Excellent credit record



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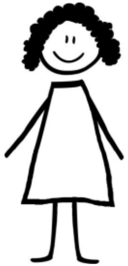

- Not a student
- 45 years old
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- Fair credit record
- ➢ Yes

- Student
- 27 years old
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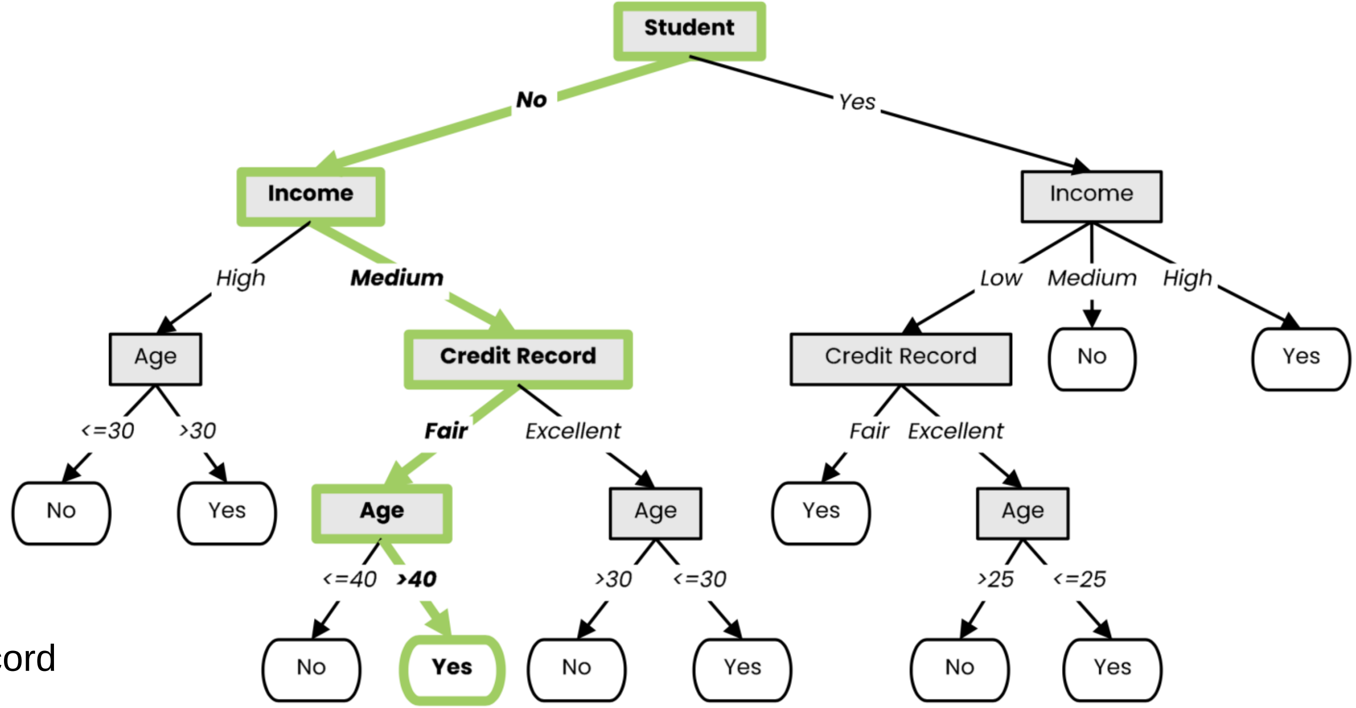

Definition

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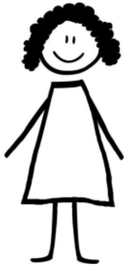
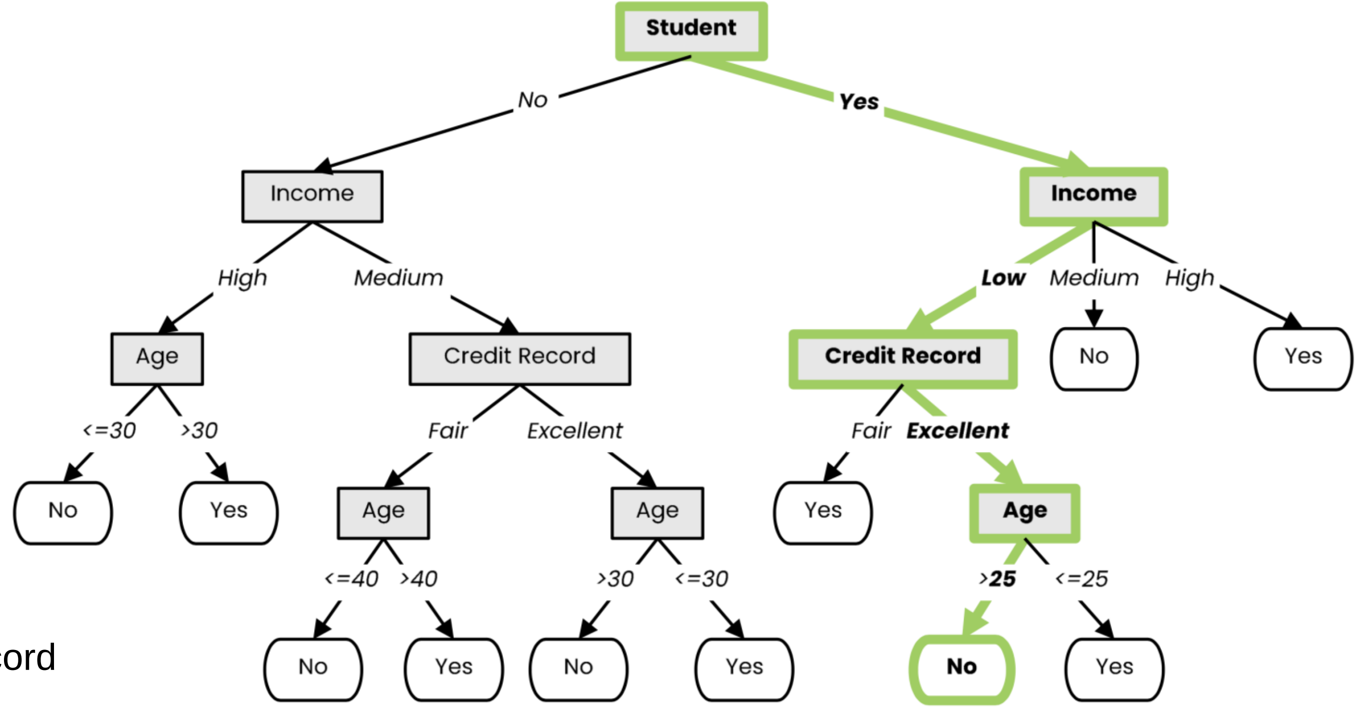
Who to loan?



- Not a student
- 45 years old
- Medium income
- Fair credit record
- ➢ Yes

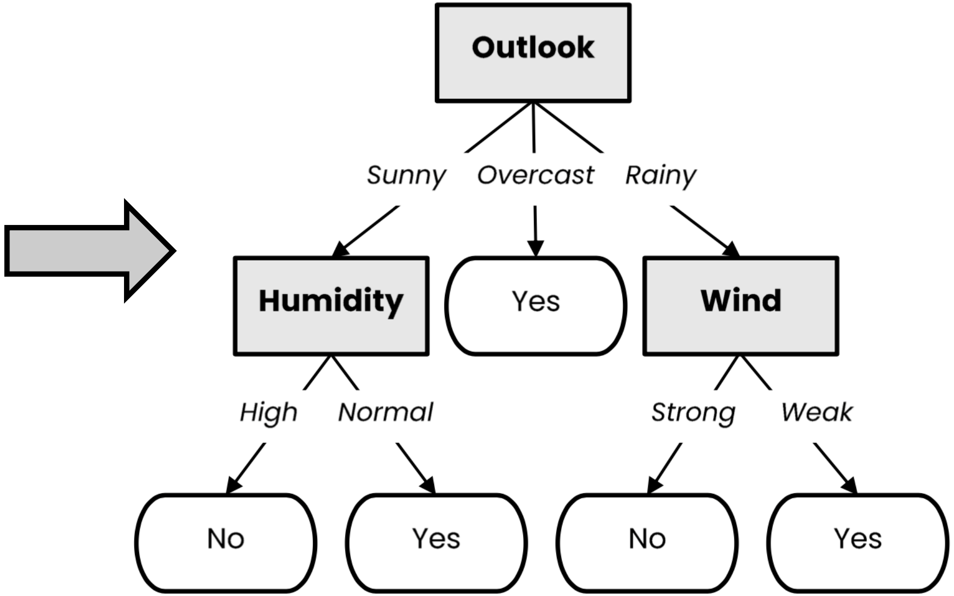
- Student
- 27 years old
- Low income
- Excellent credit record
- ➢ No



Decision Tree Learning

- We use labeled data to obtain a suitable decision tree for future predictions
  - ➢ We want a decision tree that works well on unseen data, while asking as few questions as possible

Outlook	Temperature	Humidity	Wind	Play Tennis?
Sunny	Hot	High	Weak	**No**
Sunny	Hot	High	Strong	**No**
Overcast	Hot	High	Weak	**Yes**
Rainy	Mild	High	Weak	**Yes**
Rainy	Cool	Normal	Weak	**Yes**
Rainy	Cool	Normal	Strong	**No**
Overcast	Cool	Normal	Strong	**Yes**
Sunny	Mild	High	Weak	**No**
Sunny	Cool	Normal	Weak	**Yes**
Rainy	Mild	Normal	Weak	**Yes**
Sunny	Mild	Normal	Strong	**Yes**
Overcast	Mild	High	Strong	**Yes**
Overcast	Hot	Normal	Weak	**Yes**
Rainy	Mild	High	Strong	**No**



Decision Tree Learning

- Basic step: choose an attribute and, based on its values, split the data into smaller sets
  - ➢ Recursively repeat this step until we can surely decide the label

Outlook	Temperature	Humidity	Wind	Play Tennis?
Sunny	Hot	High	Weak	**No**
Sunny	Hot	High	Strong	**No**
Overcast	Hot	High	Weak	**Yes**
Rainy	Mild	High	Weak	**Yes**
Rainy	Cool	Normal	Weak	**Yes**
Rainy	Cool	Normal	Strong	**No**
Overcast	Cool	Normal	Strong	**Yes**
Sunny	Mild	High	Weak	**No**
Sunny	Cool	Normal	Weak	**Yes**
Rainy	Mild	Normal	Weak	**Yes**
Sunny	Mild	Normal	Strong	**Yes**
Overcast	Mild	High	Strong	**Yes**
Overcast	Hot	Normal	Weak	**Yes**
Rainy	Mild	High	Strong	**No**

Outlook

Decision Tree Learning

- Basic step: choose an attribute and, based on its values, split the data into smaller sets
  - ➢ Recursively repeat this step until we can surely decide the label

Outlook = *Sunny*

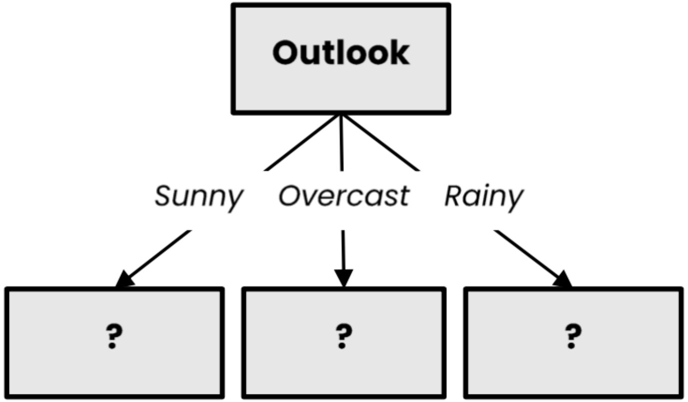
Temperature	Humidity	Wind	Play Tennis?
Hot	High	Weak	**No**
Hot	High	Strong	**No**
Mild	High	Weak	**No**
Cool	Normal	Weak	**Yes**
Mild	Normal	Strong	**Yes**

Outlook = *Overcast*

Temperature	Humidity	Wind	Play Tennis?
Hot	High	Weak	**Yes**
Cool	Normal	Strong	**Yes**
Mild	High	Strong	**Yes**
Hot	Normal	Weak	**Yes**

Outlook = *Rainy*

Temperature	Humidity	Wind	Play Tennis?
Mild	High	Weak	**Yes**
Cool	Normal	Weak	**Yes**
Cool	Normal	Strong	**No**
Mild	Normal	Weak	**Yes**
Mild	High	Strong	**No**



Decision Tree Learning

- Basic step: choose an attribute and, based on its values, split the data into smaller sets
  - ➢ Recursively repeat this step until we can surely decide the label

Outlook = *Sunny*

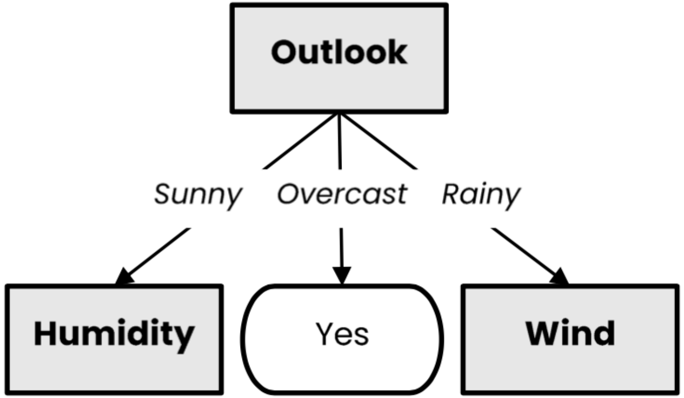
Temperature	Humidity	Wind	Play Tennis?
Hot	High	Weak	**No**
Hot	High	Strong	**No**
Mild	High	Weak	**No**
Cool	Normal	Weak	**Yes**
Mild	Normal	Strong	**Yes**

Outlook = *Overcast*

Temperature	Humidity	Wind	Play Tennis?
Hot	High	Weak	**Yes**
Cool	Normal	Strong	**Yes**
Mild	High	Strong	**Yes**
Hot	Normal	Weak	**Yes**

Outlook = *Rainy*

Temperature	Humidity	Wind	Play Tennis?
Mild	High	Weak	**Yes**
Cool	Normal	Weak	**Yes**
Cool	Normal	Strong	**No**
Mild	Normal	Weak	**Yes**
Mild	High	Strong	**No**



Decision Tree Learning

- Basic step: choose an attribute and, based on its values, split the data into smaller sets
  - ➢ Recursively repeat this step until we can surely decide the label

Outlook = *Sunny*

Humidity = High

Temperature	Wind	Play Tennis?
Hot	Weak	**No**
Hot	Strong	**No**
Mild	Weak	**No**

Humidity = Normal

Temperature	Wind	Play Tennis?
Cool	Weak	**Yes**
Mild	Strong	**Yes**

Outlook = *Overcast*

Temperature	Humidity	Wind	Play Tennis?
Hot	High	Weak	**Yes**
Cool	Normal	Strong	**Yes**
Mild	High	Strong	**Yes**
Hot	Normal	Weak	**Yes**

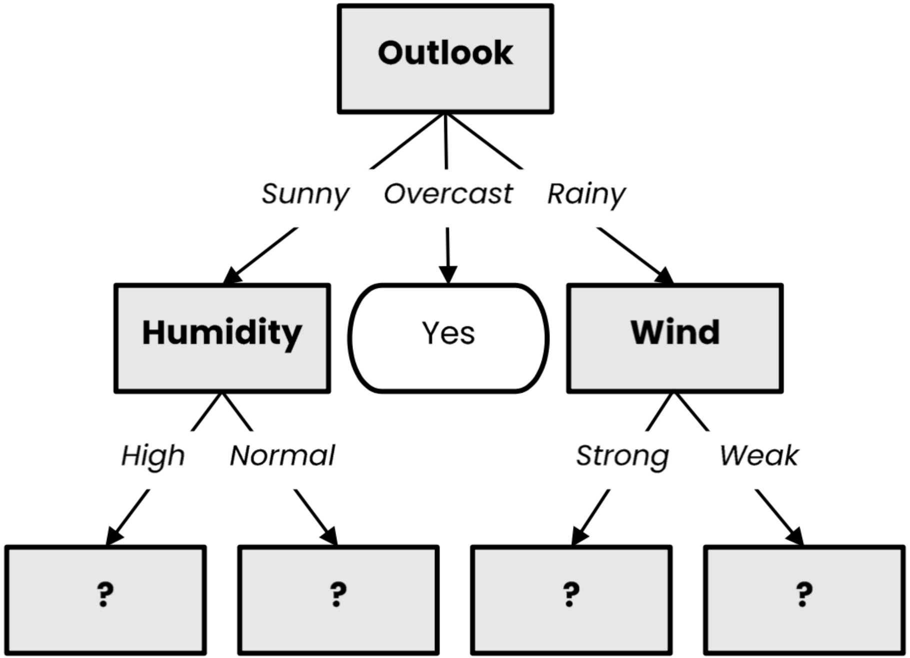
Outlook = *Rainy*

Wind = Strong

Temperature	Humidity	Play Tennis?
Cool	Normal	**No**
Mild	High	**No**

Wind = Weak

Temperature	Humidity	Play Tennis?
Mild	High	**Yes**
Cool	Normal	**Yes**
Mild	Normal	**Yes**



Decision Tree Learning

- Basic step: choose an attribute and, based on its values, split the data into smaller sets
  - ➢ Recursively repeat this step until we can surely decide the label

Outlook = *Sunny*

Humidity = High

Temperature	Wind	Play Tennis?
Hot	Weak	**No**
Hot	Strong	**No**
Mild	Weak	**No**

Humidity = Normal

Temperature	Wind	Play Tennis?
Cool	Weak	**Yes**
Mild	Strong	**Yes**

Outlook = *Overcast*

Temperature	Humidity	Wind	Play Tennis?
Hot	High	Weak	**Yes**
Cool	Normal	Strong	**Yes**
Mild	High	Strong	**Yes**
Hot	Normal	Weak	**Yes**

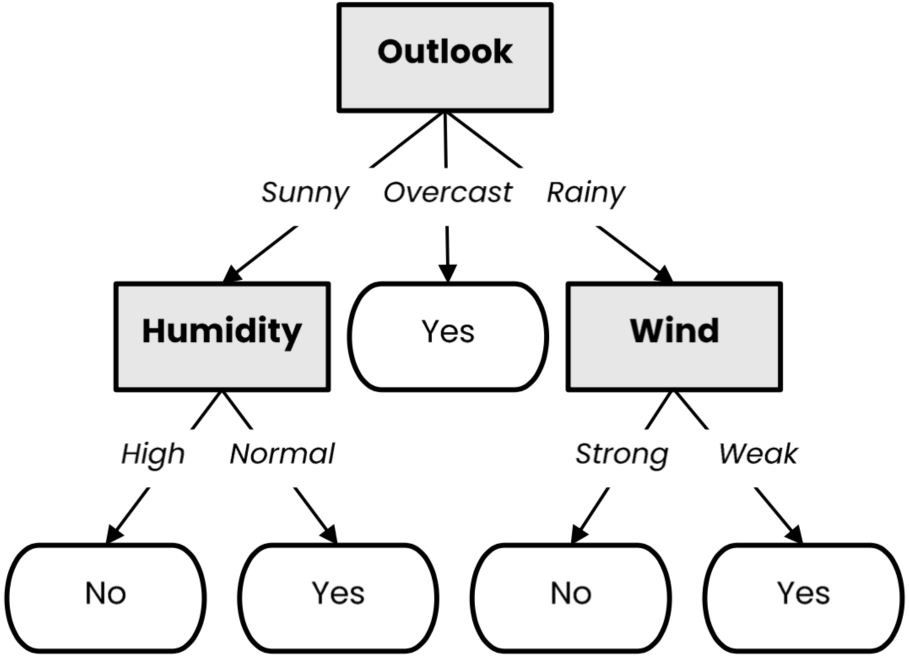
Outlook = *Rainy*

Wind = Strong

Temperature	Humidity	Play Tennis?
Cool	Normal	**No**
Mild	High	**No**

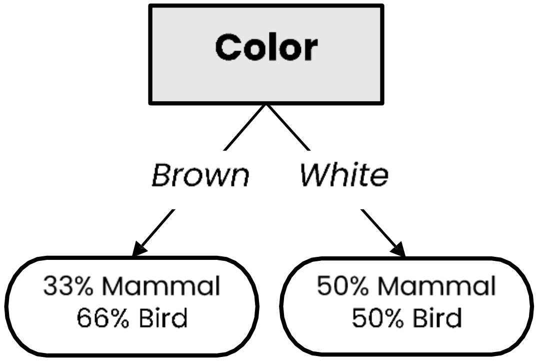
Wind = Weak

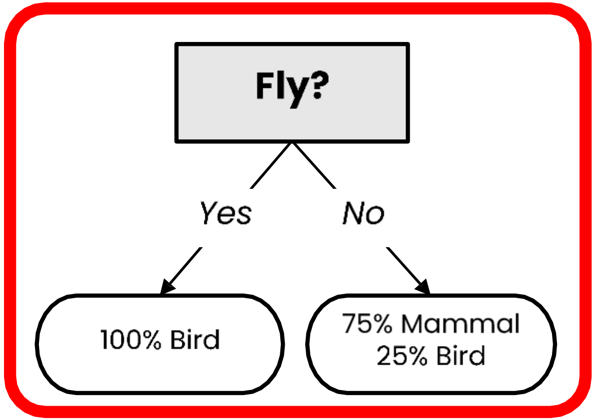
Temperature	Humidity	Play Tennis?
Mild	High	**Yes**
Cool	Normal	**Yes**
Mild	Normal	**Yes**



What is a good attribute?

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**





- Which attribute provides better splitting?
- Why?
  - ➢ Because the resulting subsets are more pure
  - ➢ Knowing the value of this attribute gives us more information about the label (the entropy of the subsets is lower)

Information Gain

Entropy

- Entropy measures the degree of randomness in data

- For a set of samples X with k classes:

$$entropy(X) = -\sum_{i=1}^{k} p_i \log_2(p_i)$$

where p_i is the proportion of elements of class i

- Lower entropy implies greater predictability!

Information Gain

- The information gain of an attribute a is the expected reduction in entropy due to splitting on values of a:

$$gain(X, a) = entropy(X) - \sum_{v \in Values(a)} \frac{|X_v|}{|X|} entropy(X_v)$$

where X_v is the subset of X for which $a = v$

Best attribute = highest information gain

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**

$$entropy\,(X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\,\log_2 \frac{3}{7} - \frac{4}{7} \log_2 \frac{4}{7} \approx 0.985$$

Best attribute = highest information gain

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
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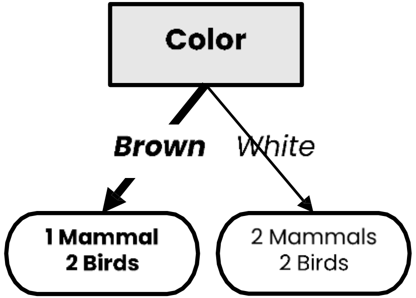
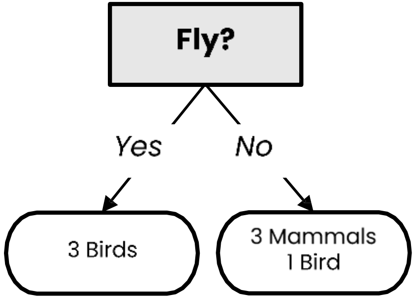


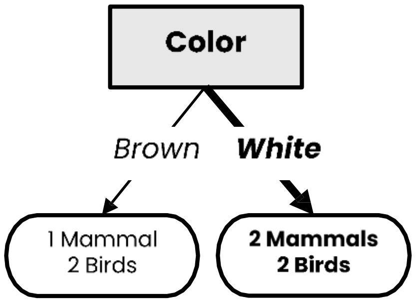


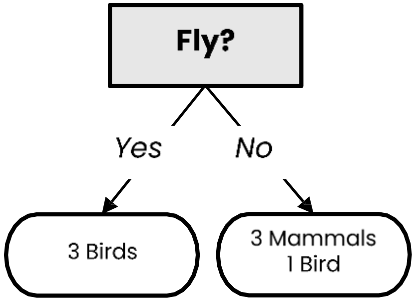
$$entropy\ (X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\ \log_2 \frac{3}{7} - \frac{4}{7} \log_2 \frac{4}{7} \approx\ 0.985$$

$$entropy\ (X_{color=brown})\ = -\frac{1}{3}\ \log_2 \frac{1}{3} - \frac{2}{3}\ \log_2 \frac{2}{3} \approx\ 0.918$$

Best attribute = highest information gain

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**



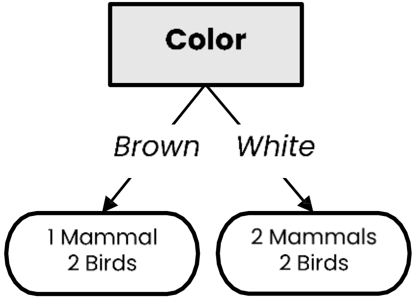


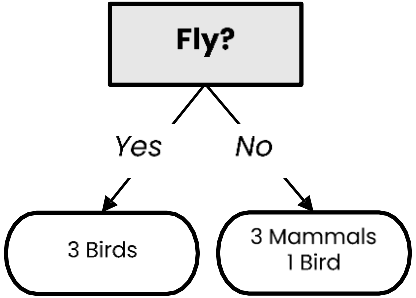
$$entropy\ (X) = -p_{\mathrm{mammal}} \log_2 p_{\mathrm{mammal}} - p_{\mathrm{bird}} \log_2 p_{\mathrm{bird}} = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} \approx 0.985$$

$$entropy\ (X_{color=brown}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad entropy\ (X_{color=white}) = 1$$

Best attribute = highest information gain

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**





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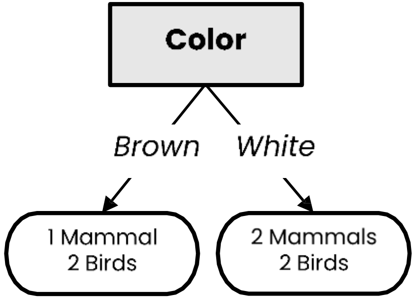
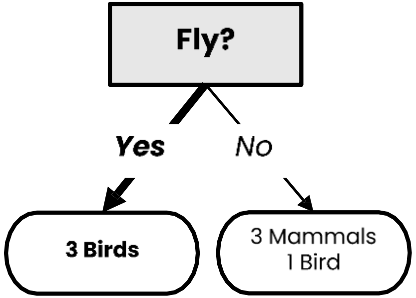
$$entropy\,(X_{color=brown}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad entropy\,(X_{color=white}) = 1$$

$$\boldsymbol{gain\,(X, color) = 0.985 - \frac{3}{7}\cdot 0.918 - \frac{4}{7}\cdot 1 \approx 0.020}$$

Best attribute = highest information gain

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**





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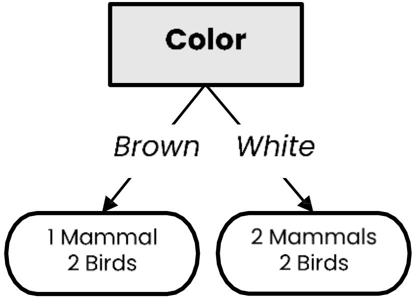
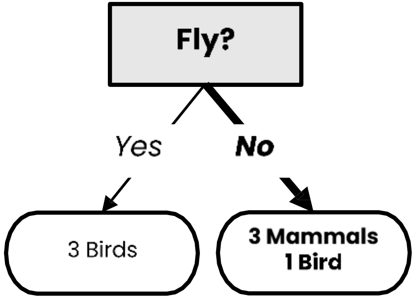
$$\boldsymbol{gain\ (X, color) = 0.985 - \frac{3}{7} \cdot 0.918 - \frac{4}{7} \cdot 1 \approx 0.020}$$

$$entropy\ (X_{fly=yes}) = 0$$

Best attribute = highest information gain

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**





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$$entropy\ (X_{color=brown}) = -\frac{1}{3} \log_2 \frac{1}{3} - \frac{2}{3} \log_2 \frac{2}{3} \approx 0.918 \qquad entropy\ (X_{color=white}) = 1$$

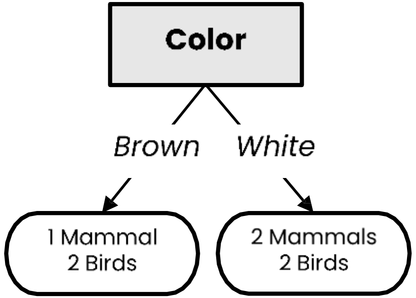
$$\boldsymbol{gain\ (X, color) = 0.985 - \frac{3}{7} \cdot 0.918 - \frac{4}{7} \cdot 1 \approx 0.020}$$

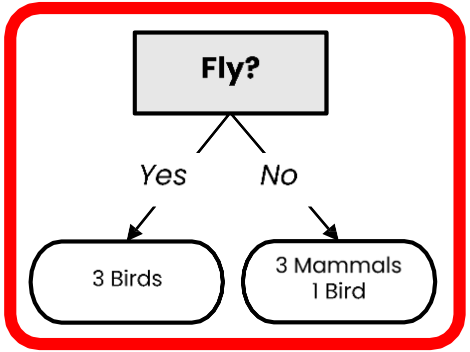
$$entropy\ (X_{fly=yes}) = 0 \qquad entropy\ (X_{fly=no}) = -\frac{3}{4} \log_2 \frac{3}{4} - \frac{1}{4} \log_2 \frac{1}{4} \approx 0.811$$

Best attribute = highest information gain

In practice, we compute $entropy(X)$ only once!

Does it fly?	Color	Class
No	Brown	**Mammal**
No	White	**Mammal**
Yes	Brown	**Bird**
Yes	White	**Bird**
No	White	**Mammal**
No	Brown	**Bird**
Yes	White	**Bird**





$$entropy\,(X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} \approx 0.985$$

$$entropy\,(X_{color=brown}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad entropy\,(X_{color=white}) = 1$$

$$\boldsymbol{gain\,(X, color) = 0.985 - \frac{3}{7}\cdot 0.918 - \frac{4}{7}\cdot 1 \approx 0.020}$$

$$entropy\,(X_{fly=yes}) = 0 \qquad entropy\,(X_{fly=no}) = -\frac{3}{4}\log_2\frac{3}{4} - \frac{1}{4}\log_2\frac{1}{4} \approx 0.811$$

$$\boldsymbol{gain\,(X, fly) = 0.985 - \frac{3}{7}\cdot 0 - \frac{4}{7}\cdot 0.811 \approx \boxed{0.521}}$$

Gini Impurity

Gini Impurity

- Gini impurity measures how often a randomly chosen example would be incorrectly labeled if it was randomly labeled according to the label distribution

Error of classifying randomly picked fruit with randomly picked label

- For a set of samples X with k classes:

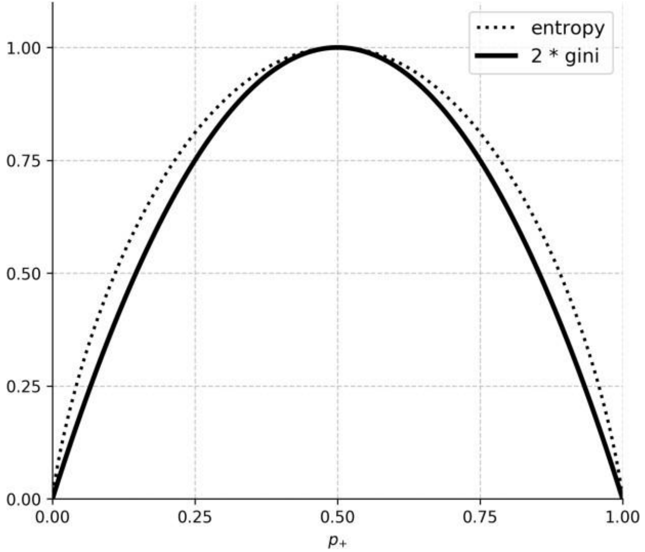
$$gini(X) = 1 - \sum_{i=1}^{k} p_i^2$$

where p_i is the proportion of elements of class i

- Can be used as an alternative to entropy for selecting attributes!

Entropy versus Gini Impurity

- Entropy and Gini Impurity give similar results in practice
  - They only disagree in about 2% of cases
    "Theoretical Comparison between the Gini Index and Information Gain Criteria" [Răileanu & Stoffel, AMAI 2004]
  - Entropy might be slower to compute, because of the log



Pruning

Pruning

- Pruning is a technique that reduces the size of a decision tree by removing branches of the tree which provide little predictive power
- It is a **regularization** method that reduces the complexity of the final model, thus reducing overfitting
  - Decision trees are prone to overfitting!

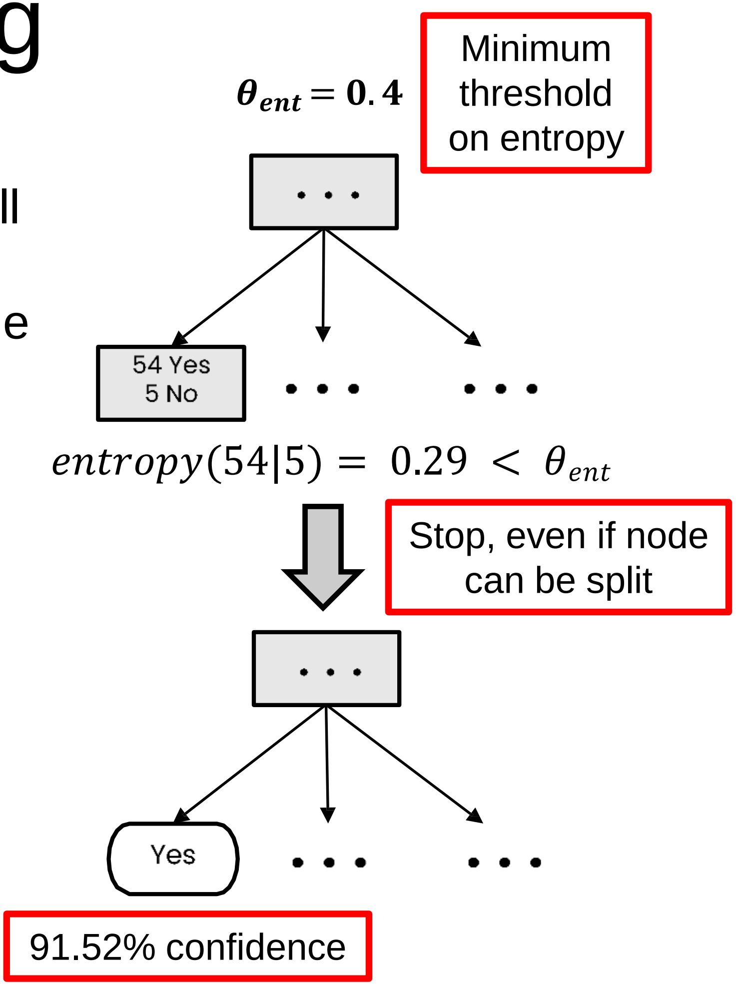
- Pruning methods:
  - Pre-pruning: Stop the tree building algorithm before it fully classifies the data
  - Post-pruning: Build the complete tree, then replace some non-leaf nodes with leaf nodes if this improves validation error

Pre-pruning

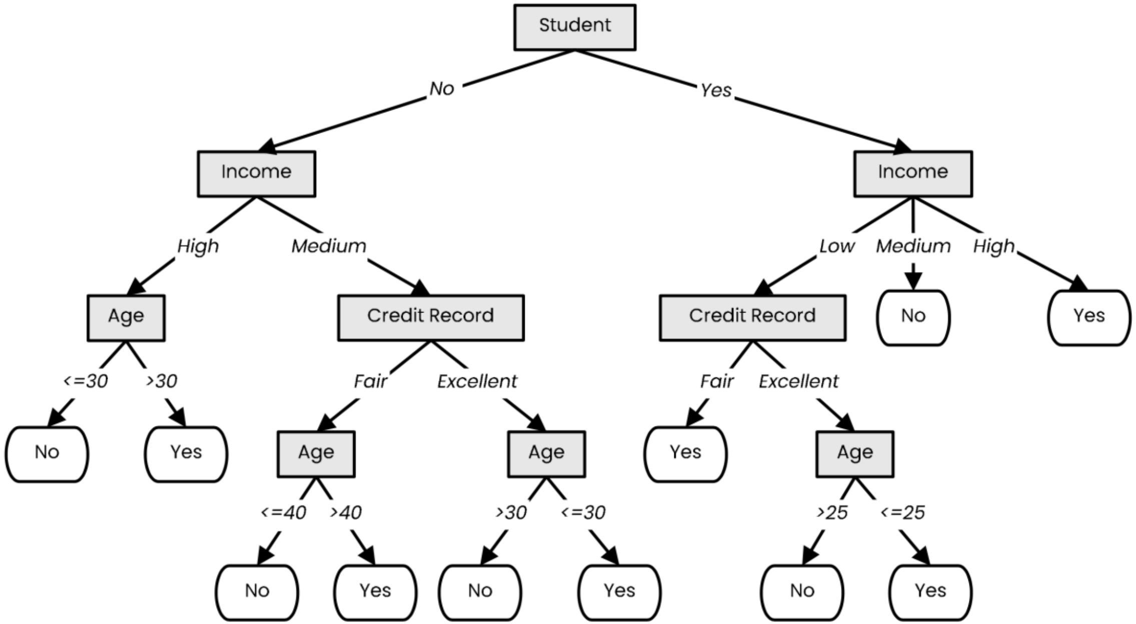
- Pre-pruning implies early stopping:
  - ➢ If some condition is met, the current node will not be split, even if it is not 100% pure
  - ➢ It will become a leaf node with the label of the majority class in the current set

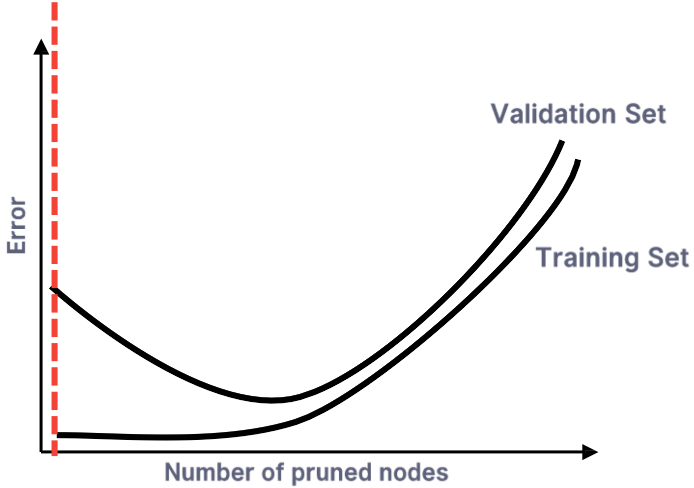
(the class distribution could be used as prediction confidence)

- Common stopping criteria include setting a threshold on:
  - ➢ Entropy (or Gini Impurity) of the current set
  - ➢ Number of samples in the current set
  - ➢ Gain of the best-splitting attribute
  - ➢ Depth of the tree



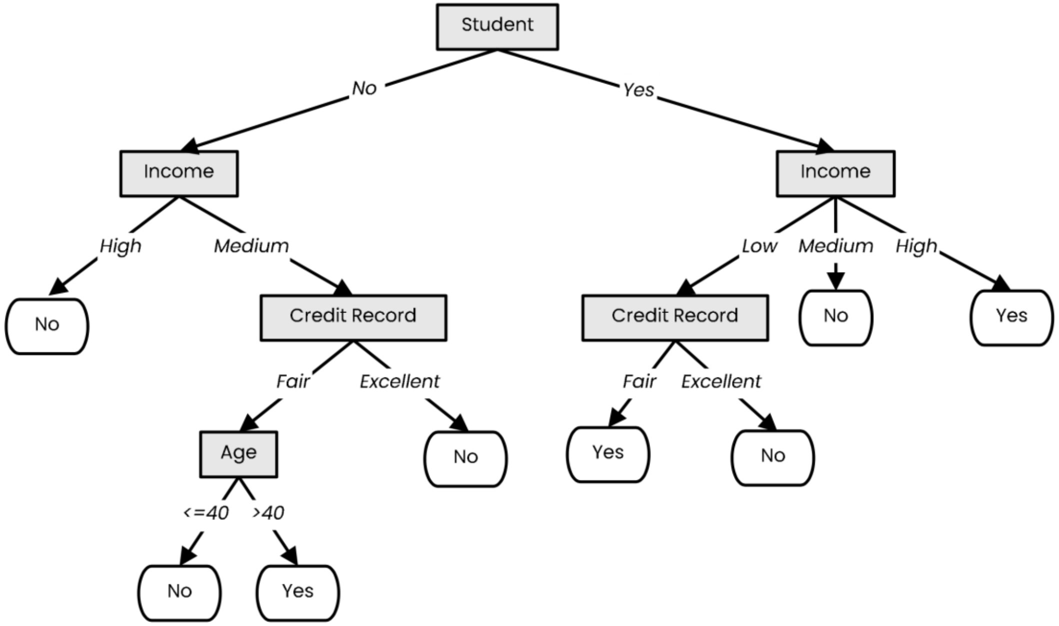
Post-pruning

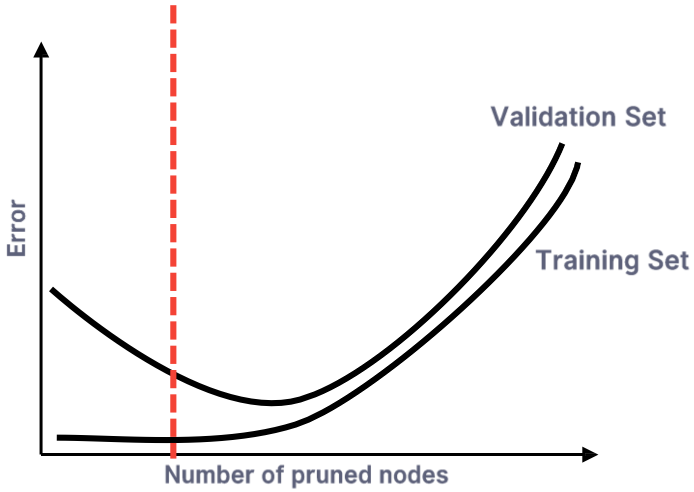




- Prune nodes in a bottom-up manner, if it decreases validation error

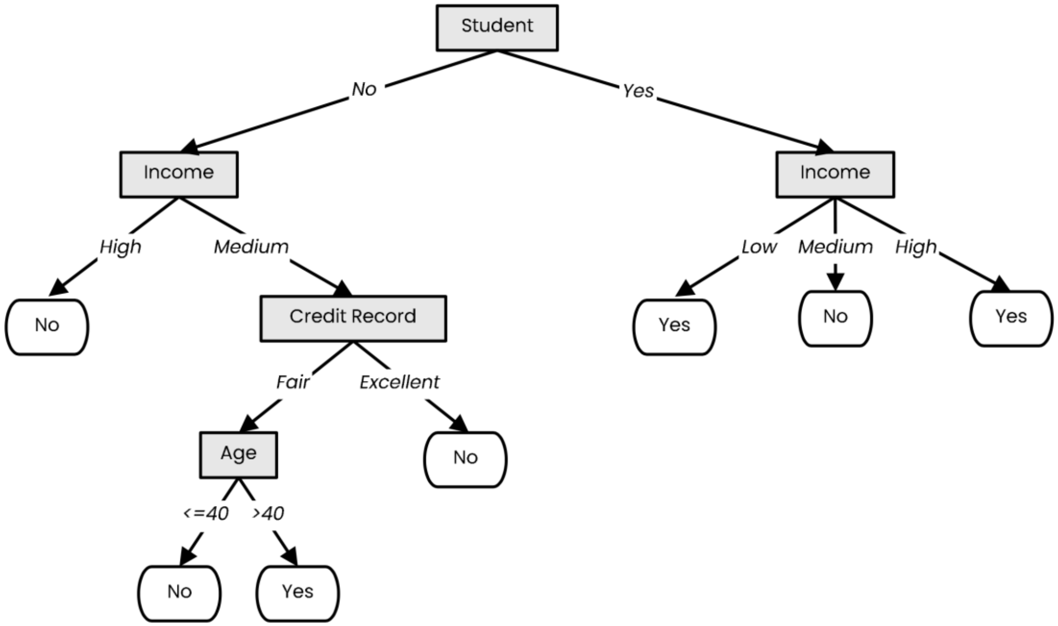
Post-pruning

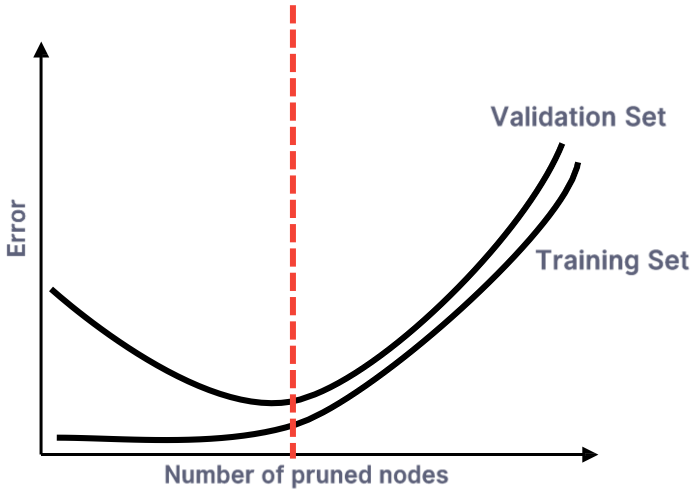




- Prune nodes in a bottom-up manner, if it decreases validation error

Post-pruning



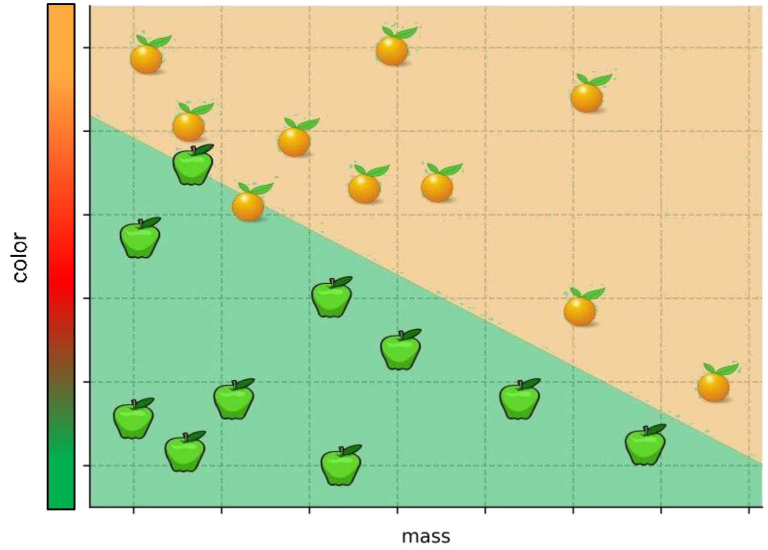


- Prune nodes in a bottom-up manner, if it decreases validation error

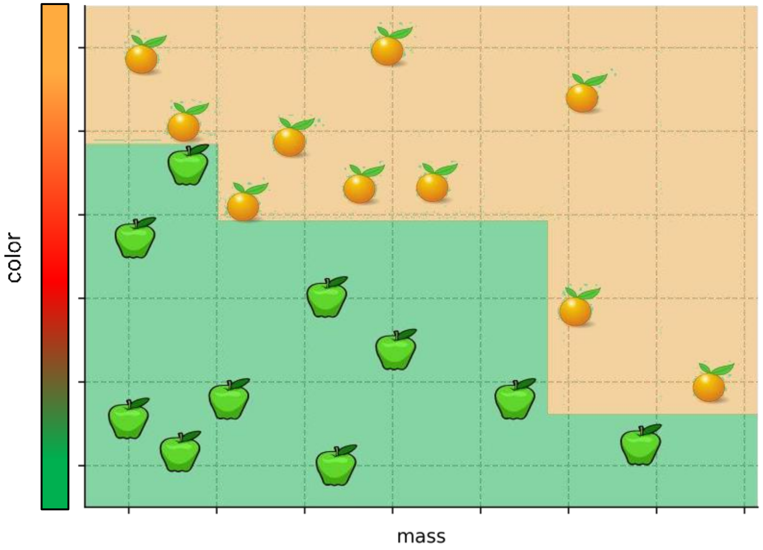
Decision Boundaries

- Decision trees produce non-linear decision boundaries

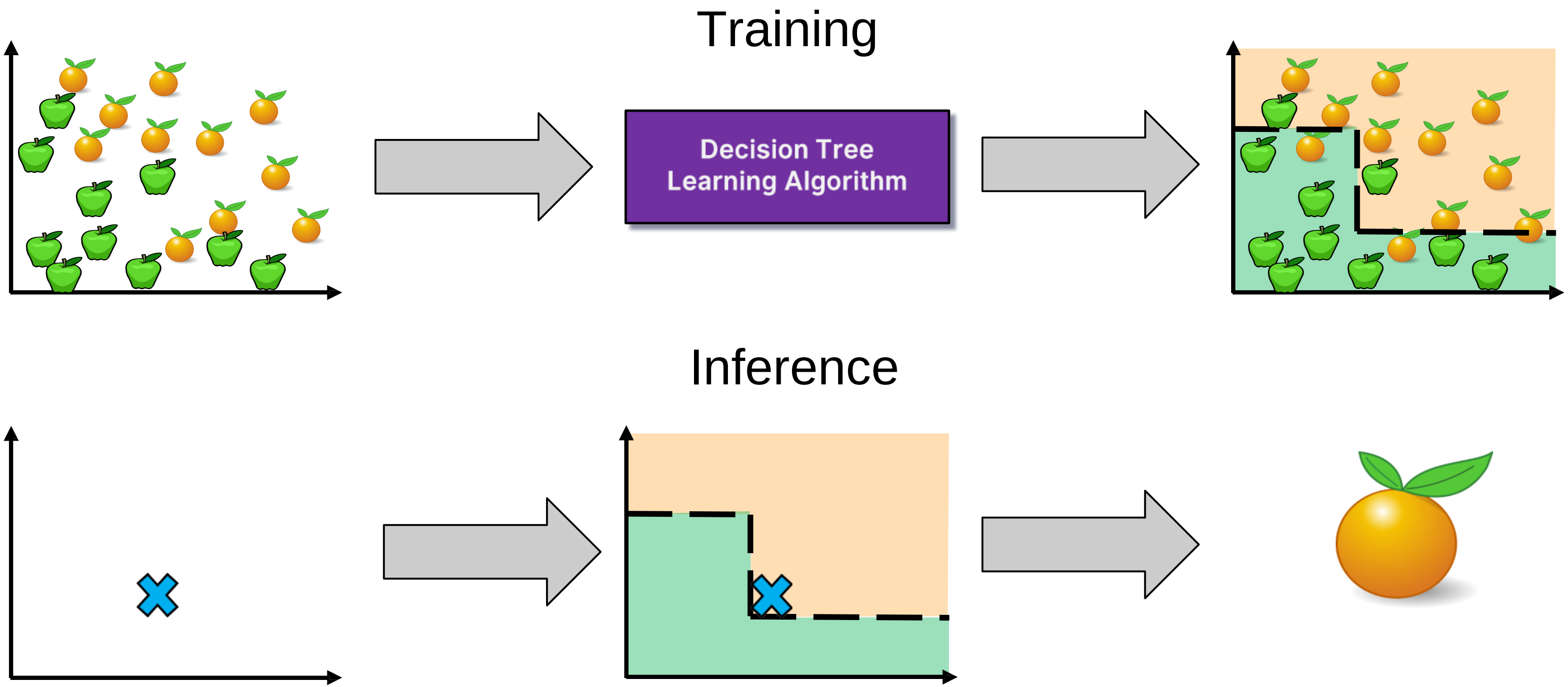
Logistec Regression



Decision Tree



Decision Trees: Training and Inference



Random Forests
(Ensemble learning with decision trees)

Gender	Age	Location	Platform	Job	Hobby	App
F	30	US	IOS	School	Games	Whatsapp
F	11	France	Android	Work	Tennis	Pokemon Go
M	16	Chile	IOS	Temp	Tennis	Snapchat
F	15	China	IOS	Retired	Chess	Whatsapp
M	25	Us	Android	School	Games	Snapchat
M	32	Us	IOS	School	Tennis	Whatsapp
F	40	Egypt	Android	Work	Chess	Snapchat
M	12	France	Android	Temp	Tennis	Whatsapp
M	14	Australia	Android	School	chess	Pokemon Go

Random Forests

Random Forests

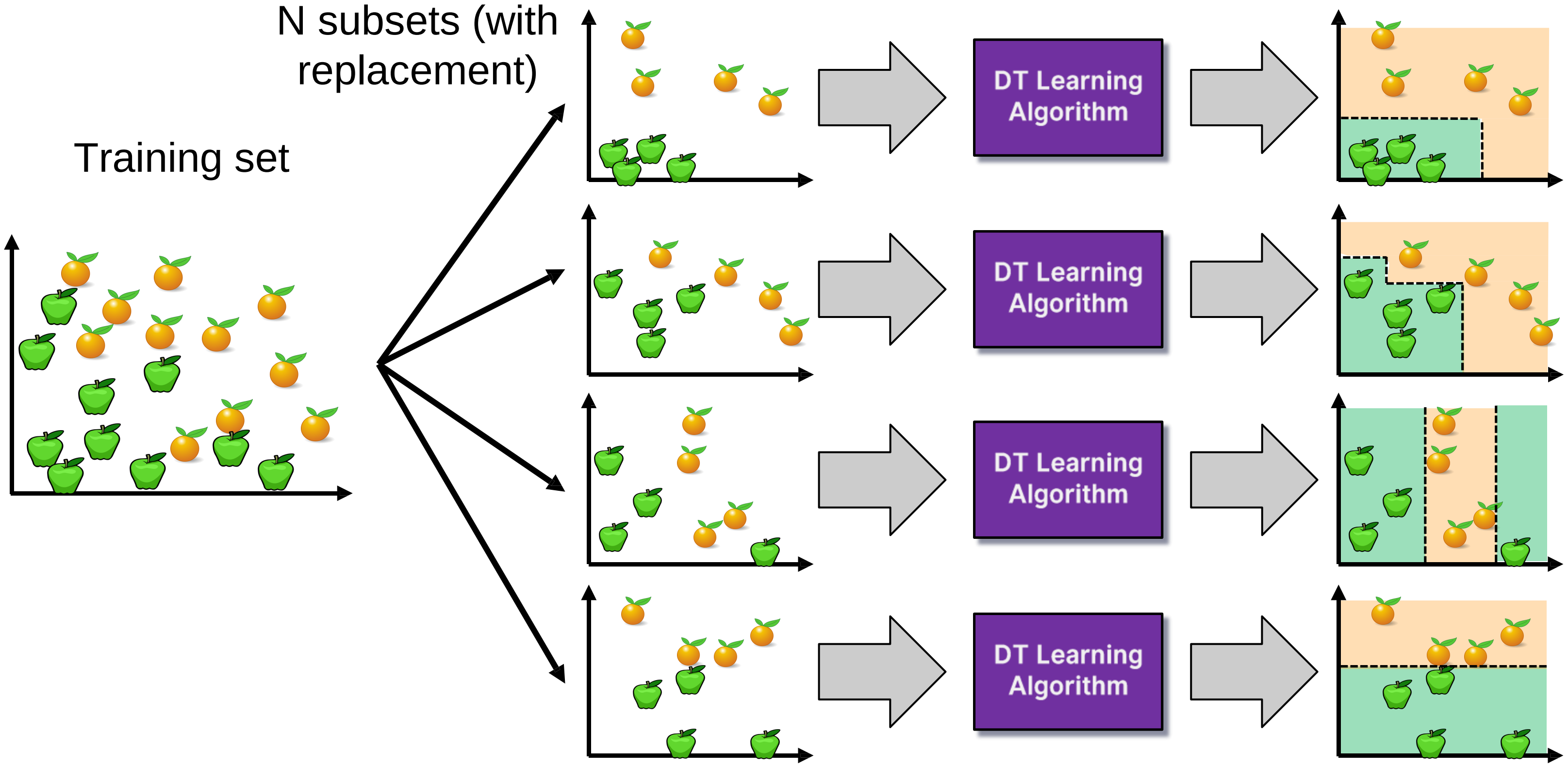
- Random Forests:
  - ➢ Instead of building a single decision tree and use it to make predictions, build many slightly different trees and combine their predictions

- We have a single data set, so how do we obtain slightly different trees?

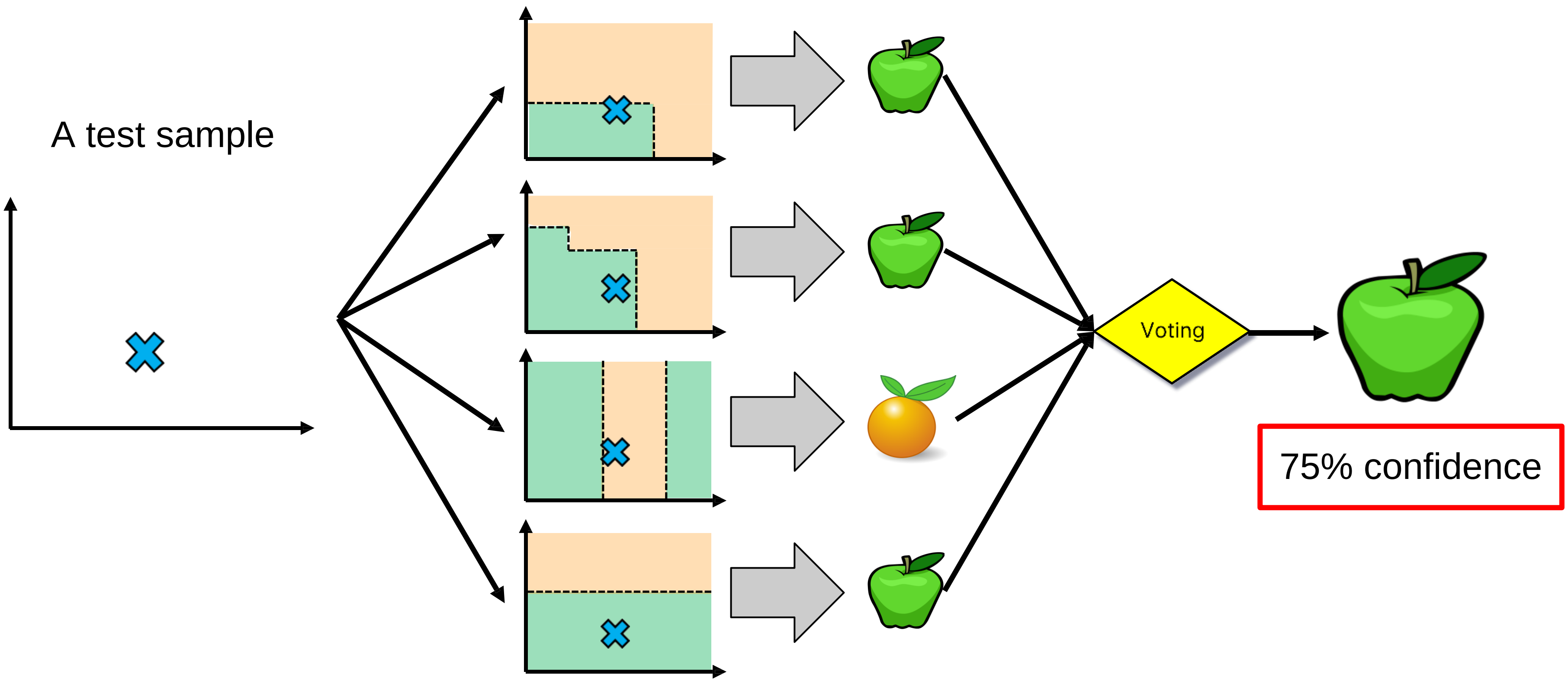
1. Bagging (**B**ootstrap **Agg**regat**ing**):
   - ➢ Take random subsets of data points from the training set to create N smaller data sets
   - ➢ Fit a decision tree on each subset

2. Random Subspace Method (also known as Feature Bagging):
   - ➢ Fit N different decision trees by constraining each one to operate on a random subset of features

Bagging at training time



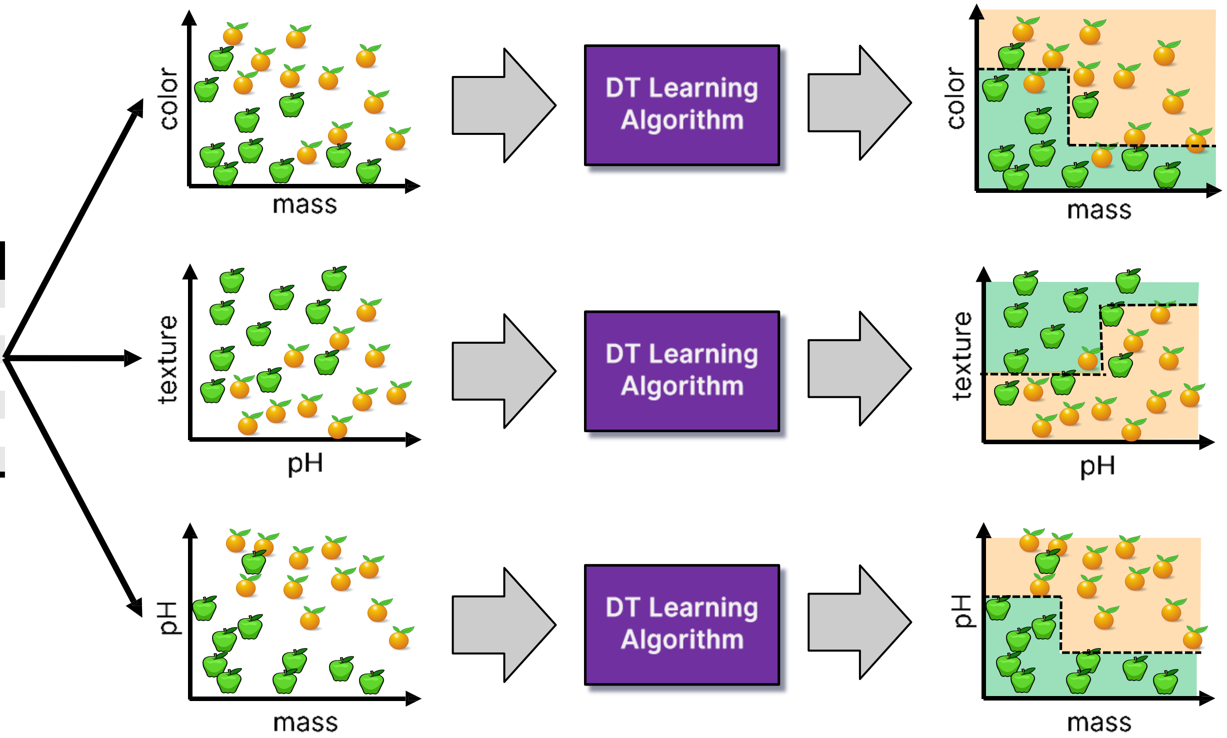
Bagging at inference time



Random Subspace Method at training time

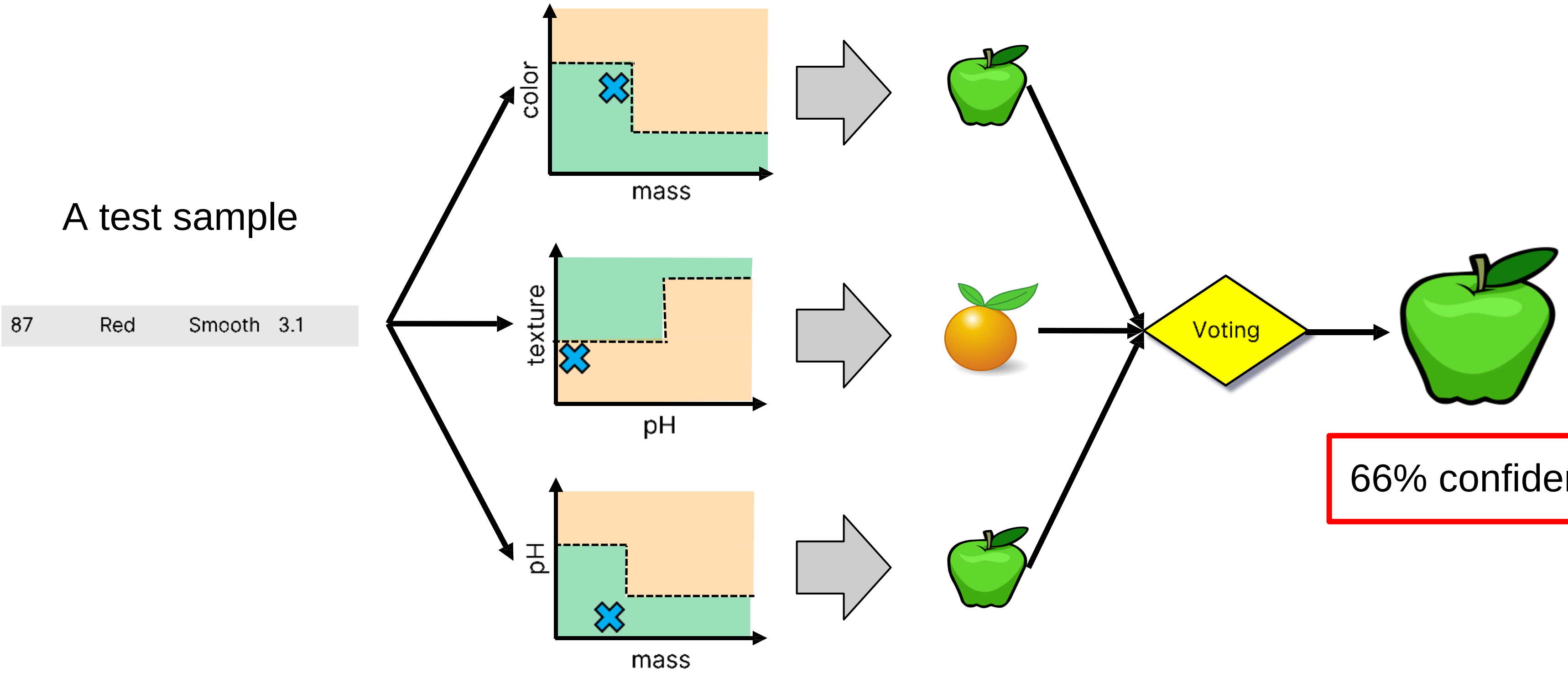
Training data

Mass (g)	Color	Texture	pH	Label
84	Green	Smooth	3.5	**Apple**
121	Orange	Rough	3.9	**Orange**
85	Red	Smooth	3.3	**Apple**
101	Orange	Smooth	3.7	**Orange**
111	Green	Rough	3.5	**Apple**
...				
117	Red	Rough	3.4	**Orange**



Random Subspace Method at inference time

A test sample



66% confidence

Random Forests

Mass (g)	Color	Texture	pH	Label
84	Green	Smooth	3.5	**Apple**
121	Orange	Rough	3.9	**Orange**
85	Red	Smooth	3.3	**Apple**
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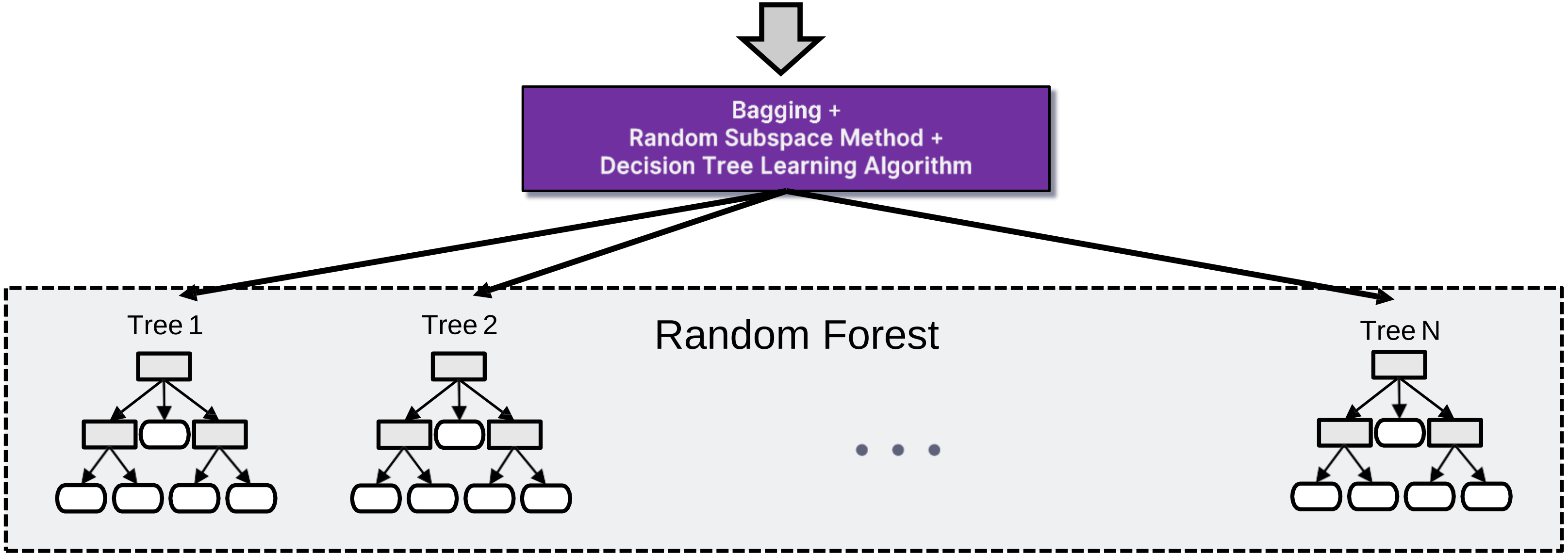
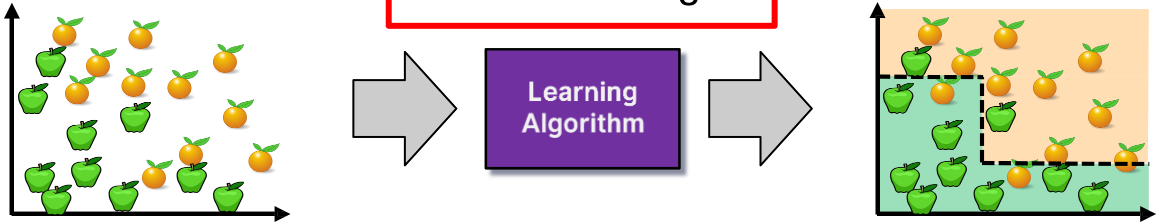


Ensemble Learning

- Ensemble Learning:
  - Method that combines multiple learning algorithms to obtain performance improvements over its components
- **Random Forests** are one of the most common examples of ensemble learning
- Other commonly-used ensemble methods:
  - Bagging: multiple models on random subsets of data samples
  - Random Subspace Method: multiple models on random subsets of features
  - Boosting: train models iteratively, while making the current model focus on the mistakes of the previous ones by increasing the weight of misclassified samples

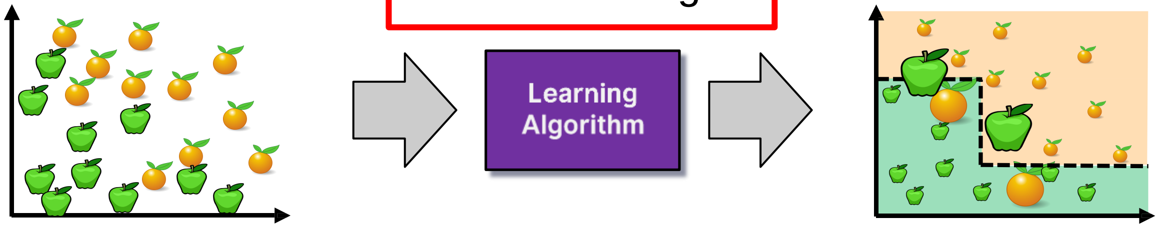
Boosting

All samples have
the same weight



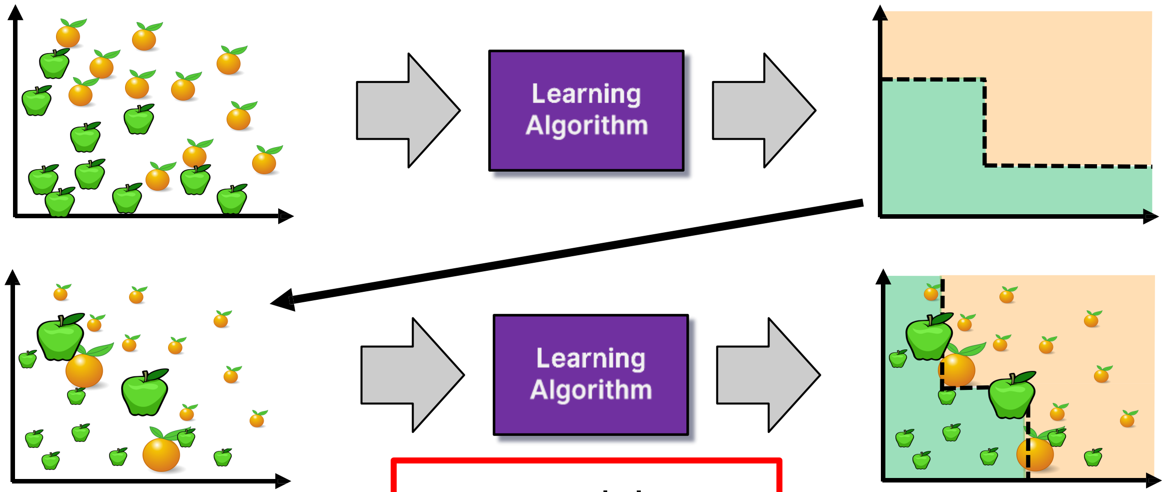
Boosting

All samples have the same weight



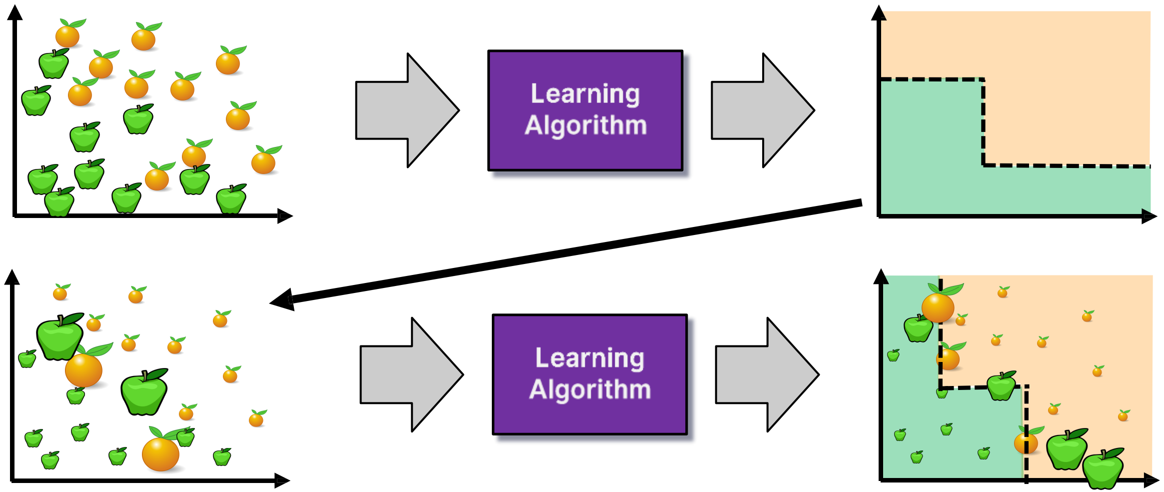
Reweight based on model’s mistakes

Boosting



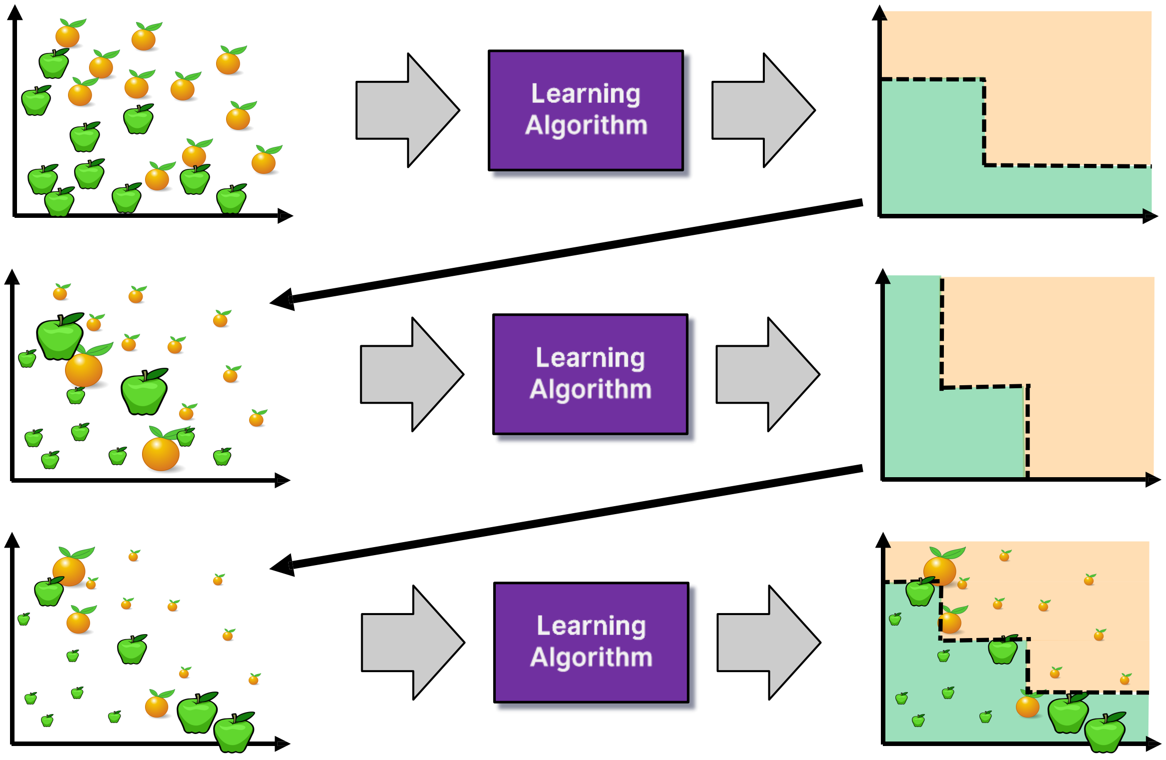
Next model sees weighted samples

Boosting

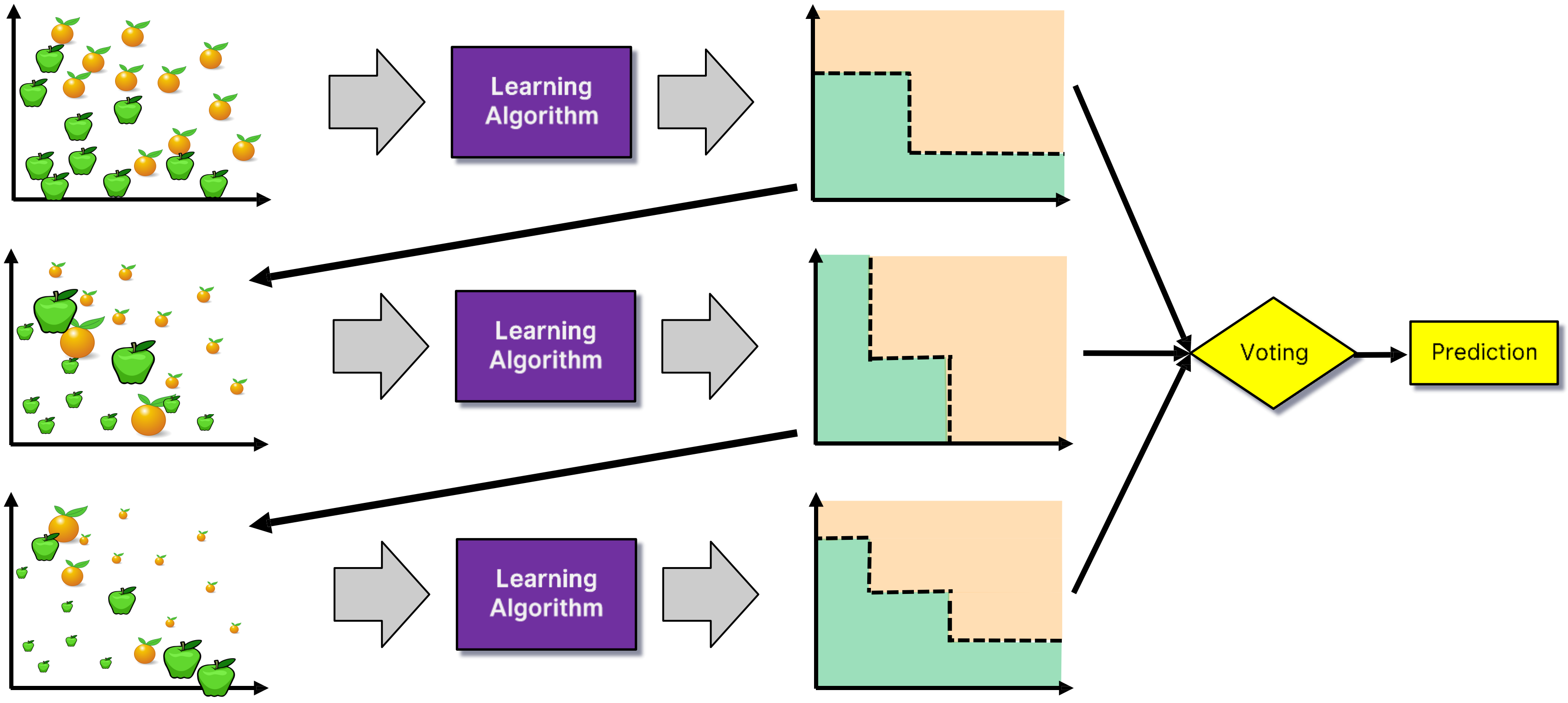


Reweight based on current model's mistakes

Boosting


Learning Algorithm
Learning Algorithm
Learning Algorithm

Boosting



Learning Algorithm
Learning Algorithm
Learning Algorithm
Voting
Prediction

Summary

- Ensemble Learning methods combine multiple learning algorithms to obtain performance improvements over its components
- Commonly-used ensemble methods:
  - Bagging (multiple models on random subsets of data samples)
  - Random Subspace Method (multiple models on random subsets of features)
  - Boosting (train models iteratively, while making the current model focus on the mistakes of the previous ones by increasing the weight of misclassified samples)
- **Random Forests** are an ensemble learning method that employ decision tree learning to build multiple trees through **bagging** and **random subspace method**.
  - They rectify the overfitting problem of decision trees!

Decision Trees and Random Forest (Python)

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier

clf = DecisionTreeClassifier(criterion = "entropy", min_samples_leaf = 3)
# Lots of parameters: criterion = "gini" / "entropy";
#                     max_depth;
#                     min_impurity_split;

clf.fit(X, y) # It can only handle numerical attributes!
# Categorical attributes need to be encoded, see LabelEncoder and OneHotEncoder

clf.predict([x]) # Predict class for x

clf.feature_importances_ # Importance of each feature
clf.tree_ # The underlying tree object

clf = RandomForestClassifier(n_estimators = 20) # Random Forest with 20 trees
```