CS 451/686-02 Data Mining
Trees – Introduction

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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.

Pros and Cons

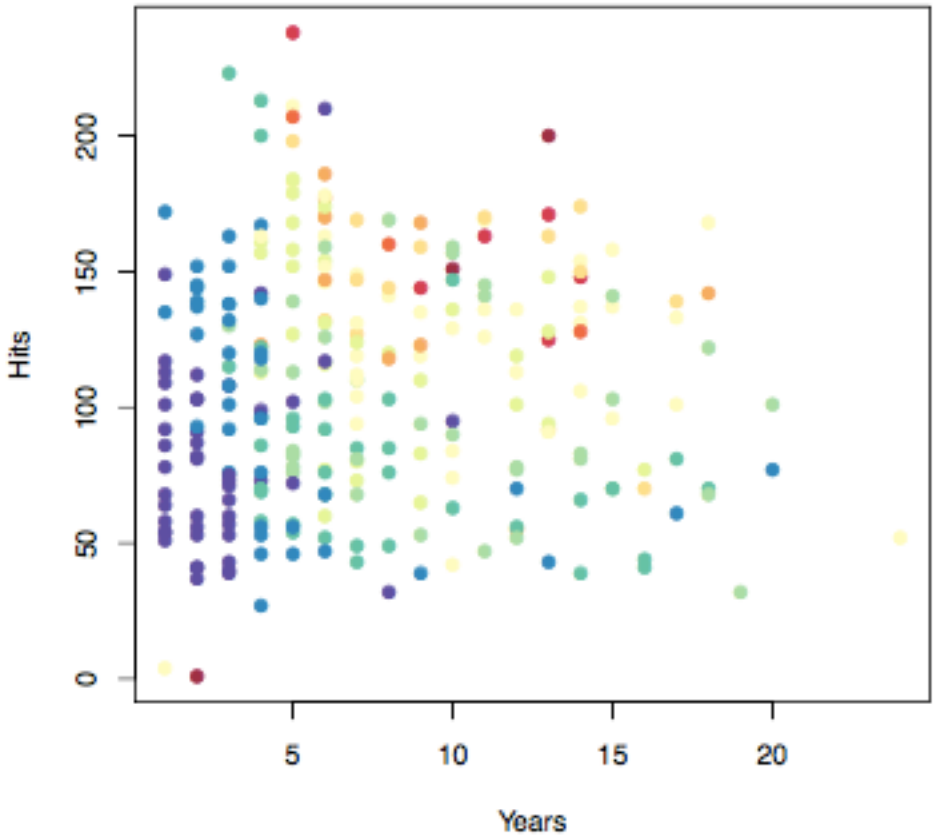
- Tree-based methods are **simple** and useful for **interpretation**.
- However they typically are not competitive with the best supervised learning approaches in terms of prediction accuracy.
- Hence we also discuss *bagging*, *random forests*, and *boosting*. These methods grow **multiple trees** 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 of interpretation.

The Basics of Decision Trees

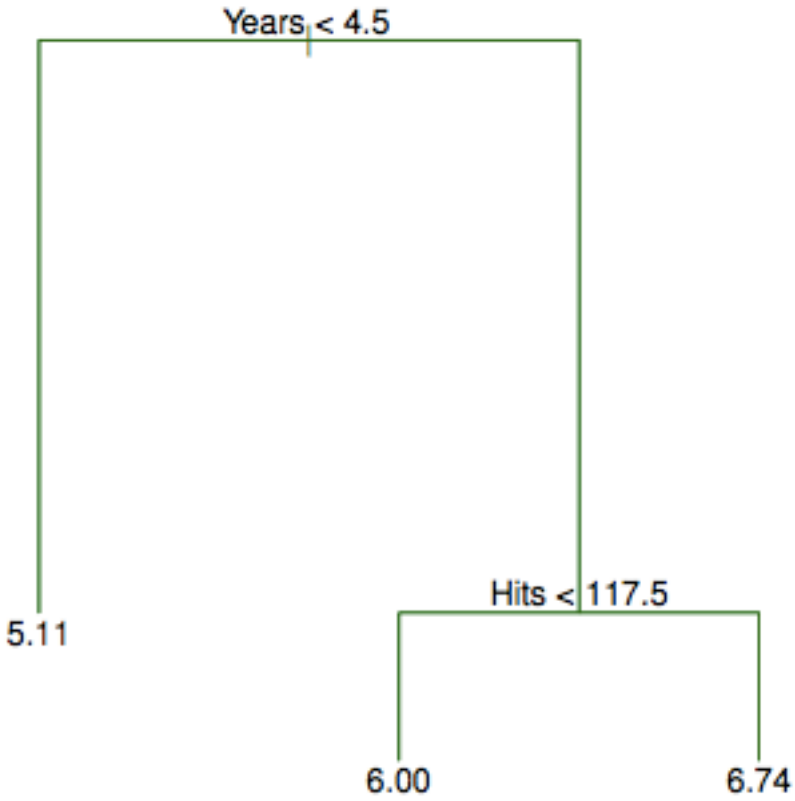
- Decision trees can be applied to **both regression and classification problems**.
- We first consider regression problems, and then move on to classification.

Baseball salary data: how would you stratify it?

Salary is color-coded from low (blue, green) to high (yellow,red)



Decision tree for these data



Details of previous figure

- For the Hitters data, we fit a regression tree for predicting the log salary of a baseball player, based on the number of years that he has played in the major leagues and the number of hits that he made in the previous year.

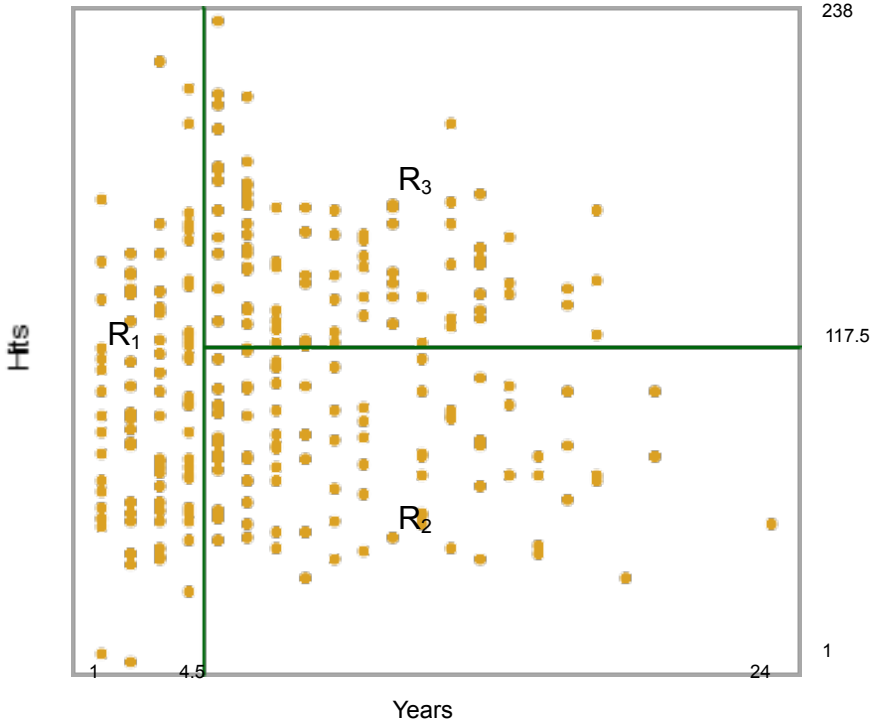
- At a given internal node:
  - the label (of the form $X_j < t_k$) indicates the left-hand branch emanating from that split, and
  - the right-hand branch corresponds to $X_j \geq t_k$.
  - For instance, the split at the top of the tree results in two large branches. The left-hand branch corresponds to Years < 4.5, and the right-hand branch corresponds to Years >= 4.5.

- The tree has two **internal nodes** and three **terminal nodes**, or **leaves**.

- The number in each leaf is **the mean of the response** for the observations that fall there.

Results

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



Terminology for Trees

- 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.

Interpretation of 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

Interpretation of Results

- Years is the most important **factor** in determining Salary, and players with less experience earn lower salaries than more experienced players. **Comment on the effect of predictor 1.**

- 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. **Comment on the effect of predictor 2.**

- 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. **Reason where weak predictors are useful.**

- Notice the steps in interpreting results of a model (a tree in this case).

Details of the tree-building process

1. We divide the **predictor space**
   — that is, the set of possible values for $X_1, X_2, \ldots, X_p$ —
   into J **distinct** and **non-overlapping regions**, $R_1, R_2, \ldots, R_J$.

2. For every observation that falls into the region R_j, we make the same **prediction**, which is simply **the mean of the response values** for the training observations in R_j.

More details of the tree-building process

- 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 j-th box.

More details of the tree-building process

- Unfortunately, it is **computationally infeasible** to consider every possible partition of the feature space into J boxes.
- For this reason, we take a *top-down*, *greedy* approach that is known as **recursive binary splitting**.
- The approach is *top-down* because it begins at the top of the tree and then successively splits the predictor space; each split is indicated via two new branches further down on the tree.
- It is *greedy* because at each step of the tree-building process, the *best* split is made *at that particular step*, rather than *looking ahead* and picking a split that will lead to a better tree in some future step.

Details— Continued

- We first select 1) **the predictor** X_j and 2) **the cut-point** s such that splitting the predictor space into the regions

$$\{X \mid X_j < s\} \text{ and } \{X \mid X_j \geq s\}$$

leads to the greatest possible reduction in RSS (**max RSS**).

- Next, we **repeat** the process, looking for the best predictor and best cut-point 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.

Details— Continued

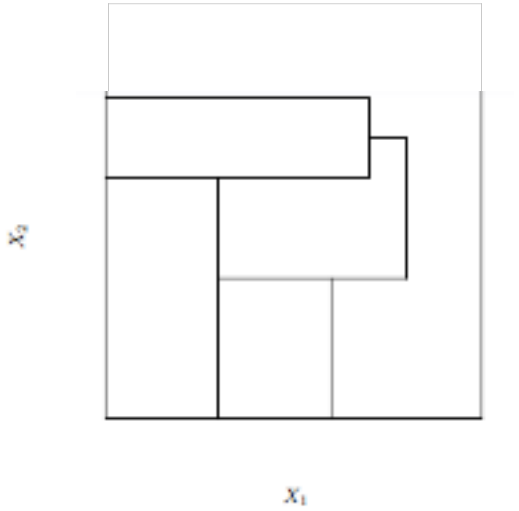
- We now have three regions. Again, we look to split **one** of these three regions further, so as to minimize the RSS.

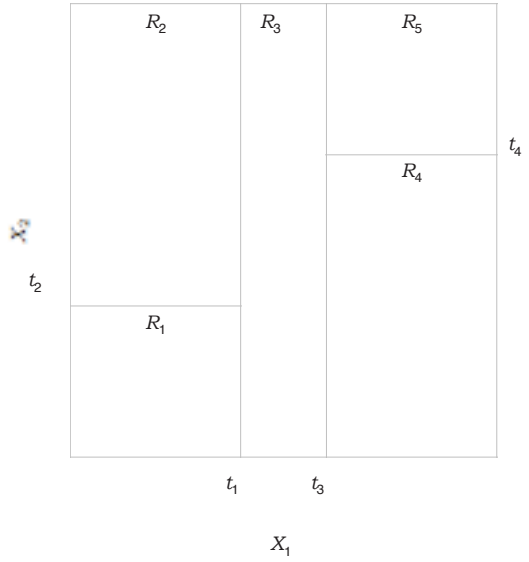
- The process continues until a **stopping criterion** is reached;
  - for instance, we may continue until no region contains more than five observations.
  - or, we may continue until the RSS reaches a lowest minimum predefined threshold
  - …

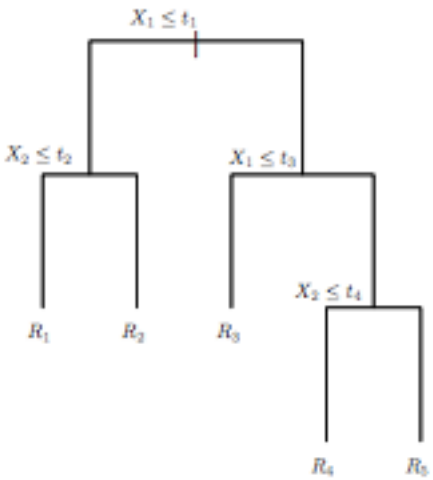
Predictions

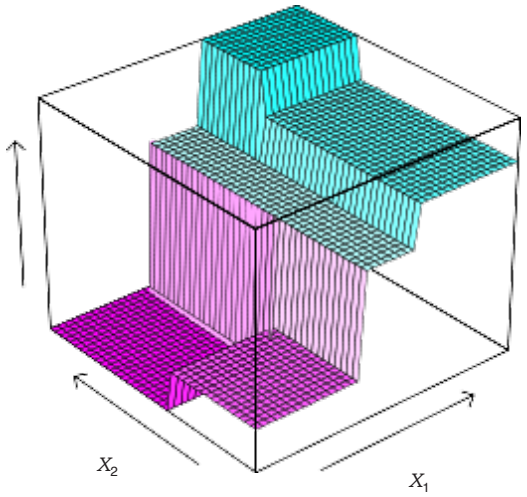
- We predict the response for a given test observation using **the mean of the training observations in the region to which that test observation belongs**.

- A five-region example of this approach is shown in the next slide.


X_2
X_1


R_2
R_3
R_5
t_4
R_4
X_2
t_2
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

Details of previous figure

Top Left: A partition of two-dimensional feature space that could not result from recursive binary splitting.

Top Right: The output of recursive binary splitting on a two-dimensional example.

Bottom Left: A tree corresponding to the partition in the top right panel.

Bottom Right: A perspective plot of the prediction surface corresponding to that tree.

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?*

- A smaller tree with **fewer splits** (that is, fewer regions $R_1, \ldots, R_J$) might lead to **lower variance** and better interpretation **at the cost of a little bias**.
- One possible alternative to the process described above is to grow the tree only so long as the **decrease in the RSS** due to each split exceeds some **(high) threshold**.

- This strategy will result in smaller trees, but is too *short-sighted:* a seemingly worthless split (by tolerating a high RSS) early on in the tree might be followed by a very good split — that is, a split that leads to a large reduction in RSS later on.

Pruning a tree– continued

- 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 m-th terminal node, and $\hat{y}_{R_m}$ is the mean of the training observations in R_m.

Choosing the best subtree

- 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 $\hat{\alpha}$.

Summary: tree algorithm

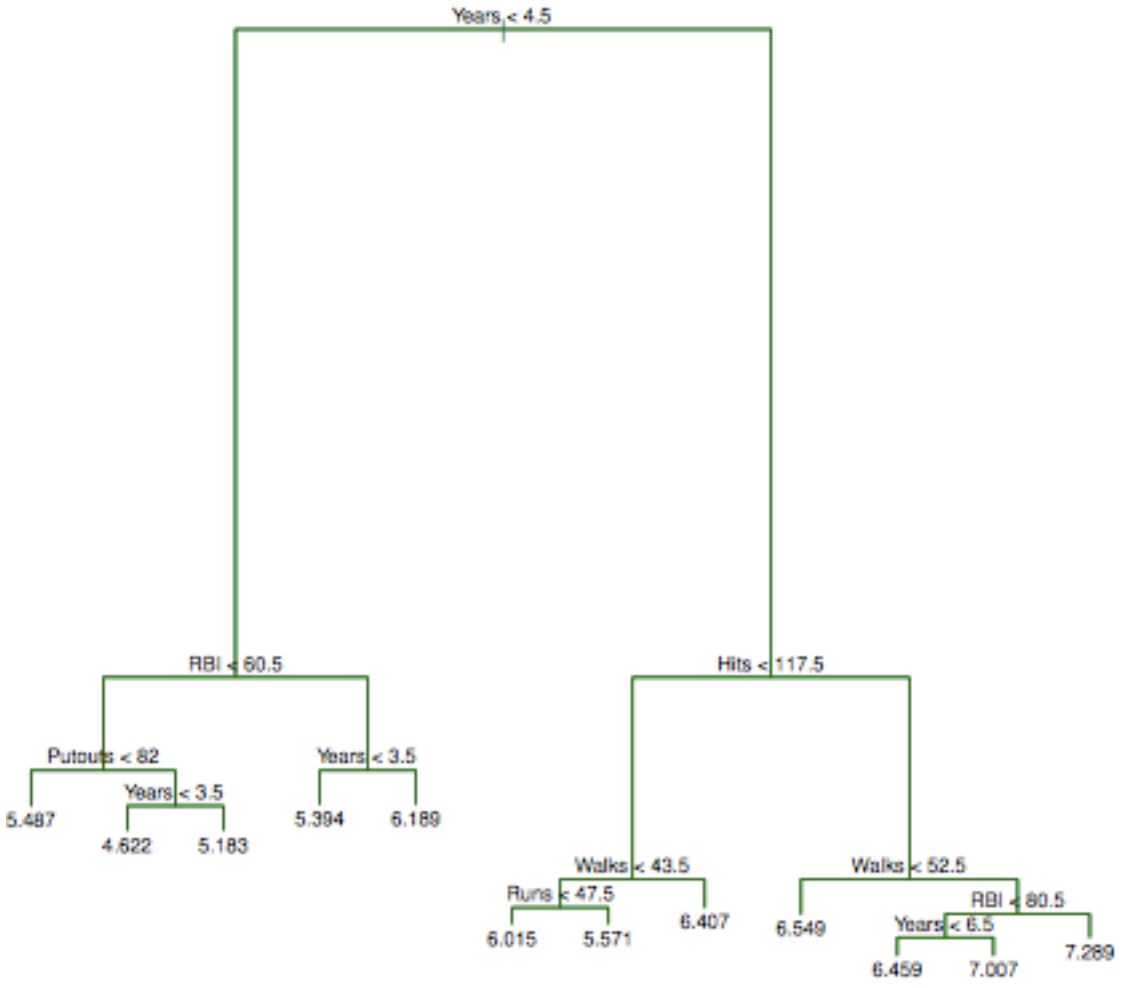
1. Use **recursive binary splitting** to grow a large tree on the training data, stopping only when each terminal node has fewer than some **minimum number of observations**.
2. Apply **cost complexity pruning** to the large tree in order to obtain a sequence of best subtrees, as a function of α.
3. Use K-fold **cross-validation** to choose α. For each $k = 1, \ldots, K$:
   - 3.1 Repeat Steps 1 and 2 on the $\frac{K-1}{K}$ th fraction of the training data, excluding the k-th fold.
   - 3.2 Evaluate the mean squared prediction error on the data in the left-out k- th fold, as a function of α.

   Average the results, and pick α to minimize the average error.
4. Return the subtree from Step 2 that corresponds to the chosen value of α.

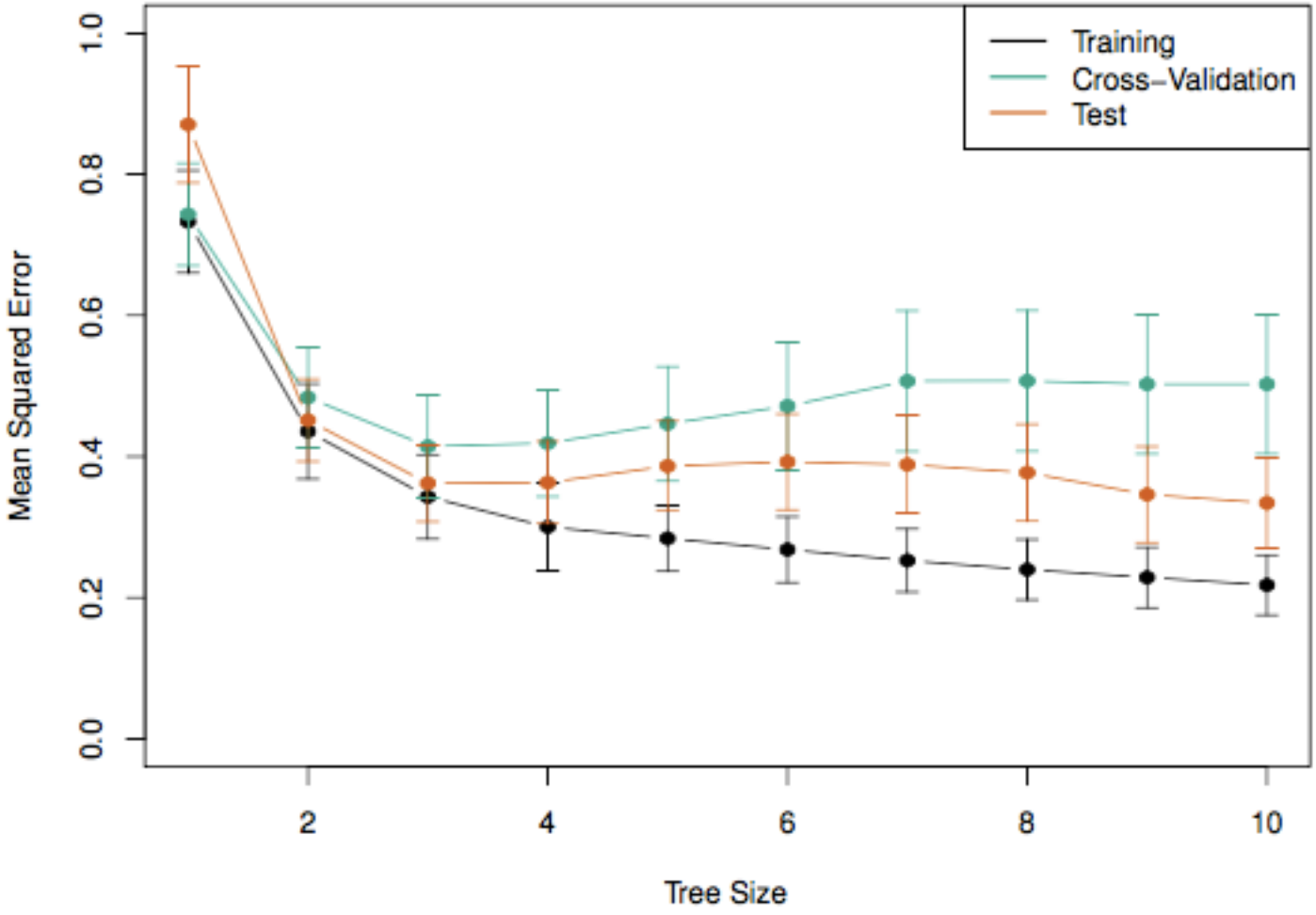
Baseball example continued

- 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 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.

Baseball example continued



Baseball example continued



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.

Details of classification trees

- Just as in the regression setting, we use recursive binary splitting to grow a classification tree.
- 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**:

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

Here $\hat{p}_{mk}$ represents the proportion of training observations in the m-th region that are from the k-th class.

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

Gini index and Deviance

- The *Gini index* is defined by

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

  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**.

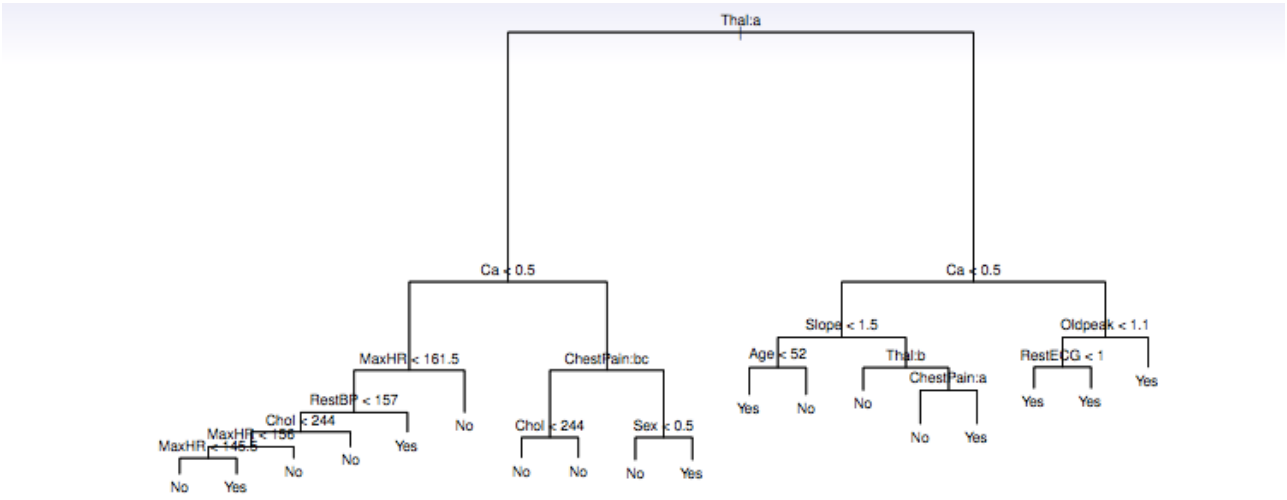
- An alternative to the Gini index is *cross-entropy*, given by

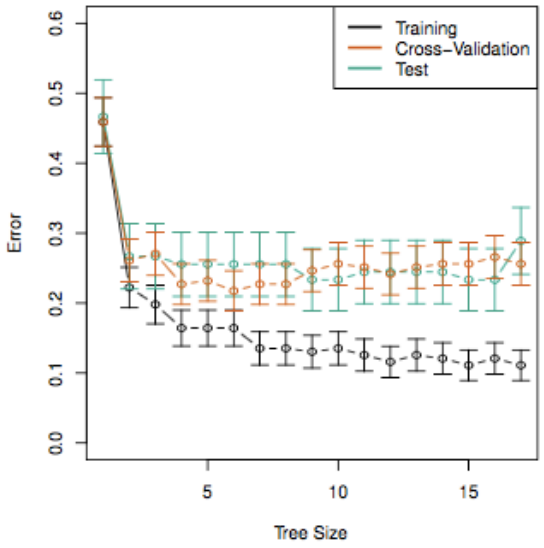
$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$$

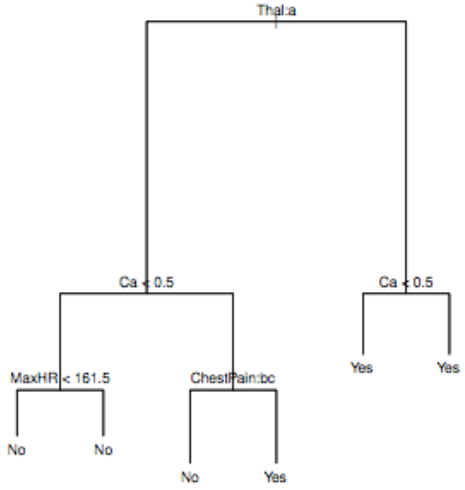
- It turns out that the Gini index and the cross-entropy are very **similar numerically**.

Example: heart data

- 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.


Thal:a
Ca < 0.5
Ca < 0.5
MaxHR < 161.5
ChestPain:bc
Slope < 1.5
Oldpeak < 1.1
RestBP < 157
Chol < 244
Chol < 244
Sex < 0.5
Age < 52
Thal:b
RestECG < 1
ChestPain:a
MaxHR < 156
MaxHR < 145.5
No
Yes


Training
Cross-Validation
Test
Error
Tree Size
0.0
0.1
0.2
0.3
0.4
0.5
0.6
5
10
15


Thal:a
Ca < 0.5
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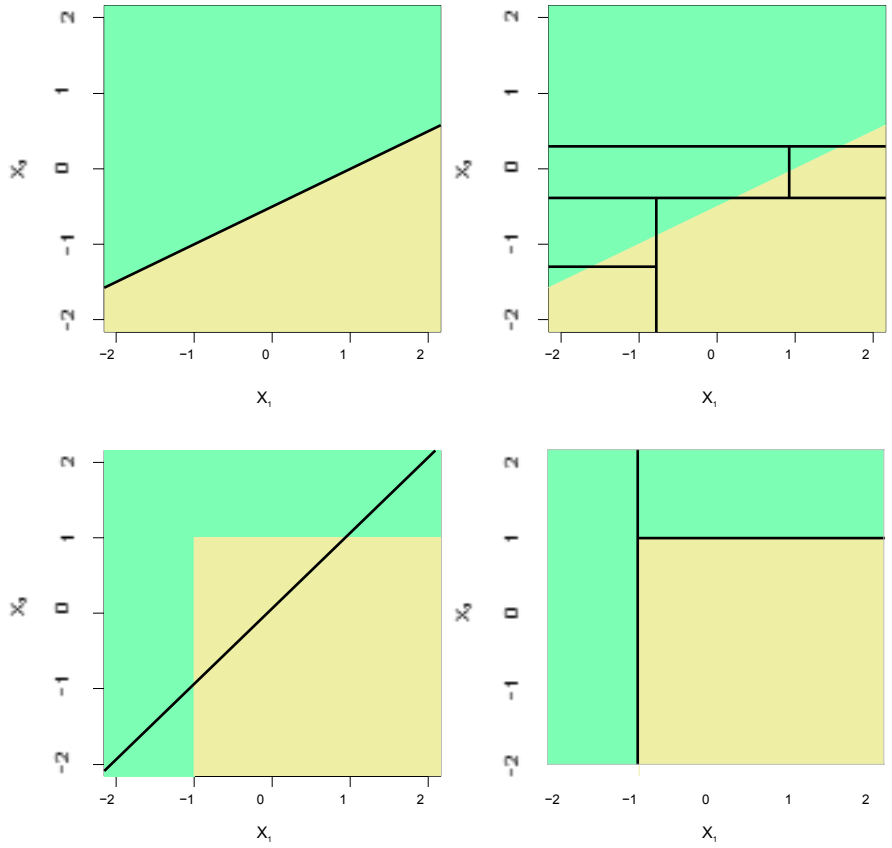
MaxHR < 161.5
ChestPain:bc
Yes
No

Trees Versus Linear Models



Top Row: True linear boundary; Bottom row: true non-linear boundary.

Left column: linear model; Right column: tree-based model

Advantages and Disadvantages of Trees

- ▲ Trees are very **easy to explain** to people. In fact, they are even easier to explain than linear regression!
- ▲ Some people believe that decision trees more closely **mirror human decision-making** than do the regression and classification approaches seen in previous chapters.
- ▲ 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.