START Tuesday 3/1/22 (Week 7, Lecture 12)

Thursday 3/3/22 (Week 8, Lecture 15)

- R implementation of trees

Tree based methods[1]

[1] Based on materials in ISLR Ch 8

Tree-based Methods

- 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 **tree-based** or **decision-tree** methods.

Pros and Cons

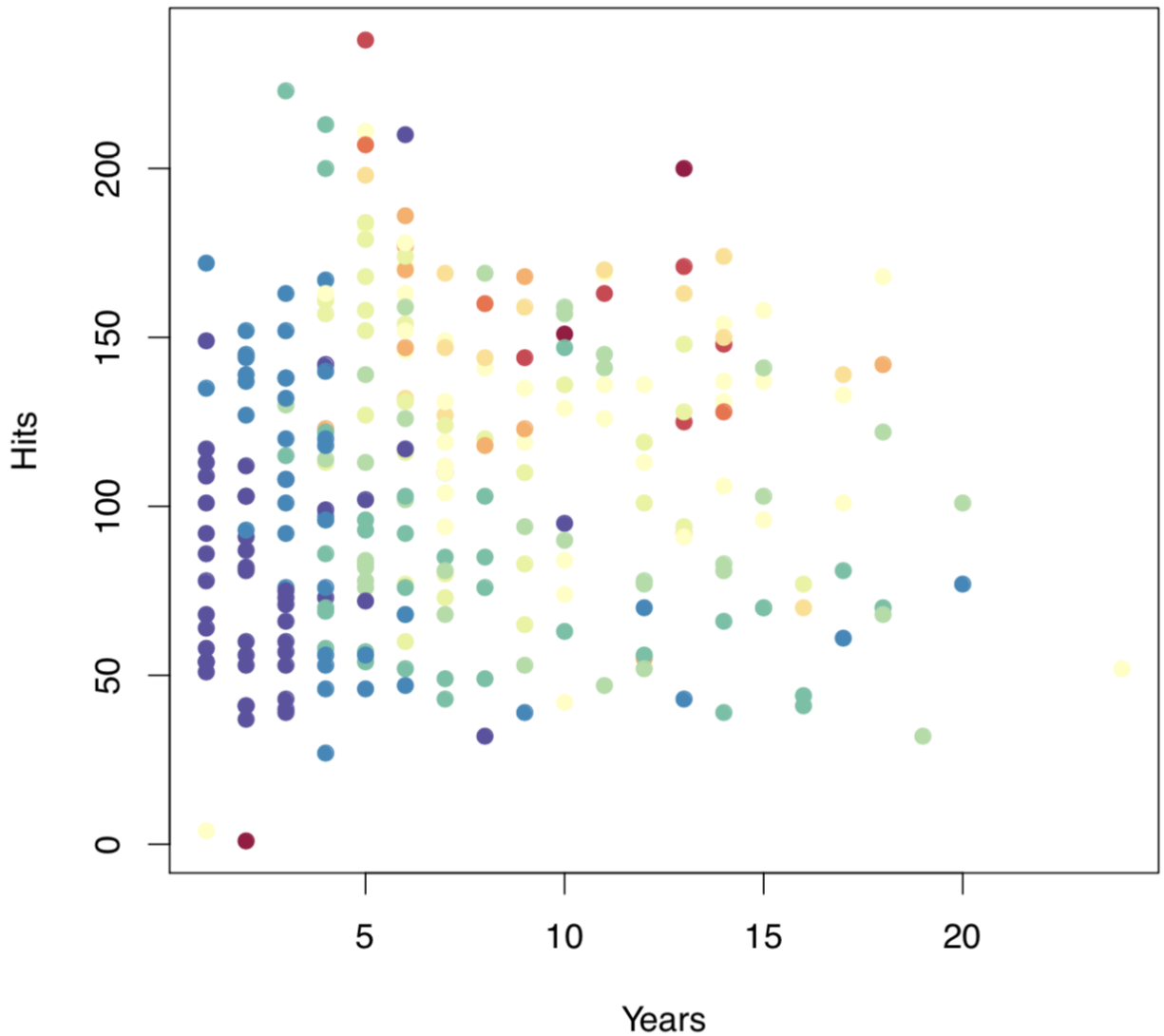
- Tree-based methods are simple and useful for interpretation.
- However they typically are not competitive with the best supervised learning approaches in terms of prediction accuracy.
- Hence we also discuss **bagging, random forests**, and **boosting**. These methods grow multiple trees which are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



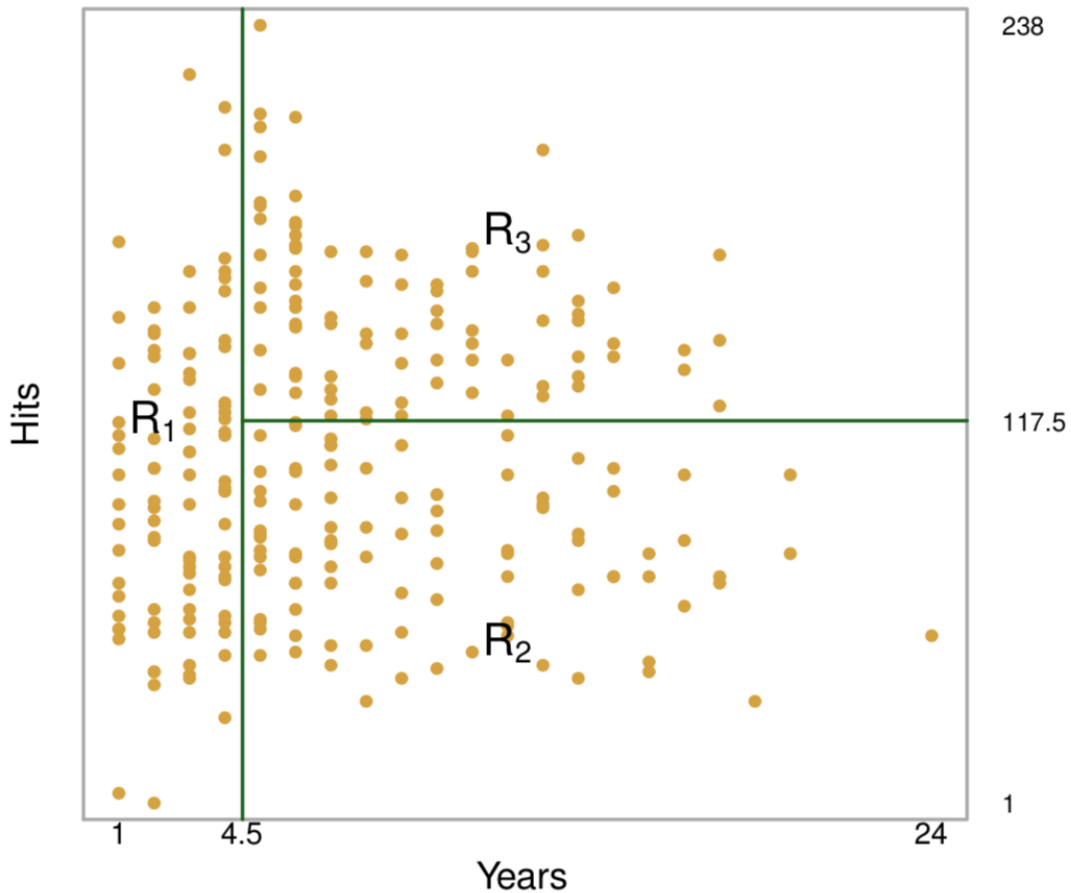
Decision tree for these data

Details of the tree

- For the Hitters data, 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 condition satisfied on the left-hand branch of the split, and the right-hand branch corresponds to $X_j \geqslant t_k$. 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: $R_1 = \{X | Years < 4.5\}$, $R_2 = \{X | Years >= 4.5, Hits < 117.5\}$, and $R_3 = \{X | Years >= 4.5, Hits >= 117.5\}$.



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.

Details of the tree-building process

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

More details of the tree-building process

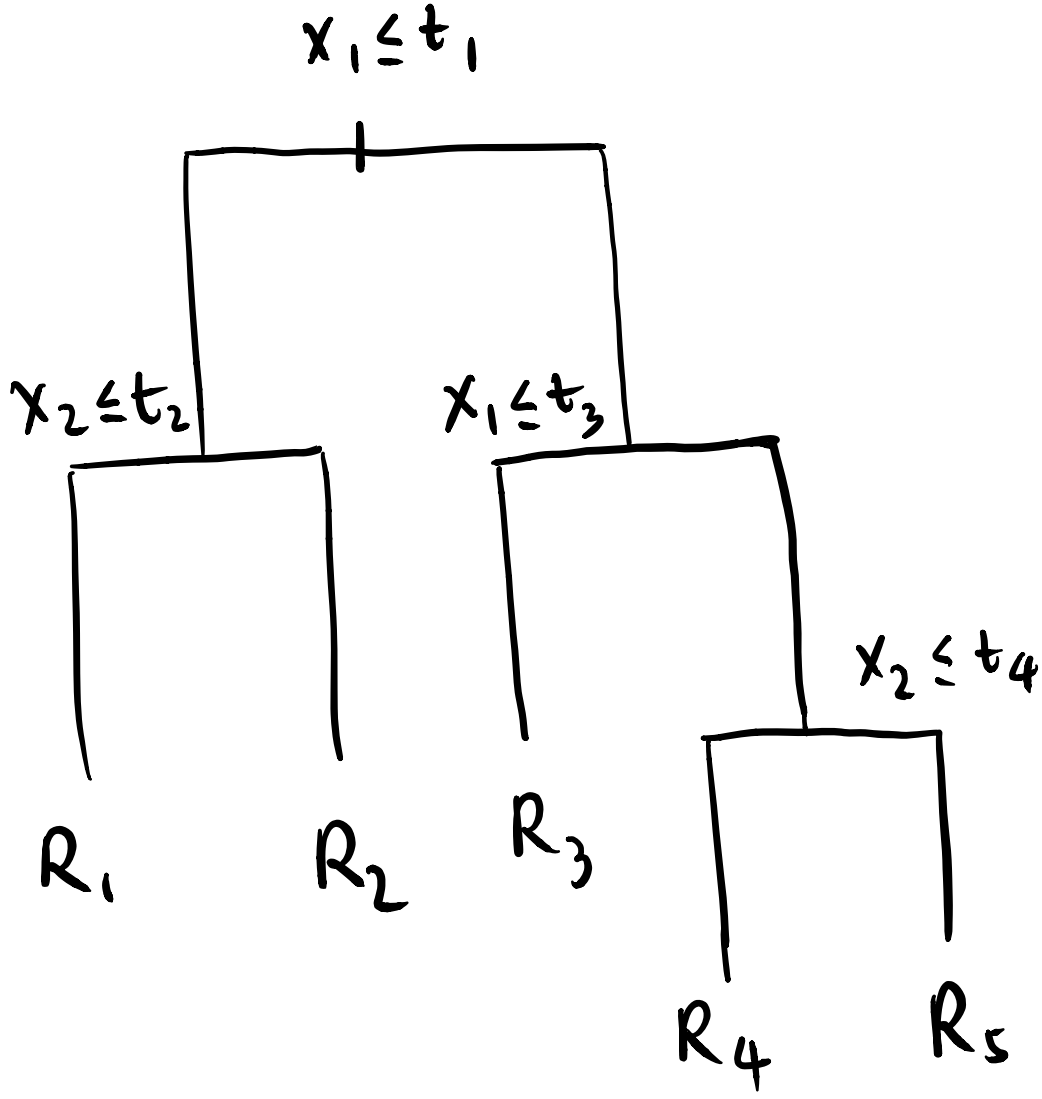
- Unfortunately, it is computationally infeasible to consider every possible partition of the feature space into J boxes.
- For this reason, we take a **top-down**, **greedy** approach that is known as recursive binary splitting.
- The approach is **top-down** because it begins at the top of the tree 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.

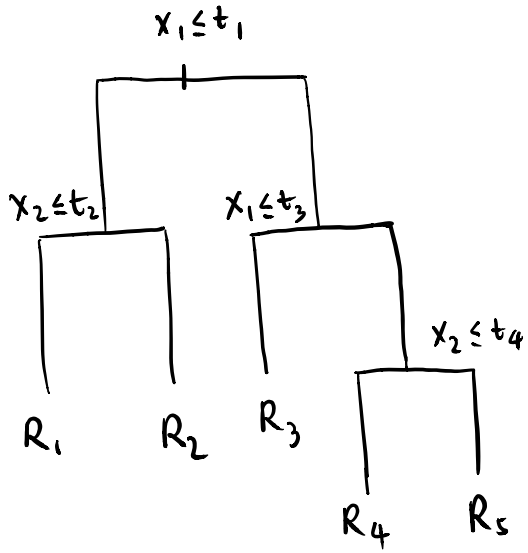
Details– Continued

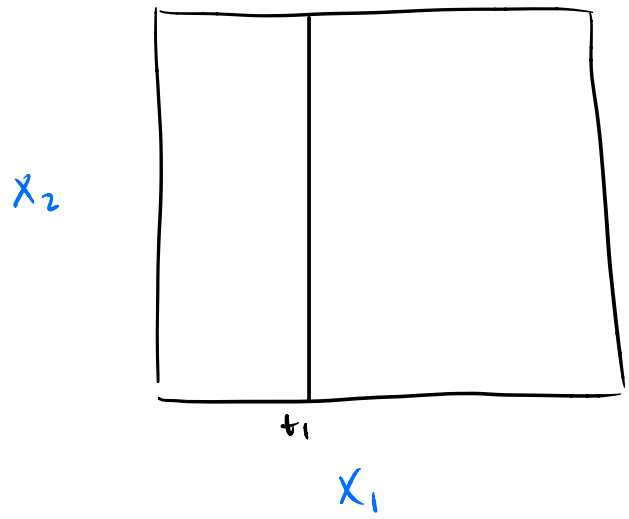
- We first select the predictor X_j and the cutpoint s such that splitting the predictor space into the regions $\{X|X_j < s\}$ and $\{X|X_j \geqslant s\}$ leads to the greatest possible reduction in RSS.
- Next, we repeat the process, looking for the best predictor and best cutpoint in order to split 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.

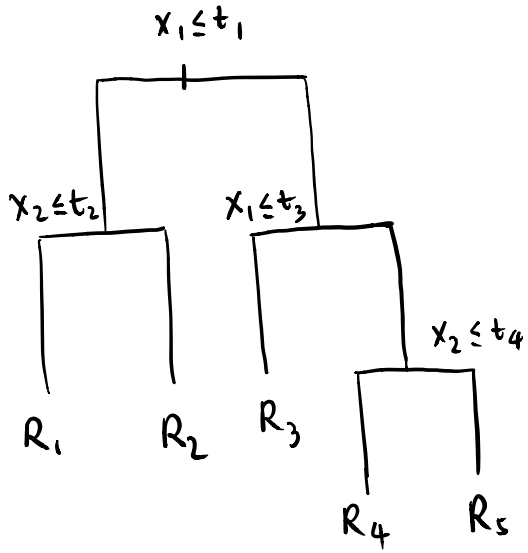
Predictions

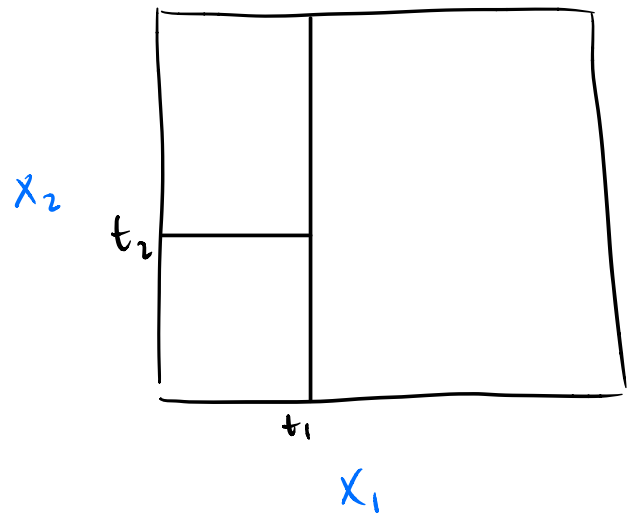
- We predict the response for a given test observation using the mean of the training observations in the region to which that test observation belongs.
- A five-region example of this approach is shown next.

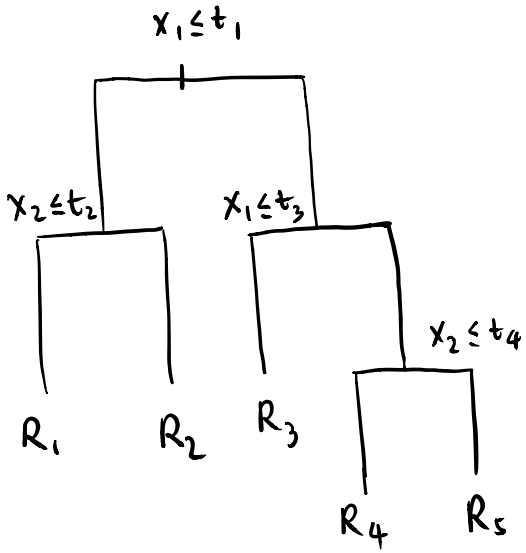

$X_1 \leq t_1$
$X_2 \leq t_2$
$X_1 \leq t_3$
$X_2 \leq t_4$
R_1
R_2
R_3
R_4
R_5

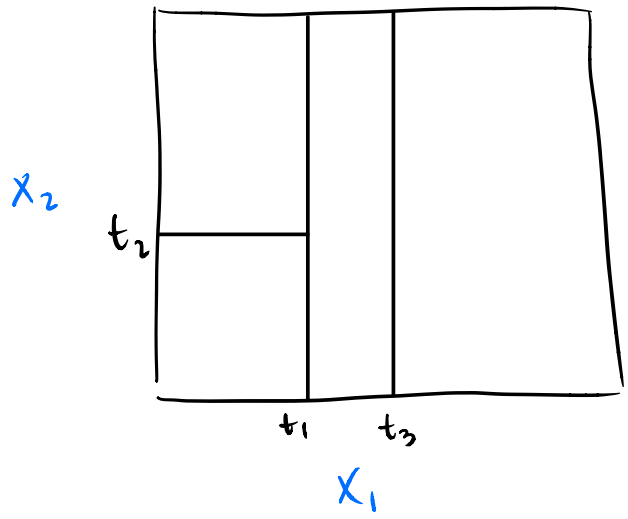

$X_1 \le t_1$
$X_2 \le t_2$
$X_1 \le t_3$
$X_2 \le t_4$
R_1
R_2
R_3
R_4
R_5

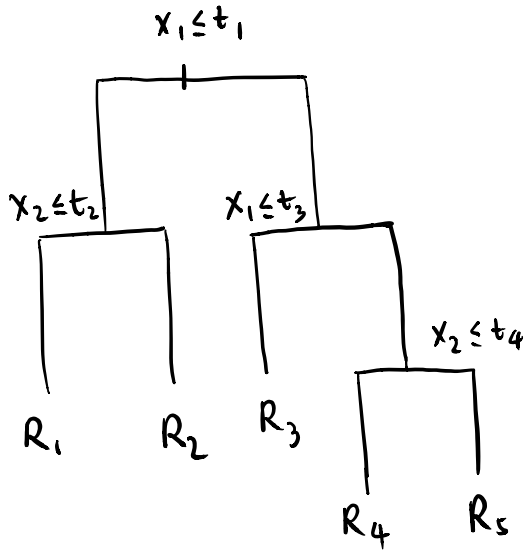

X_2
t_1
X_1

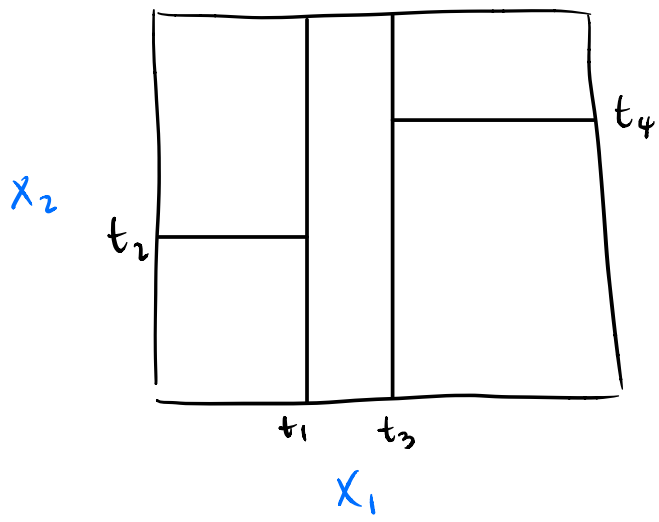

$X_1 \le t_1$
$X_2 \le t_2$
$X_1 \le t_3$
$X_2 \le t_4$
R_1
R_2
R_3
R_4
R_5

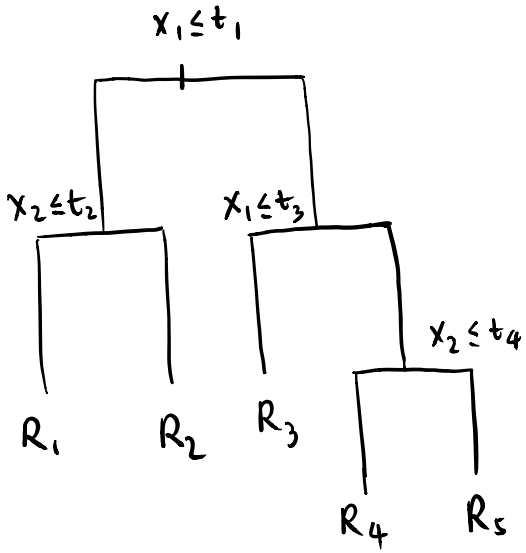

X_2
t_2
t_1
X_1

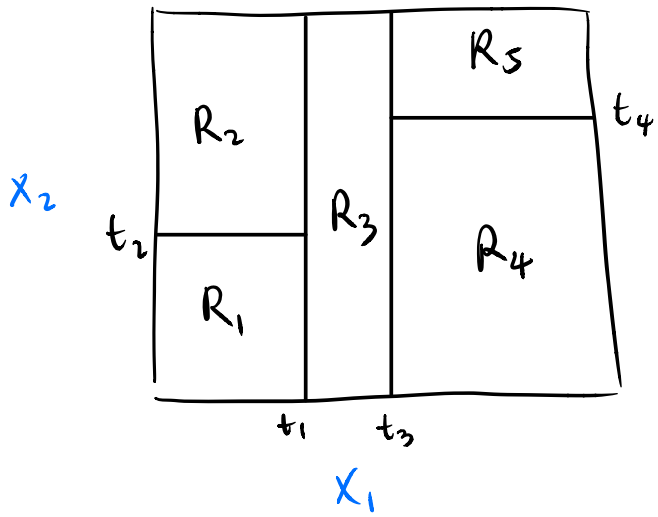

$X_1 \le t_1$
$X_2 \le t_2$
$X_1 \le t_3$
$X_2 \le t_4$
R_1
R_2
R_3
R_4
R_5


X_2
t_2
t_1
t_3
X_1

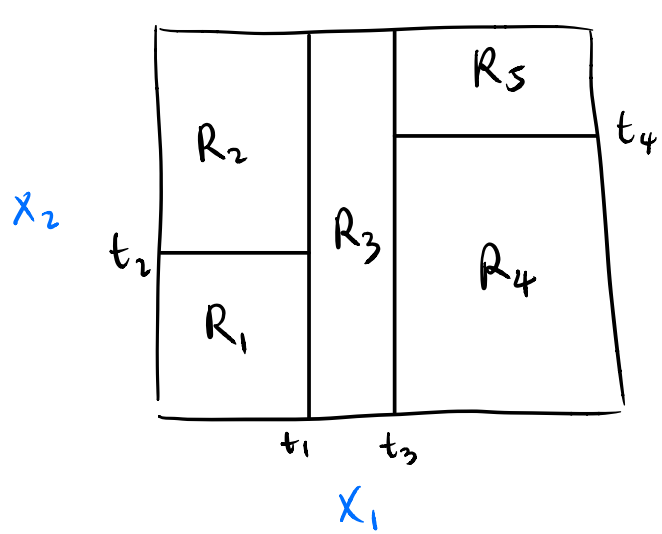

$x_1 \le t_1$
$x_2 \le t_2$
$x_1 \le t_3$
$x_2 \le t_4$
R_1
R_2
R_3
R_4
R_5

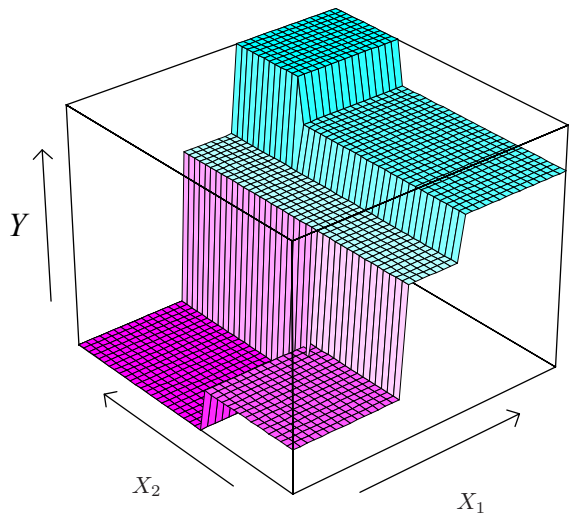

X_2
t_4
t_2
t_1
t_3
X_1


$x_1 \le t_1$
$x_2 \le t_2$
$x_1 \le t_3$
$x_2 \le t_4$
R_1
R_2
R_3
R_4
R_5


x_2
R_2
R_5
t_4
t_2
R_3
R_4
R_1
t_1
t_3
x_1

Prediction





To predict Y^* at $X^* = (X_1^*, X_2^*)$:

1. Find the region that X^* belongs to according to the tree or partition.
2. Suppose the region is R_j. Let $Y^* = Ave_{i \in R_j}(y_i)$.

Pruning a tree

We can always keep growing a tree until the is only one observation in each region, thus our training error will be 0, model will be too flexible.

- 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 $R_1, \cdots, R_J$) 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 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. We will come back to this point after discussing classification tree.

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

$$\min_{T \subset T_0} \sum_{j=1}^{J_T} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2 + \alpha J_T$$

Here J_T is the number of regions or terminal nodes of the tree T, R_j is the rectangle (i.e. the subset of predictor space) corresponding to the jth terminal node, and $\hat{y}_{R_j}$ is the mean of the training observations in R_j.

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 for a range of α values.

3. Use K-fold cross-validation to choose α. For each $k = 1, \cdots, K$:
   - Repeat Steps 1 and 2 on the $\frac{K-1}{K}$th fraction of the training data, excluding the kth fold.
   - Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

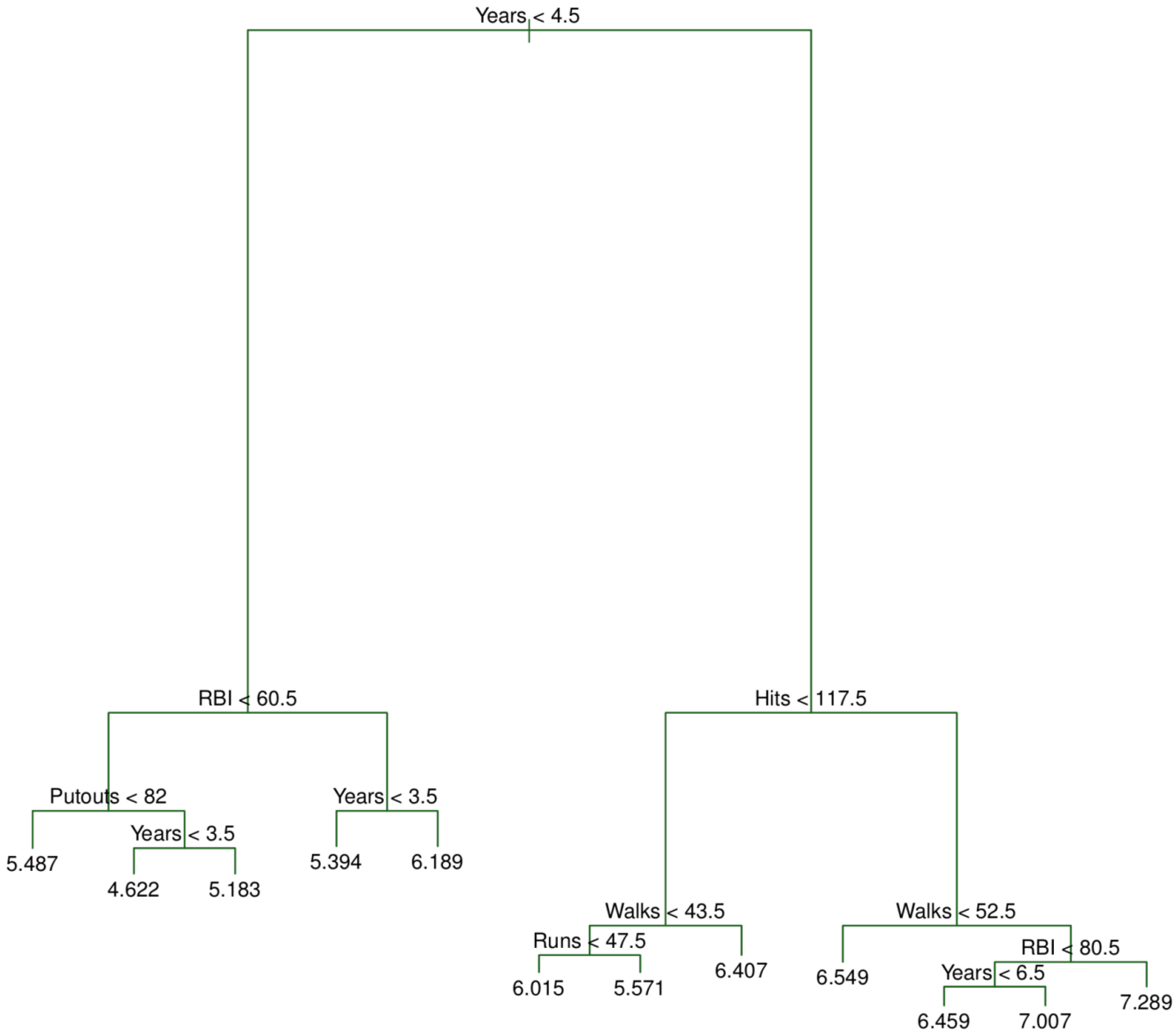
   Average the results, and pick α to minimize the average error.

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.

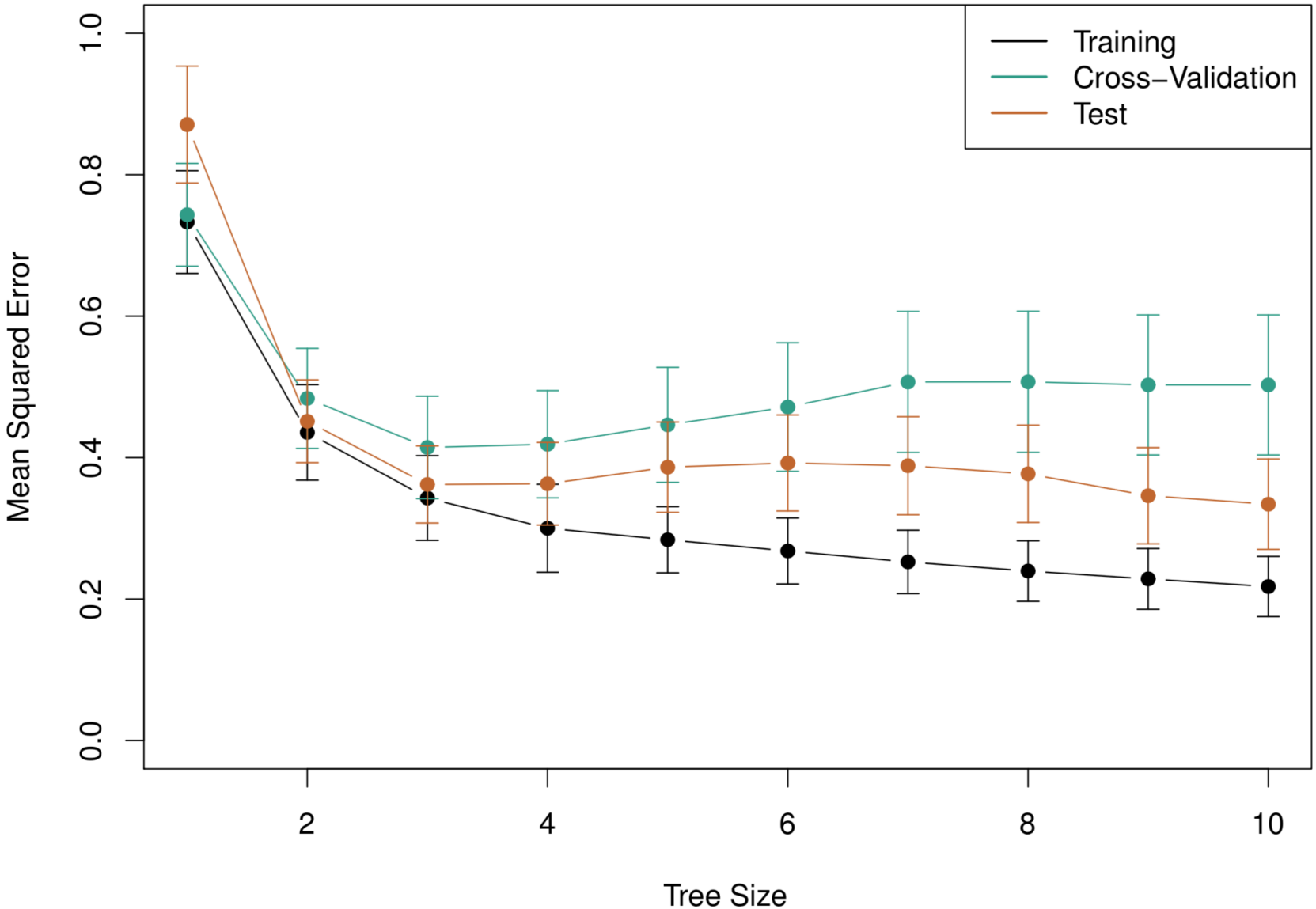
Unpruned tree



Pruned tree

Baseball example continued

STOP Tuesday 3/1/22 (week 7, Lecture 12)



START Thursday 3/4/22 (Week 7, Lecture 13)

- 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:

$$E_j = 1 - \max_k(\hat{p}_{jk}).$$

  Here $\hat{p}_{jk}$ represents the proportion of training observations in the jth 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. Will explain later.

↳ however, when we prune a classification tree you can change your criteria from Gini index or Entropy back to classification error rate.

Gini index and Deviance

- The **Gini index** is defined by

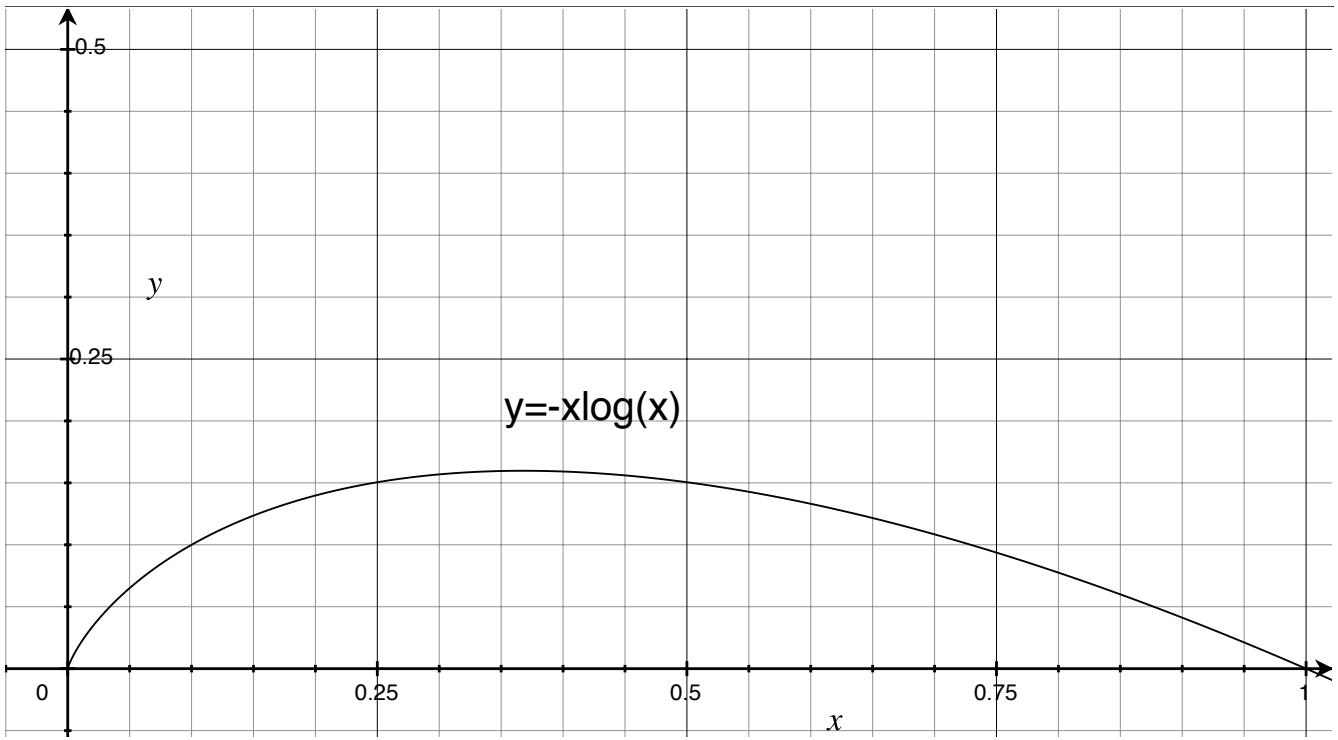
$$G_j = \sum_{k=1}^{K} \hat{p}_{jk}(1 - \hat{p}_{jk}),$$

  a measure of total variance across the K classes. The Gini index takes on a small value if all of the $\hat{p}_{jk}$'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.
- The overall purity of a tree is a weighted average $\frac{1}{n}\sum_{j=1}^{J} n_j G_j$ with n_j being the number of training observations in region R_j.

Entropy

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

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



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

Comparison of classification error rate vs Gini index

Consider two scenarios for three-class classification

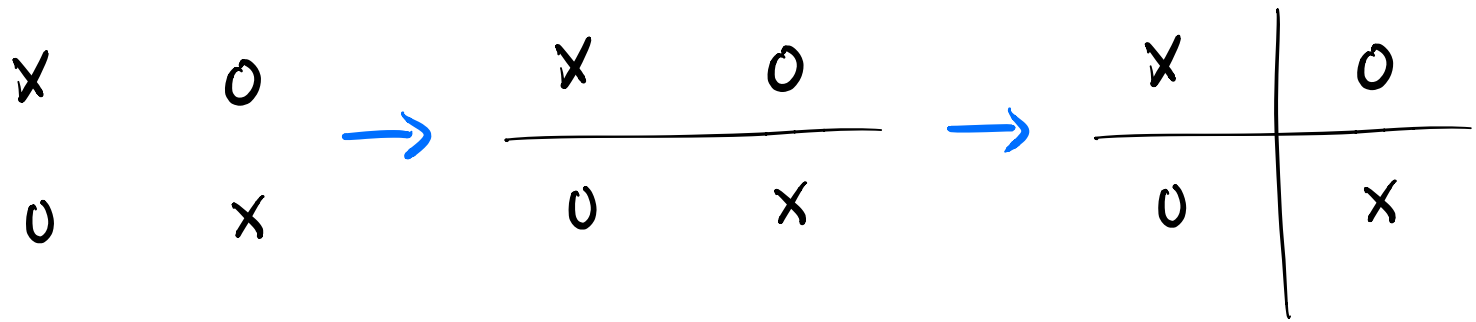
1. $p_1 = 50\%, p_2 = 25\%, p_3 = 25\%$
   - Classification error 0.5 vs Gini index 0.625
2. $p_1 = 50\%, p_2 = 50\%, p_3 = 0\%$
   - Classification error 0.5 vs Gini index 0.5

Gini index would favor second scenario as it is more pure whereas classification error rate cannot distinguish between the two.

- We would want our classifier to be different for the two scenarios (b/c they are different) but the classification error rate is the same for both.
- Gini index is different under the two scenarios.
  - ↳ more sensitive to the actual configuration of our regions (so is entropy) than the classification error rate

Why stopping growing a tree at some threshold is short-sighted?

e.g. stop growing tree when RSS < C where C is our threshold. (for regression tree)



Gini 50% → 50% → 0%

- Free stop growing when Gini index stops shrinking we never reach the last stage.

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.

↳ need to go back and cover this. Very important!!!

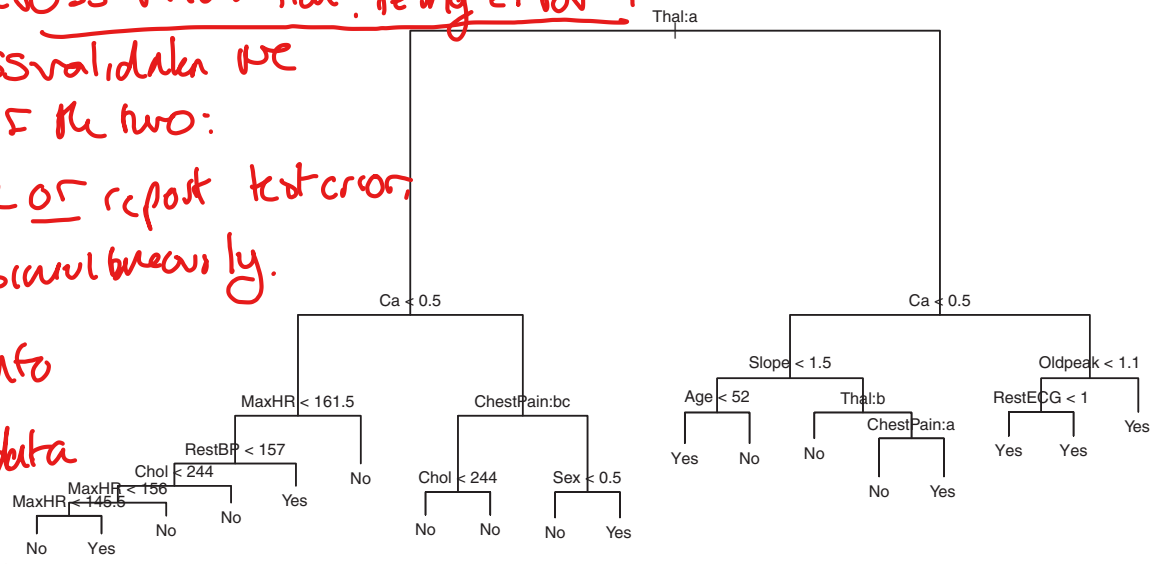
Why do we need cross-validation than testing error?

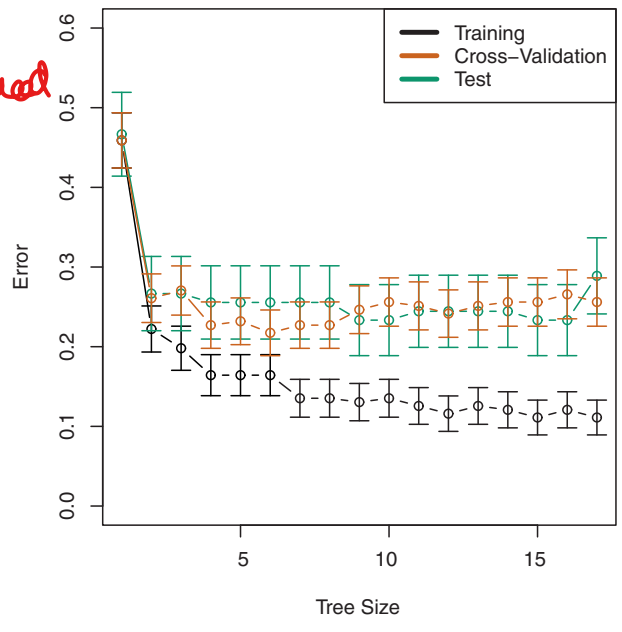
- If we just do cross validation we can achieve 1 of the two:
  choose tree size OR report test error
  Can't do both simultaneously.

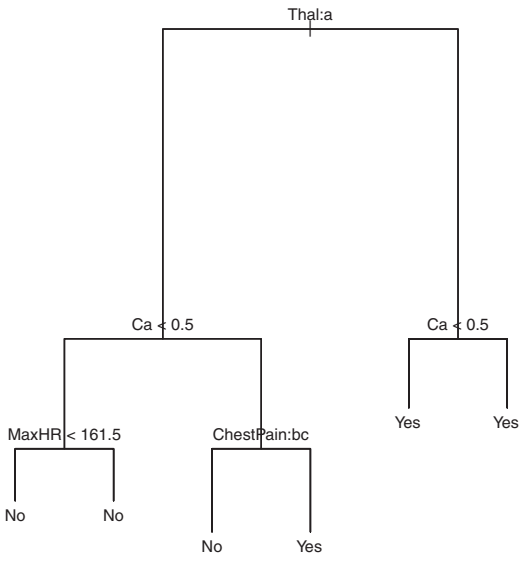
⇒ Most split data into training & testing data

- run cross validation on training then run model on test data & report test error.

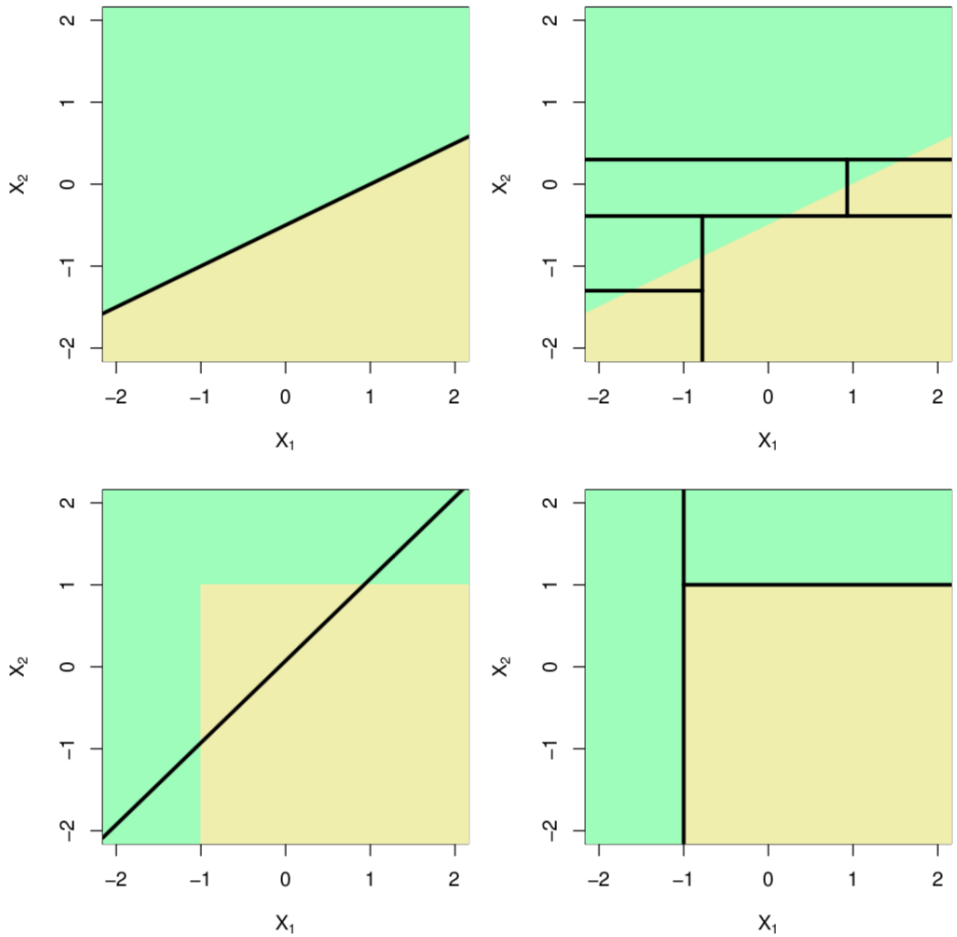
OR more advanced techniques (nested-CV).







Trees Versus Linear Models



* Linear boundary: linear model better
* nonlinear boundary tree is better

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 (single tree based methods)

- 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.
- Unfortunately, trees generally do not have the same level of predictive accuracy as some other regression and classification approaches.

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.
- Recall that given a set of n independent observations $Z_1, \cdots, Z_n$, each with variance σ^2, the variance of the mean $\bar{Z}$ of the observations is given by σ^2/n.
- In other words, **averaging a set of observations reduces variance**. Of course, this is not practical because we generally do not have access to multiple training sets.

Bagging– continued

- Instead, we can bootstrap, by taking repeated samples from the (single) training data set.
- 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

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

This is called **bagging**.

* no need to worry about pruning *

Bagging classification trees

- The above prescription applies 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.

Out-of-Bag Error Estimation

• no need for cross-validation when bagging automatically get error estimation (OOB)

- It turns out that there is a very straightforward way to estimate the test error of a bagged model.
- Recall that the key to bagging is that trees are repeatedly fit to bootstrapped subsets of the observations. One can show that on average, each bagged tree makes use of around two-thirds of the observations. (subsets selected by sampling w/ replacement)
- The remaining one-third of the observations not used to fit a given bagged tree are referred to as the **out-of-bag**(OOB) observations.
- We can predict the response for the ith observation using each of the trees in which that observation was OOB. This will yield around $B/3$ predictions for the ith observation, which we average.
- This estimate is essentially the leave-one-out (LOO) cross-validation error for bagging, if B is large.

code to check:

```
x = null, for (i in 1:100000){
  sample_temp = sample(1:1000, replace = True)
  x[i] = length(unique(sample_temp))/length(sample_temp)
}
mean(x) ≈ 0.63 ≈ 4/5
```

Out-of-Bag Error Estimation

* There is a package in R to get OOB Es trees, but we can use this algorithm for any prediction method.

1. For $b = 1, \ldots, B$:
   - Take a bootstrap sample z^{*b} (of n observations) to use as a training set
   - Fit a regression tree $\hat{f}^{*b}$

2. For $i = 1, \ldots, n$:
   - Set $S = \{b : (y_i, x_i) \notin z^{*b}\}$
   - Calculate

$$OOB_{SE}[i] = \left(y_i - \frac{1}{|S|} \sum_{b \in S} \hat{f}^{*b}(x_i) \right)^2$$

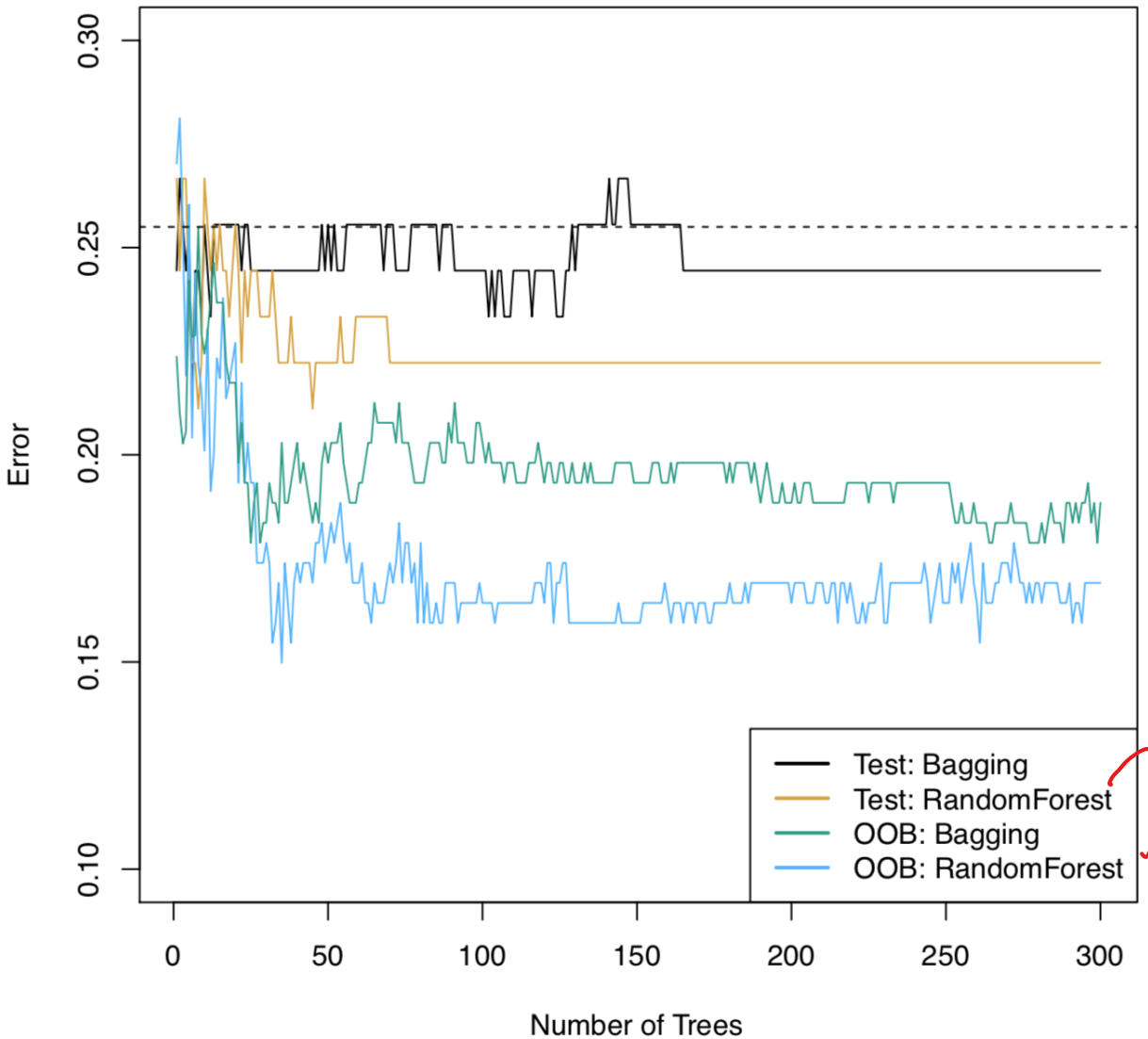
3. Final OOB MSE estimate $= \frac{1}{n} \sum_{i=1}^{n} OOB_{SE}[i]$

Note: if B (and hence $|S|$) is large then $OOB_{SE}[i]$ is approximately the same as $LOO_{SE}[i]$ i.e. removing sample i and finding squared error of the bagging prediction based on the $n - 1$ remaining observations

STOP Thursday 3/3/22 (Week 7, lecture 13)

Bagging the heart data

START Tuesday 3/7/22 (week 8, lecture 14)



come back to random forest later.

Details of previous figure

* when we bag, the trees are not independent (b/c we're drawing from the same sample) Random forest tries to make the trees as independent as possible.

Bagging and random forest results for the Heart data.

- The test error (black and orange) is shown as a function of B, the number of bootstrapped training sets (or equivalently the number of trees) used.
- Random forests were applied with $m = \sqrt{p}$. *
- The dashed line indicates the test error resulting from a single classification tree.
- The green and blue traces show the OOB error, which in this case is considerably lower.
- Note that the error does not increase as $B \to \infty$.

↳ we never have to worry about overfitting w/ bagging & random forests

(no bias variance trade off)

• when we average R.V. we get variance reduction for free

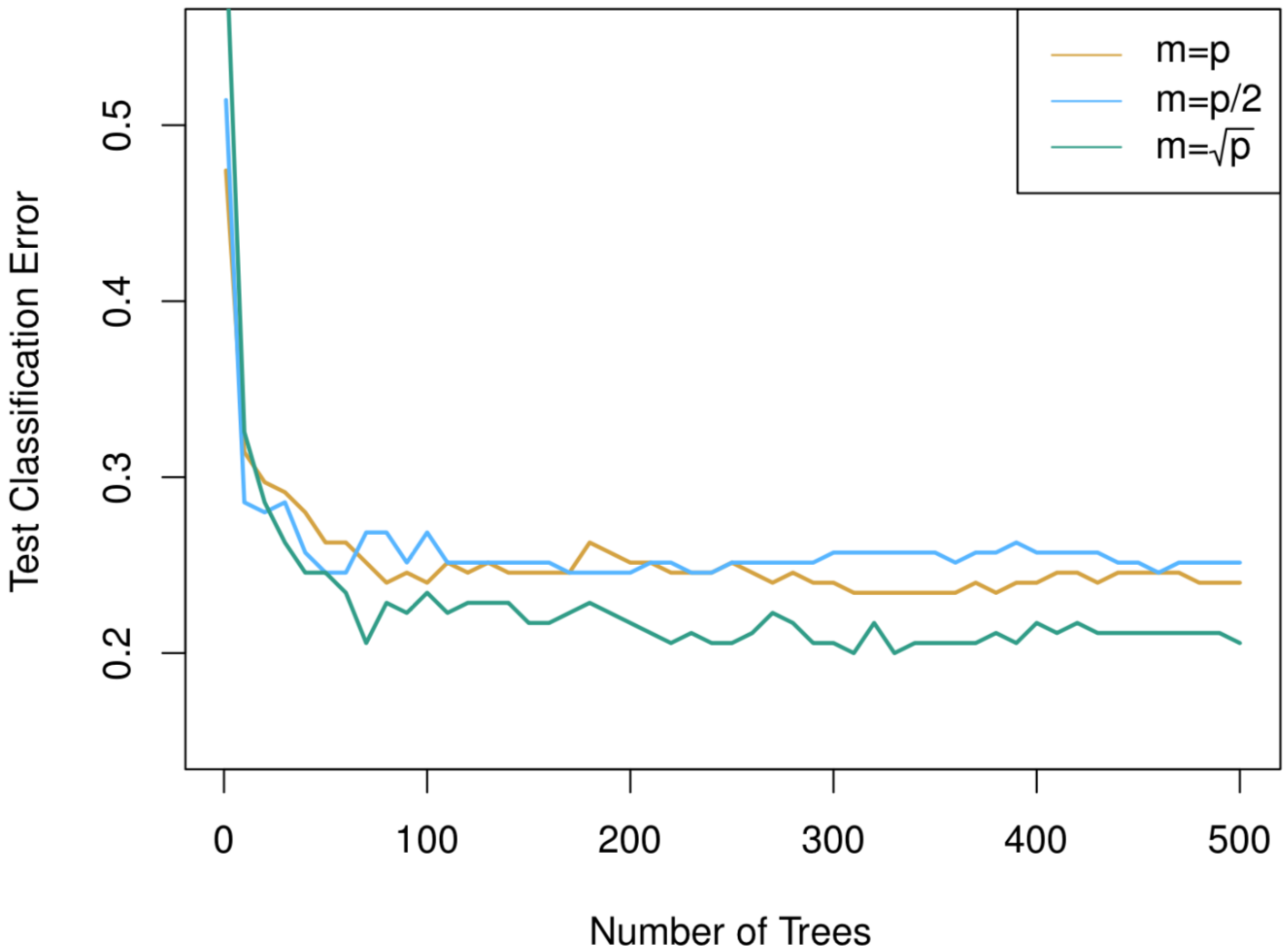
Random Forests

- **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.
- 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).

Example: gene expression data

- Now we apply random forests to a high-dimensional biological data set consisting of expression measurements of 4,718 genes measured on tissue samples from 349 patients.
- There are around 20,000 genes in humans, and individual genes have different levels of activity, or expression, in particular cells, tissues, and biological conditions.
- 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.

Results: gene expression data



Details of previous figure

- Results from random forests for the fifteen-class gene expression data set with $p = 500$ predictors.
- The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m, the number of predictors available for splitting at each interior tree node.
- Random forests ($m < p$) lead to a slight improvement over bagging ($m = p$). A single classification tree has an error rate of 45.7%.

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 algorithm for regression trees

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \cdots, B$, repeat:
   - Fit a tree $\hat{f}^b$ with d splits ($d + 1$ terminal nodes) to the training data (X, r).
   - Update $\hat{f}$ by adding in a shrunken version of the new tree:

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

   - Update the residuals,

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

3. Output the boosted model,

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

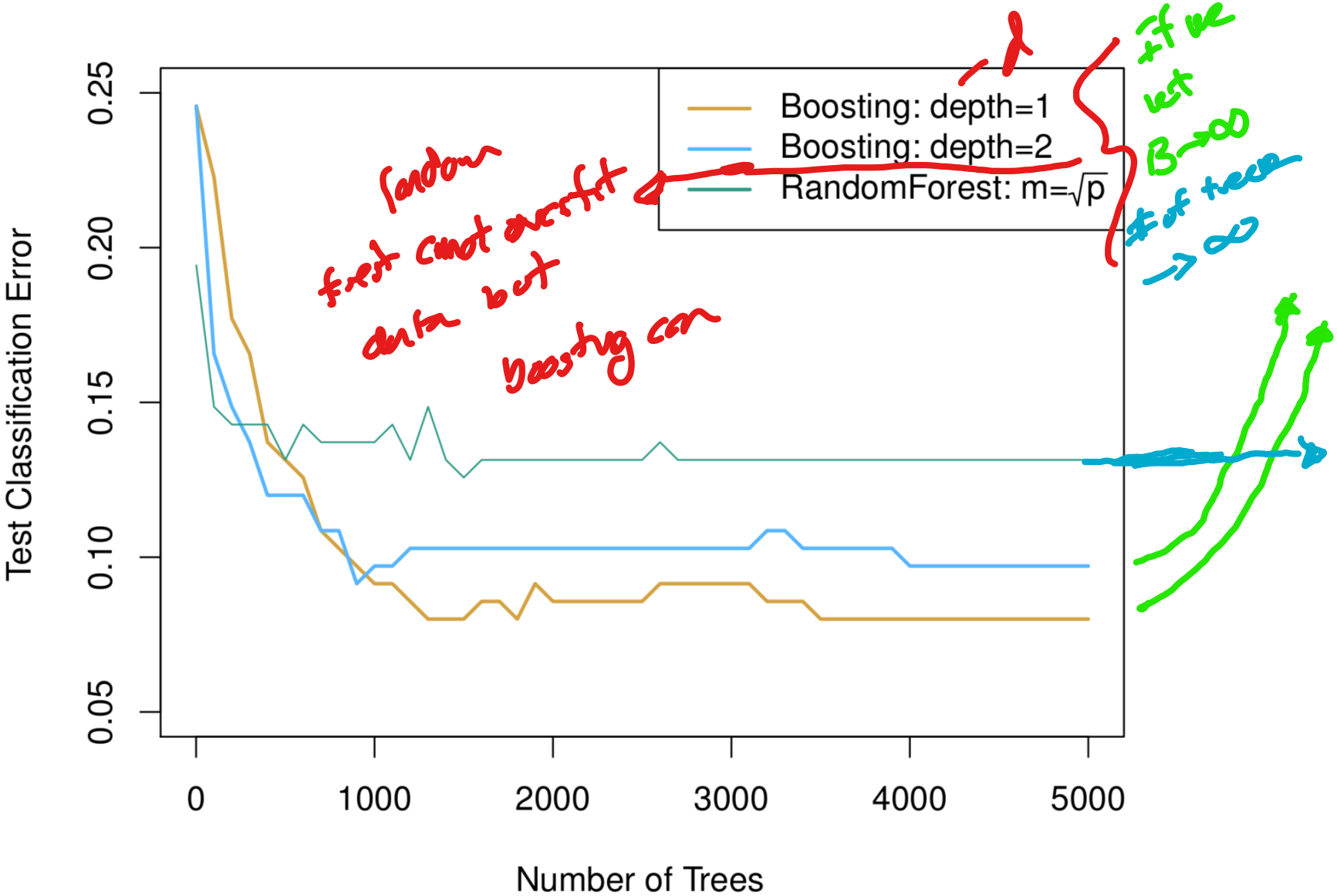
What is the idea behind this procedure?

- 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**.
- Given the current model, we fit a decision tree to the residuals from the model. We then add this new decision tree into the fitted function in order to update the residuals.
- Each of these trees can be rather small, with just a few terminal nodes, determined by the parameter d in the algorithm.
- By fitting small trees to the residuals, we slowly improve $\hat{f}$ in areas where it does not perform well. The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals.

Boosting for classification

- Boosting for classification is similar in spirit to boosting for regression, but is a bit more complex. We will not go into detail here.
- You can learn about the details in **Elements of Statistical Learning, chapter 10**.
- The R package gbm (gradient boosted models) handles a variety of regression and classification problems.

Gene expression data continued



Details of previous figure

- Results from performing boosting and random forests on the fifteen-class gene expression data set in order to predict **cancer** versus **normal**.
- The test error is displayed as a function of the number of trees. For the two boosted models, $\lambda = 0.01$. Depth-1 trees slightly outperform depth-2 trees, and both outperform the random forest, although the standard errors are around 0.02, making none of these differences significant.
- The test error rate for a single tree is 24%.

Tuning parameters for boosting

→ do CV to choose B.

1. The **number of trees** B. Unlike bagging and random forests, boosting can overfit if B is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select B.

– usually don't do CV for this, just choose 0.01 or 0.001

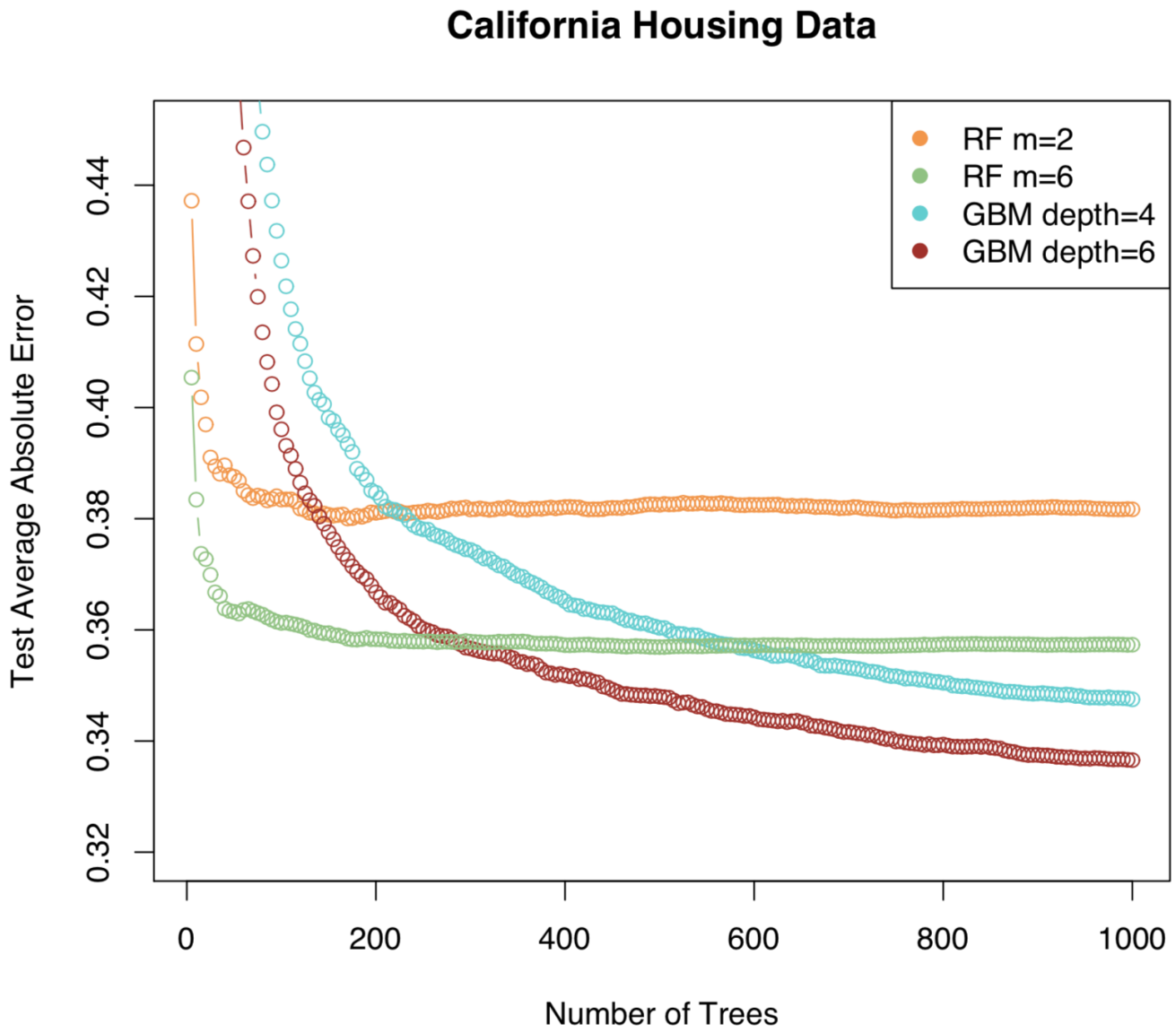
2. The **shrinkage parameter** λ, a small positive number. This controls the rate at which boosting learns. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ can require using a very large value of B in order to achieve good performance.

Low will affect the # of trees needed to obtain the same result.

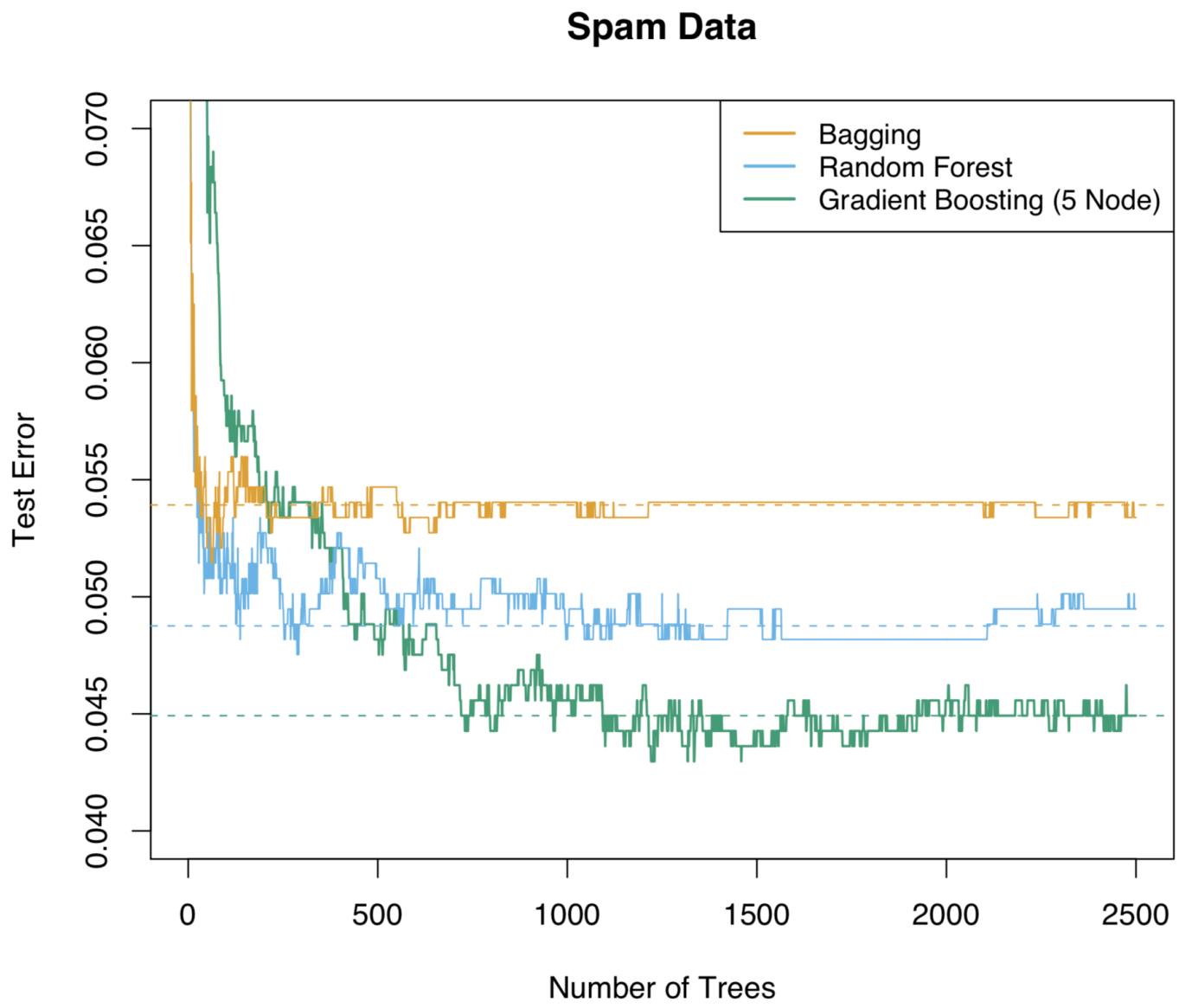
3. The **number of splits** d in each tree, which controls the complexity of the boosted ensemble. Often $d = 1$ works well, in which case each tree is a **stump**, consisting of a single split and resulting in an additive model. More generally d is the **interaction depth**, and controls the interaction order of the boosted model, since d splits can involve at most d variables.

→ can in principle do CV to choose. If we suspect interactions can choose d=2 or higher

Another regression examples

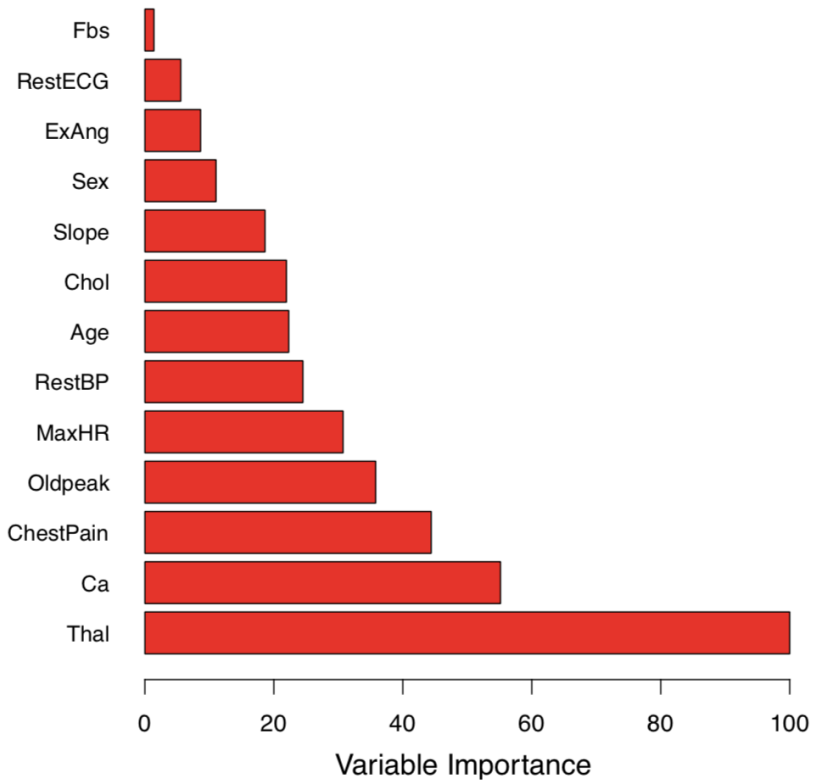


Another classification example



Variable importance measure

- For bagged/RF regression trees, we record the total amount that the RSS is decreased due to splits over a given predictor, averaged over all B trees. A large value indicates an important predictor.
- Similarly, for bagged/RF classification trees, we add up the total amount that the Gini index is decreased by splits over a given predictor, averaged over all B trees.



Variable importance plot for the **Heart** data

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.

Tuesday

STOP 3/7/22 (week 8, lecture 17)