Topic 6. Tree-Based Methods

Outline

- Regression tree
- Classification tree
- Tree Pruning
- Improving Trees

Regression Tree

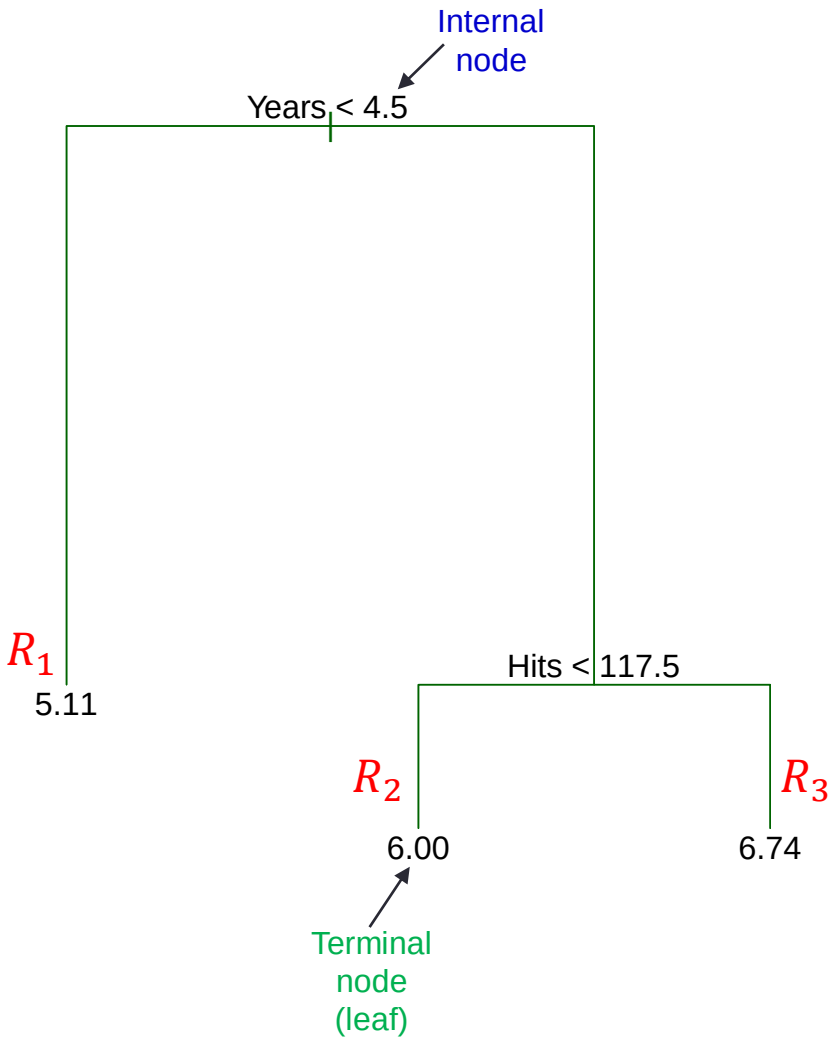
Partitioning the Predictor Space

- One way to make predictions/classification is to divide the predictor space (i.e. all the possible values for $X_1, X_2, \ldots, X_p$) into distinct regions, say $R_1, R_2, \ldots, R_k$.

- Then for every $\boldsymbol{X}$ that falls in a particular region (say R_j) we make the prediction using data in that region as training data. For example, when the response is numerical, we can use the mean of data in that region as prediction.

Regression Tree Example

- In the **Hitters** dataset, the predicted baseball player Salary is the number in each terminal node. It is the mean of the response for the observations that fall there.
- Note that Salary is measured in 1000s, and log-transformed
- The predicted salary for a player who played in the league for more than 4.5 years and had less than 117.5 hits last year is $\$1000 \times e^{6.00} = \$402,834$



Regions of Predictor Space

- The tree segments the players into three regions of predictor space:

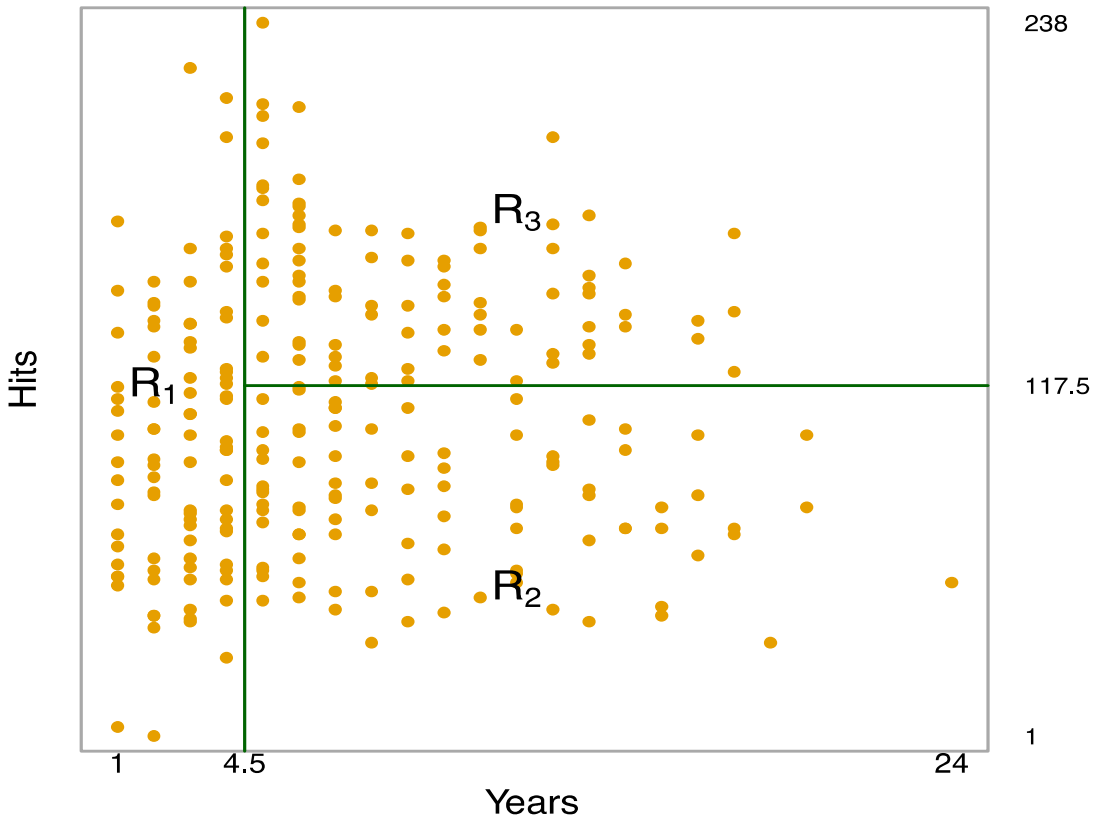
  R_1: players who have played for 4.5 or fewer years

  R_2: players who have played for 4.5 or more years and made fewer than 117.5 hits last year

  R_3: players who have played for five or more years and made at least 117.5 hits last year

- Prediction is made in each region separately

Another Way of Visualizing the Decision Tree



Linear regression

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$$

Regression tree

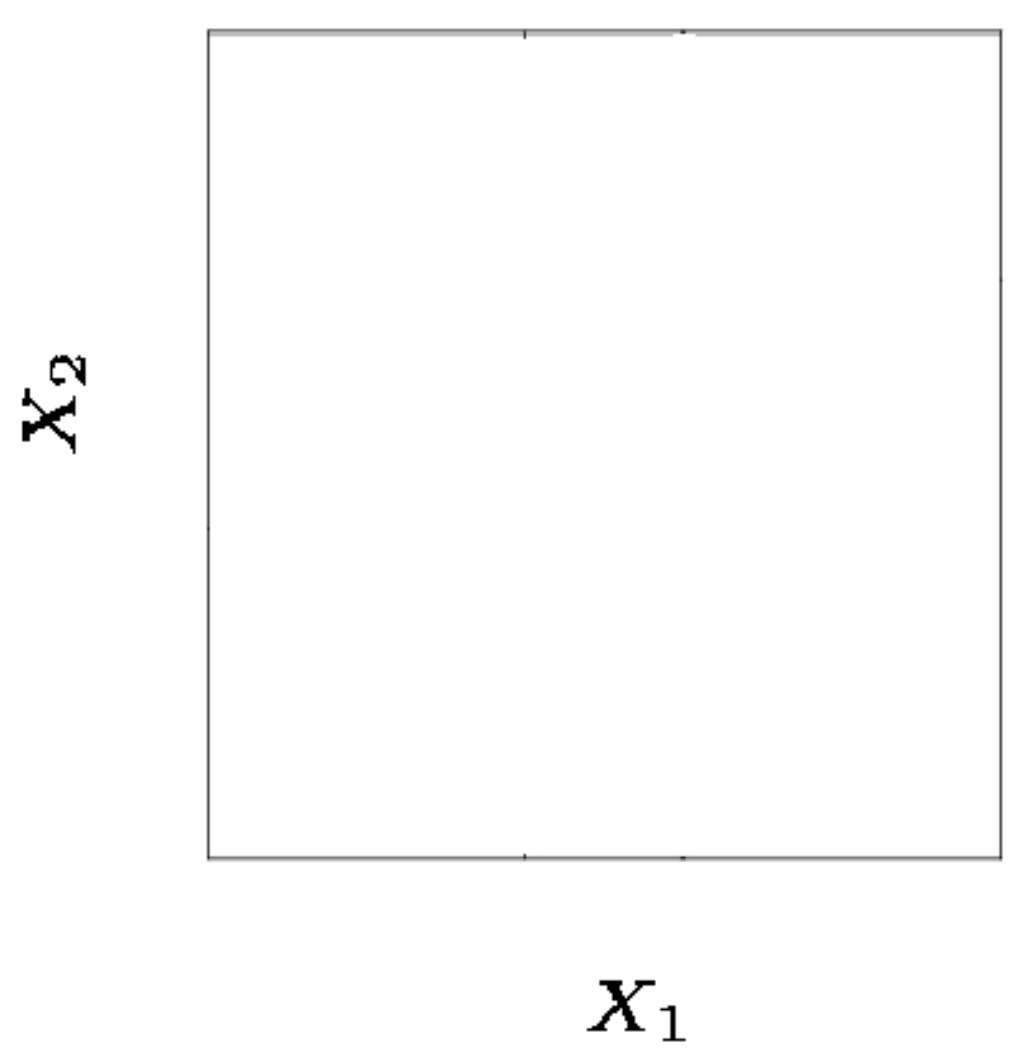
$$f(X) = \sum_{m=1}^{M} c_m \cdot 1_{(X \in R_m)}$$

Some Natural Questions

1. Where to split? i.e., how do we decide on the regions $R_1, R_2, \ldots, R_k$, or equivalently, what tree structure should we use?

2. What values should we use for the prediction in each region $\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_k$?

1. Where to Split?

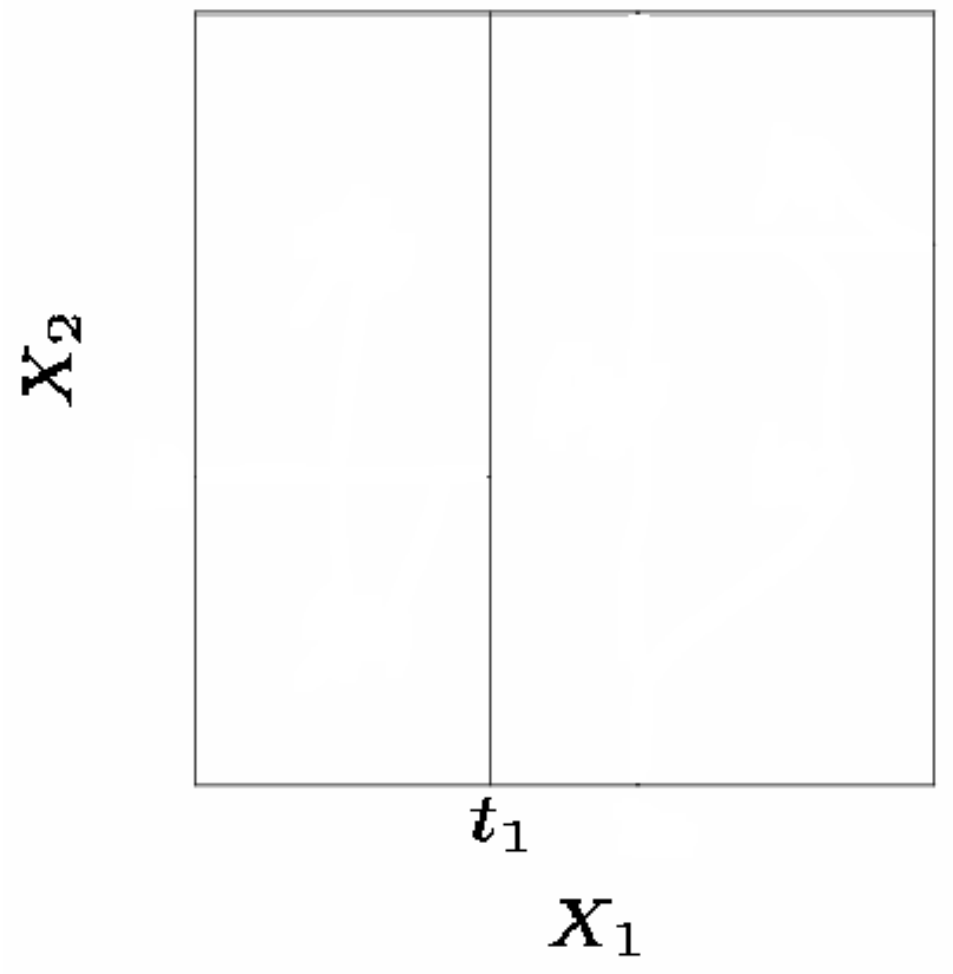


Recursive Binary Splitting—Step 1

- We consider splitting the predictor space into two regions, $X_j > s$ and $X_j < s$ for all possible values of j and s (i.e., all predictors and possible cutpoints).
- We then choose the j and s that result in the lowest RSS on the training data.

Result of Step 1

- Here the optimal split was on X_1 at point t_1.

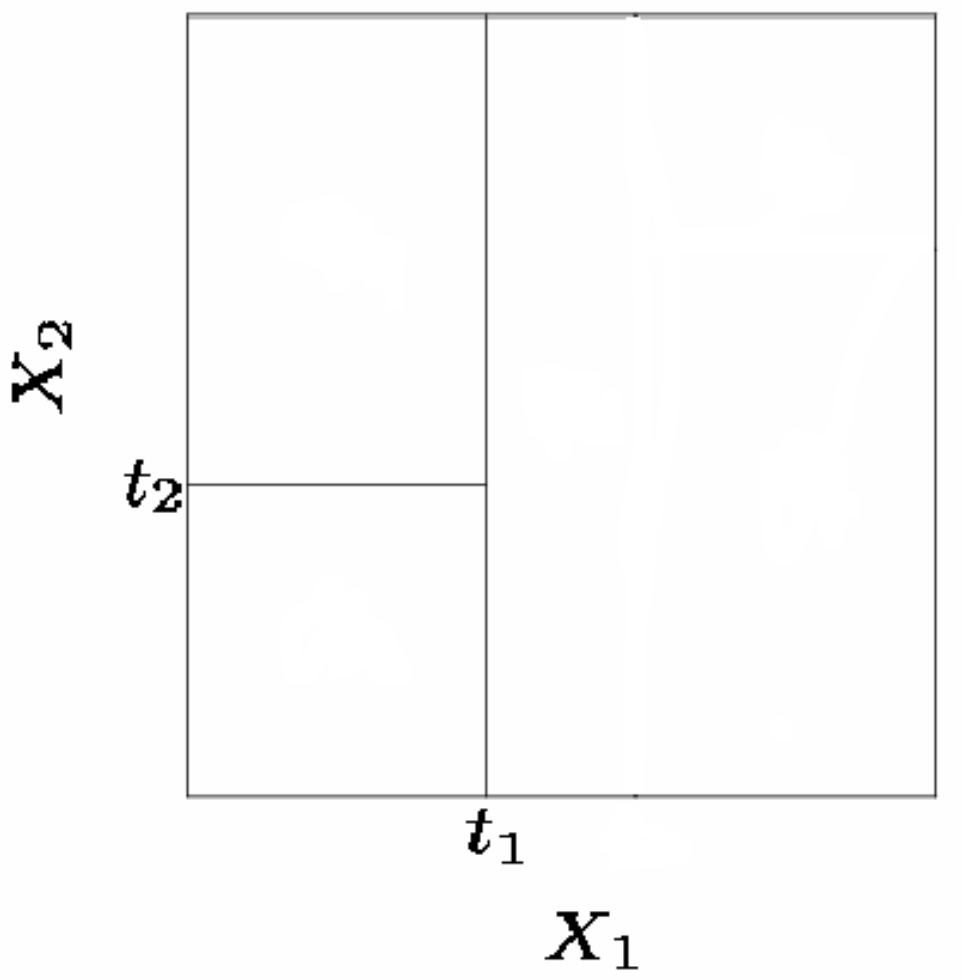


Recursive Binary Splitting—Step 2

- Now we repeat the process looking for the next best split except that we must also consider whether to split the first region or the second region.
- Again the criteria is smallest RSS.

Result of Step 2

- Here the optimal split was the left region on X_2 at point t_2.

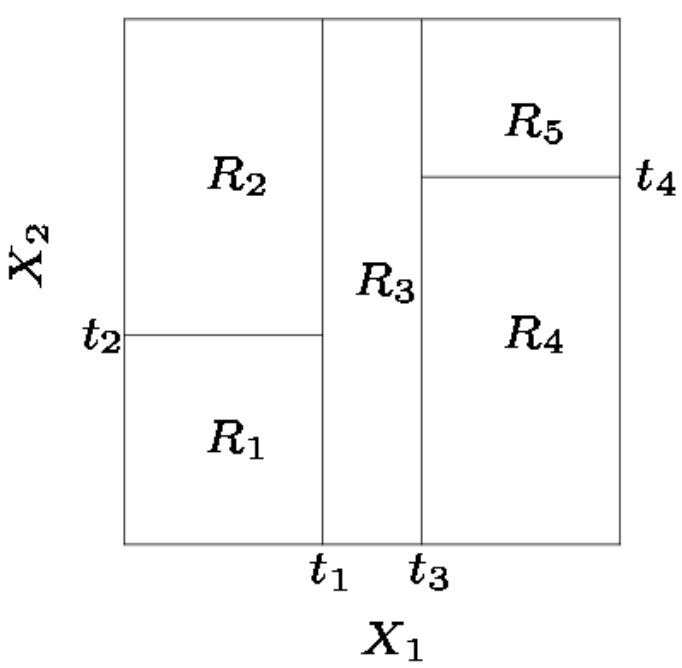


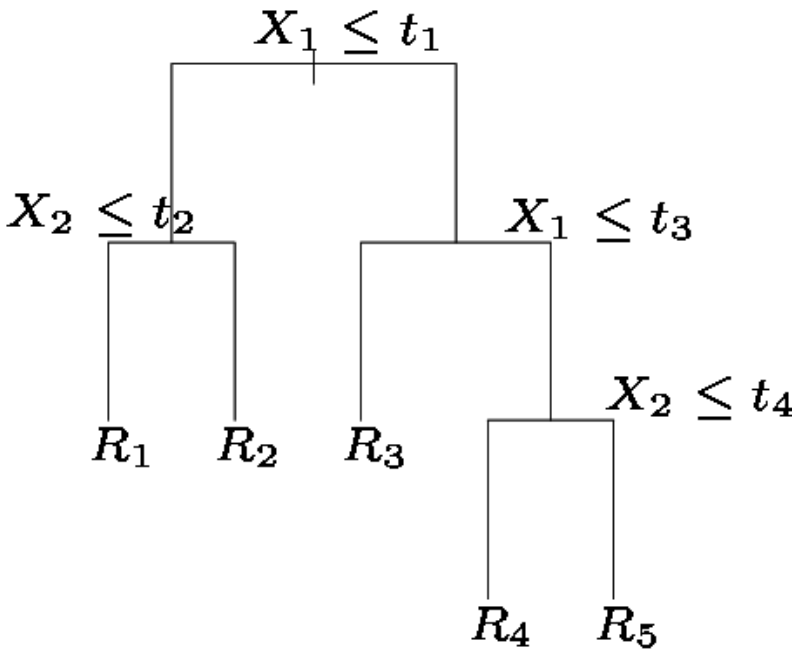
Recursive Binary Splitting—Step 3

- This process continues until our regions have too few observations to continue, e.g., all regions have 5 or fewer points.

Final Output

- When we create partitions this way we can always represent them using a tree structure.
- This provides a very simple way to explain the model to a non-expert.



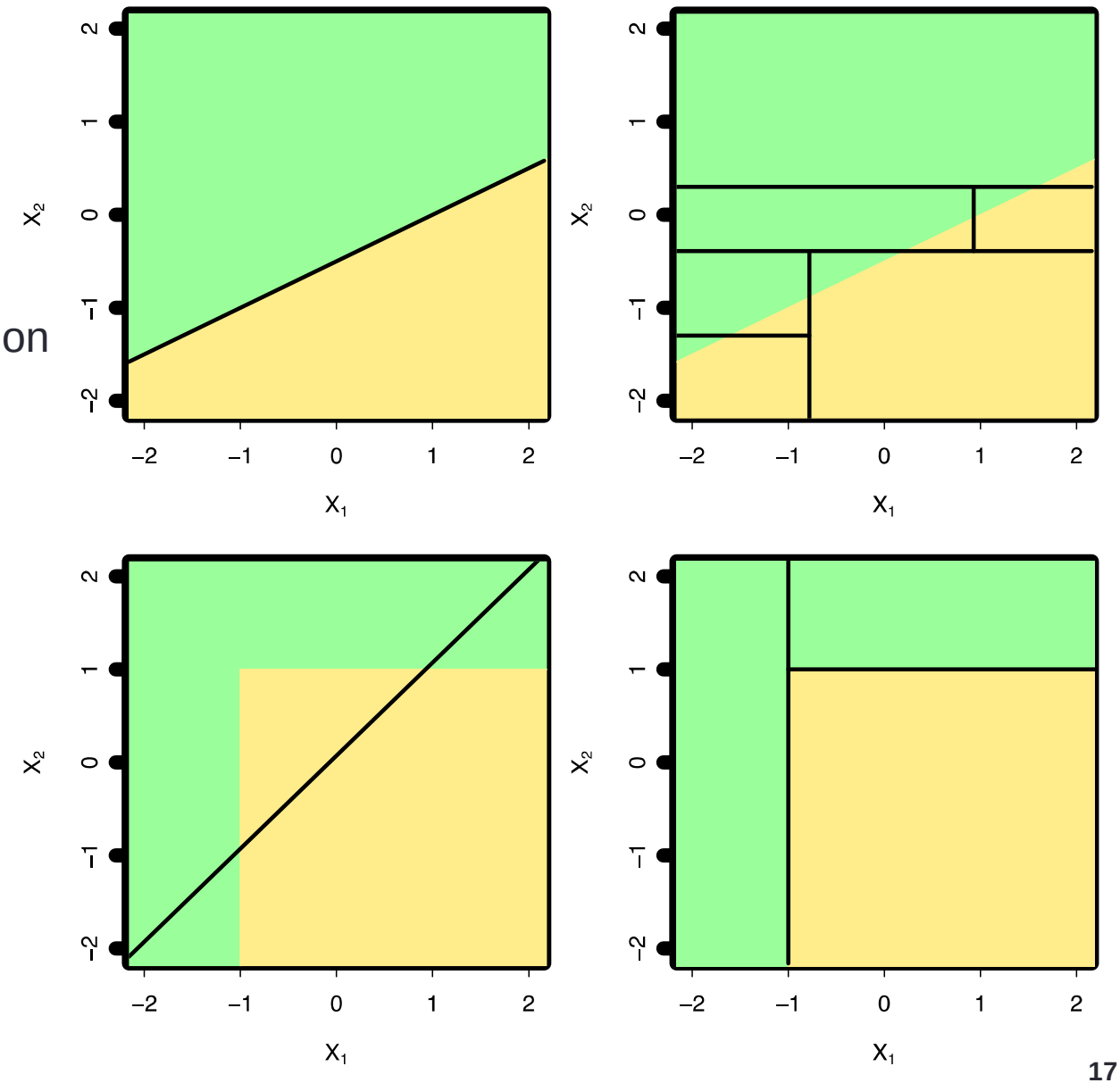


2. What Values Used for Predictions?

- Find Predictions $\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_k$
- Simple!
- For region R_j, the best prediction is simply the *average* of all the responses in the training data that fell in this region.

Trees vs. Linear Model: Classification Example

- Top row: the true decision boundary is linear
  - Left: linear model (good)
  - Right: decision tree
- Bottom row: the true decision boundary is non-linear
  - Left: linear model
  - Right: decision tree (good)



Trees vs. Linear Models

- Which model is better?
  - If the relationship between the predictors and response is linear, then classical linear models such as linear regression would outperform regression trees.
  - On the other hand, if the relationship between the predictors is highly non-linear and complex, then decision trees would outperform classical approaches.

Pros of Decision Trees

- Trees are very easy to explain to people, probably even easier than linear regression!
- Some people believe that decision trees more closely mirror human decision-making than do classical regression and classification approaches.
- Trees can be displayed graphically, and are easily interpreted even by non-expert (especially if they are small).
- They can easily handle qualitative predictors without the need to create dummy variables.

Cons of Decision Trees

- Trees don’t have the same prediction accuracy as some of the more complicated approaches that we examine in this course.

- Trees can be very non-robust. A small change in the data can cause a large change in the final estimated tree.

Classification Tree

Classification Trees

- Suppose for example we have two regions R_1 and R_2 with $\hat{y}_1 = 0$, $\hat{y}_2 = 1$.

- Then for any value of $\boldsymbol{X}$ such that $\boldsymbol{X} \in R_1$, we would predict 0, otherwise if $\boldsymbol{X} \in R_2$, we would predict 1.

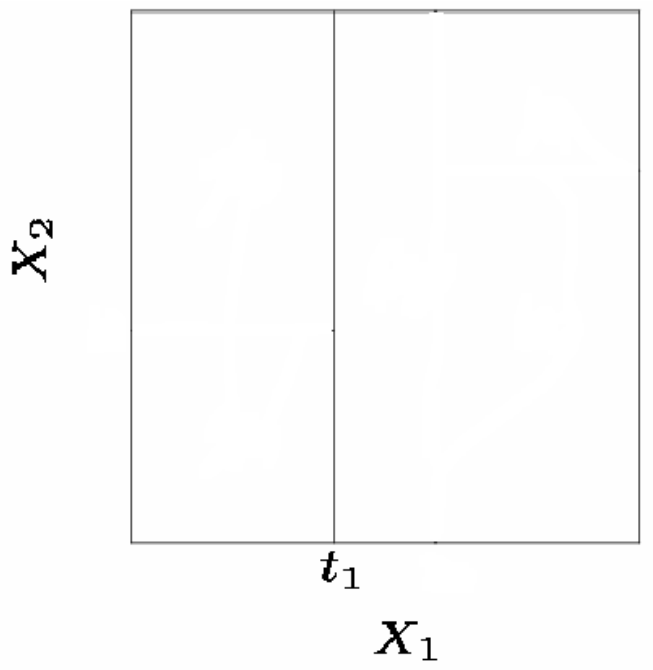
- The two questions:

  (1) how to split the predictor space?

  (2) what is used for prediction in each region?

1. Recursive Binary Splitting

- Follow the same procedure as in regression tree
- The only difference is that *RSS will not be used for making the binary splits. Criteria defined for classification will be used*.



Performance Measures in Classification Trees

- **Classification error rate**

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

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

Classification error is not sufficiently sensitive for tree-growing.

Performance Measures (Cont')

- **Gini index**

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

It is a measure of *node purity*. A small value indicates that a node contains predominantly observations from a single class.

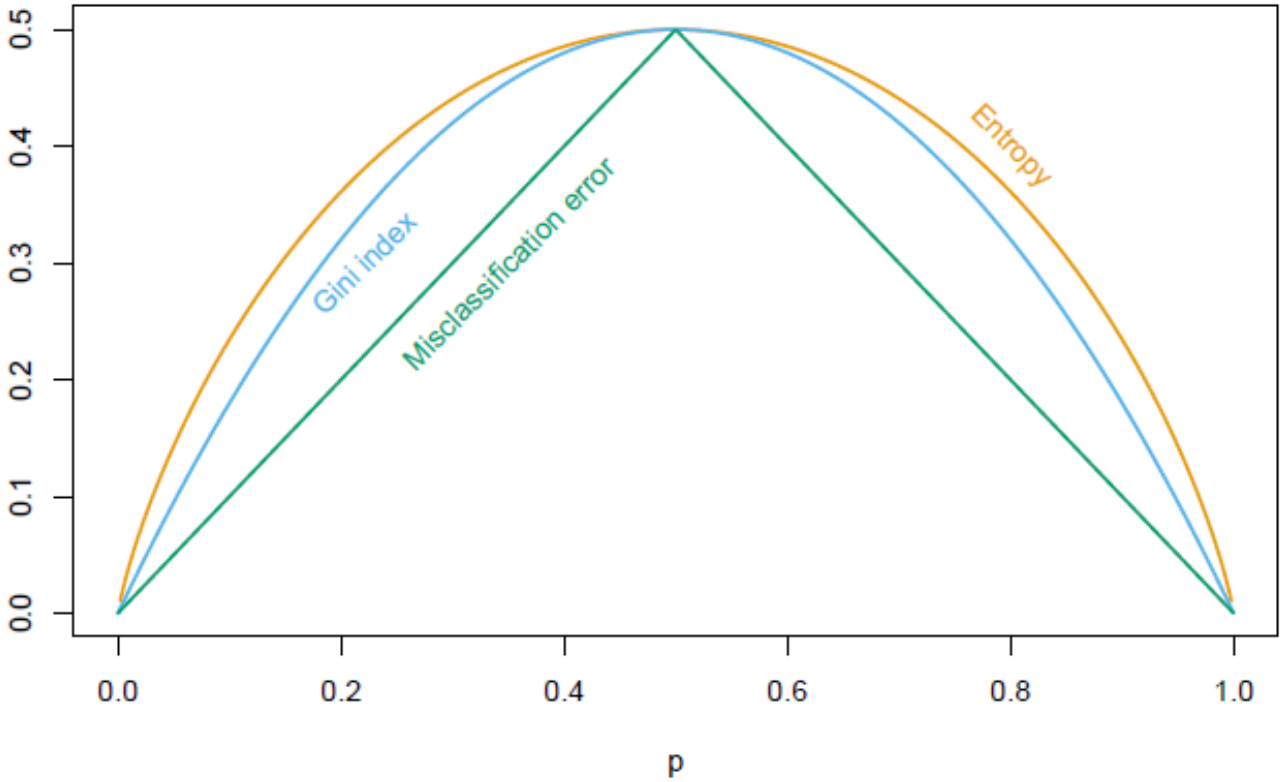
- **Cross-entropy**

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

It is quite similar to the Gini index numerically.

Comparison of Performance Measures

- **For a 2-class problem**



Gini index and cross-entropy are differentiable, and thus more amenable to numerical optimization.

Comparison of Performance Measures (Cont.)

- Gini index and cross-entropy are more sensitive to changes in the node probabilities than the misclassification error rate.

2. Predictions

- Find Predictions $\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_k$
- For region R_j, the best prediction is the *most commonly occurring class* of training observations in that region.

True Pruning

Improving Tree Accuracy

- A large tree (i.e., one with many terminal nodes) may tend to overfit the training data.
- A small tree tends to have lower variance and better interpretation.
- Generally, we can improve accuracy by "pruning" the tree, i.e., cutting off some of the terminal nodes.

(allthingsclipart.com)

Tree Pruning

- Grow a very large tree and then prune it back to obtain a subtree.
- Find a number of subtrees in this way.
- Use cross validation to estimate test error of each subtree.
- Choose the subtree that has lowest test error.

Cost Complexity Pruning

- Also known as weakest link pruning. Rather than considering every possible subtree, we consider a sequence of trees indexed by a nonnegative tuning parameter α.
- For each value of α there is a subtree $T \subset T_0$ such that

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

- The tuning parameter α controls a trade-off between the subtree's complexity and its fit to training data.
- Obtain a sequence of subtrees as a function of α. Select a value of α using cross validation, and then return to the full data set and obtain the subtree corresponding to α.

Algorithm for Tree Pruning

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.

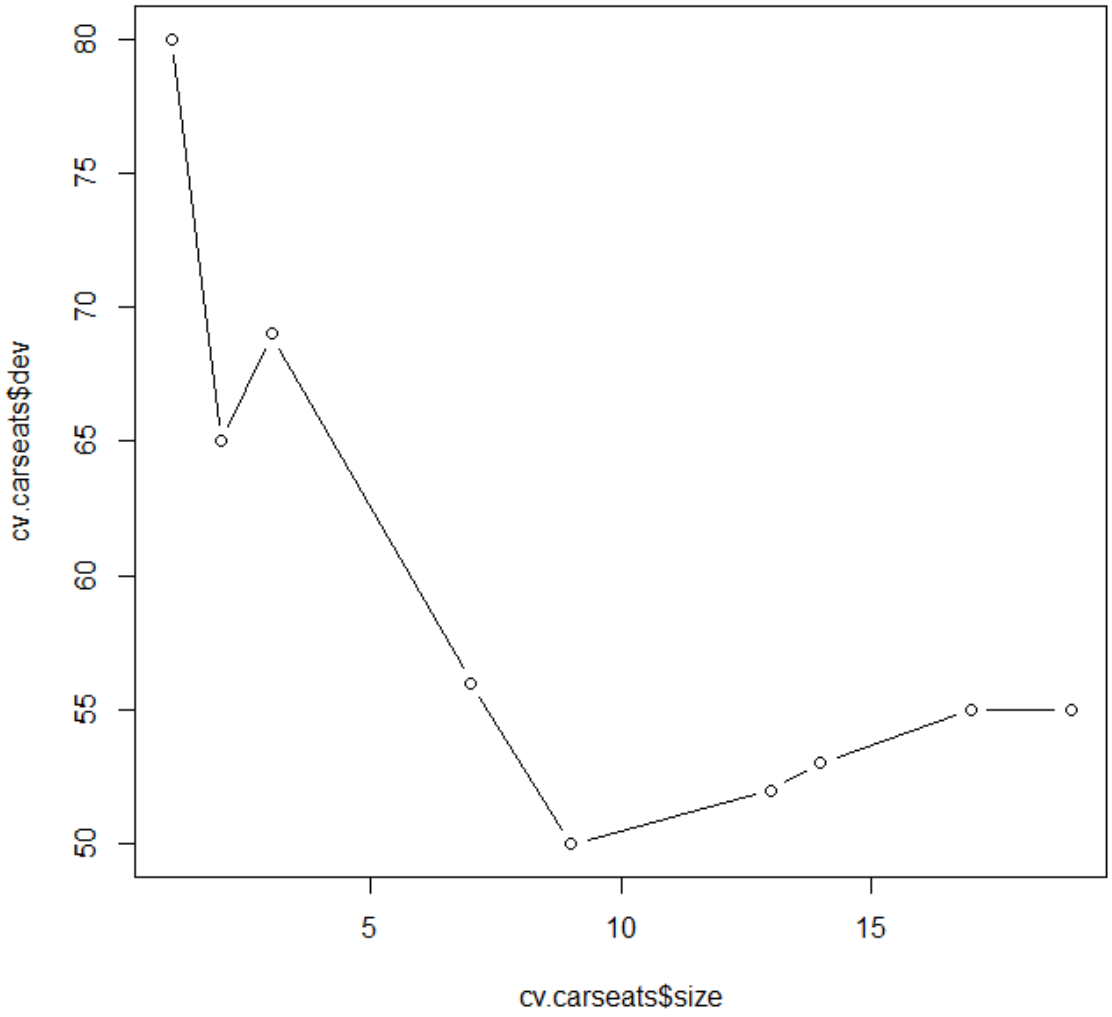
4. Return the subtree from Step 2 that corresponds to the chosen value of α.

Carseats Data Set

- Carseats data set in the ISLR library
- Sales (child car seat sales) in 400 locations with potential predictors such as Price, Urban (No/Yes, indicate whether the store is in an urban or rural location), US (No/Yes, indicate whether the store is in the US or not) and ShelveLoc (*Bad/Medium/Good*, indicate the quality of the shelving location, i.e., the space within a store in which the car seat is displayed).
- Use ifelse() function to create a binary response variable, which takes on Yes if Sales>8, and No otherwise. Then a classification tree is fit for the data.

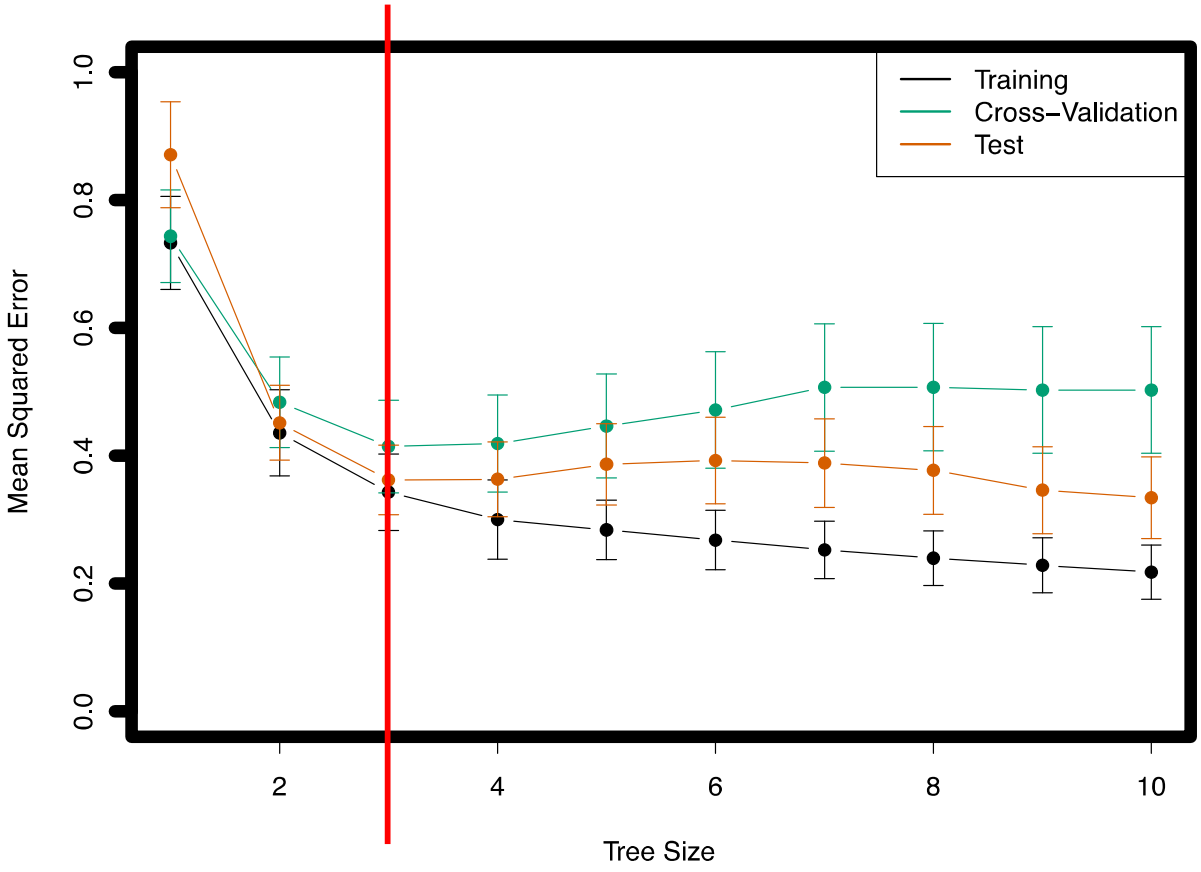
(**Note:** the purpose of creating a binary response from the continuous response Sales is only to illustrate how to build a classification tree!)

Tree Pruning (Cont'd)

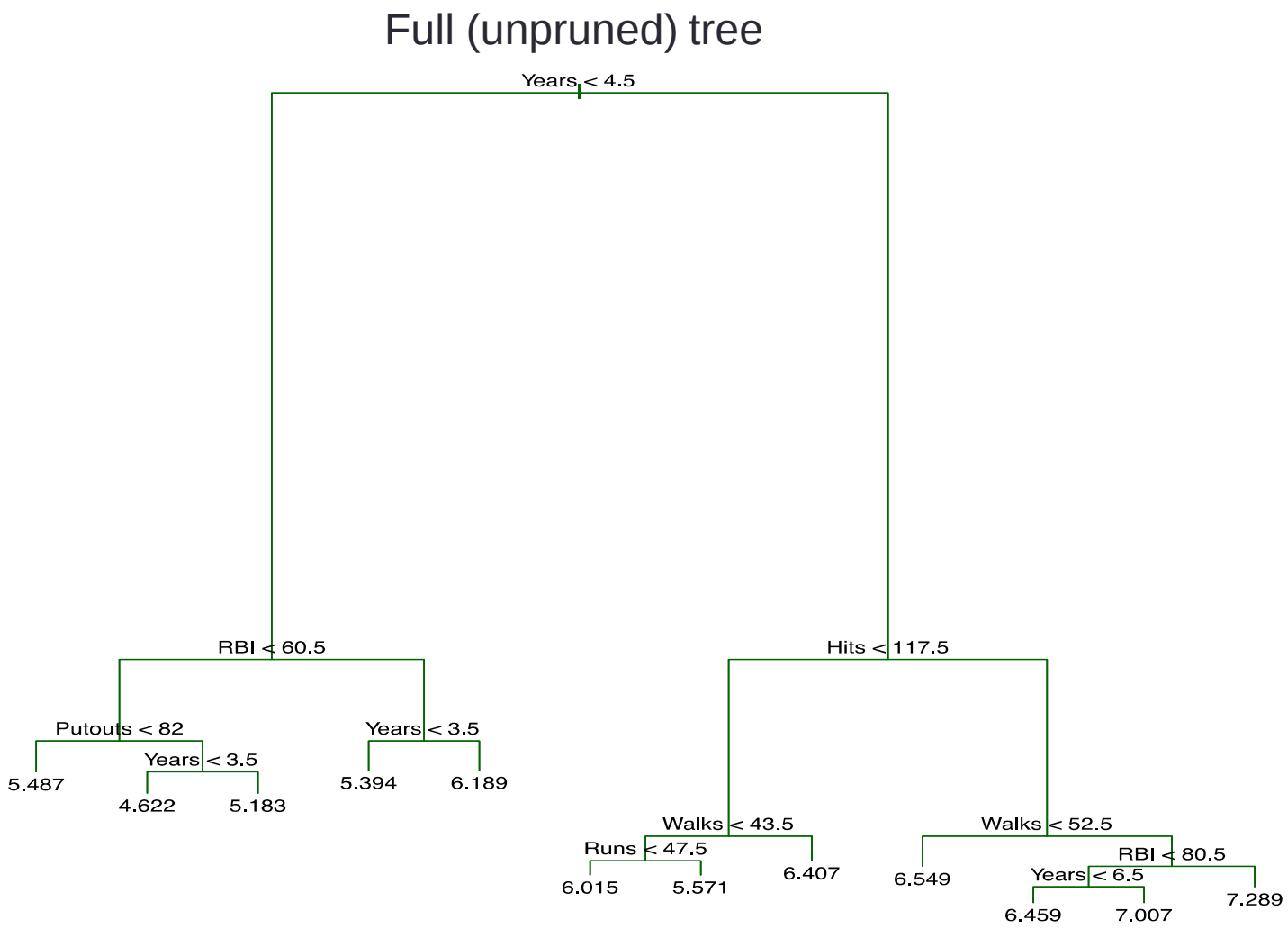


Example: Baseball Players' Salaries

The minimum cross validation error occurs at a tree size of 3



Example: Baseball Players' Salaries

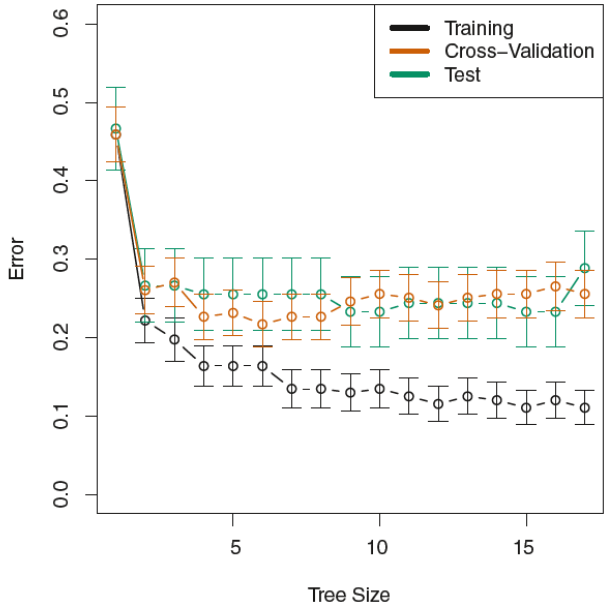


Example: Baseball Players' Salaries

- Cross validation indicated that the best test error is achieved when the tree size is three (i.e., there are 3 terminal nodes).

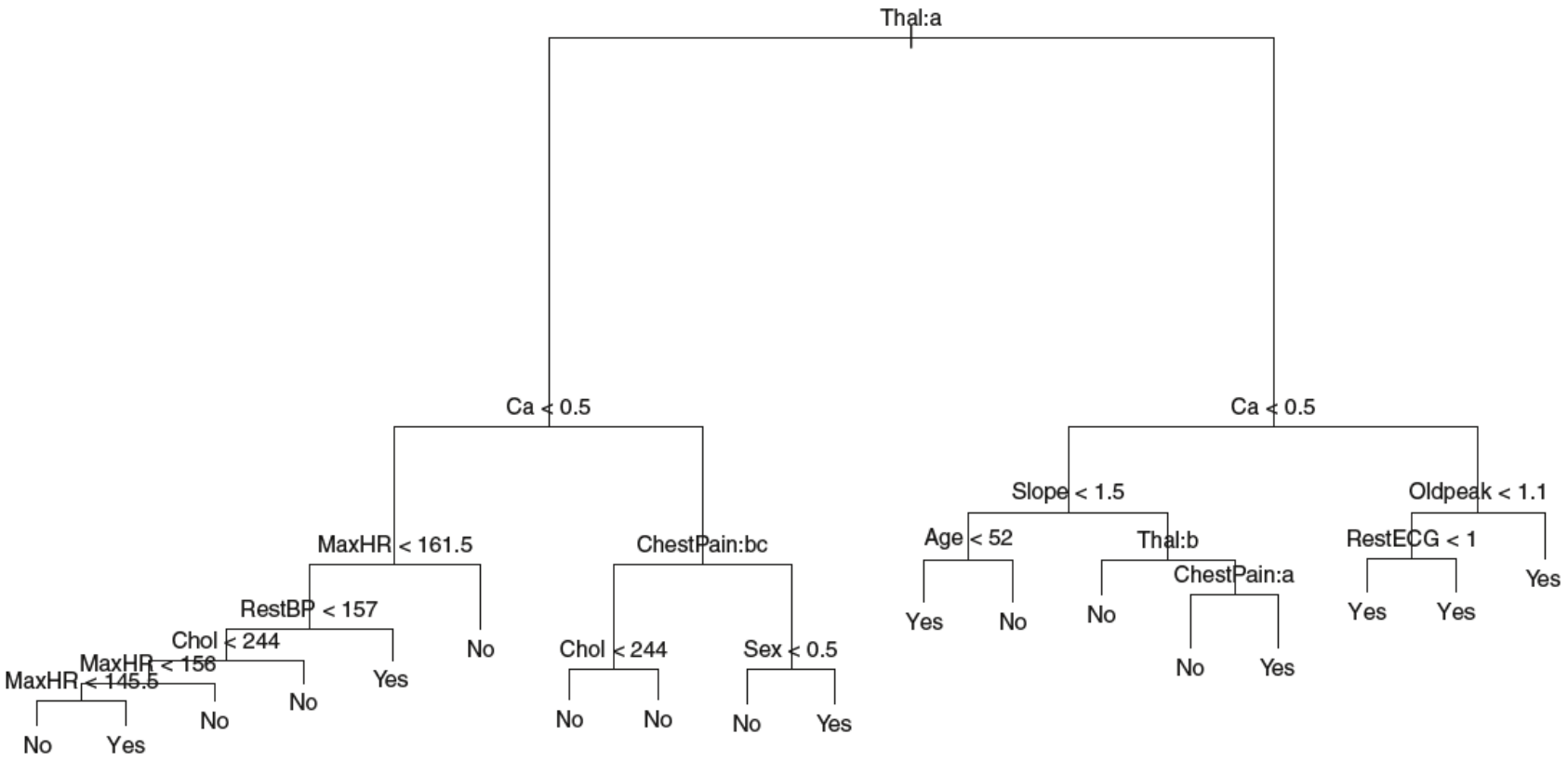
Another Example: Classification on Heart Disease

- Heart data set
- A binary outcome HD (whether to have heart disease) of 303 patients with potential predictors such as Age, Sex, Chol (a cholesterol measurement) and other heart and lung function measurements
- Cross validation results (tree with 6 terminal nodes is chosen)



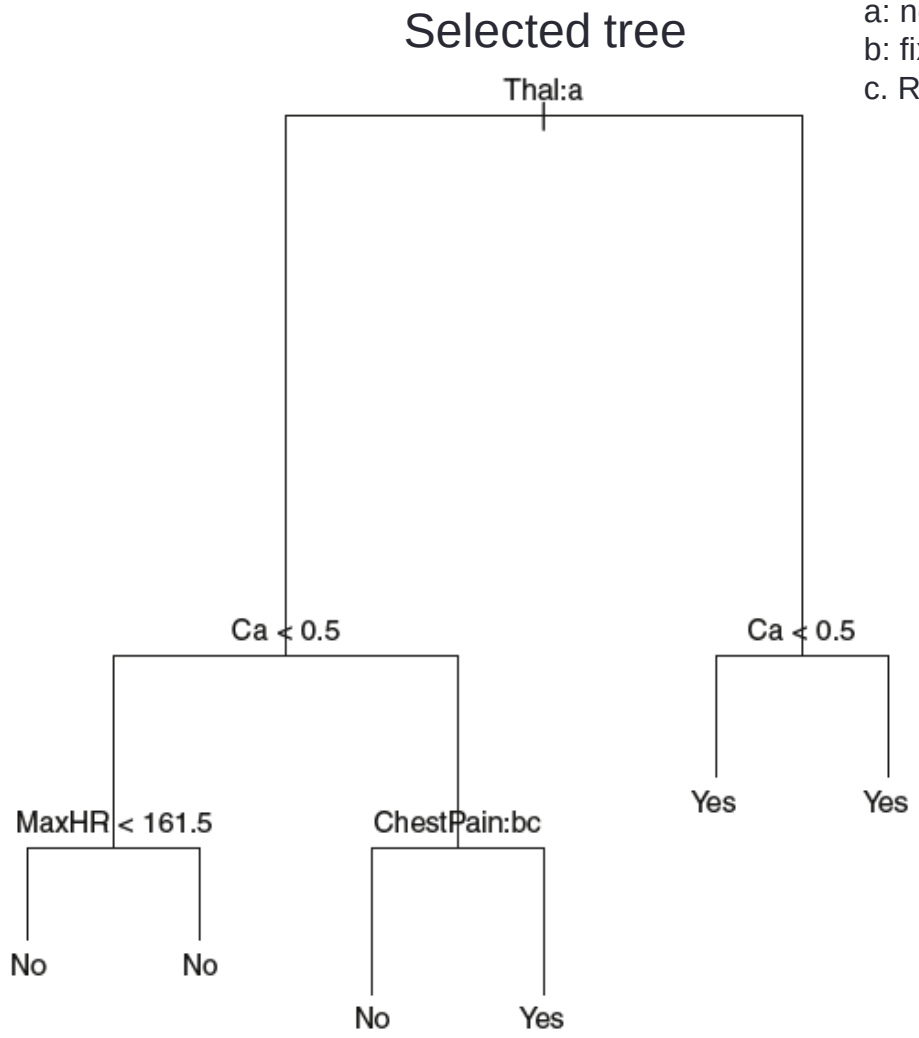
Another Example

Full (unpruned) tree



Another Example

Thal (Thallium stress test)
a: normal
b: fixed
c. Reversible defects



Improving Trees

Motivation

- Decision trees discussed earlier suffer from high variance!
  - If we randomly split the training data into 2 parts, and fit decision trees on both parts, the results could be quite different.
- We would like to have models with low variance (and thus high prediction accuracy).
- Ensemble method: Combine many simple "building block" models in order to obtain a single and potentially very powerful model. Simple building block models are sometimes known as *weak learners*.
- Three ensemble methods to improve trees: *Bagging*, *Random forests*, *Boosting*

Background: The Bootstrap

- A powerful tool to quantify the uncertainty associated with a given estimator or statistical learning method
- The power of the bootstrap lies in the fact that it can be easily applied to a wide range of statistical learning methods, including those for which a measure of variability is otherwise difficult to obtain and is not automatically output by software.

Example: the Problem

- Suppose that we wish to invest a fixed sum of money in two financial assets that yield returns of X and Y, which are two random variables.
- We will invest a fraction α in X, and the remaining $1 - \alpha$ in Y.
- We wish to choose α to minimize the total risk, or variance, of our investment; that is, to minimize $Var(\alpha X + (1 - \alpha)Y)$.
- One can show that the value minimizing the risk is

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}$$

- **Problem:** how to estimate α?

Example: Estimating the Optimal α

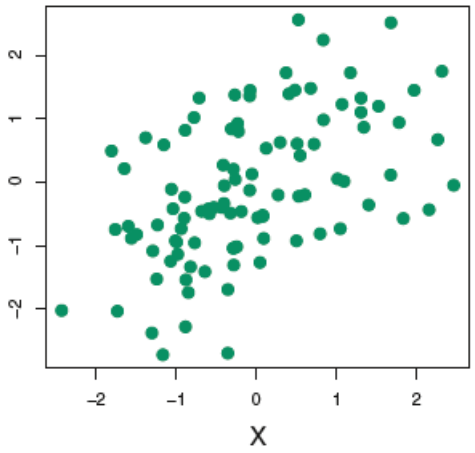
- In reality, the quantities $\sigma_X^2, \sigma_Y^2, \sigma_{XY}$ are unknown.
- We can compute estimates for them, $\hat{\sigma}_X^2, \hat{\sigma}_Y^2, \hat{\sigma}_{XY}$, using a data set that contains past measurements for X and Y.
- We then estimate the value of the optimal α by

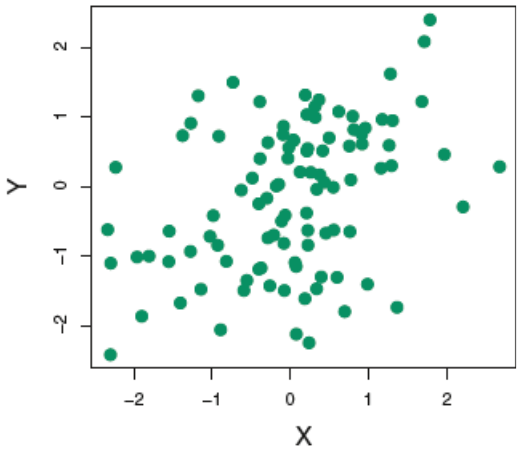
$$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}$$

Example: Simulation Study

- Each panel contains 100 pairs of observations for X and Y

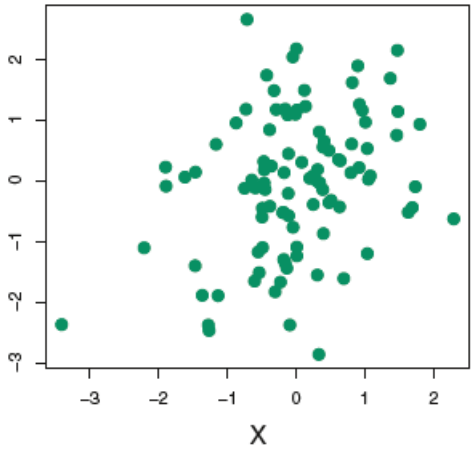
$\hat{\alpha} = 0.576$

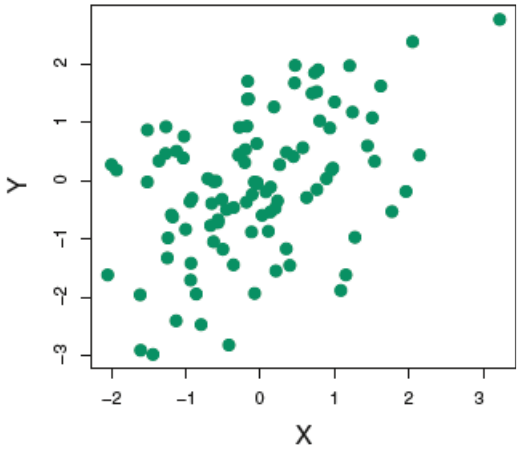




$\hat{\alpha} = 0.532$

$\hat{\alpha} = 0.657$





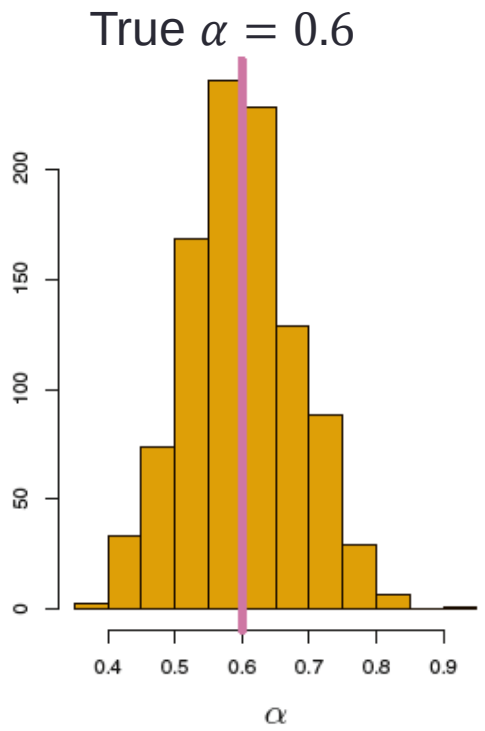
$\hat{\alpha} = 0.651$

Example: Quantifying Accuracy of Estimates

- Generate 1000 simulations, each of which yields one estimate of α. Calculate mean and standard deviation of these estimates.

$$\bar{\alpha} = \frac{1}{1,000} \sum_{r=1}^{1,000} \hat{\alpha}_r = 0.5996$$

$$\sqrt{\frac{1}{1,000-1} \sum_{r=1}^{1,000} (\hat{\alpha}_r - \bar{\alpha})^2} = 0.083$$



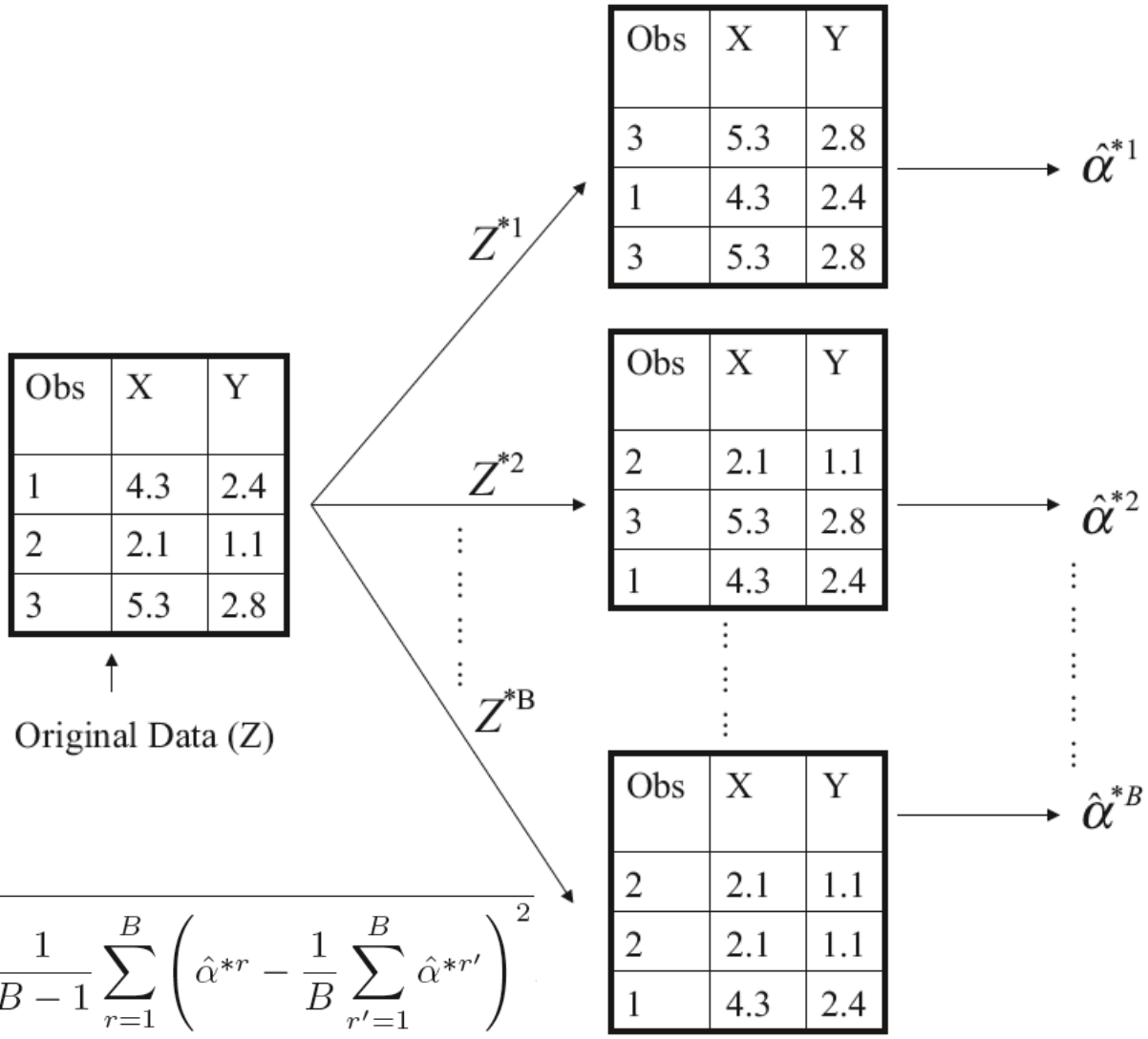
However…

- This procedure needs 1000 data sets from the true population to quantify the accuracy (or uncertainty) of the estimate of α.
- However, in practice, it is usually not possible to generate new samples from the true population.
- Consider the case where only one data set is available, how can we quantify the accuracy of $\hat{\alpha}$?

Idea of The Bootstrap

- The bootstrap approach uses a computer to emulate the process of obtaining new sample sets, so that we can estimate the variability of $\hat{\alpha}$ without generating additional samples.
- Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets by repeatedly sampling observations from the original data set.

Illustration on A Dataset with $n = 3$

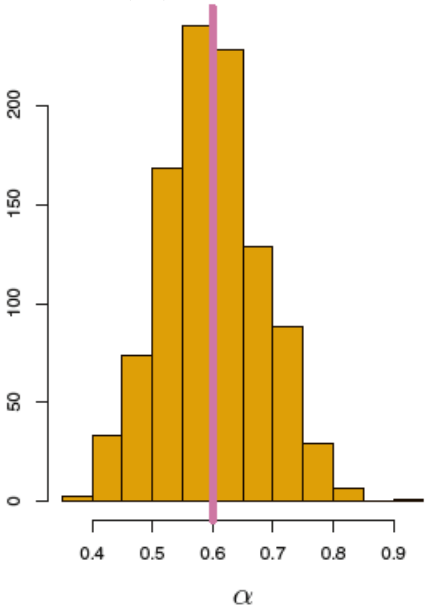


$$\mathrm{SE}_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1}\sum_{r=1}^{B}\left(\hat{\alpha}^{*r} - \frac{1}{B}\sum_{r'=1}^{B}\hat{\alpha}^{*r'}\right)^2}$$

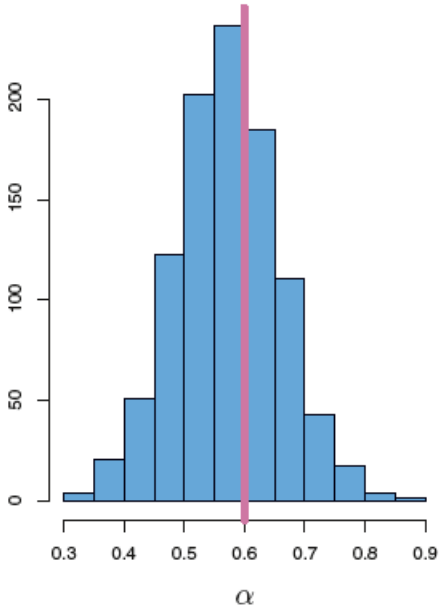
Example: Results from the Bootstrap

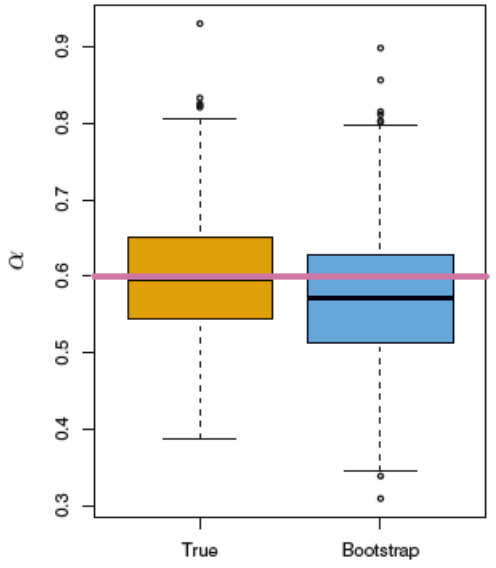
- Left: histogram of estimates obtained by generating 1000 simulated data sets from the true population.
- Center: histogram obtained from 1000 bootstrap samples from a single data set.

$SE(\hat{\alpha}) = 0.083$



$SE(\hat{\alpha}) = 0.087$





Example: Summary of Results

- The bootstrap estimate of $SE(\hat{\alpha})$ is very similar to the estimate based on 1000 data sets.
- The left is based on 1000 simulated data sets from the true population, while the right is based on only a single data set.
- The left represents the idealized situation, and the right is for real data.

Advantages of The Bootstrap

- One of the great advantages of the bootstrap approach is that it can be applied in almost all situations (for various statistical learning methods and various types of data).
- No complicated mathematical calculations are required.

1. Bagging

- Bagging: **b**ootstrap **agg**regat**ing**.
- Bagging is an extremely powerful idea based on two things:
  - Bootstrapping: plenty of training datasets!
  - Averaging: reduces variance!
- Why does averaging reduces variance?
  - Averaging a set of observations reduces variance. Recall that given a set of n independent observations $Z_1, \ldots, Z_n$, each with variance σ^2, the variance of the mean $\bar{Z}$ of the observations is given by σ^2/n.

Bagging for Regression Trees

- Generate B different bootstrapped training datasets
- Construct B regression trees using the training datasets
- Average the resulting predictions

Note: These trees are not pruned, so each individual tree has low bias but high variance. Averaging these trees reduces variance, and thus we end up lowering both variance and bias.

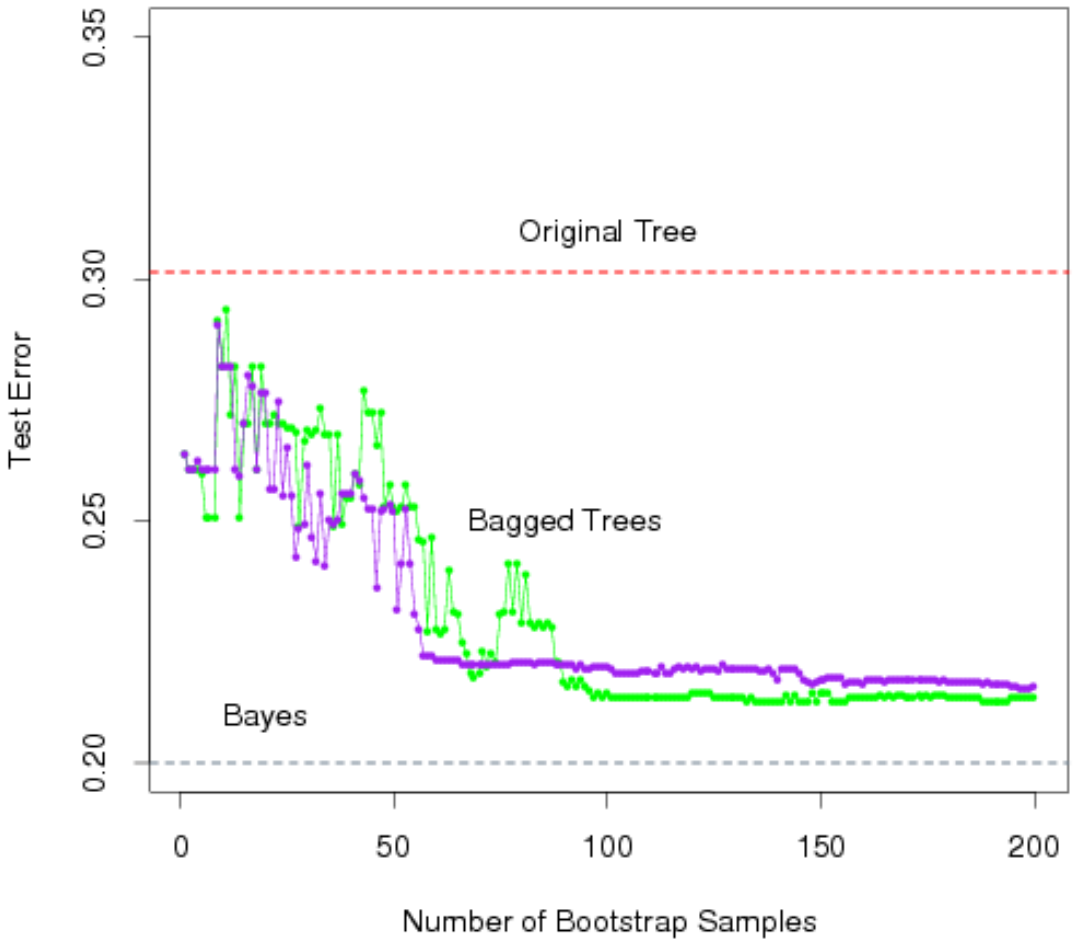
Bagging for Classification Trees

- Generate B different bootstrapped training datasets
- Construct B classification trees using the training datasets
- For prediction, there are two approaches:
  1. Record the class that each bootstrapped data set predicts and provide an overall prediction to the most commonly occurring one (majority vote).
  2. If our classifier produces probability estimates we can just average the probabilities and then predict to the class with the highest probability

Both methods work well.

A Comparison of Error Rates

- Here the green line represents a simple majority vote approach
- The purple line corresponds to averaging the probability estimates.
- Both do far better than a single tree (dashed red) and get close to the Bayes error rate (dashed grey).



Advantage/Disadvantage of Bagging

- Bagging typically improves the accuracy over prediction using a single tree, but it is now *hard to interpret* the model!
- When we bag a large number of trees, it is no longer possible to represent the resulting statistical learning procedure using a single tree, and it is no longer clear which variables are most important to the procedure.
- Thus bagging improves prediction accuracy at the expense of interpretability.

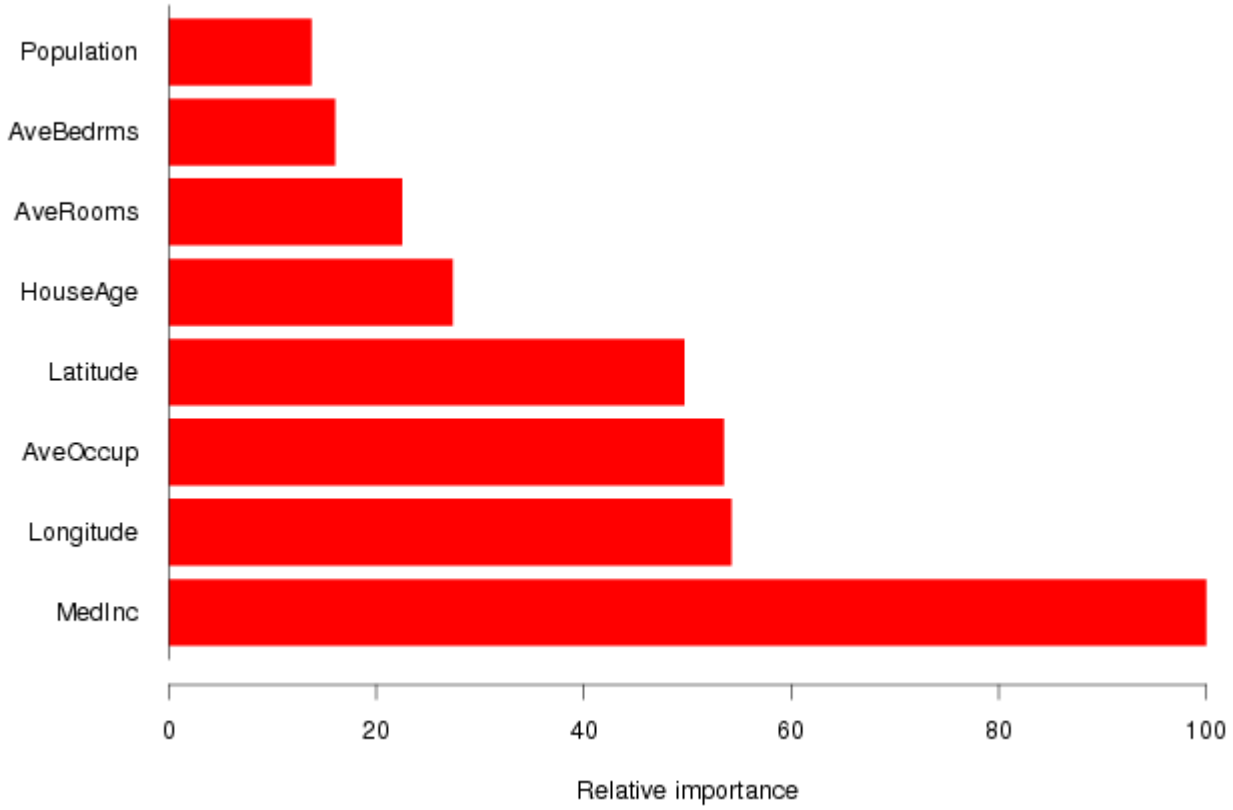
Variable Importance Measures

- Although the collection of bagged trees is much more difficult to interpret than a single tree, we can obtain an overall summary of the importance of each predictor.
- **How**: use the amount of RSS (for bagging regression trees) or the Gini index (for bagging classification trees) decreased due to splits over the predictor.
- A large value indicates an important predictor.

```
bag.boston$importance
```

Example: Boston Data

- Median income is the most important variable.
- Longitude, Latitude and Average occupancy are the next most important.



2. Random Forests

- It is a very efficient statistical learning method.
- It builds on the idea of bagging, but it provides an improvement because it de-correlates the trees.
- How does it work?
  - Build a number of decision trees on bootstrapped training sample,
  - For each tree, each time a split in a tree is considered, **a random sample of m predictors** is chosen as split candidates from among the p predictors.

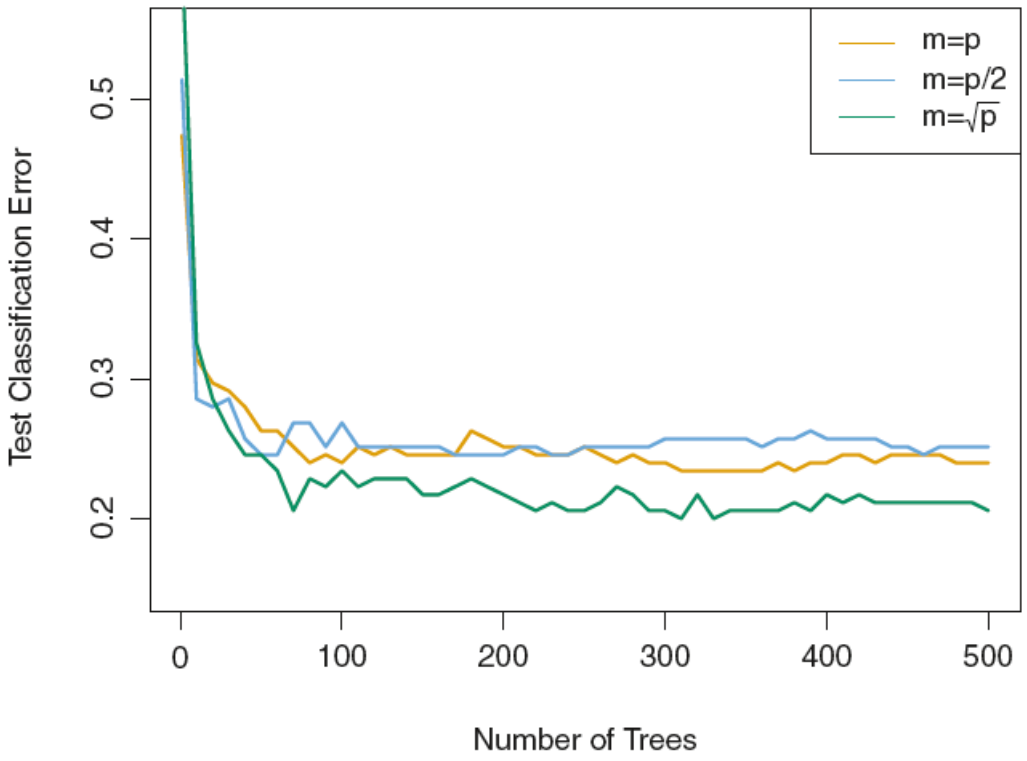
  (Usually $m = \sqrt{p}$ is used for classification)

Why *m* Predictors in Splitting?

- Suppose that we have a very strong predictor in the data set along with a number of other moderately strong predictor, then in the collection of bagged trees, most or all of them will use the very strong predictor for the first split!
- All bagged trees will look similar. Hence all the predictions from the bagged trees will be highly correlated.
- Averaging many highly correlated quantities does not lead to a large variance reduction, and thus random forests "de-correlates" the bagged trees leading to more reduction in variance.

Random Forest with different values of “m”

- Notice when random forests are built using $m = p$, then this amounts simply to bagging.



3. Boosting

- Bagging grow trees simultaneously:
  1. creating multiple copies of the original training data set using the bootstrap
  2. fitting a separate decision tree to each copy
  3. combining all the trees to generate a single predictive model

- Boosting grows trees sequentially: each tree is grown using information from previously grown trees.

- Boosting does not involve bootstrap sampling: each tree is fit on a modified version of the original data set.

Algorithm of Boosting for Regression Trees

Algorithm 8.2 *Boosting for Regression Trees*

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.

2. For $b = 1, 2, \ldots, B$, repeat:

   (a) Fit a tree $\hat{f}^b$ with d splits ($d+1$ terminal nodes) to the training data (X, r).

   (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:

   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \tag{8.10}$$

   (c) Update the residuals,

   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \tag{8.11}$$

3. Output the boosted model,

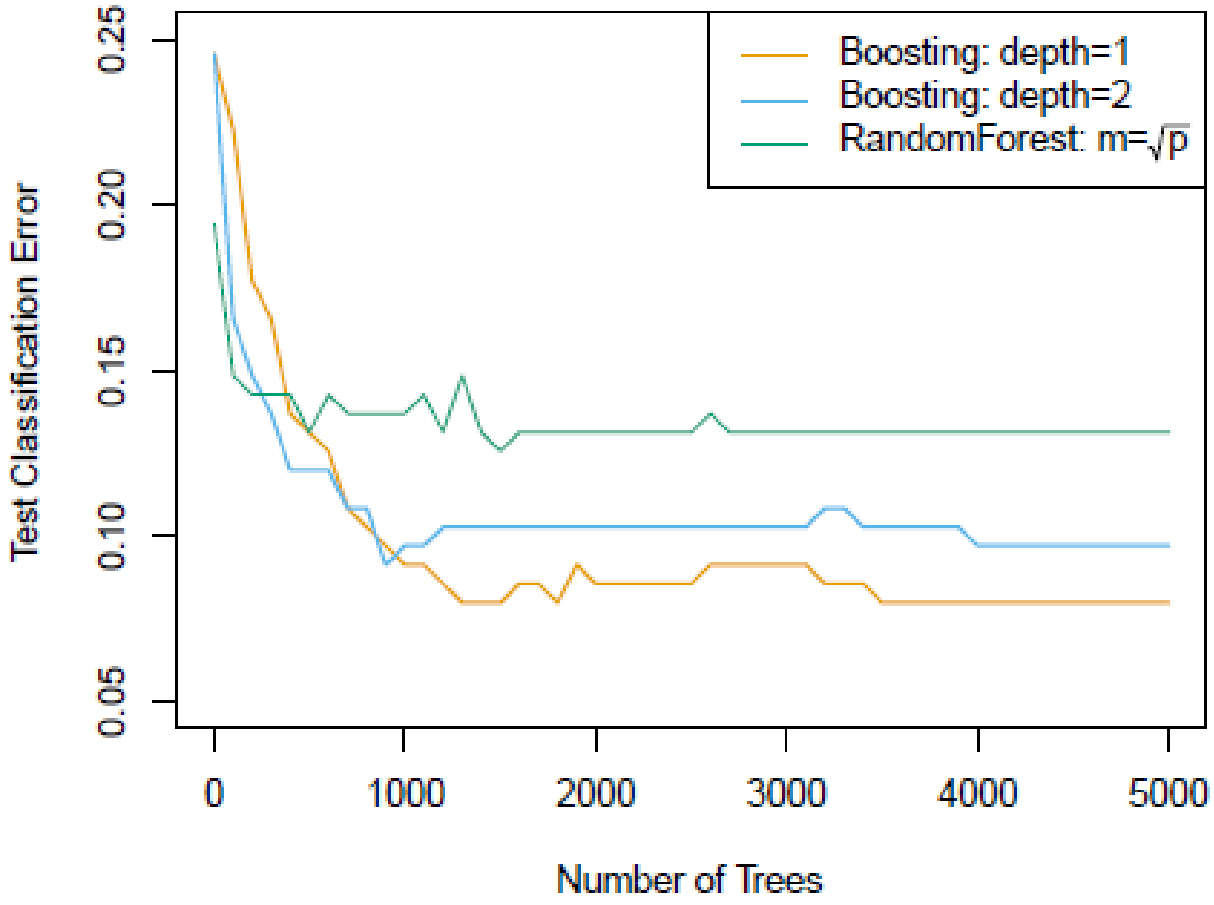
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x). \tag{8.12}$$

Tuning Parameters

- Boosting has three tuning parameters:
  1. The number of trees B
  2. The shrinkage parameter λ, a small positive number
  3. The number d of splits
- B: Unlike bagging and random forests, boosting can overfit if B is too large. We use cross validation to select B.
- λ: This controls the rate at which boosting learns. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ can require using a very large value of B in order to achieve good performance.
- d: This controls the complexity of the boosted ensemble. Often $d = 1$ works well, in which case each tree consists of a single split. More generally d is the interaction depth and controls the interaction order of the boosted model, since d splits can involve at most d variables.

Boosting vs. Random Forests

- Depth-1 trees slightly outperforms depth-2 trees, and both outperform random forests.



Idea behind Boosting

- Fitting a single large tree may cause overfitting.
- Boosting *learns slowly*: in each step, fit a very small tree to the residuals, so that improve $\hat{f}$ in areas where it does not perform well.
- In general, statistical learning approaches that learn slowly tend to perform well.

Summary of Tree Ensemble Methods

- **Bagging**: trees are grown independently on random samples of the observations. Consequently, the trees tend to be quite similar to each other. Thus, bagging can get caught in local optima and fail to thoroughly explore the model space.
- **Random forests**: trees are once again grown independently on random samples of the observations. However, each split on each tree is performed using a random subset of the features, thereby decorrelating the trees, and leading to a more thorough exploration of model space relative to bagging.
- **Boosting**: only the original data are used. The trees are grown successively, using a “slow” learning approach: each new tree is fit to the signal that is left over from the earlier trees, and shrunken down before it is used.

Questions (1)

Read slides of Topic 6. Then answer the following questions.

- In a regression tree, what is an internal node, and what is a terminal node?
- In a regression tree, what is the prediction in each region of the predictor space?
- In building a regression tree, what is the criteria used in each splitting?
- Compared with linear regression, when should we choose regression tree?
- What are the pros and cons of tree methods?

Questions (2)

- In a classification tree, what is the prediction in each region of the predictor space?
- In building a classification tree, what is the criteria used in each splitting?
- What are differences of classification trees vs. regression trees?
- Why can pruning improve tree accuracy?
- How to conduct tree pruning?
- If several tree models have similar CV errors, which one will you choose?

Questions (3)

- What is the purpose of using bagging, random forests and boosting methods?
- What is bagging? Why can it improve tree models?
- What is random forests? Why can it improve tree models?
- What is the relationship of bagging and random forests?
- Does random forests perform better than bagging?
- What value of m should be used in applying random forests?
- What is the key difference of boosting vs. bagging and random forests?