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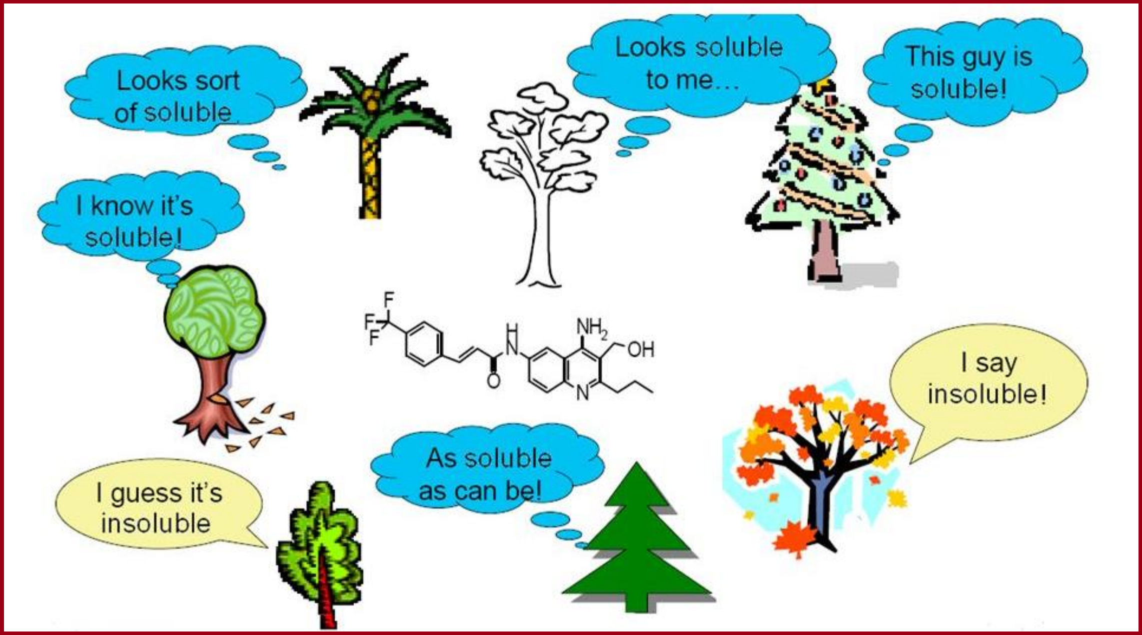

Decision Trees and Random Forests

Machine Learning 2023-24
UML book chapter 18
Slides P. Zanuttigh

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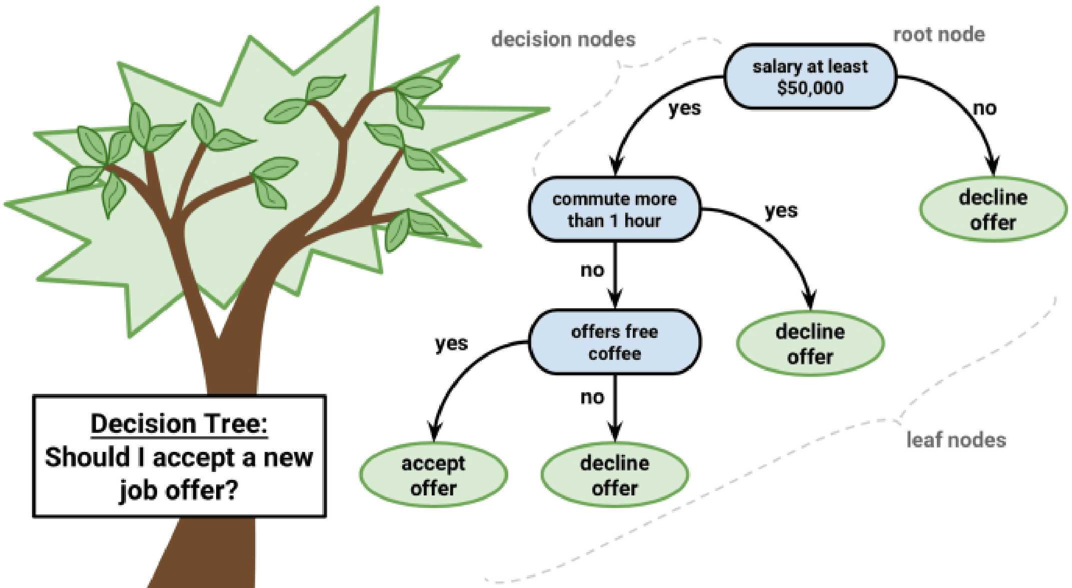
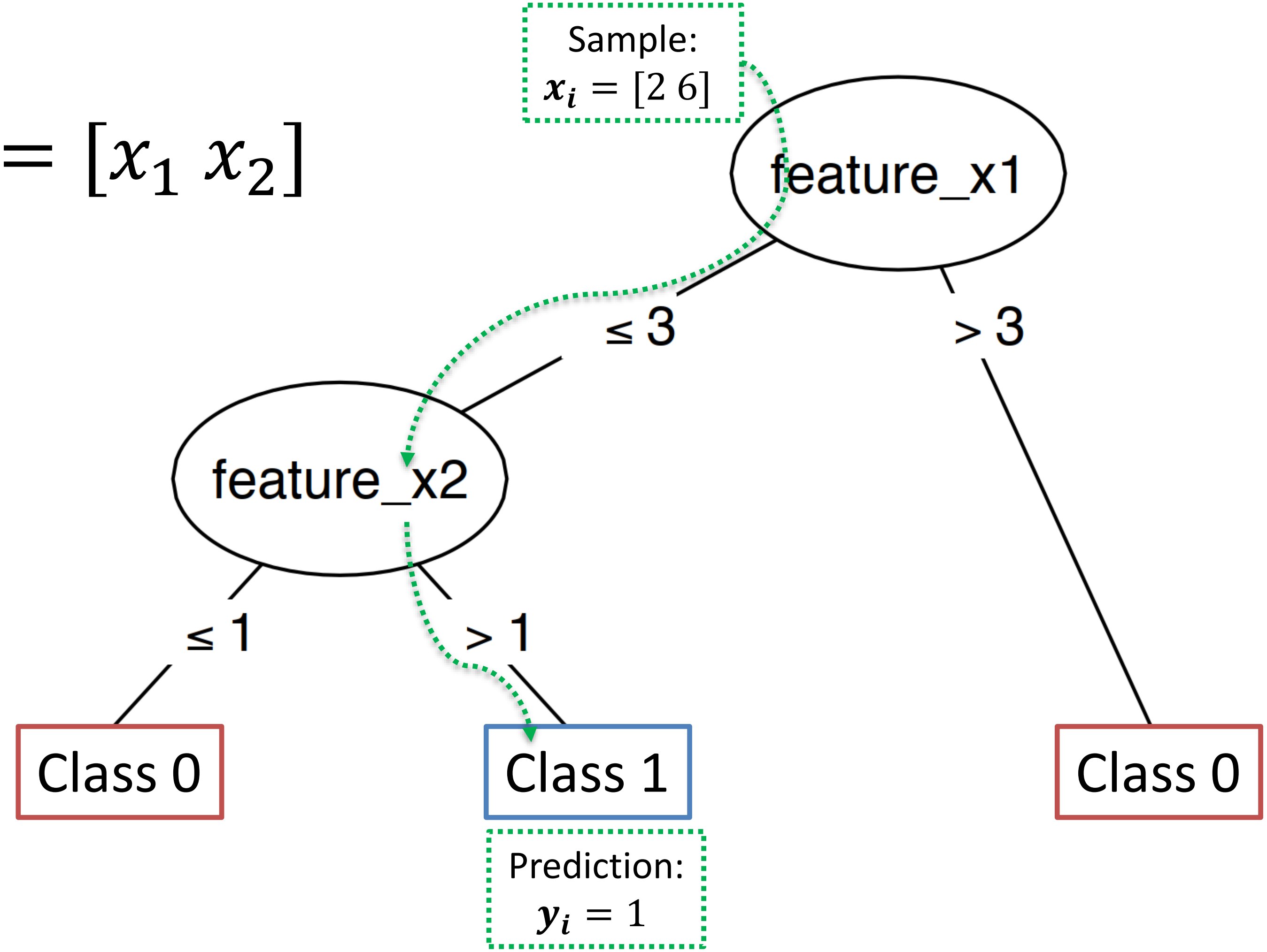
Decision Trees



- ❑ A decision tree is a model that predicts the label associated with a sample $\boldsymbol{x}$ by traveling along a tree from the root to a leaf
  - ➢ In this lecture we'll focus on binary trees
- ❑ At each internal node we make a decision based on features of $\boldsymbol{x}$
  - ➢ It corresponds to splitting the input space
  - ➢ Simplest idea, split on the basis of a threshold on one of the features, i.e., $x_i < \theta$ or $x_i \geq \theta$
- ❑ Each leaf is associated to a label

Example: Decision Tree

$$\boldsymbol{x} = [x_1 \; x_2]$$



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Grow a Decision Tree

Consider a binary classification setting and assume to have a gain (performance) measure:

Start

- A single leaf assigning the most common of the two labels
  i.e., the one of the majority of the samples

At each iteration

- Analyze the effect of splitting a leaf
- Among all possible splits select the one leading to a larger gain in the performance measure and split the corresponding leaf (or choose not to split)

Iterative Dichotomizer 3 (ID3)

$\mathtt{ID3}(S, A)$

INPUT: training set S, feature subset $A \subseteq [d]$

Assume binary features, i.e., $\mathcal{X} = \{0,1\}^d$

if all examples in S are labeled by 1, return a leaf 1

if all examples in S are labeled by 0, return a leaf 0

No more features to use

if $A = \emptyset$, return a leaf whose value = majority of labels in S

else :

Let $j = \text{argmax}_{i \in A}\, \mathtt{Gain}(S, i)$

Find which split (i.e. splitting over which feature) leads to the maximum gain

x_j: selected feature for the split

if all examples in S have the same label

Return a leaf whose value = majority of labels in S

else

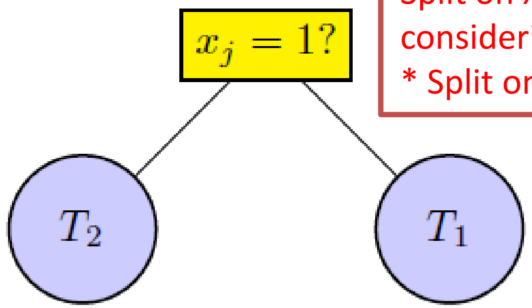
call recursively removing feature used for the split

Let T_1 be the tree returned by $\mathtt{ID3}(\{(\mathbf{x}, y) \in S : x_j = 1\}, A \setminus \{j\})$.

Let T_2 be the tree returned by $\mathtt{ID3}(\{(\mathbf{x}, y) \in S : x_j = 0\}, A \setminus \{j\})$.

Return the tree:

Split on xj and recursively call the algorithm considering the remaining features*
* Split on a feature only once: they are binary



If real valued features: need to find threshold, can split on same feature with different thresholds

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Gain Measure

Training error

- Define the gain as the decrease in the training error

Gini Index $G = \sum_{i=1}^{C} p(i)(1 - p(i)) = 1 - \sum_{i=1}^{C} [p(i)]^2$

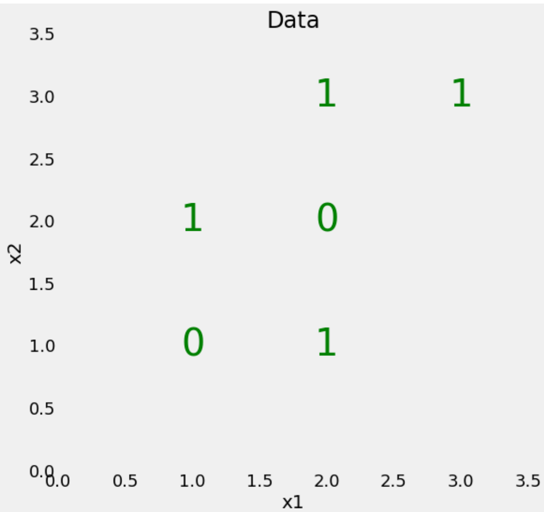
$i = 1, \ldots, C$: classes $\quad p(i)$: probability of class i

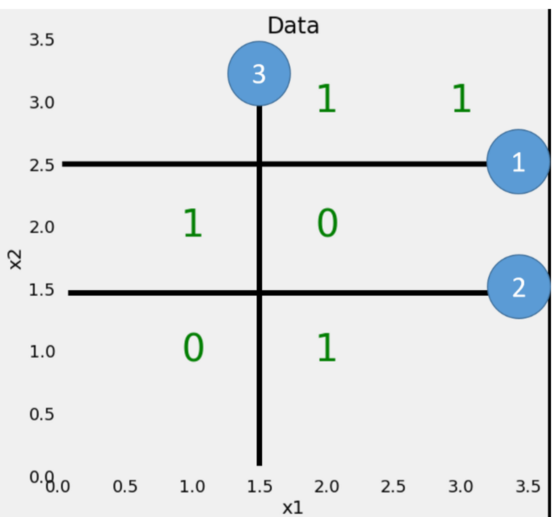
- It is a measure of statistical dispersion in a frequency distribution
  - For binary classification case: $G = 2p(0)p(1)$, i.e, *G=0* if all samples in the same class, *G=1/2* if 50% split
- *Measure of variance*: higher variance more misclassifications
- It measures how "*pure*" is the distribution after the split
- Gini Index is a smooth and concave upper bound of the train error

Threshold based splitting rules for real valued features

- Extend by creating a set of thresholds and testing all the various combination of features and thresholds

Example

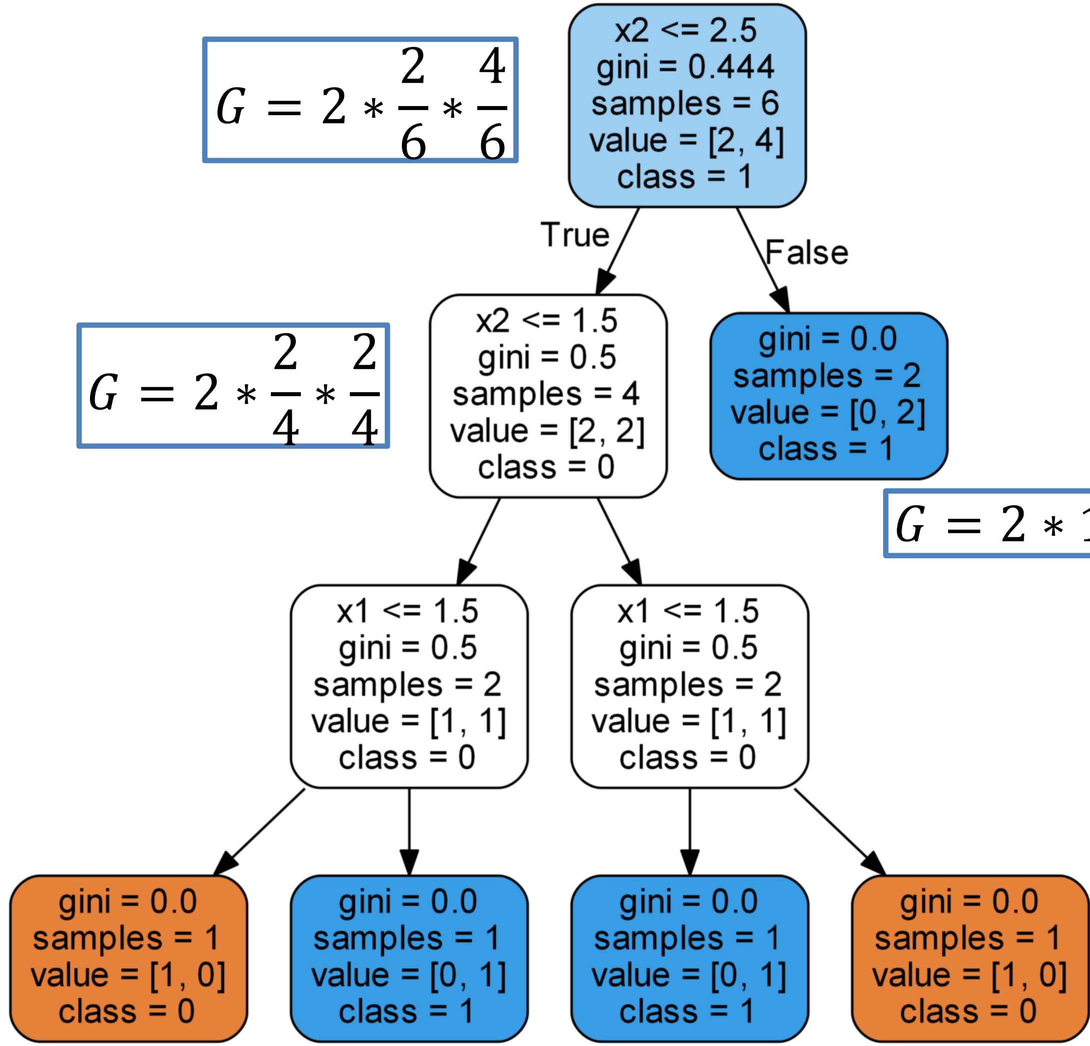




$$G = 2 * \frac{2}{6} * \frac{4}{6}$$

$$G = 2 * \frac{2}{4} * \frac{2}{4}$$

$$G = 2 * 1 * 0$$



Pruning

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Generic Tree Pruning Procedure
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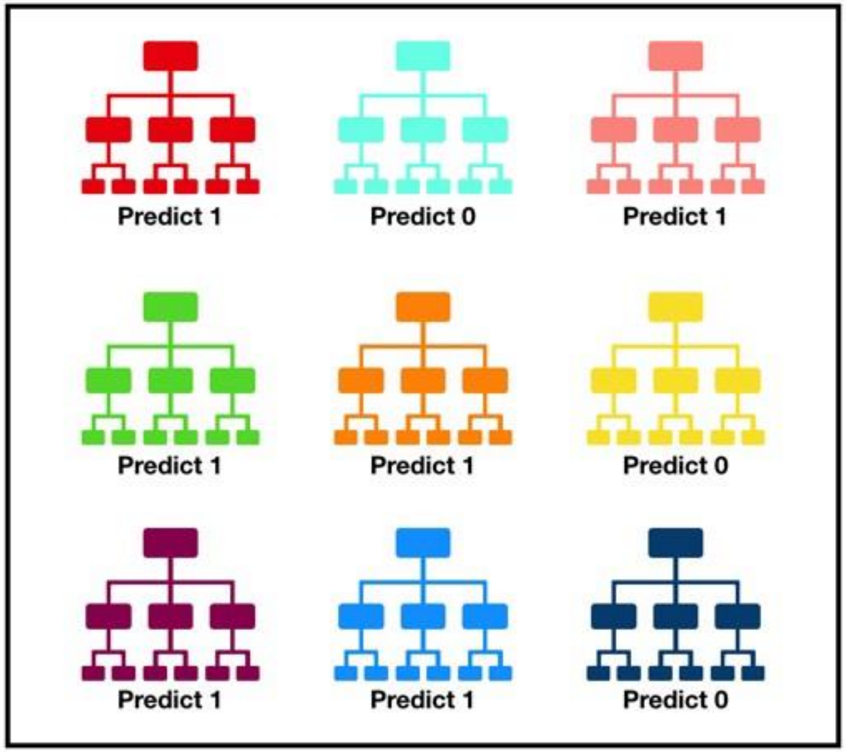
input:
  function $f(T, m)$ (bound/estimate for the generalization error
    of a decision tree T, based on a sample of size m),
  tree T.
foreach node j in a bottom-up walk on T (from leaves to root):
  find T' which minimizes $f(T', m)$, where T' is any of the following:
    the current tree after replacing node j with a leaf 1.
    the current tree after replacing node j with a leaf 0.
    the current tree after replacing node j with its left subtree.
    the current tree after replacing node j with its right subtree.
    the current tree.
  let $T := T'$.

- *Key issue of ID3:* The tree is typically very large with high risk of overfitting
  - Prune the tree to reduce its size without affecting too much the performances

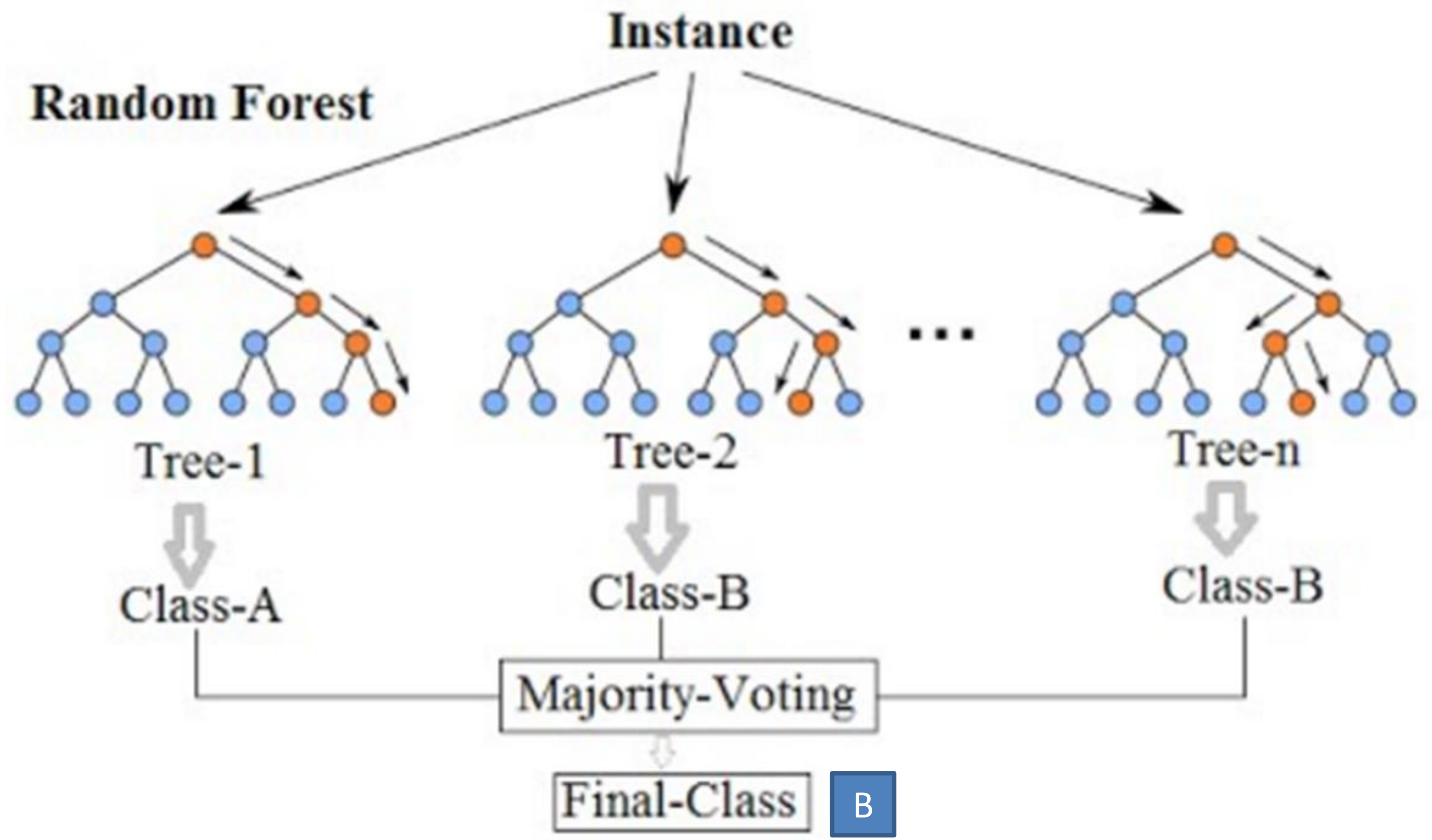
Random Forests (RF)



Tally: Six 1s and Three 0s
Prediction: 1

- Introduced by Leo Breiman in 2001
- Instead of using a single large tree construct an ensemble of simpler trees
- A Random Forest (RF) is a classifier consisting of a collection of decision trees
- The prediction is obtained by a majority voting over the prediction of the single trees

Random Forest: Example



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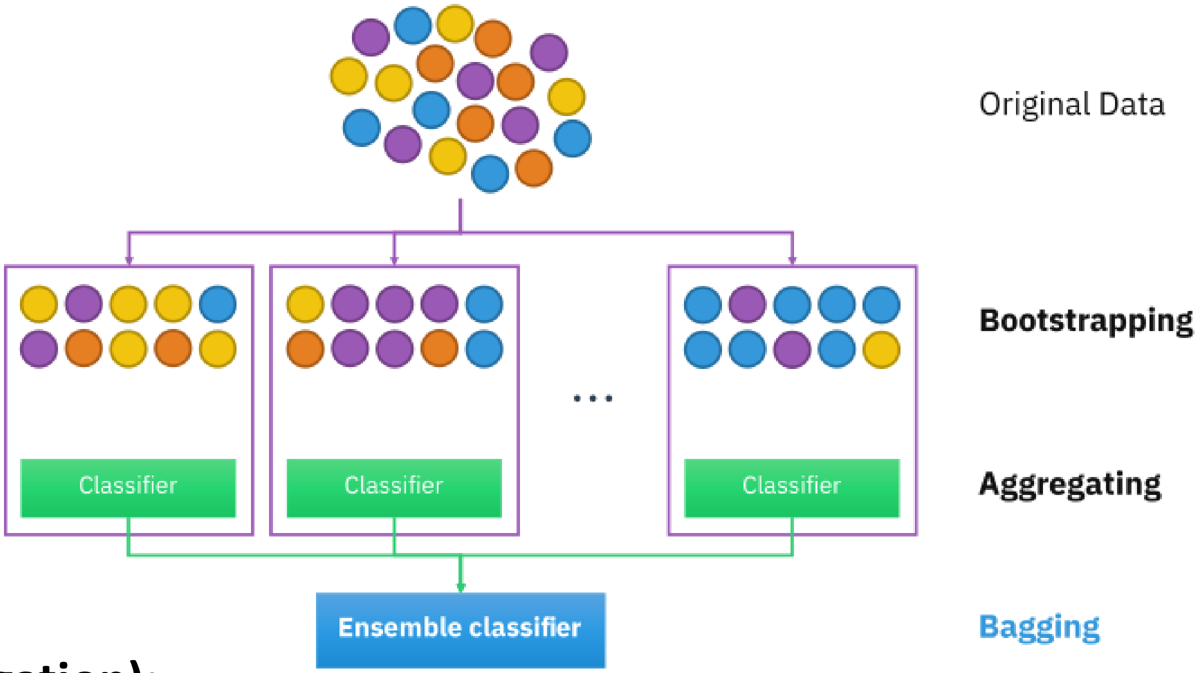
Random Sampling with Replacement

Idea: randomly sample from a training dataset with replacement

- Assume a training set S of size m: we can build new training sets by taking at random m samples from S with replacement (i.e., the same sample can be selected multiple times)
  - For example, if our training data is [1, 2, 3, 4, 5, 6] then we might sample sets like [1, 2, 2, 3, 6, 6], [1, 2, 4, 4, 5, 6], [1 1 1 1 1 1], etc.....
  - i.e., all lists have a length of six but some values can be repeated in the random selection
- Notice that we are not subsetting the training data into smaller chunks

Bootstrap Aggregation (Bagging)



Bagging (Bootstrap Aggregation):

- Decisions trees are very sensitive to the data they are trained on: small changes to the training set can result in significantly different tree structures
- *Random Forest* takes advantage of this by allowing each individual tree to randomly sample with replacement from the dataset, resulting in different training sets producing different trees
- This process is known as bagging

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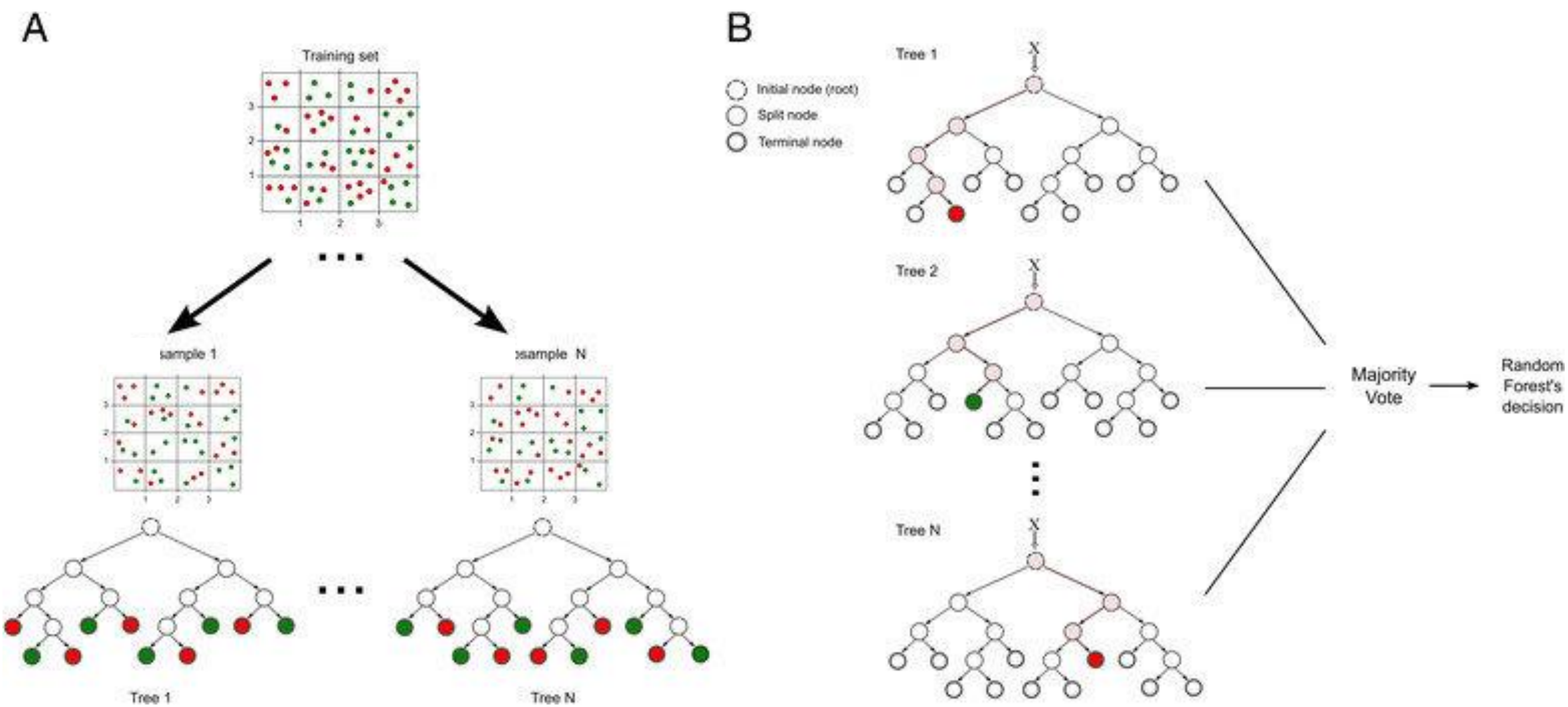
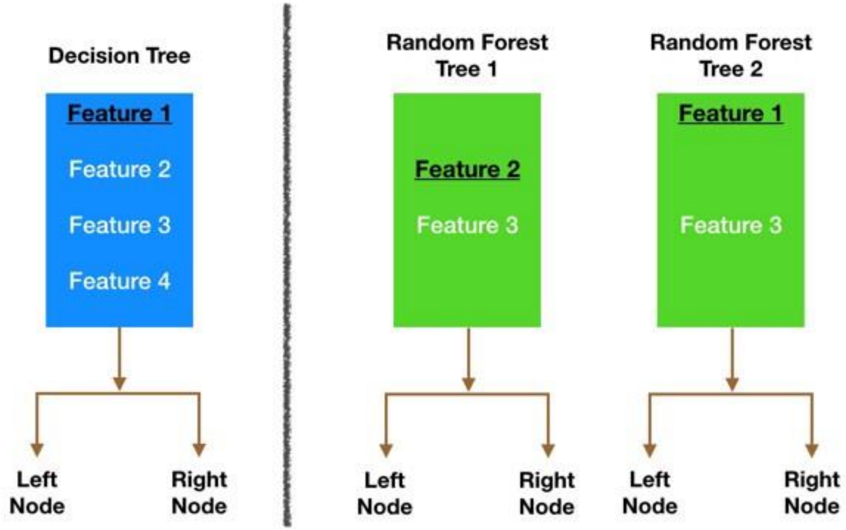
Bagging: Example



Randomization: Feature Randomnsess



- In a normal decision tree, when it is time to split a node, we consider every possible feature and pick the one that produces the largest gain
- In contrast, each tree in a random forest can pick only from a random subset of features (*Feature Randomness*)
- I.e., node splitting in a random forest model is based on a random subset of features for each tree
- This forces even more variation amongst the trees in the model and ultimately results in lower correlation across trees and more diversification