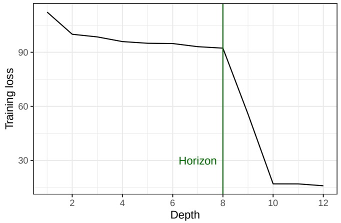
# Introduction to Machine Learning

# CART: Stopping Criteria & Pruning

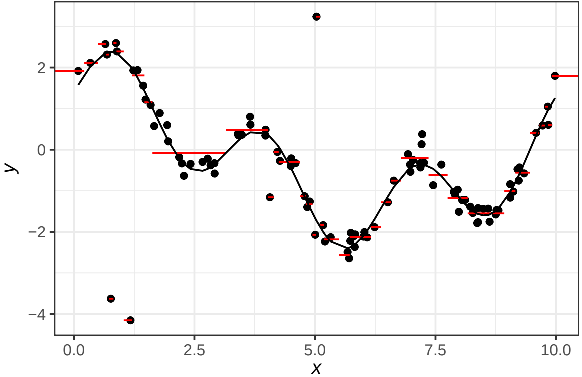



## Learning goals

- Understand which problems arise when growing the tree until the end
- Know different stopping criteria
- Understand the idea of pruning

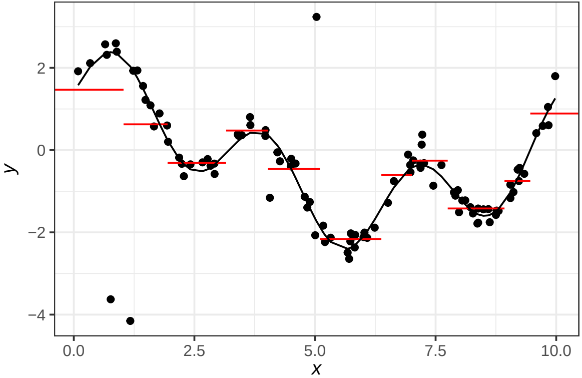
# OVERFITTING TREES

The recursive partitioning procedure used to grow a CART could run until every leaf only contains a single observation. Problem: Very complex trees will *overfit the training data.* At some point we should stop splitting nodes into ever smaller child nodes:

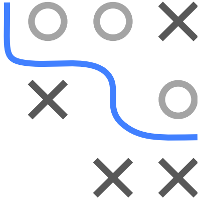


# OVERFITTING TREES

We can reduce overfitting to some extent with a less deep tree:



# STOPPING CRITERIA

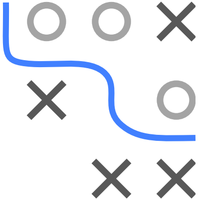


We can define different **stopping criteria**, e.g.: Don’t split a node if

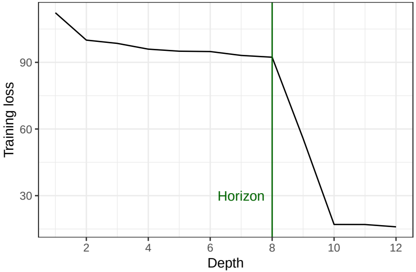
- a certain number of leaves if reached,
- it contains too few observations,
- splitting results in children with too few observations,
- splitting does not achieve a certain minimal improvement of the risk in the children, compared to the risk in the parent node,
- it already has the same target value (**pure node**) or identical feature values for all observations.

Selection of a stopping criterion and its concrete values are hyperparameters of CART.

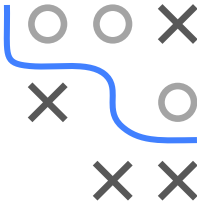
# HORIZON EFFECT



It is hard to tell where we should stop while we're growing the tree: Before we have actually tried all possible additional splits further down a branch, we can't know whether any one of them will be able to reduce the risk by a lot (*horizon effect*).



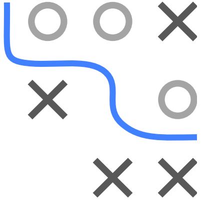
# PRUNING



We try to tackle the horizon effect by **pruning**, a method to select the optimal size of a tree:

- Finding a combination of suitable strict stopping criteria ("pre-pruning") is a hard problem (see chapter on **tuning**).
- Alternative: Grow a large tree, then remove branches so that the resulting smaller tree has lower risk ("post-pruning").
- Often, post-pruning is meant when referring to pruning.

# POST-PRUNING: CCP

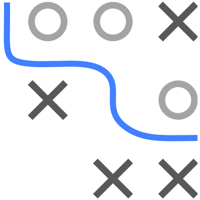


- Prominent pruning method: Cost-complexity pruning (CCP)
- Idea: Grow a large tree and remove the least informative leaves
- CCP is steered with a regularization parameter $\alpha$ that penalizes the number of leaves in a sub tree

$$\mathcal{R}_{\text{reg}}(T) = \sum_{m=1}^{|T|} \sum_{i:x^{(i)} \in Q_m} L(y^{(i)}, c_m) + \alpha |T|,$$

where $|T|$ is the number of leaves of sub tree $T$, $Q_m$ is the subset of the feature space related to the $m$-th terminal node, with its prediction $c_m$, and $T_0$ is the complete tree.

# CCP

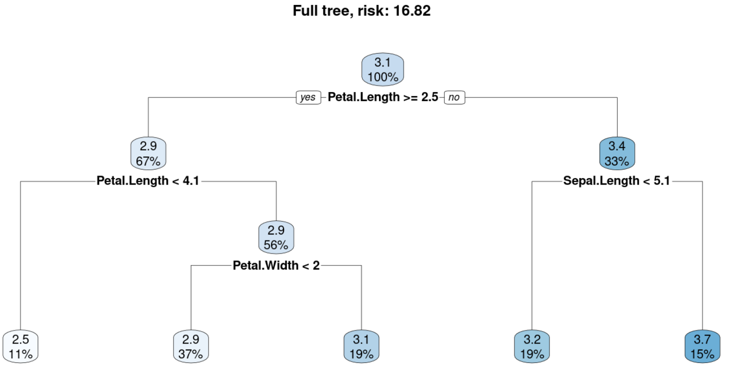


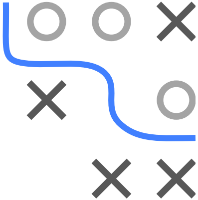
CCP performs a greedy backward search:

- Computes $\mathcal{R}_{\text{reg}}(T)$ with a fixed $\alpha$ for all possible sub trees that can be created by replacing one internal node with a leaf.
- By replacing a node we also eliminate all subsequent nodes.
- We select the sub tree with lowest risk and repeat the procedure.
- We stop if pruning does not further reduce the risk.
- This is proven to result in the pruned tree with the lowest risk.
- For $\alpha = 0$, we would obviously select $T_0$.
- Hyperparameter $\alpha$ is typically selected via cross-validation.
- Other prominent post-pruning methods include, e.g., reduced error pruning (REP) or pessimistic error pruning (PEP).

# CCP

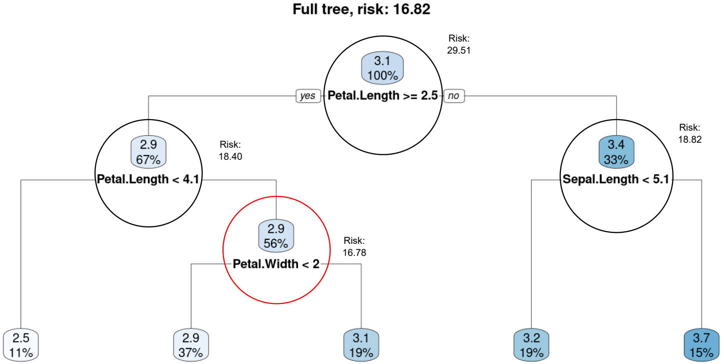
We run the CCP algorithm step-by-step with $\alpha = 1.2$:

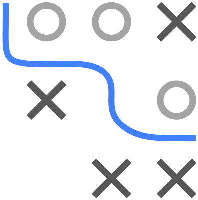


# CCP

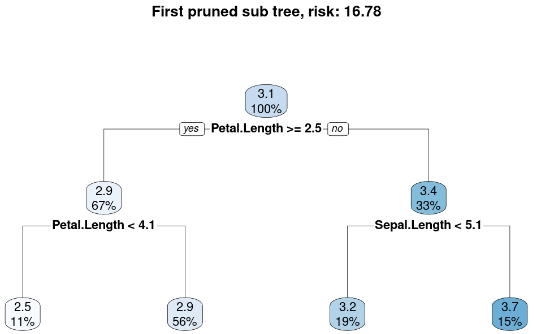
There are four possible nodes that we can eliminate to prune the tree.
We take the one replacement that results in the lowest risk (red).

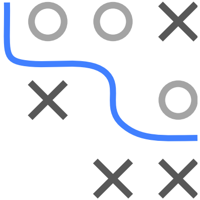


# CCP

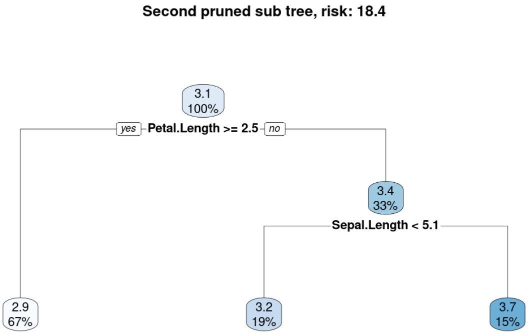
The first pruned sub tree has a lower risk than the full tree. Thus, we prefer it over the full tree.

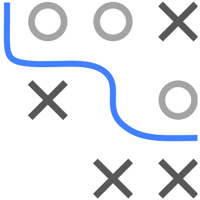


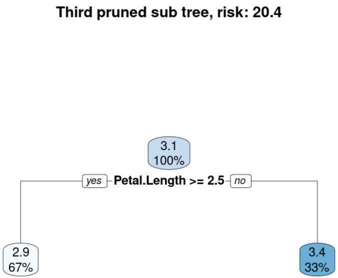
# CCP

From here on, the risk increases.



# CCP


Third pruned sub tree, risk: 20.4
3.1
100%
yes
Petal.Length >= 2.5
no
2.9
67%
3.4
33%

# CCP

We select the first sub tree as it results in the lowest risk in the complete sequence of sub trees.

**Fully pruned sub tree, risk: 29.51**