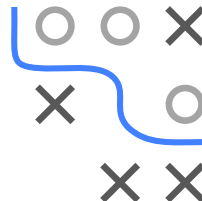


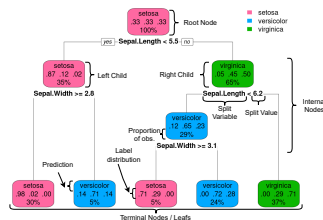
Introduction to Machine Learning

CART: Predictions with CART

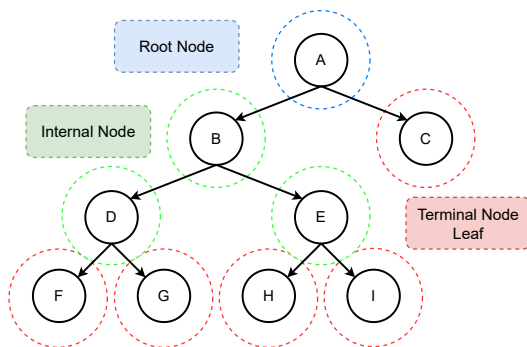


Learning goals

- Understand the basic structure of a tree model
- Understand that the basic idea of a tree model is the same for classification and regression
- Understand how the label of a new observation is predicted via CART
- Know hypothesis space of CART

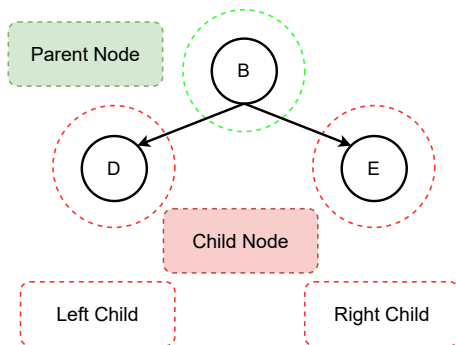


BINARY TREES



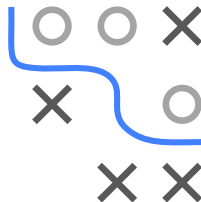
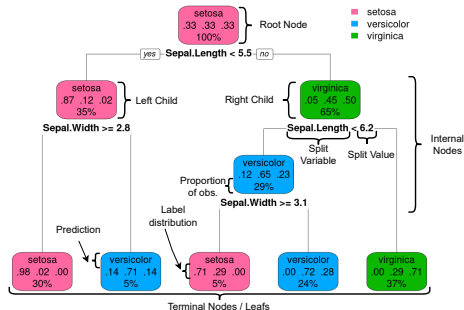
- Binary trees represent a top-down hierarchy with binary splits
- A tree is composed of different node types: a) the root node, b) internal nodes, and c) terminal nodes (also leaves).

BINARY TREES



- Nodes have relative relationships, they can be:
 - Parent nodes
 - Child nodes
- Root nodes don't have parents – leaves don't have children

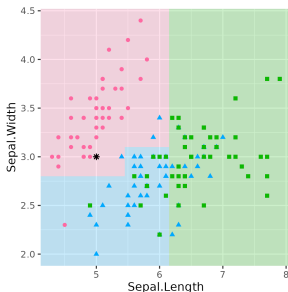
CLASSIFICATION TREES



- Classification trees use the structure of a binary tree
- Binary splits are constructed top-down in a *data optimal* way
- Each split is a threshold decision for a single feature
- Each node contains the training points which follow its path
- Each leaf contains a constant prediction

CLASSIFICATION TREE MODEL AND PREDICTION

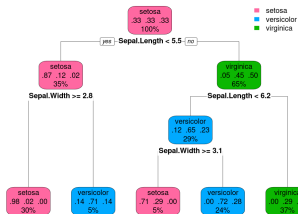
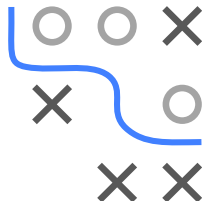
- When predicting new data (here*: `Sepal.Length = 5`, `Sepal.Width = 3`) we use the learned split points and pass an observation through the tree
- Each observation is assigned to exactly one leaf
- Classification trees can make hard-label predictions (here: `setosa`) or predict probabilities (here: 0.98, 0.02, 0.00)



CART AS A RULE BASED MODEL

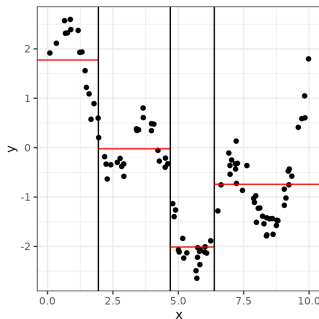
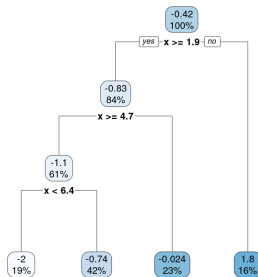
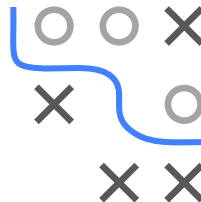
Leaf nodes can be expressed by a set of rules (left to right):

| Hard label prediction | Label distribution | Sepal.Width | Sepal.Length |
|-----------------------|--------------------|-------------|-------------------------|
| setosa | 0.98, 0.02, 0.00 | ≥ 2.8 | < 5.5 |
| versicolor | 0.14, 0.71, 0.14 | < 2.8 | < 5.5 |
| setosa | 0.71, 0.29, 0.00 | ≥ 3.1 | $\geq 5.5 \ \& \ < 6.2$ |
| versicolor | 0.00, 0.72, 0.28 | < 3.1 | $\geq 5.5 \ \& \ < 6.2$ |
| virginica | 0.00, 0.29, 0.71 | — | ≥ 6.2 |



REGRESSION TREE MODEL AND PREDICTION

- Works the same way as for classification
- But predictions in leaf nodes are a numerical scalar



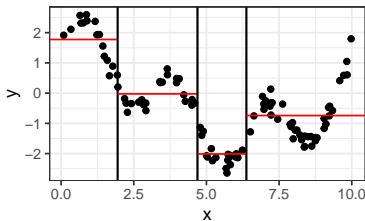
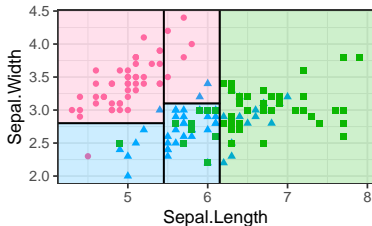
TREE AS AN ADDITIVE MODEL

Trees divide the feature space \mathcal{X} into **rectangular regions**:

$$f(\mathbf{x}) = \sum_{m=1}^M c_m \mathbb{I}(\mathbf{x} \in Q_m),$$

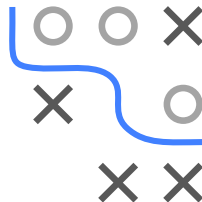
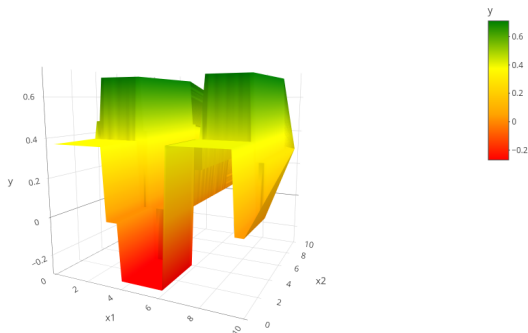
where a tree with M leaf nodes defines M “rectangles” Q_m .

c_m is the predicted numerical response, class label or class distribution in the respective leaf node.



TREE AS AN ADDITIVE MODEL

A 2D regression example:



(For binary classification with probabilities, 2D surface looks similar.)