Introdução à Inteligência Computacional

Capítulo 8: Métodos baseados em Árvore

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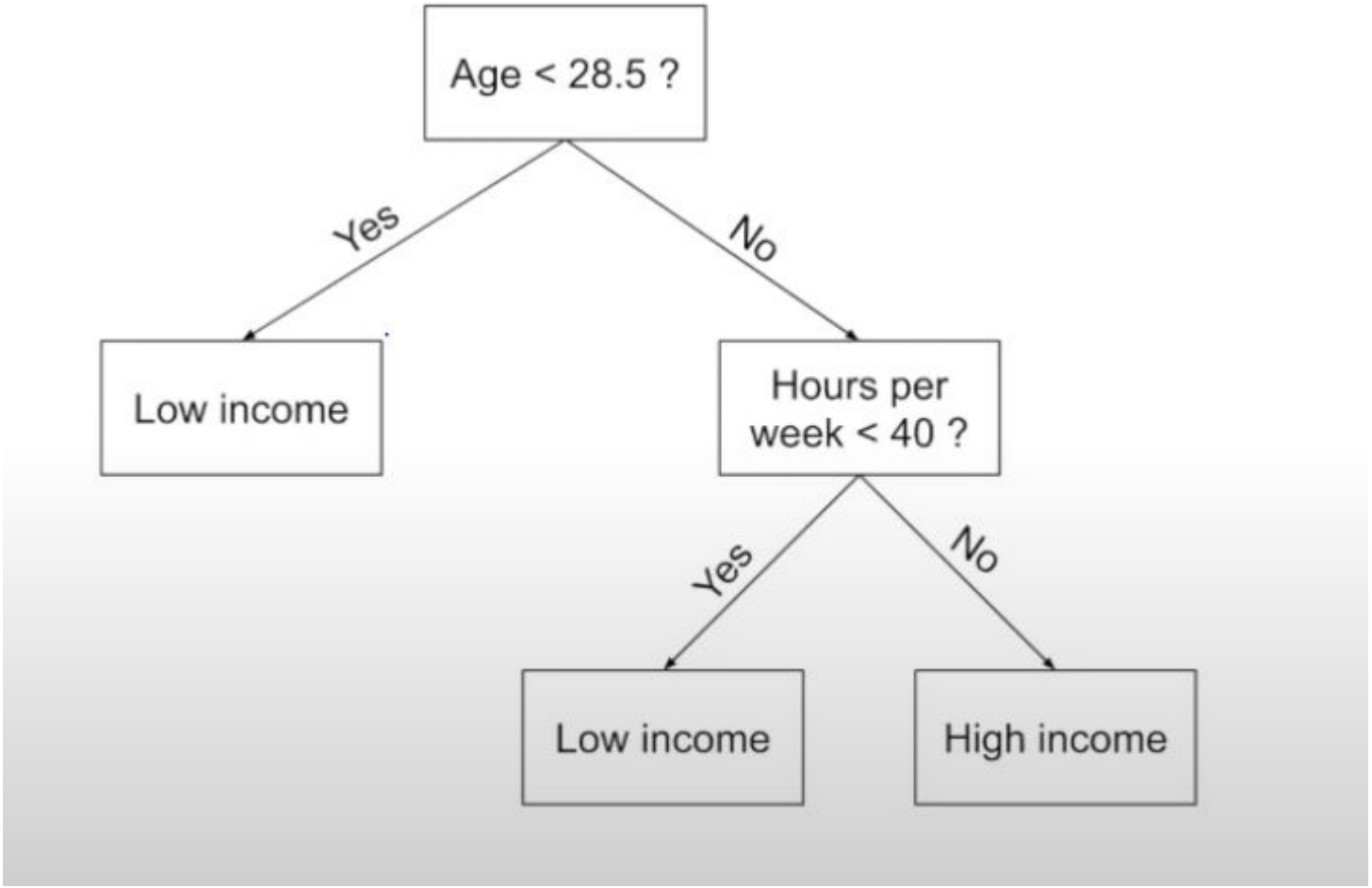
Intro

- Here we describe *tree-based* methods for regression and classification.
- These involve *stratifying* or *segmenting* the predictor space into a number of simple regions.
- Since the set of splitting rules used to segment the predictor space can be summarized in a tree, these types of approaches are known as *decision-tree* methods.

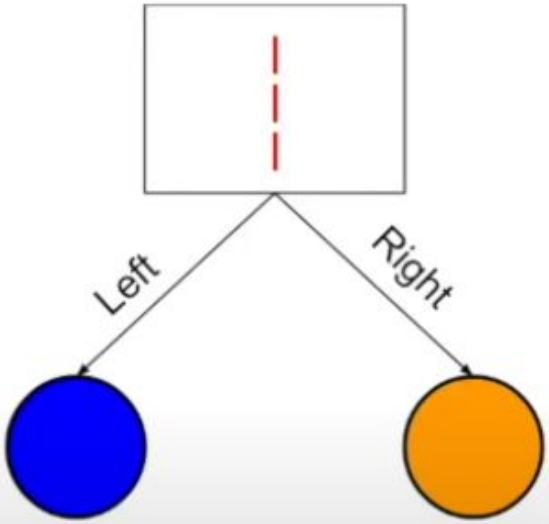
Example of a Decision Tree

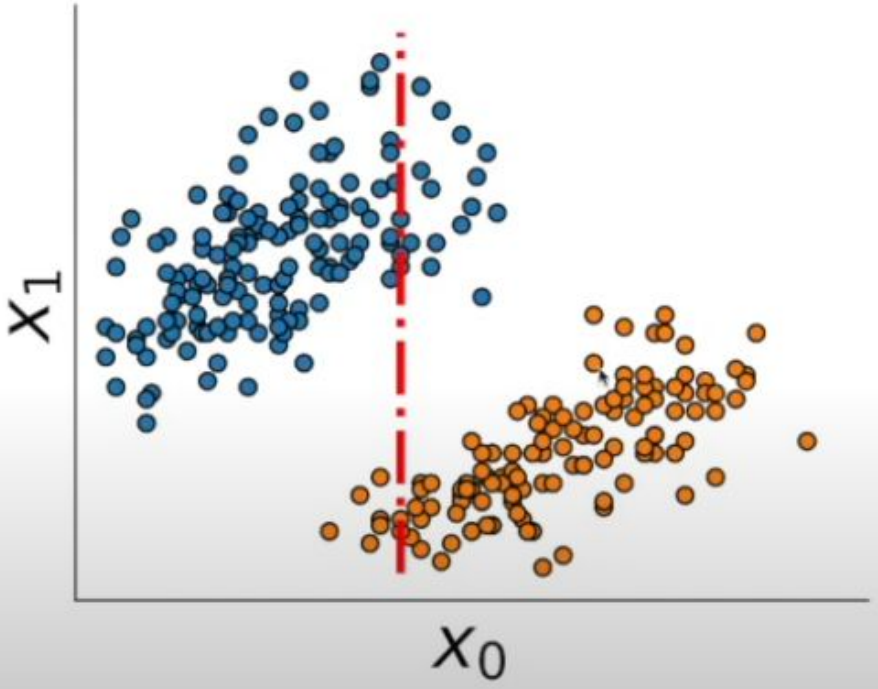


Intro

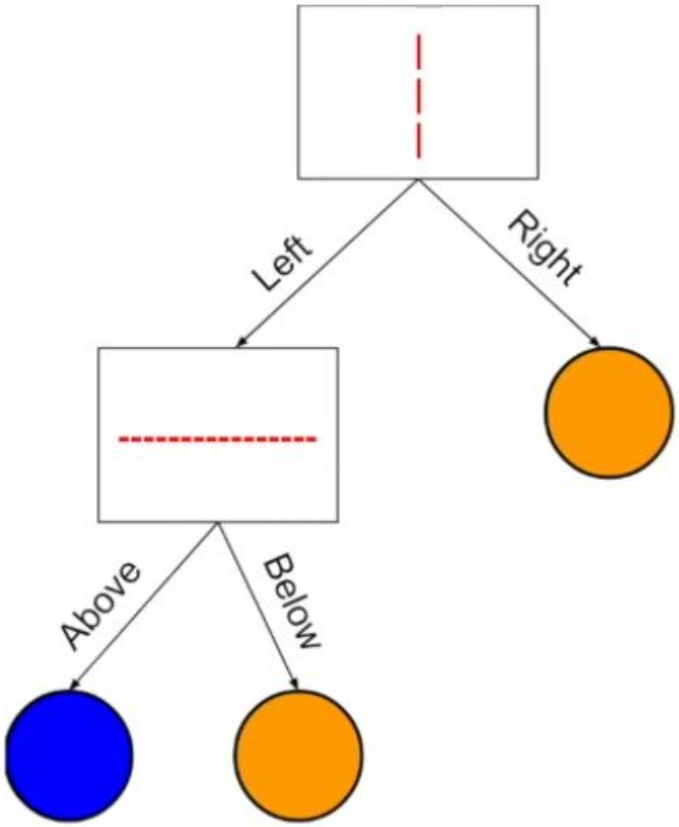
- Tree-based methods are simple and useful for interpretation.
- However they typically are not competitive with the best supervised learning approaches in terms of prediction accuracy.
- Hence we also discuss *bagging*, *random forests*, and *boosting*. These methods grow multiple trees which are then combined to yield a single consensus prediction.
- Combining a large number of trees can often result in dramatic improvements in prediction accuracy, at the expense of some loss interpretation.

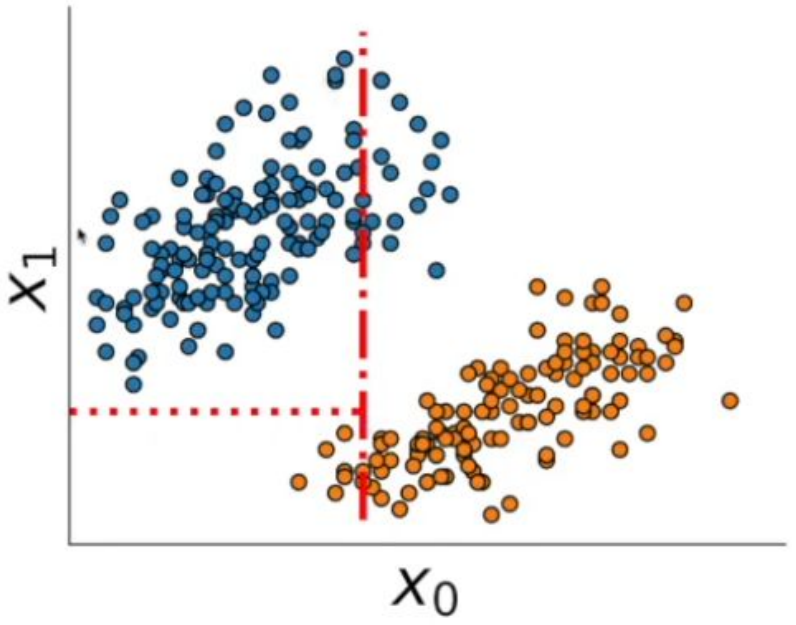
Intuition - Classification



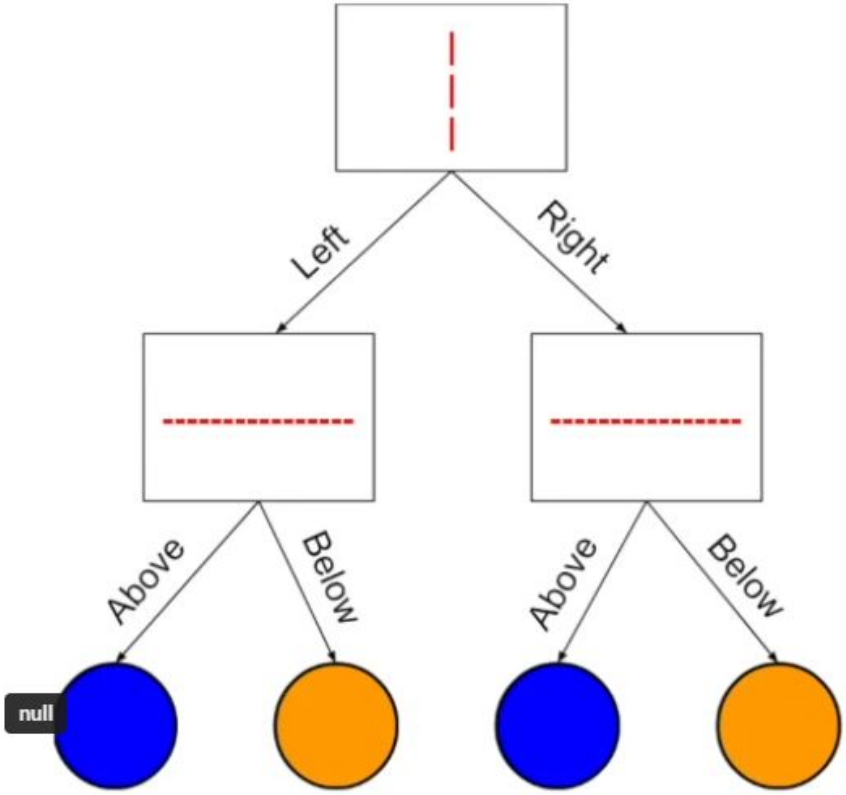


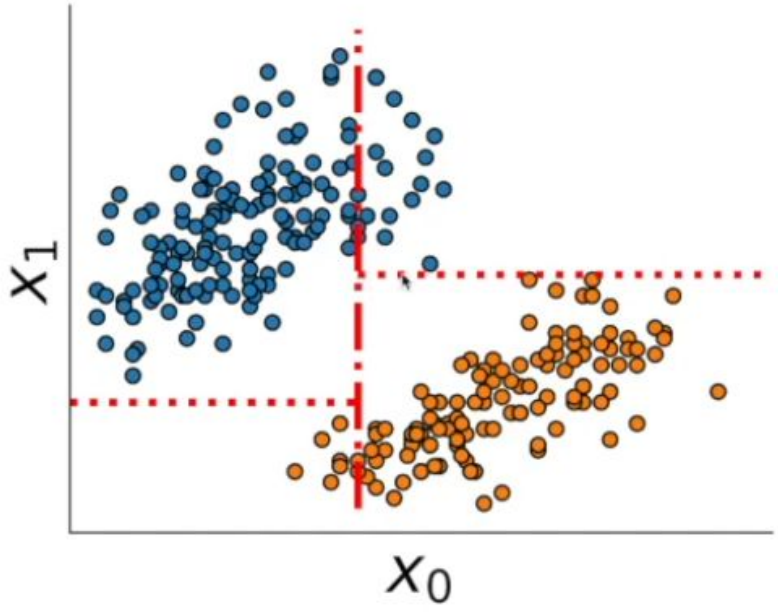
Intuition - Classification



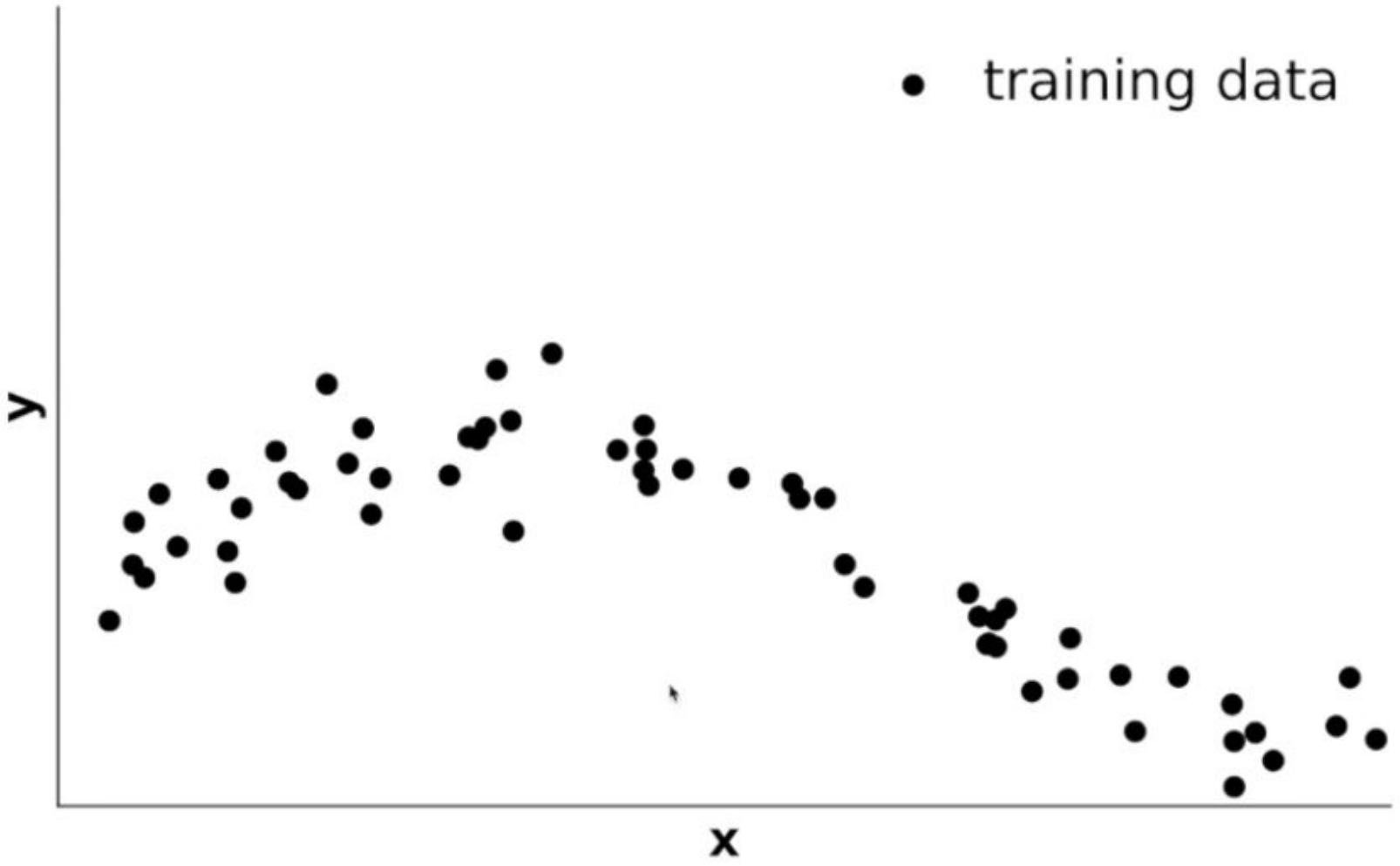


Intuition- Classification

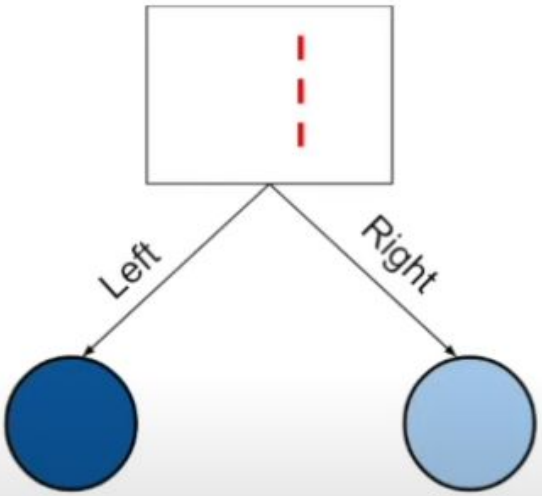


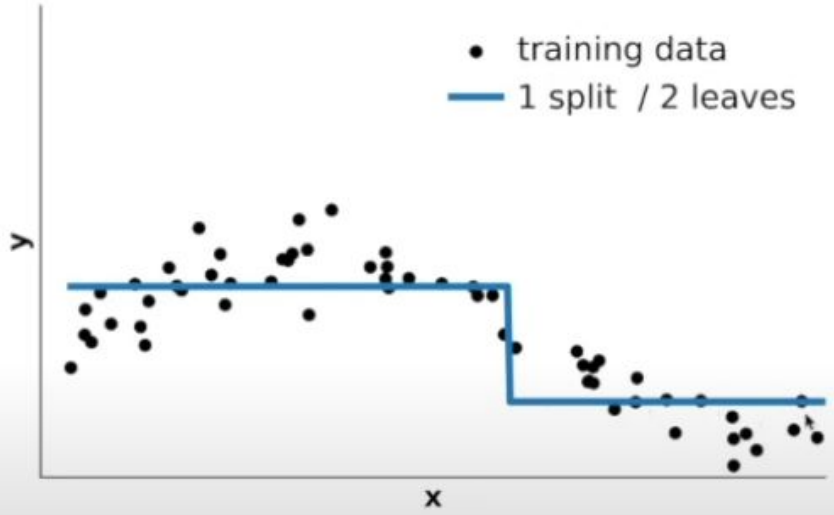


Intuition - Regression

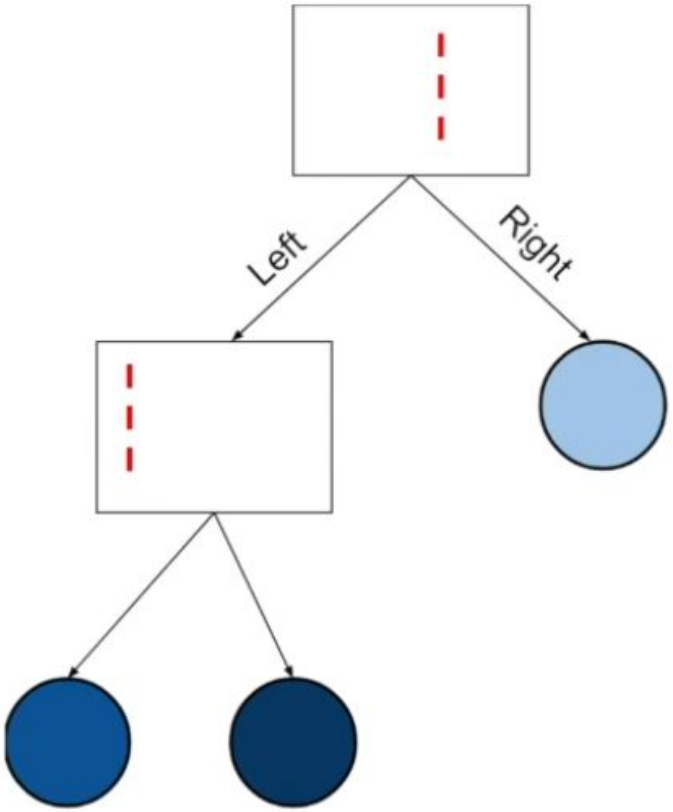


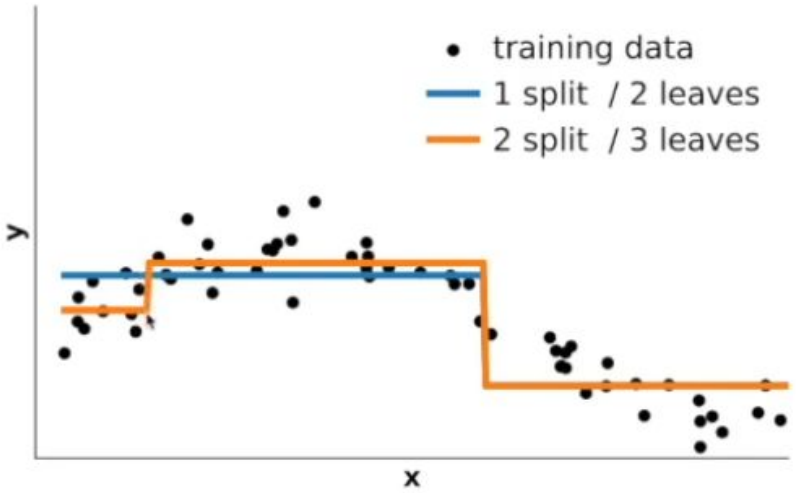
Intuition - Regression



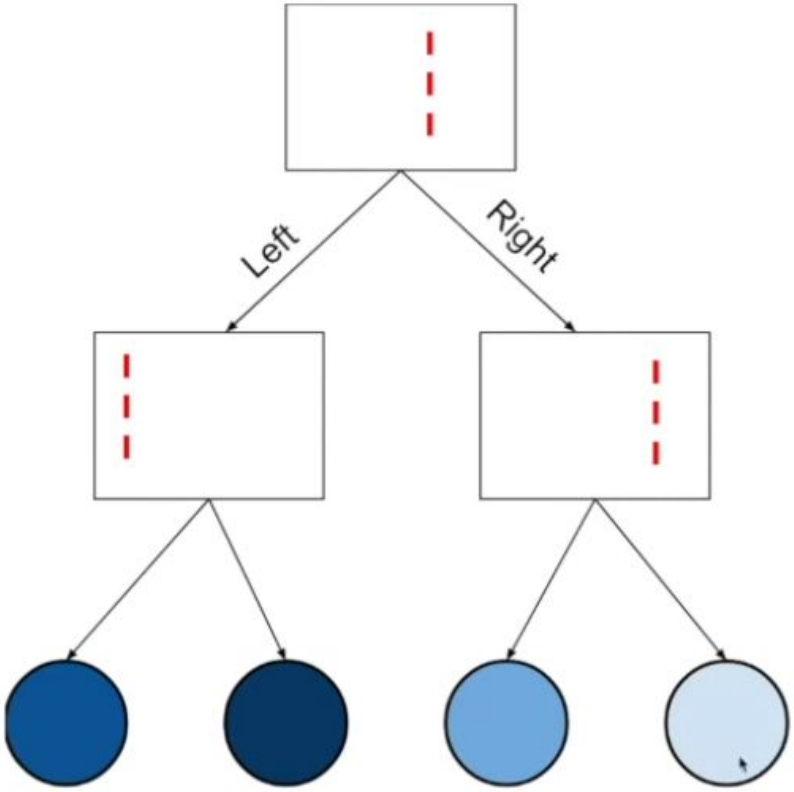


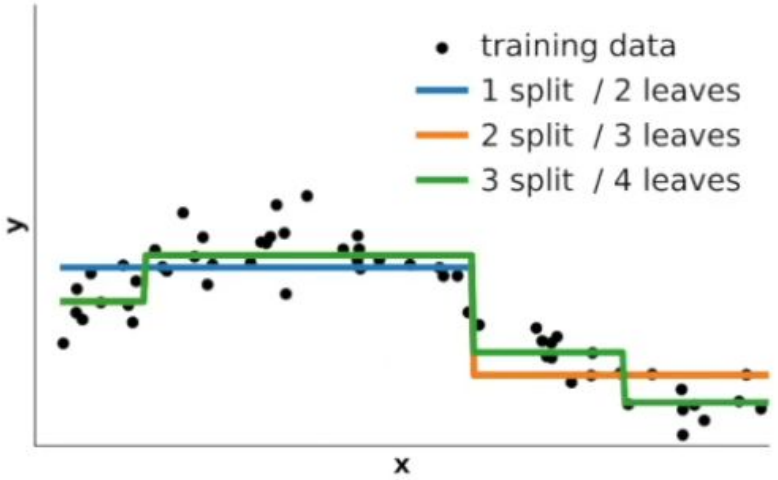
Intuition - Regression



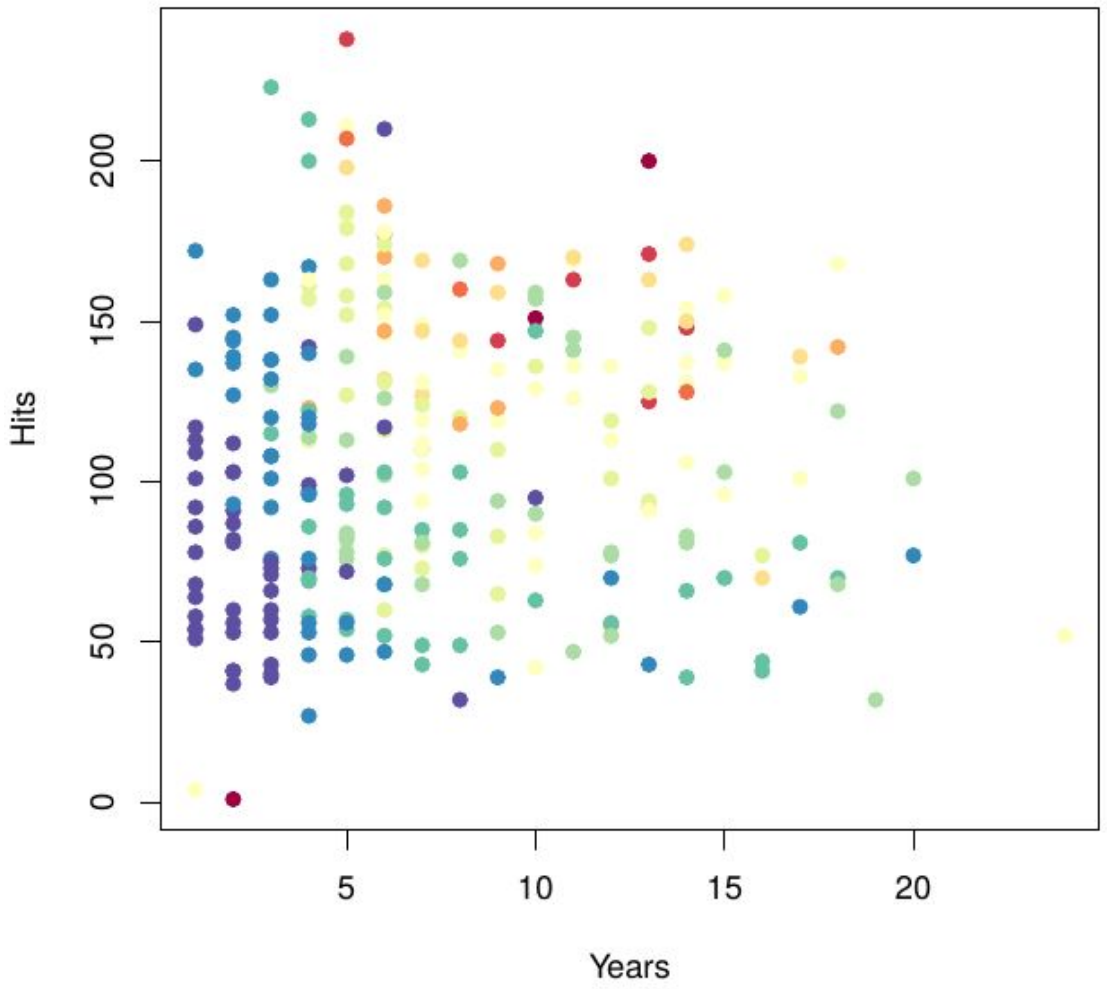


Intuition - Regression



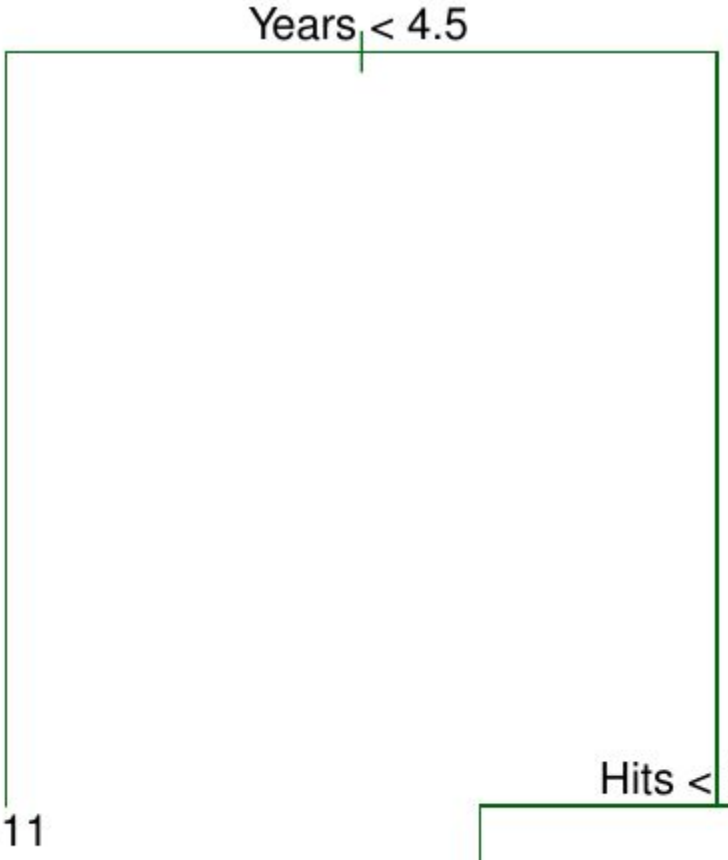


Hitters Data



X_1 = the number of years that he has played in the major leagues
X_2 = the number of hits that he made in the previous year
Y = salary in thousands of dollars: $\log_e$(salary)

Regression Tree for Hitters Data

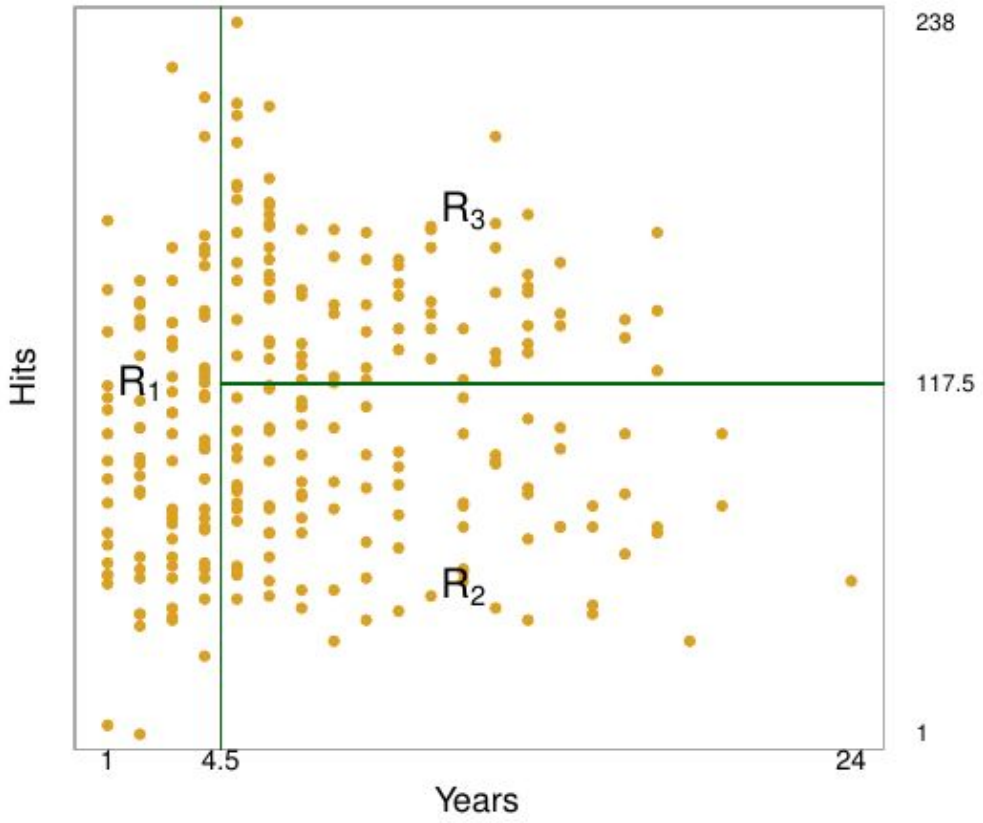


$$Y_1 = 10^3 * e^{5.11}$$

$$Y_2 = 10^3 * e^{6}$$

$$Y_3 = 10^3 * e^{6.74}$$

- Overall, the tree stratifies or segments the players into three regions of predictor space: $R_1 = \{\mathrm{X} \mid \texttt{Years} < 4.5\}$, $R_2 = \{\mathrm{X} \mid \texttt{Years} >= 4.5, \texttt{Hits} < 117.5\}$, and $R_3 = \{\mathrm{X} \mid \texttt{Years} >= 4.5, \texttt{Hits} >= 117.5\}$.



Interpretation of the Results

- `Years` is the most important factor in determining `Salary`, and players with less experience earn lower salaries than more experienced players.
- Given that a player is less experienced, the number of `Hits` that he made in the previous year seems to play little role in his `Salary`.
- But among players who have been in the major leagues for five or more years, the number of `Hits` made in the previous year does affect `Salary`, and players who made more `Hits` last year tend to have higher salaries.
- Surely an over-simplification, but compared to a regression model, it is easy to display, interpret and explain

Terminology

- In keeping with the *tree* analogy, the regions R_1, R_2, and R_3 are known as *terminal nodes*
- Decision trees are typically drawn *upside down*, in the sense that the leaves are at the bottom of the tree.
- The points along the tree where the predictor space is split are referred to as *internal nodes*
- In the hitters tree, the two internal nodes are indicated by the text `Years`<4.5 and `Hits`<117.5.

How do we construct the regions ($R_1, R_2, \ldots, R_J$)?

- In theory, the regions could have any shape. However, we choose to divide the predictor space into high-dimensional rectangles, or *boxes*, for simplicity and for ease of interpretation of the resulting predictive model.
- The goal is to find boxes $R_1, \ldots, R_J$ that minimize the RSS, given by

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2,$$

where $\hat{y}_{R_j}$ is the mean response for the training observations within the jth box.

Recursive Binary Splitting Algorithm - Part One

- We first select the predictor X_j and the cutpoint s such that splitting the predictor space into the regions $\{X|X_j < s\}$ and $\{X|X_j \geq s\}$ leads to the greatest possible reduction in RSS.

For any j and s, we define the pair of half-planes

$$R_1(j,s) = \{X|X_j < s\} \text{ and } R_2(j,s) = \{X|X_j \geq s\},$$

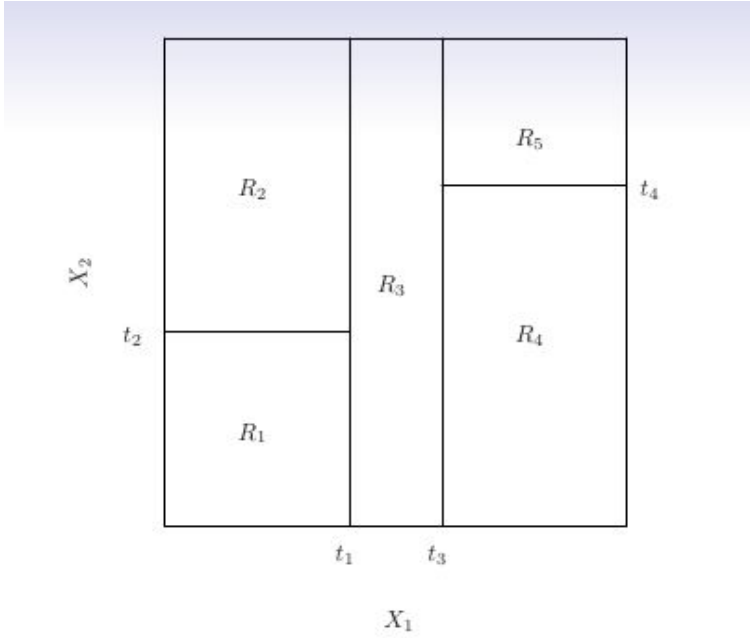
and we seek the value of j and s that minimize the equation

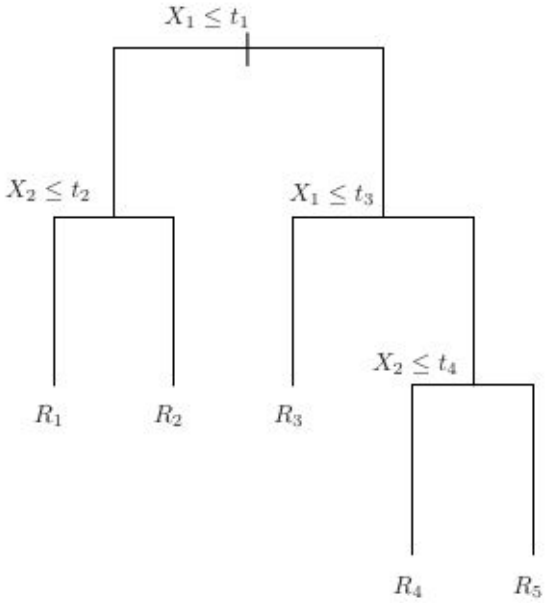
$$\sum_{i:\, x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:\, x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2,$$

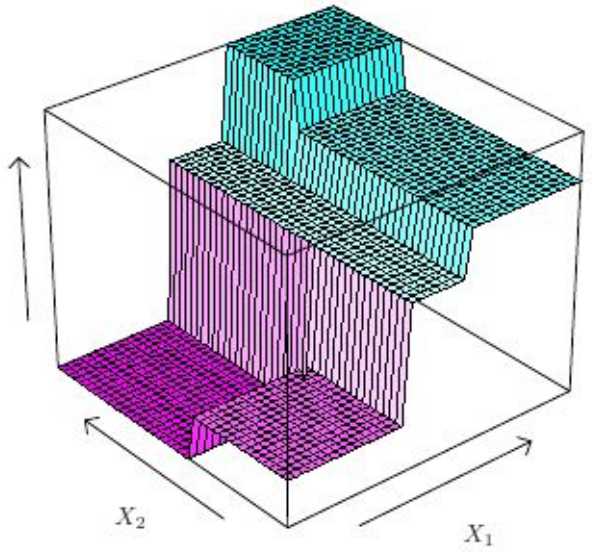
Recursive Binary Splitting Algorithm - Part Two

- Next, we repeat the process, looking for the best predictor and best cutpoint in order to split the data further so as to minimize the RSS within each of the resulting regions.
- However, this time, instead of splitting the entire predictor space, we split one of the two previously identified regions. We now have three regions.
- Again, we look to split one of these three regions further, so as to minimize the RSS. The process continues until a stopping criterion is reached; for instance, we may continue until no region contains more than five observations.

Example


R_5
R_2
t_4
X_2
R_3
t_2
R_4
R_1
t_1
t_3
X_1


$X_1 \leq t_1$
$X_2 \leq t_2$
$X_1 \leq t_3$
$X_2 \leq t_4$
R_1
R_2
R_3
R_4
R_5

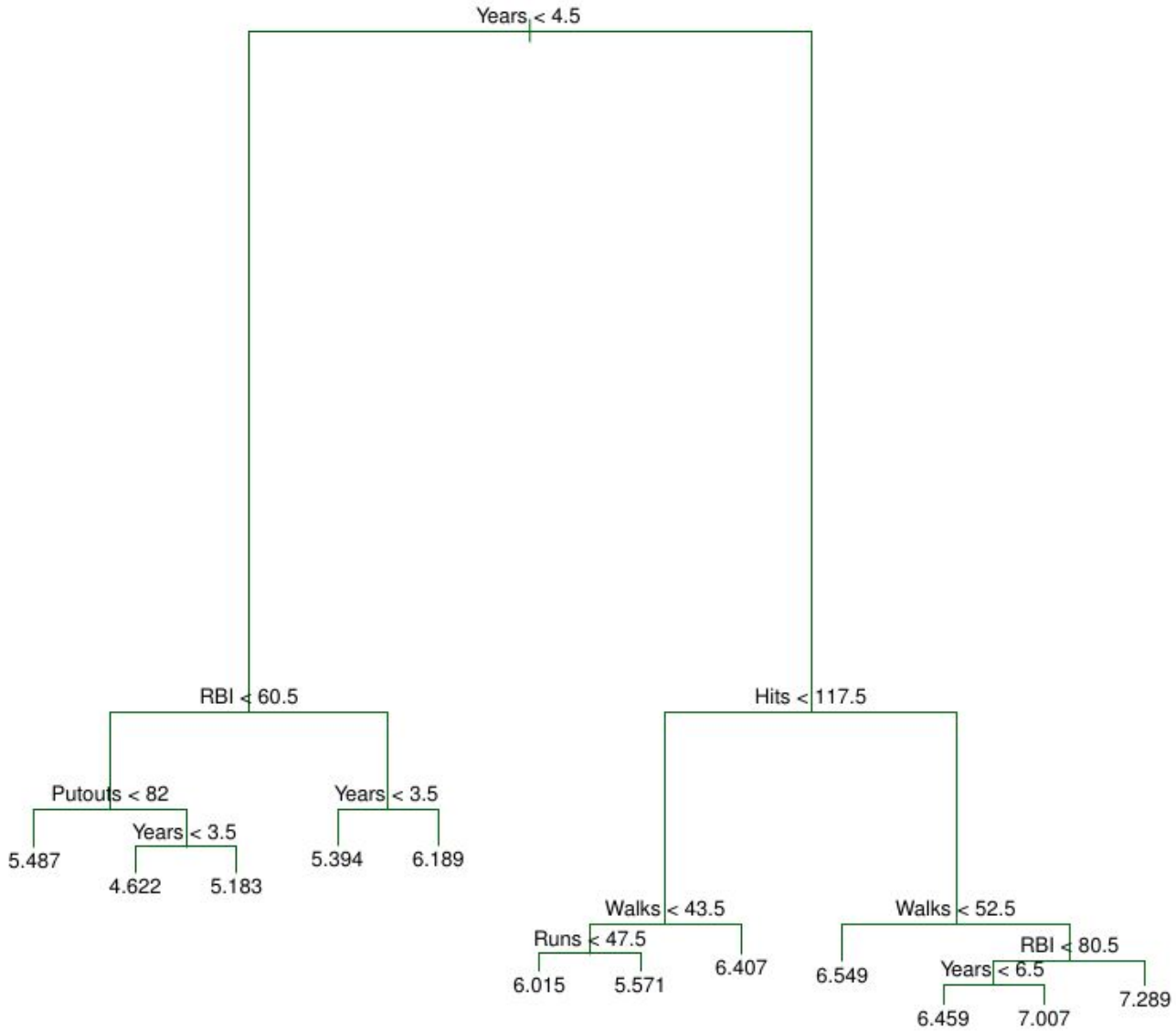

X_2
X_1

Pruning a Tree

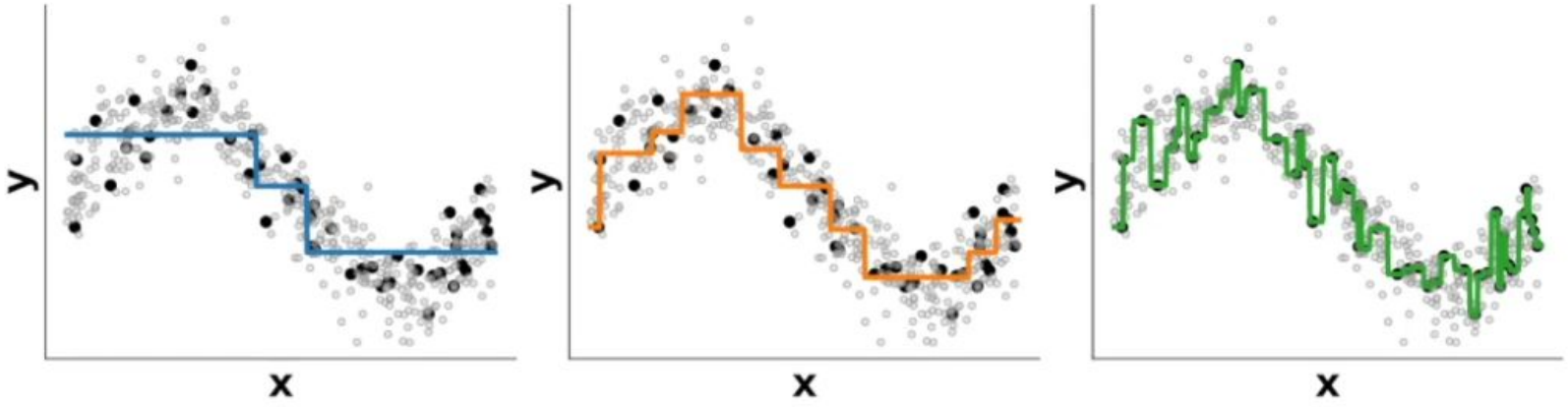
- The process described above may produce good predictions on the training set, but is likely to *overfit* the data, leading to poor test set performance. *Why?*

This is because the resulting tree might be too complex.

Hitters Data without Pruning



Tree Depth and Overfitting



Underfitting

`max_depth` or
`max_leaf_nodes`
too small

Best trade-off

Overfitting

`max_depth` or
`max_leaf_nodes`
too large

Pruning a Tree

- A better strategy is to grow a very large tree T_0, and then *prune* it back in order to obtain a *subtree*
- *Cost complexity pruning* — also known as *weakest link pruning* — is used to do this
- we consider a sequence of trees indexed by a nonnegative tuning parameter α. For each value of α there corresponds a subtree $T \subset T_0$ such that

$$\sum_{m=1}^{|T|} \sum_{i:\, x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

is as small as possible. Here $|T|$ indicates the number of terminal nodes of the tree T, R_m is the rectangle (i.e. the subset of predictor space) corresponding to the mth terminal node, and $\hat{y}_{R_m}$ is the mean of the training observations in R_m.

Choosing the best subtree

$$\sum_{m=1}^{|T|} \sum_{i:\, x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

- The tuning parameter α controls a trade-off between the subtree's complexity and its fit to the training data.
- We select an optimal value $\hat{\alpha}$ using cross-validation.
- We then return to the full data set and obtain the subtree corresponding to $\hat{\alpha}$.

Algorithm 8.1 *Building a Regression Tree*

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.

2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.

3. Use K-fold cross-validation to choose α. That is, divide the training observations into K folds. For each $k = 1, \ldots, K$:

   (a) Repeat Steps 1 and 2 on all but the kth fold of the training data.

   (b) Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

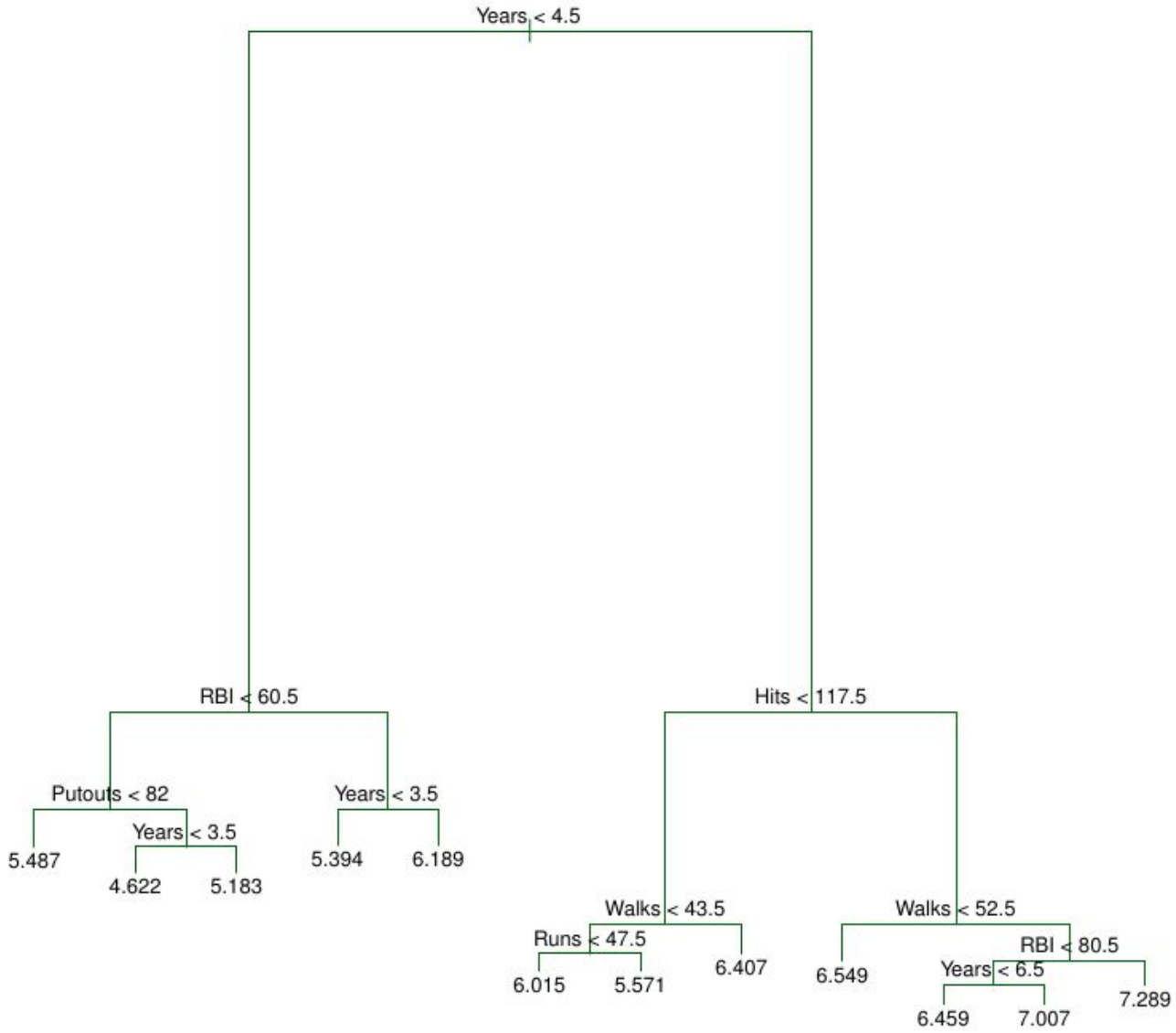
   Average the results for each value of α, and pick α to minimize the average error.

4. Return the subtree from Step 2 that corresponds to the chosen value of α.

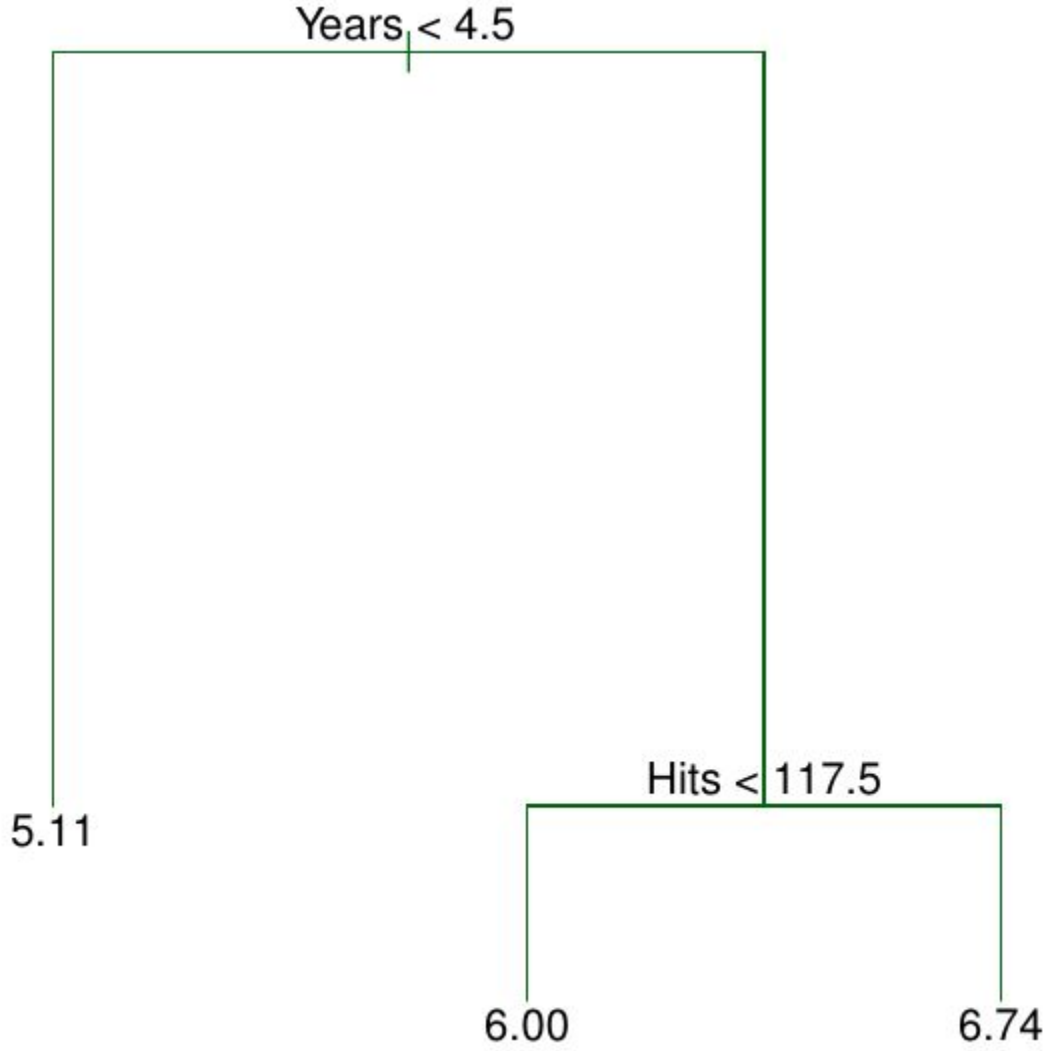
Hitters Data Continued

- First, we randomly divided the data set in half, yielding 132 observations in the training set and 131 observations in the test set.
- We then built a large regression tree on the training data and varied α in in order to create subtrees with different numbers of terminal nodes.
- Finally, we performed six-fold cross-validation in order to estimate the cross-validated MSE of the trees as a function of α.

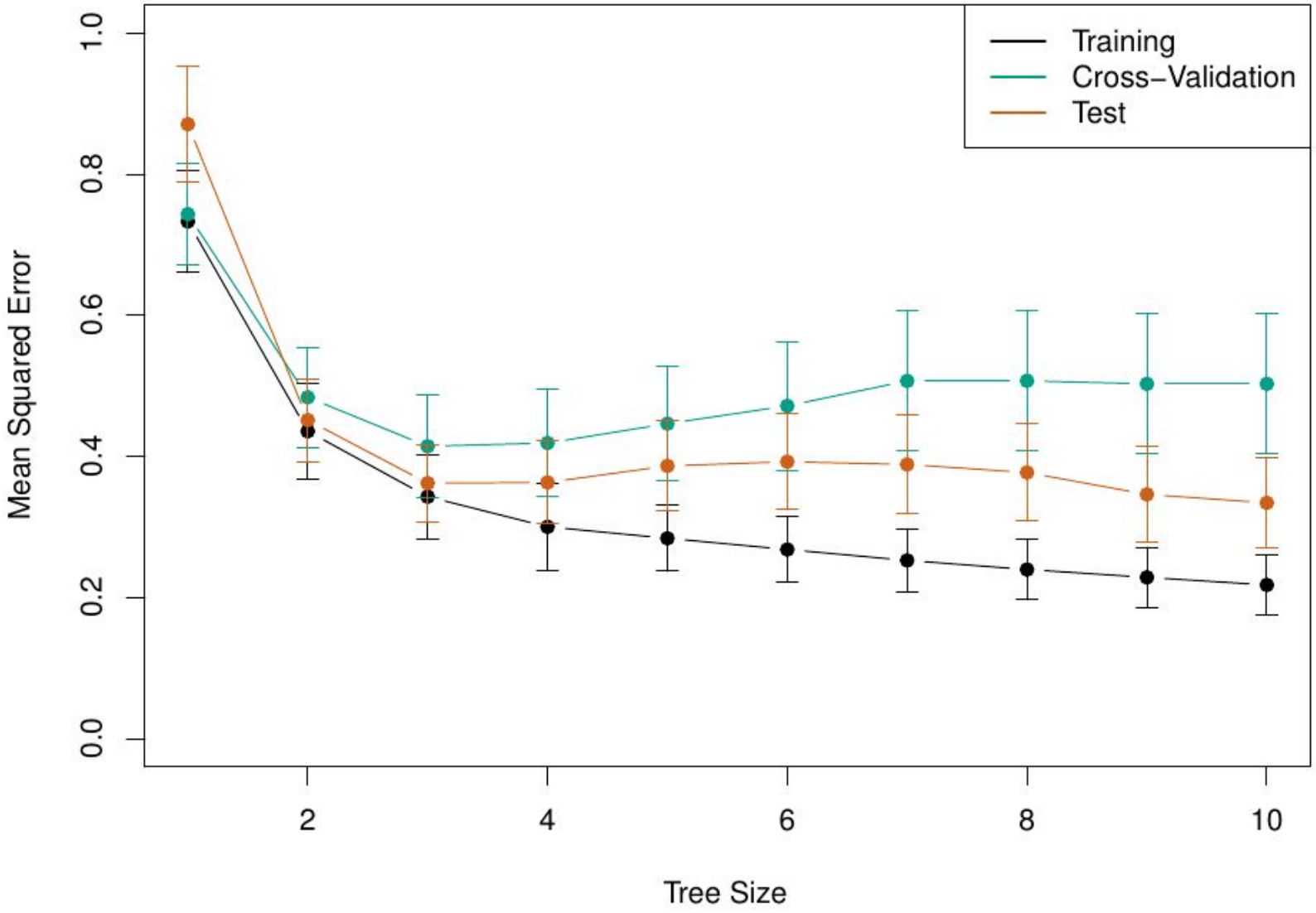
Unpruned Decision Tree for Hitters Data



Pruned Decision Tree for Hitters Data



Choosing best subtree via Cross Validation



Classification Trees

- Very similar to a regression tree, except that it is used to predict a qualitative response rather than a quantitative one.
- For a classification tree, we predict that each observation belongs to the *most commonly occurring class* of training observations in the region to which it belongs.

Criterion for Making Splits (1)

- In the classification setting, RSS cannot be used as a criterion for making the binary splits
- A natural alternative to RSS is the *classification error rate*. this is simply the fraction of the training observations in that region that do not belong to the most common class:

$$E_m = 1 - \max_k(\hat{p}_{mk})$$

Here $\hat{p}_{mk}$ represents the proportion of training observations in the mth region that are from the kth class.

- However classification error is not sufficiently sensitive for tree-growing, and in practice two other measures are preferable.

Criterion for Making Splits (2)

- The *Gini index* is defined by

$$G_m = \sum_{k-1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

a measure of total variance across the K classes. The Gini index takes on a small value if all of the $\hat{p}_{mk}$'s are close to zero or one.

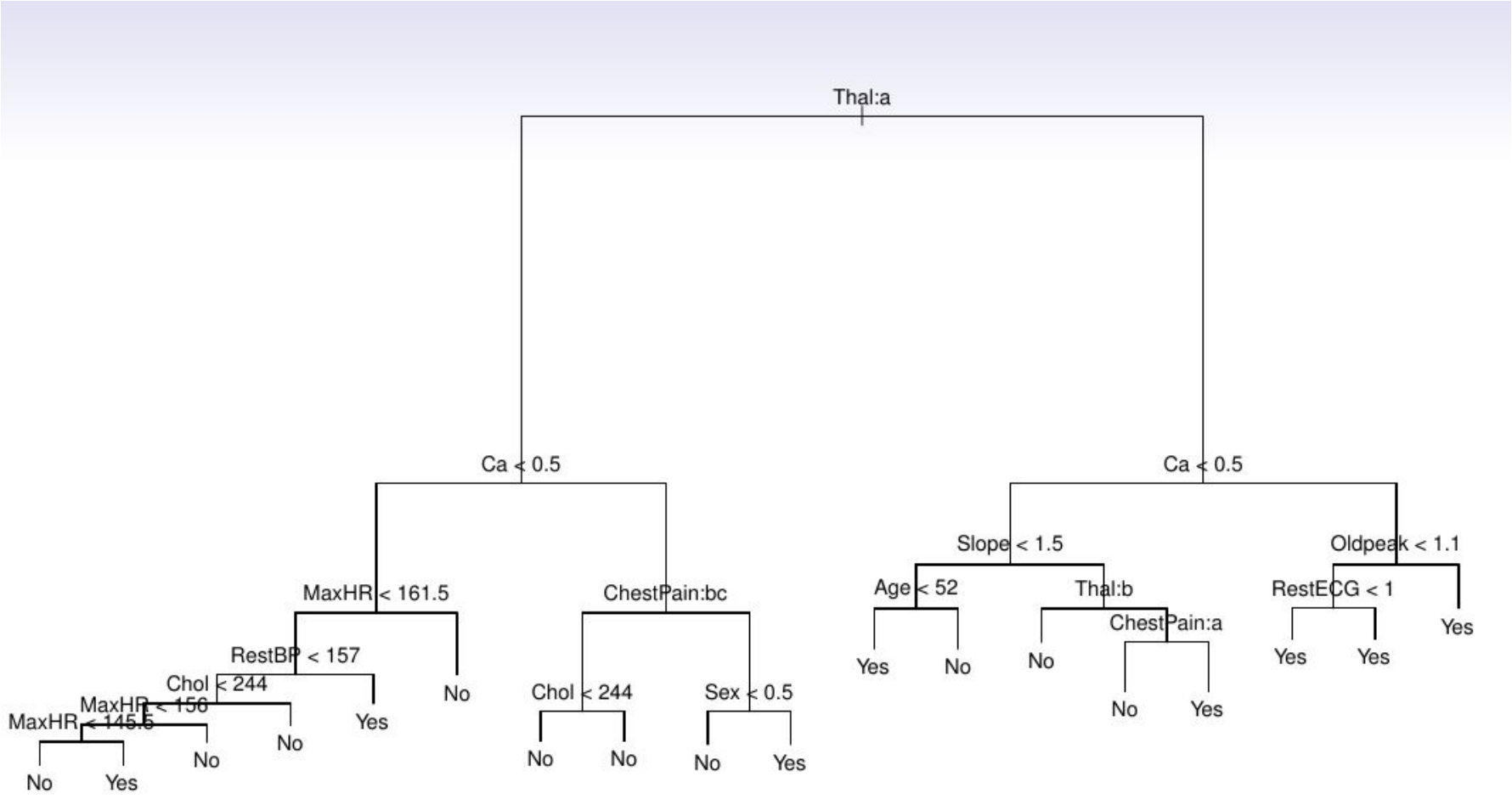
- For this reason the Gini index is referred to as a measure of node *purity* — a small value indicates that a node contains predominantly observations from a single class.

$$0 \leq G_m \leq 0.5$$

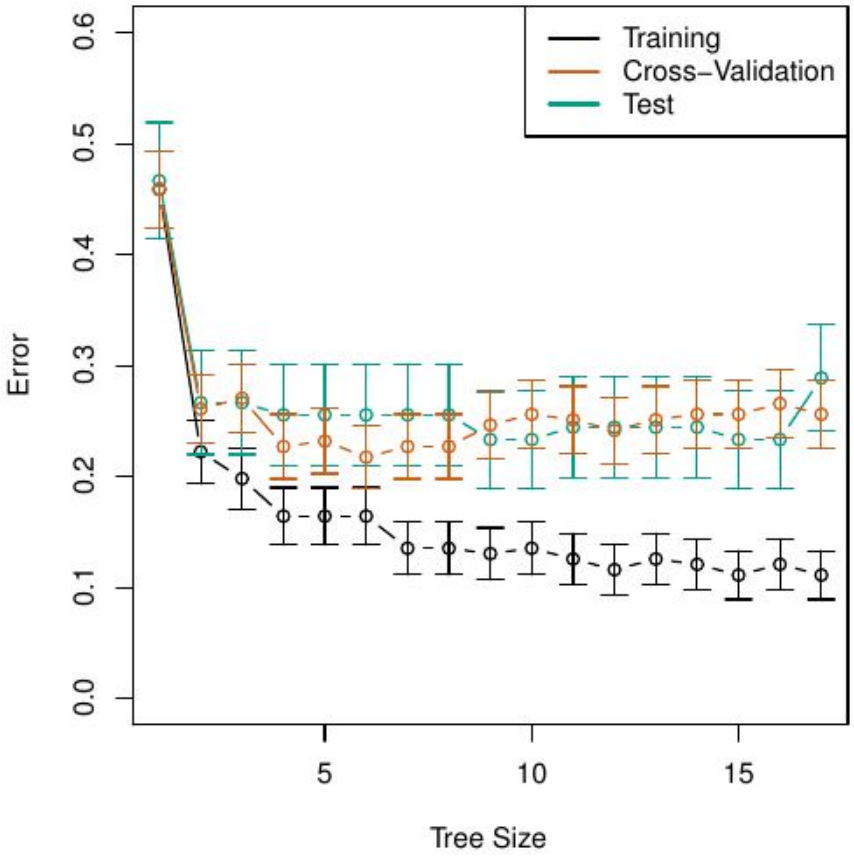
Heart Data - Example

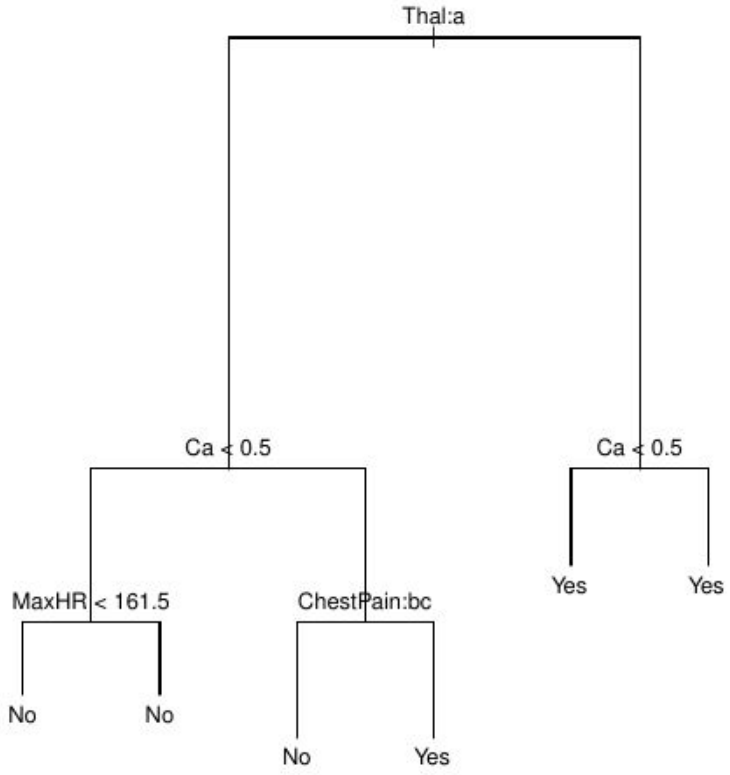
- These data contain a binary outcome `HD` for 303 patients who presented with chest pain.
- An outcome value of `Yes` indicates the presence of heart disease based on an angiographic test, while `No` means no heart disease.
- There are 13 predictors including `Age`, `Sex`, `Chol` (a cholesterol measurement), and other heart and lung function measurements.
- Cross-validation yields a tree with six terminal nodes. See next figure.

Heart Data - Unpruned Classification Tree

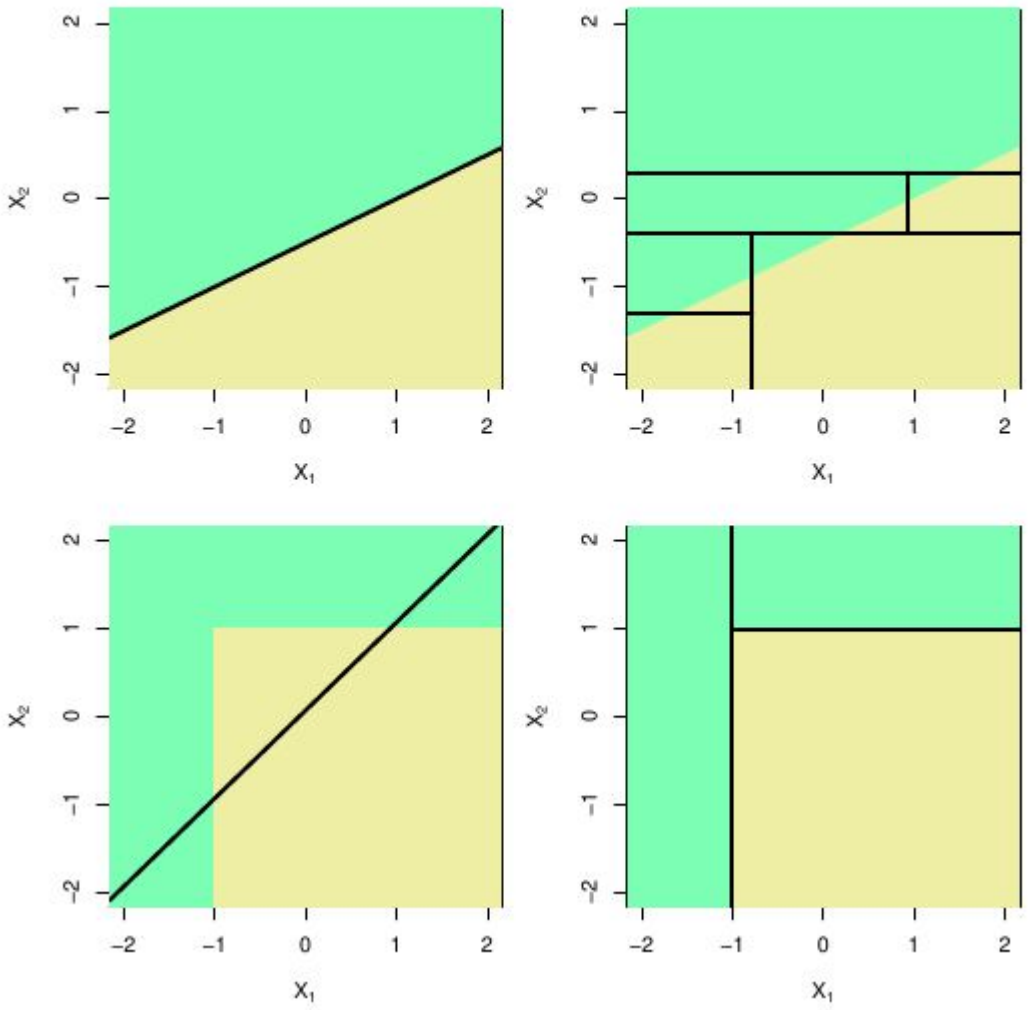


Heart Data - Pruned Classification Tree





Trees Versus Linear Models



Advantages and Disadvantages of Trees

- ▲ Trees are very easy to explain to people. In fact, they are even easier to explain than linear regression!
- ▲ Trees can be displayed graphically, and are easily interpreted even by a non-expert (especially if they are small).
- ▲ Trees can easily handle qualitative predictors without the need to create dummy variables.
- ▼ Unfortunately, trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches seen in this book.

However, by aggregating many decision trees, the predictive performance of trees can be substantially improved. We introduce these concepts next.

Bagging

- *Bootstrap aggregation*, or *bagging*, is a general-purpose procedure for reducing the variance of a statistical learning method; we introduce it here because it is particularly useful and frequently used in the context of decision trees.

- In this approach we generate B different bootstrapped training data sets. We then train our method on the bth bootstrapped training set in order to get $\hat{f}^{*b}(x)$, the prediction at a point x. We then average all the predictions to obtain

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^{*b}(x).$$

  This is called *bagging*.

Bagging classification trees

- The above prescription applied to regression trees
- For classification trees: for each test observation, we record the class predicted by each of the B trees, and take a *majority vote*: the overall prediction is the most commonly occurring class among the B predictions.

Random Forests (1)

- *Random forests* provide an improvement over bagged trees by way of a small tweak that *decorrelates* the trees. This reduces the variance when we average the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, *a random selection of m predictors* is chosen as split candidates from the full set of p predictors. The split is allowed to use only one of those m predictors.

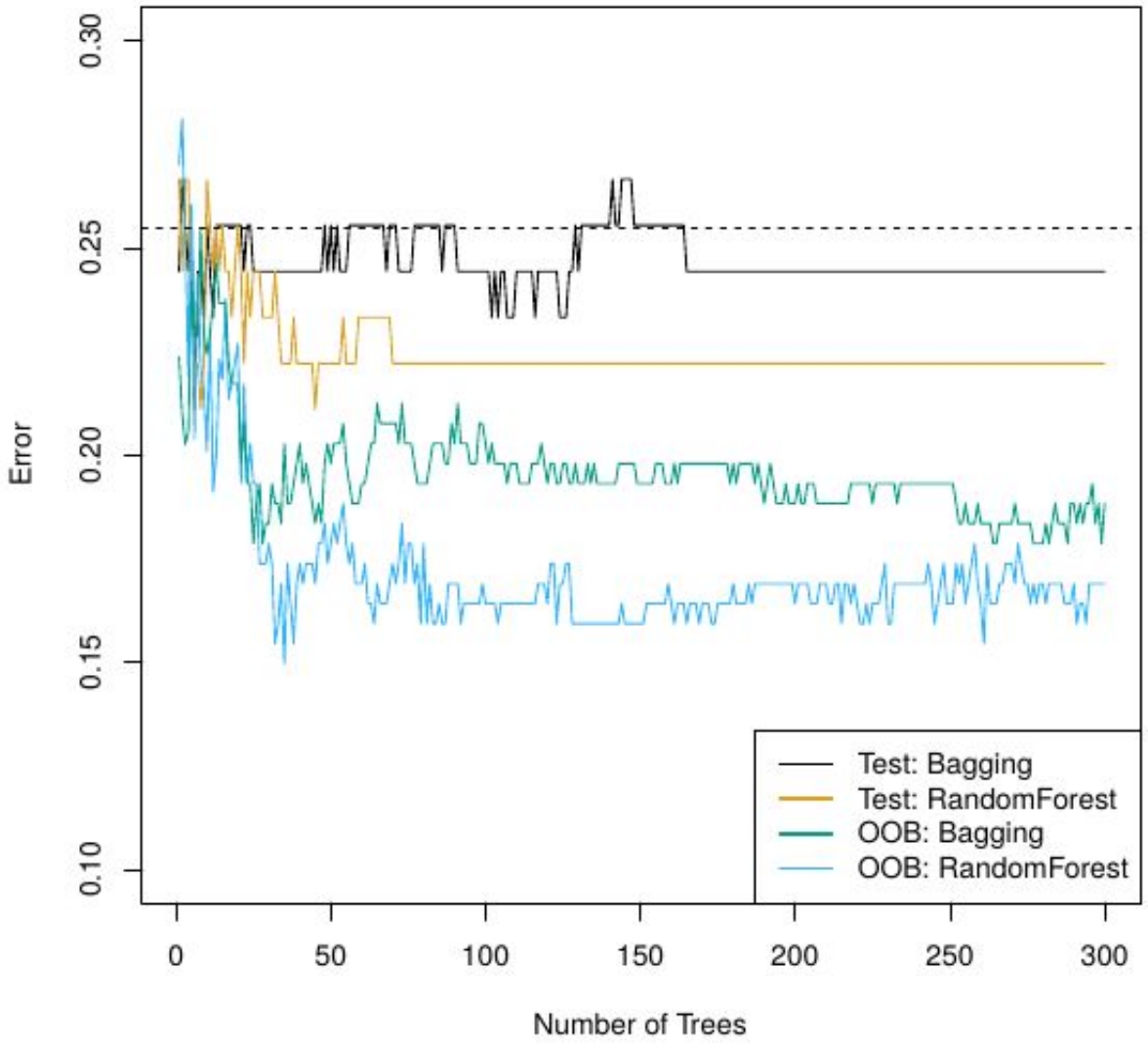
Random Forests (2)

- A fresh selection of m predictors is taken at each split, and typically we choose $m \approx \sqrt{p}$ — that is, the number of predictors considered at each split is approximately equal to the square root of the total number of predictors (4 out of the 13 for the Heart data).

Why Random Forests can be better that Bagging?

- Random Forests force splits to consider only a subset of predictors. In contrast to Bagging, this tends to generate uncorrelated trees and can lead to a larger reduction in variance.

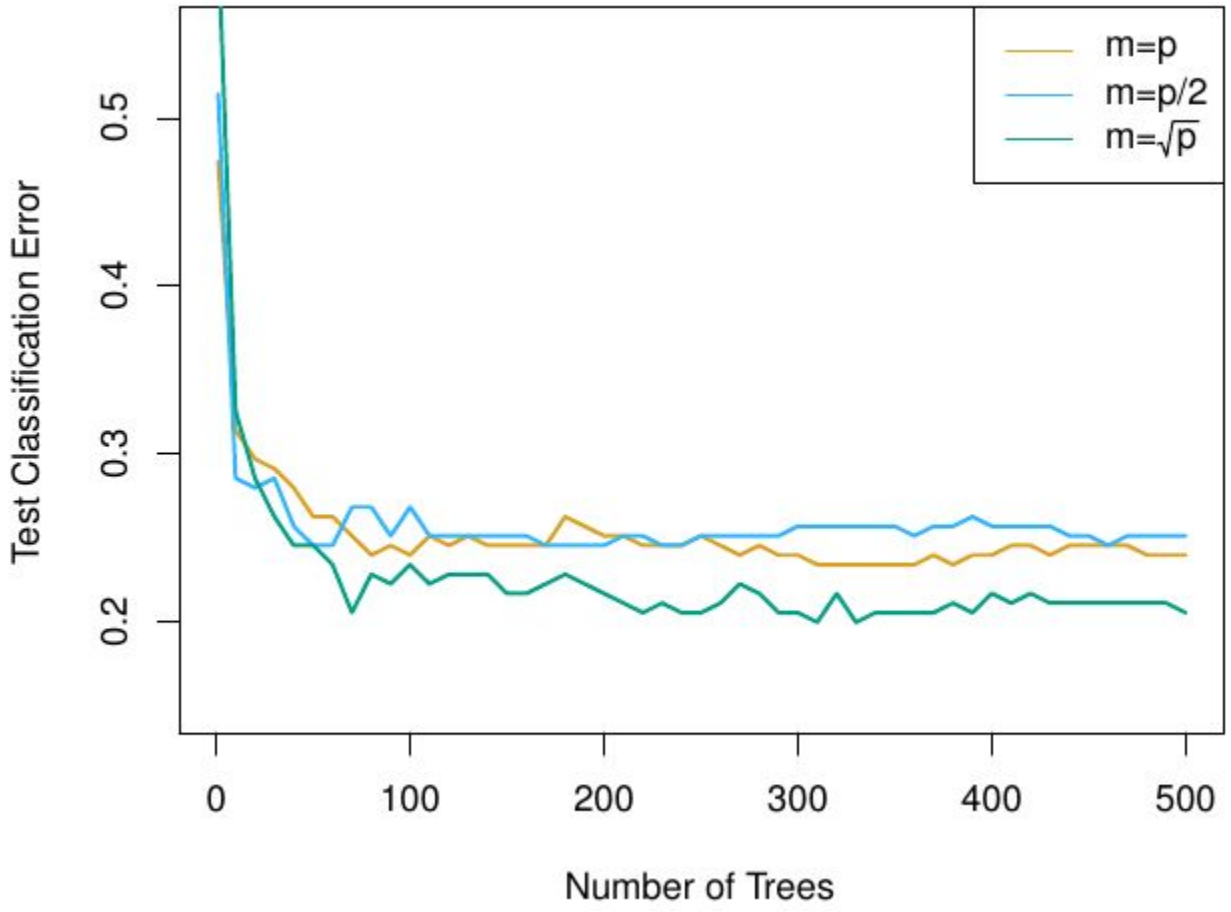
Heart Data - Example



Gene Expression Data - Example (1)

- We applied random forests to a high-dimensional biological data set consisting of expression measurements of 4,718 genes measured on tissue samples from 349 patients.
- Each of the patient samples has a qualitative label with 15 different levels: either normal or one of 14 different types of cancer.
- We use random forests to predict cancer type based on the 500 genes that have the largest variance in the training set.
- We randomly divided the observations into a training and a test set, and applied random forests to the training set for three different values of the number of splitting variables m.

Gene Expression Data - Example (2)



Boosting

- Like bagging, boosting is a general approach that can be applied to many statistical learning methods for regression or classification. We only discuss boosting for decision trees.
- Recall that bagging involves creating multiple copies of the original training data set using the bootstrap, fitting a separate decision tree to each copy, and then combining all of the trees in order to create a single predictive model.
- Notably, each tree is built on a bootstrap data set, independent of the other trees.
- Boosting works in a similar way, except that the trees are grown *sequentially*: each tree is grown using information from previously grown trees.

Boosting for Classification - Algorithm

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X$, $y_i \in Y = \{-1, +1\}$

Initialize $D_1(i) = 1/m$.

distribution of weights over the training set

For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.

Decision Tree trained over D_t

- Get weak hypothesis $h_t : X \to \{-1, +1\}$ with error

$$\epsilon_t = \Pr_{i \sim D_t} \left[h_t(x_i) \neq y_i \right].$$

obtém o erro sobre D_t

- Choose $\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$.

measures the importance that is assigned to h_t. \alpha_t gets larger as e_t gets smaller.

- Update:

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases}$$

$$= \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

increase the weight of misclassified examples and decrease of the correct ones

where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Output the final hypothesis:

$$H(x) = \text{sign} \left(\sum_{t=1}^{T} \alpha_t h_t(x) \right).$$

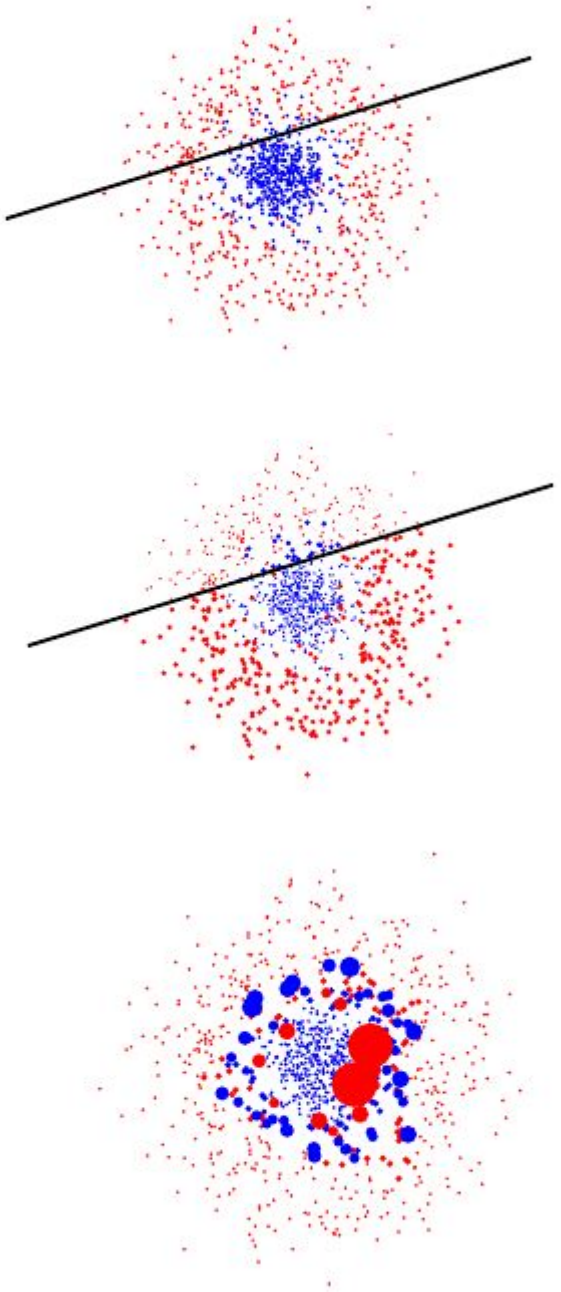
weighted majority vote of the T weak hypotheses.

Boosting

Reweighting formula:

$$D_{t+1}(i) = \frac{D_t(i) exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

$$exp(-\alpha_t y_i h_t(x_i)) \begin{cases} < 1, & y_i = h_t(x_i) \\ > 1, & y_i \neq h_t(x_i) \end{cases}$$



What is the idea behind Boosting? (1)

- Unlike fitting a single large decision tree to the data, which amounts to fitting the data hard and potentially overfitting, the boosting approach instead learns slowly.

- weak learner = rather small trees, with just a few terminal nodes. (Ex: depth-1 Trees)

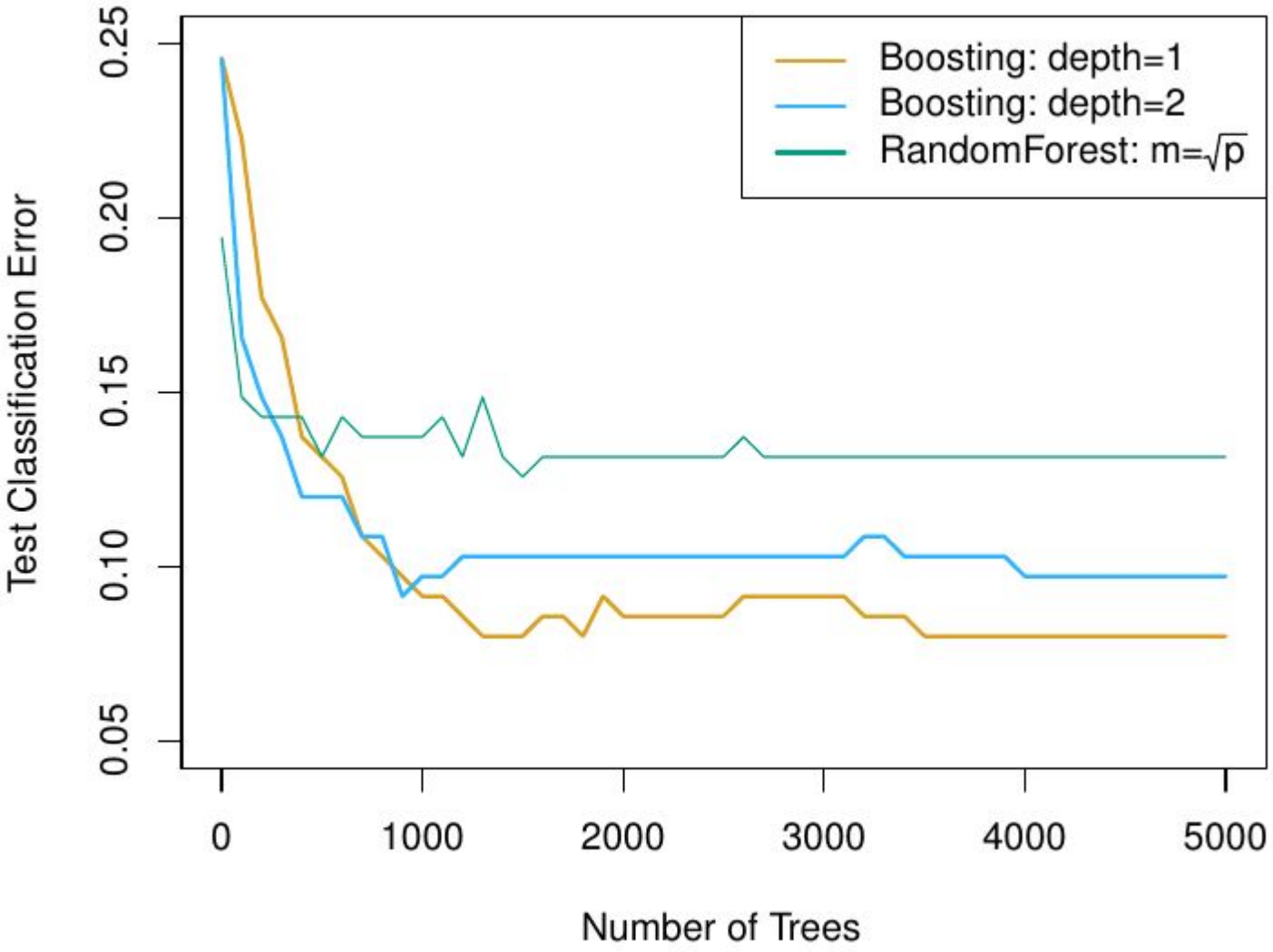
- AdaBoost is adaptive in the sense that subsequent weak learners are tweaked in favor of those instances misclassified by previous classifiers.

What is the idea behind Boosting? (2)

- the outputs of the decision trees ('weak learners') are combined into a weighted sum that represents the final output of the boosted classifier.

- the individual learners can be weak, but as long as the performance of each one is slightly better than random guessing (e.g., their error rate is smaller than 0.5 for binary classification), the final model can be proven to converge to a strong learner.

Gene Expression Data - Example



Summary

- Decision trees are simple and interpretable models for regression and classification
- However they are often not competitive with other methods in terms of prediction accuracy
- Bagging, random forests and boosting are good methods for improving the prediction accuracy of trees. They work by growing many trees on the training data and then combining the predictions of the resulting ensemble of trees.
- The latter two methods— random forests and boosting— are among the state-of-the-art methods for supervised learning. However their results can be difficult to interpret.