NYC DATA SCIENCE ACADEMY

Trees, Bagging, Random Forests, & Boosting

Data Science with R: Machine Learning

Outline

- Part 1: Decision Trees
- Part 2: Bagging
- Part 3: Random Forests
- Part 4: Boosting
- Part 5: Variable Importance

PART 1

Decision Trees

What are Tree-Based Methods?

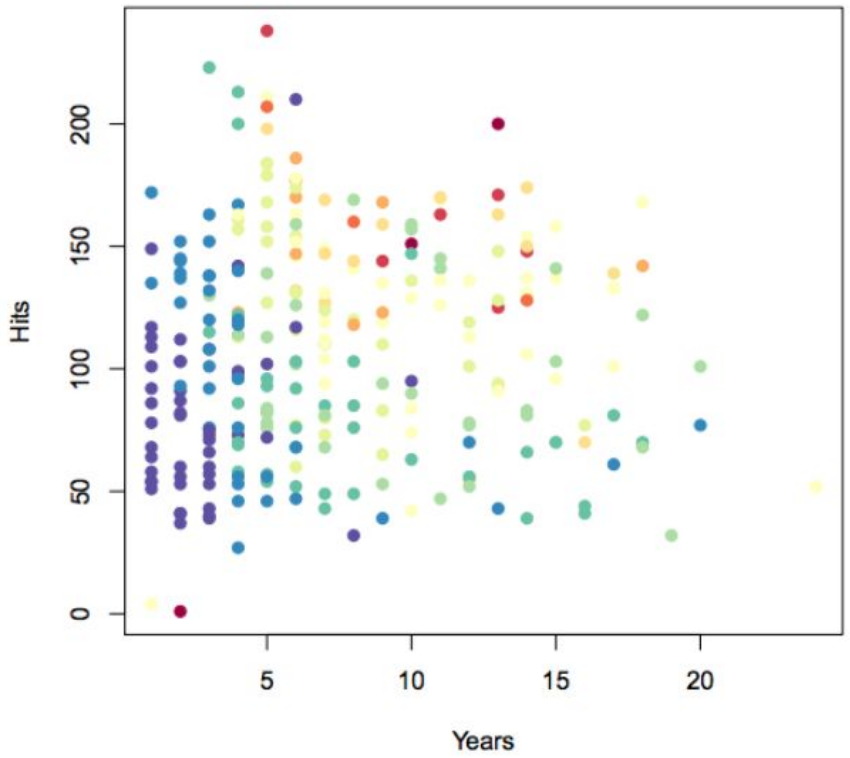
- Tree-based methods are supervised learning procedures that aid in both regression and classification settings.

- The models aim to construct solutions that stratify the feature space into relatively easy to describe regions.

- Essentially, if we can get an idea of the general characteristics of observations that fall within particular regions of space, we can inform the characteristics of new observations that fall within the same regions.

Regression Trees: Visually

- Let's return to the baseball player salary data. How might we segment the following graph into regions?
  - Color corresponds to salary: red/orange = high, blue/violet = low.



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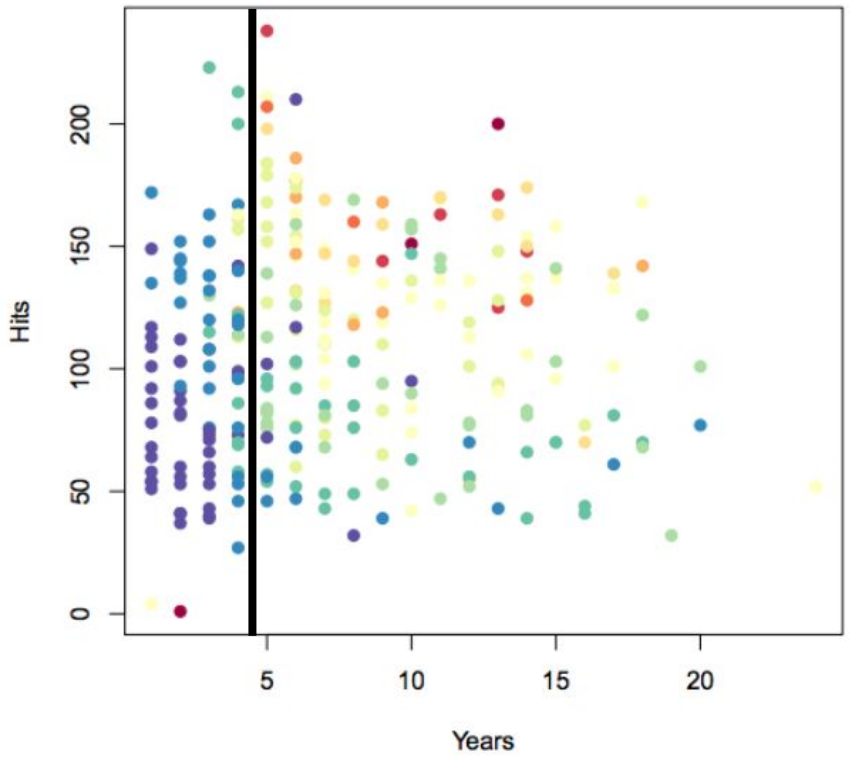

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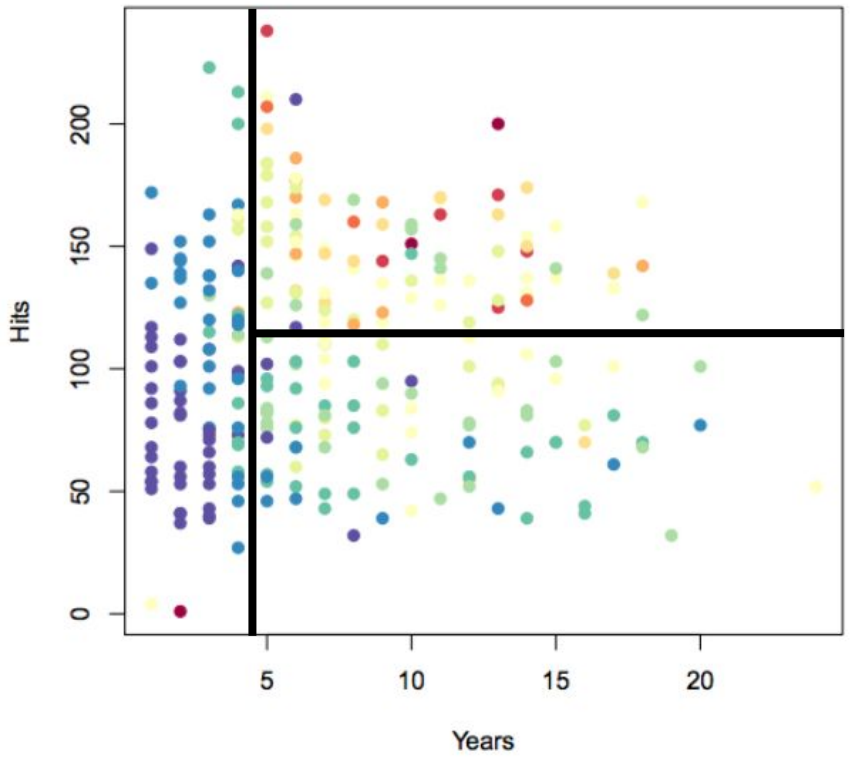


Regression Trees: Visually

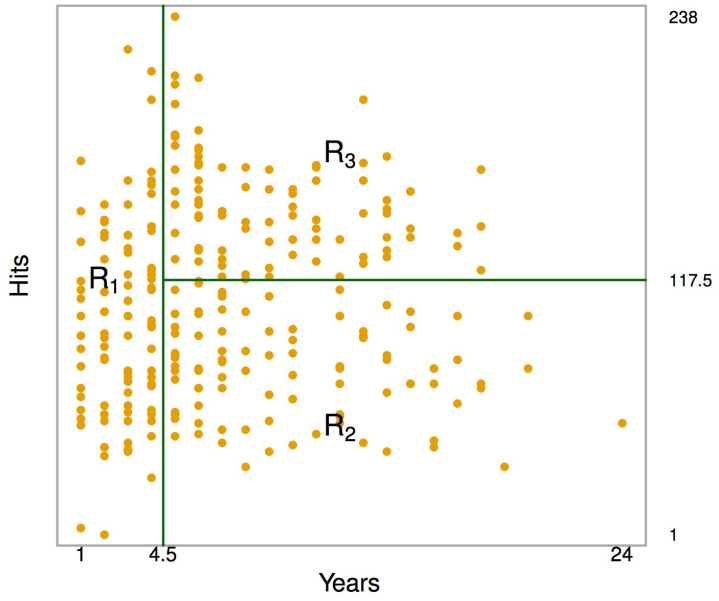
- The decision tree that corresponds to cuts similar to what we've created is given below:

How to Interpret a Decision Tree

- What is the decision tree actually saying? How do we interpret this tree?
  - We start from the top of the tree and pass a new observation through the various internal nodes.
  - At each internal node, we make a decision of how to proceed based on the characteristics of the observation at hand.
    - If the listed condition is satisfied, we move down the left branch.
    - If the listed condition is not satisfied, we move down the right branch.
  - Continue this process until you reach a terminal node/leaf (i.e., a node for which there is no further decision to be made).
    - The number within the terminal node is the mean response value for the observations that fell within that region; this is also the prediction for future observations that fall within that region.

How to Interpret a Decision Tree

- The decision tree ended up partitioning the feature space into three regions:
  - R_1: Where players have less than 4.5 years of experience.
  - R_2: Where players have greater than 4.5 years of experience and had fewer than 117.5 hits.
  - R_3: Where players have greater than 4.5 years of experience and had greater than 117.5 hits.



Regression Trees: Mathematically

- The process of building a regression tree can be simplified into the following two steps:
  1. Segment the predictor space (all possible values of $X_1, X_2, \ldots, X_p$) into J distinct and non-overlapping regions. Call these regions $R_1, R_2, \ldots, R_J$.
  2. For every observation that falls into a specific region R_j, predict the mean of the response values for the training observations that fell within R_j.

- This is a bit of an over-simplification:
  - How do we decide where exactly to segment the predictor space?
  - How do we come upon the regions $R_1, R_2, \ldots, R_J$?

Regression Trees: Mathematically

- Theoretically, it is possible that regions in the feature space could have any shape; however, if the region splits were to not follow some specific pattern, it would be difficult to represent the resulting model by a decision tree.
  - For ease of interpretation, rectangular/box-like segments will allow us to construct a decision tree for our predictive model.

- The goal now becomes much simpler; find rectangular boxes $R_1, R_2, \ldots, R_J$ such that the RSS is minimized, given by:

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

  - We aim to minimize the squared differences of the response as compared to the mean response for the training observations within the j^{th} region.

Regression Trees: Mathematically

- While the goal itself seems straightforward, it is computationally infeasible to consider every possible segmentation of the feature space into J regions.
  - The minimization problem isn't as easily solvable as we have seen with other machine learning methods, especially as the number of regions increases.

- Tree-based methods provide an approximation by implementing both a top-down and a greedy approach called recursive binary splitting:
  - The method is top-down because the feature space is split into binary components in a successive fashion, creating new branches of the tree to potentially be split themselves.
  - The method is greedy because splits are made at each step of the process based on the best result possible at that given step.
    - The splits are not made based on what might eventually lead to a better segmentation in future steps.

Recursive Binary Splitting: Mathematically

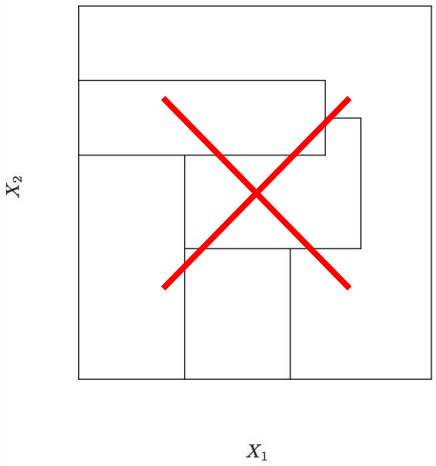
- The recursive binary splitting process depends on the greatest reduction in the RSS based on the predictor X_j and the cutpoint s that end up partitioning the space into the regions:
  - $R_1(j, s) = \{X \mid X_j < s\}$
  - $R_2(j, s) = \{X \mid X_j \geq s\}$

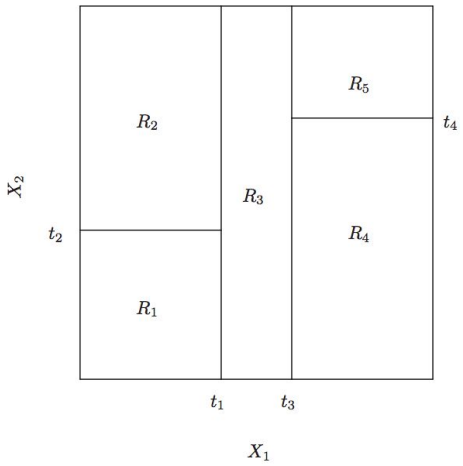
- In other words, the splitting process seeks the values of j and s that will end up minimizing the following:

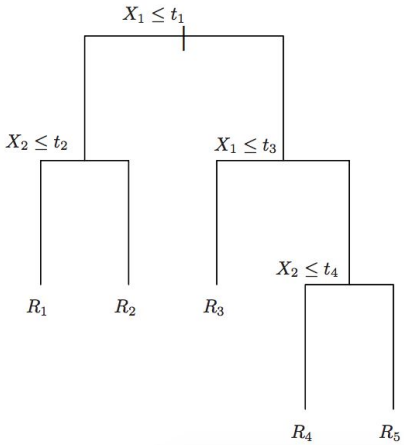
$$\sum_{i:x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

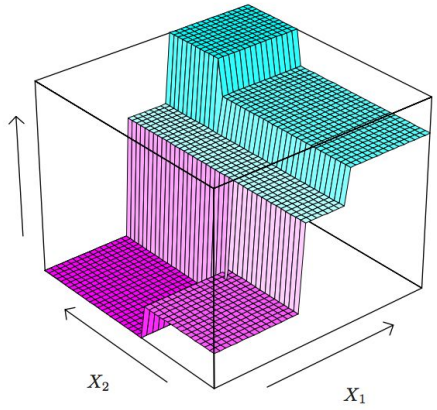
- This process is repeated by considering each of the newly created regions as the new overall feature spaces to segment.

Recursive Binary Splitting: Visually









Image

When do we Stop Splitting?

- The recursive binary splitting process as described above is likely to induce overfitting, thus leading to poor predictive performance on new observations.
  - Consider the extreme case in which each observation has its own terminal node (this model will have high variance). The RSS will be exactly 0 on the training set.

- What if we try fitting a tree with fewer regions? Theoretically, this should lead to lower variance with a cost of some bias, but ultimately lead to better prediction.
  - Grow the tree to a certain extent until the reduction in the RSS at a split doesn't surpass a certain threshold.
  - Problem: Although a split might not be incredibly valuable in reducing the RSS early on in a tree, it might lead to a future split that does reduce the RSS to a large extent. What is one possible solution?

Tree Pruning

- We've seen that deciding on the number of splits prior to building a tree isn't the best strategy.
  - What if we first built a tree that is very large and then pruned it back in order to obtain a suitable subtree?

- The best subtree will be the one that yields the lowest test error rate.
  - Given a subtree, we can estimate the test error by implementing the cross-validation process, but this is too cumbersome because the large number of possible subtrees. We still need a better process!

- In practice, rather than checking every single possible subtree, the process of cost complexity pruning (i.e., weakest link pruning) allows us to select a smaller set of subtrees for consideration.

Cost Complexity Tree Pruning

- Consider a sequence of trees indexed by a non-negative tuning parameter α. For each value of α there corresponds a subtree T such that the following is criterion minimized:

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

- Where:
  - $|T|$ indicates the total number of terminal nodes of subtree T.
  - R_m is the subset region of the feature space corresponding to the m^{th} terminal node.

Cost Complexity Tree Pruning

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

- The tuning parameter α helps balance the tradeoff between the overall complexity of the tree and its fit to the training data:
  - Small values of α yield trees that are quite extensive (have many terminal nodes).
  - Large values of α yield trees that are quite limited (have few terminal nodes).

- This process is very similar to the shrinkage/regularization method utilized in ridge and lasso regression!

Cost Complexity Tree Pruning

- It can be shown that as the value of the tuning parameter α increases, branches of the overall tree are pruned in a nested manner.
  - Thus, it is possible to obtain a sequence of subtrees as a function of α.

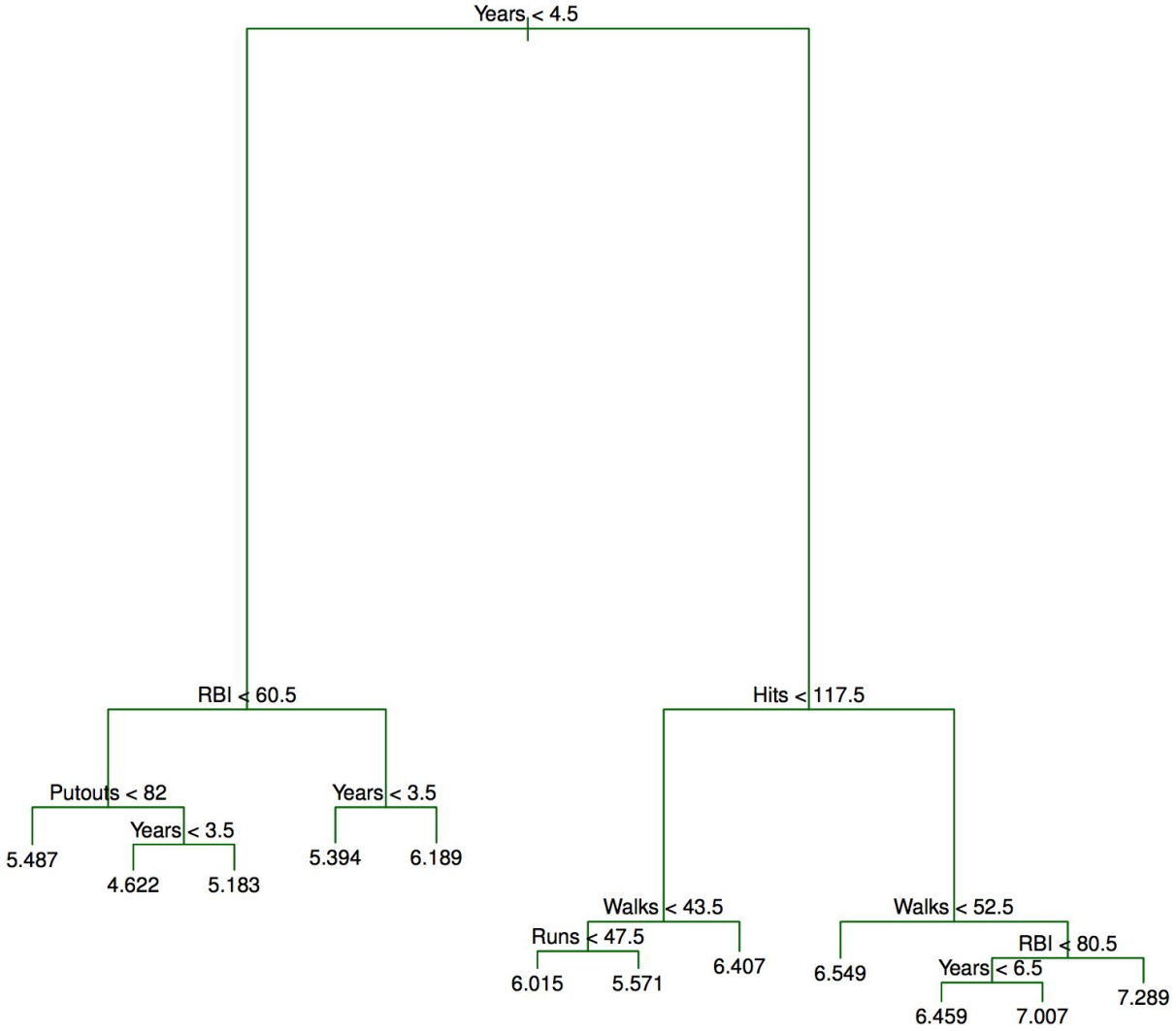
- As with any other tuning parameter, in order to select the optimal value of α we implement cross-validation.

- Ultimately, the subtree that is used for prediction is built using all of the available data with the determined optimal value of α.

Building a Regression Tree

- Incorporating these ideas, the algorithm for building a regression tree is as follows:
  1. Use recursive binary splitting to build a large tree on the training data; stop before each observation falls into its own leaf (e.g., when each terminal node has fewer than 5 observations, etc.).
  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 the best α.
     a. For each of the K folds:
        i. Repeat steps 1 and 2 on all but the k^{th} fold of the training data.
        ii. Evaluate the mean squared prediction error on the data in the left-out k^{th} fold as a function of α.
     b. Average the errors for each α; select the α that minimizes this criterion.
  4. Return the subtree of the overall tree from step 2 that corresponds to the best α.

Building a Regression Tree



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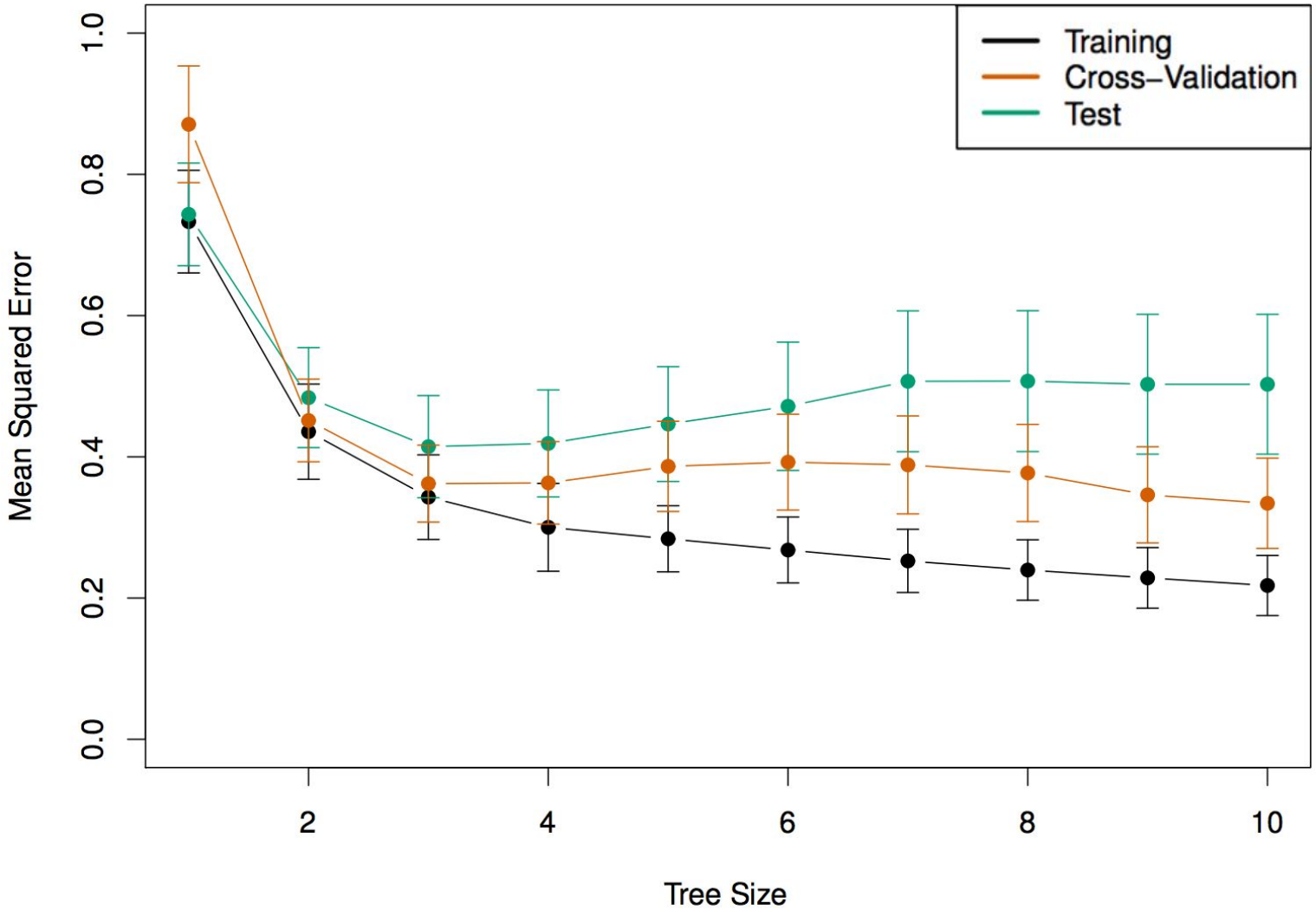

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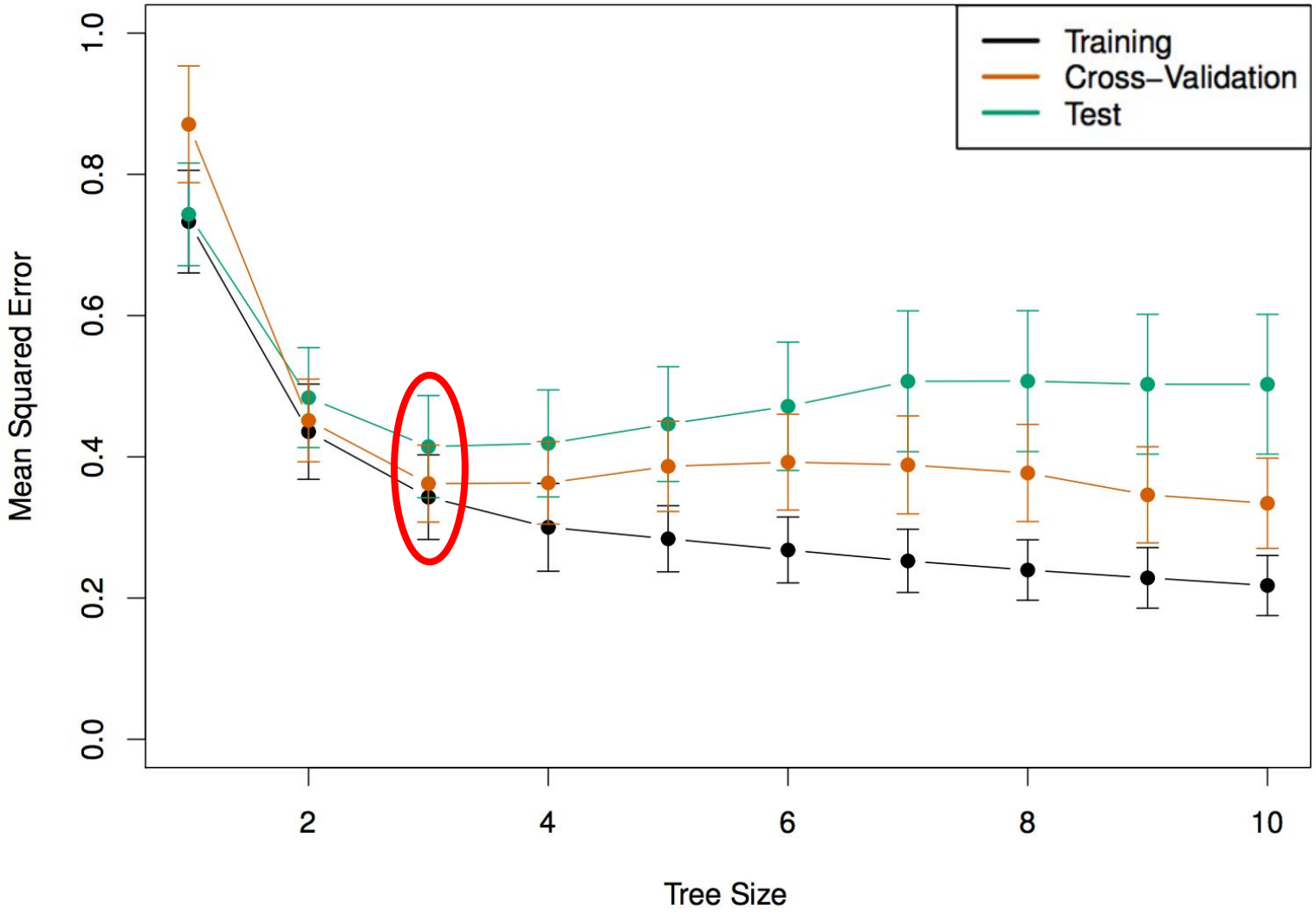
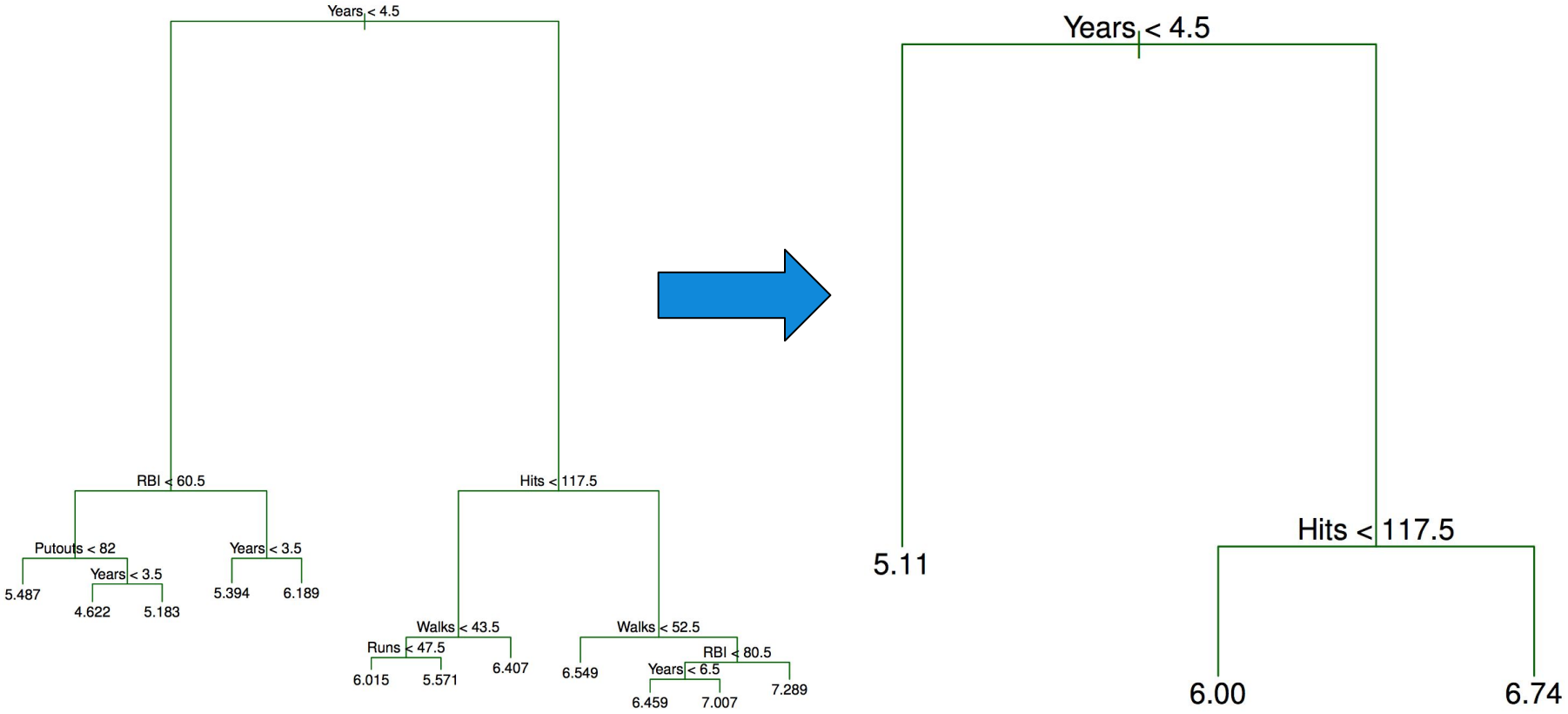


Building a Regression Tree



Classification Trees

- Classification trees are very similar to regression trees; they are the analogous output of the aforementioned process when we try to predict a qualitative (categorical) response rather than a quantitative (numerical) response.

- For each of the subregions created, we predict that an observation belongs to the most commonly occurring class of training observations in its associated region.

- In this setting, we still implement the process of recursive binary splitting to create various subregions of our feature space.
  - Unfortunately, the RSS no longer makes sense for the categorical setting. What criterion can we use instead?

Classification Trees: The Gini Index

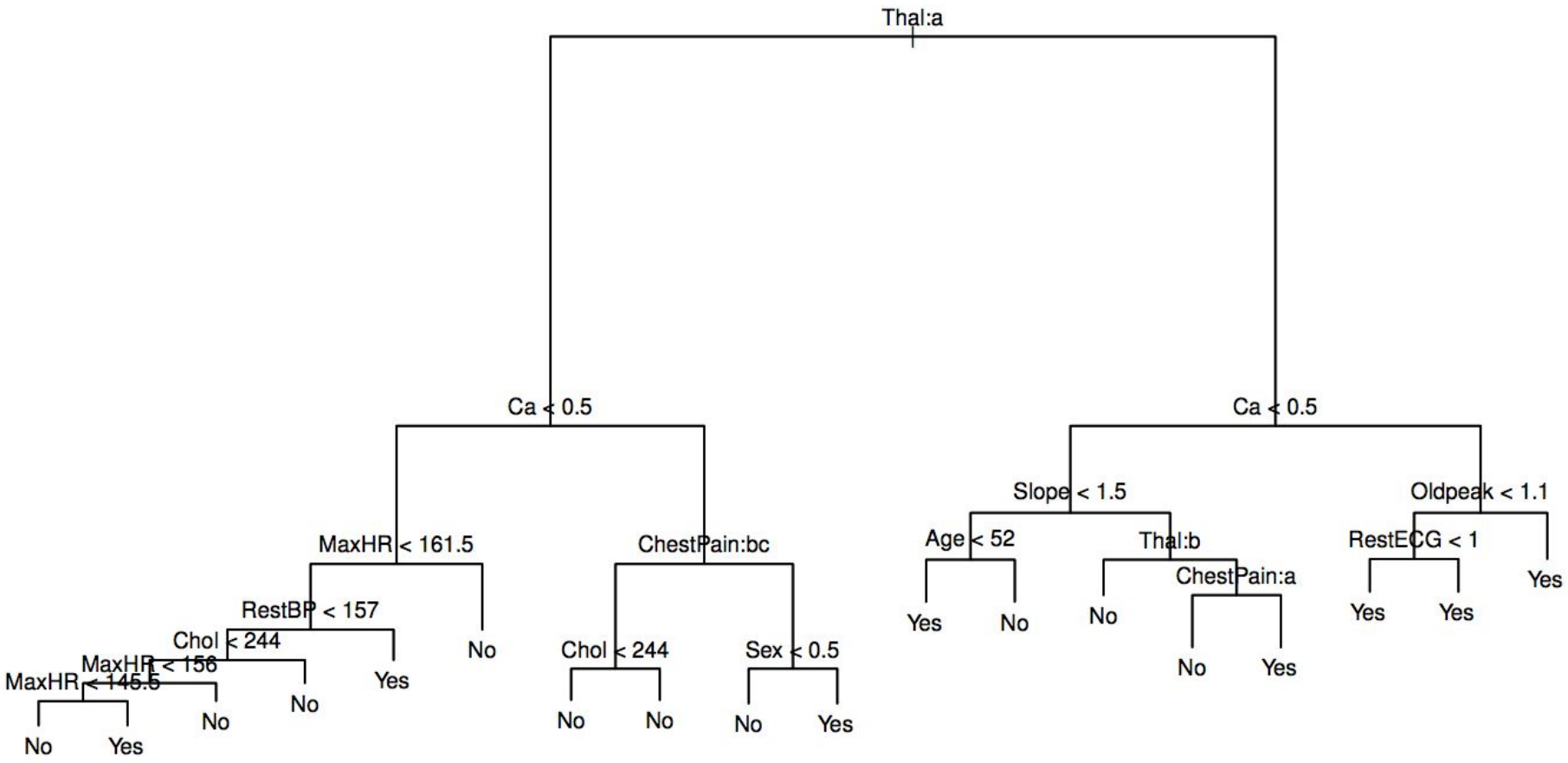
- A simple alternative is the misclassification rate (i.e., the fraction of training observations in a region that do not belong to the most common class).
  - It turns out that the misclassification rate can end up not being sufficiently sensitive; it's too choppy doesn't lead to a smooth tree building process.

- The typical criterion used instead is called the Gini index, defined as:

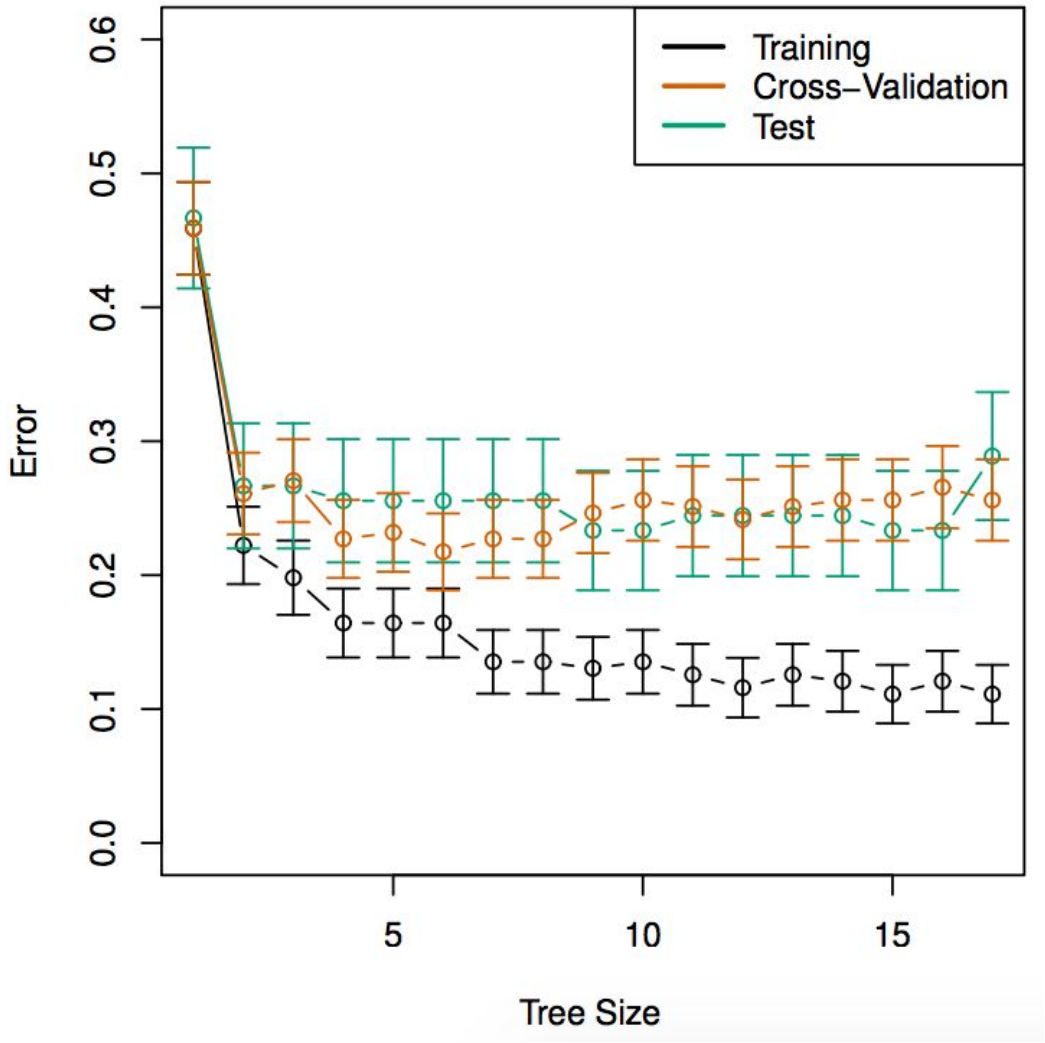
$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

  - Here, the proportions of interest denote the fraction of training observations in the m^{th} region that are from the k^{th} class.
  - The index measures the total variance among the K classes; it is often referenced as a measure of terminal node purity.

Classification Trees



Classification Trees



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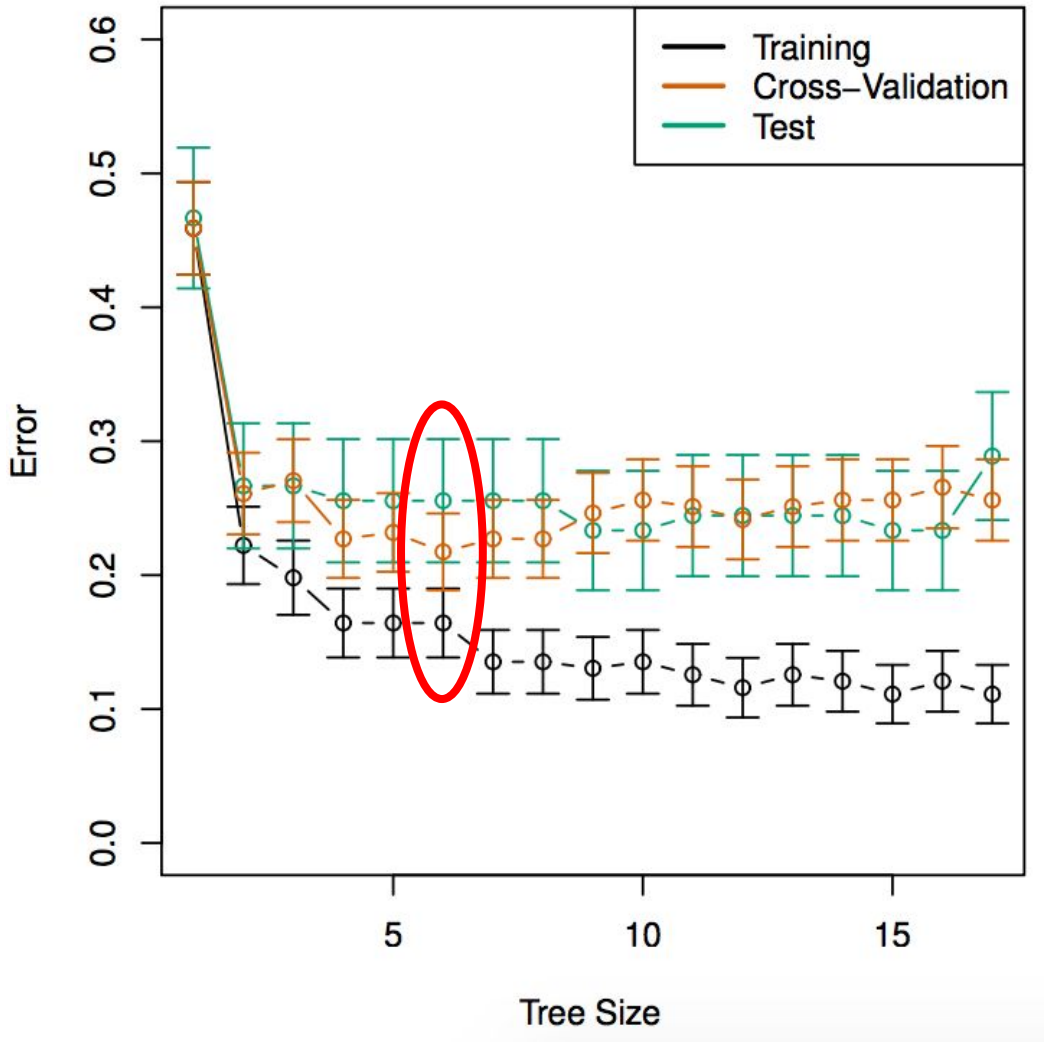

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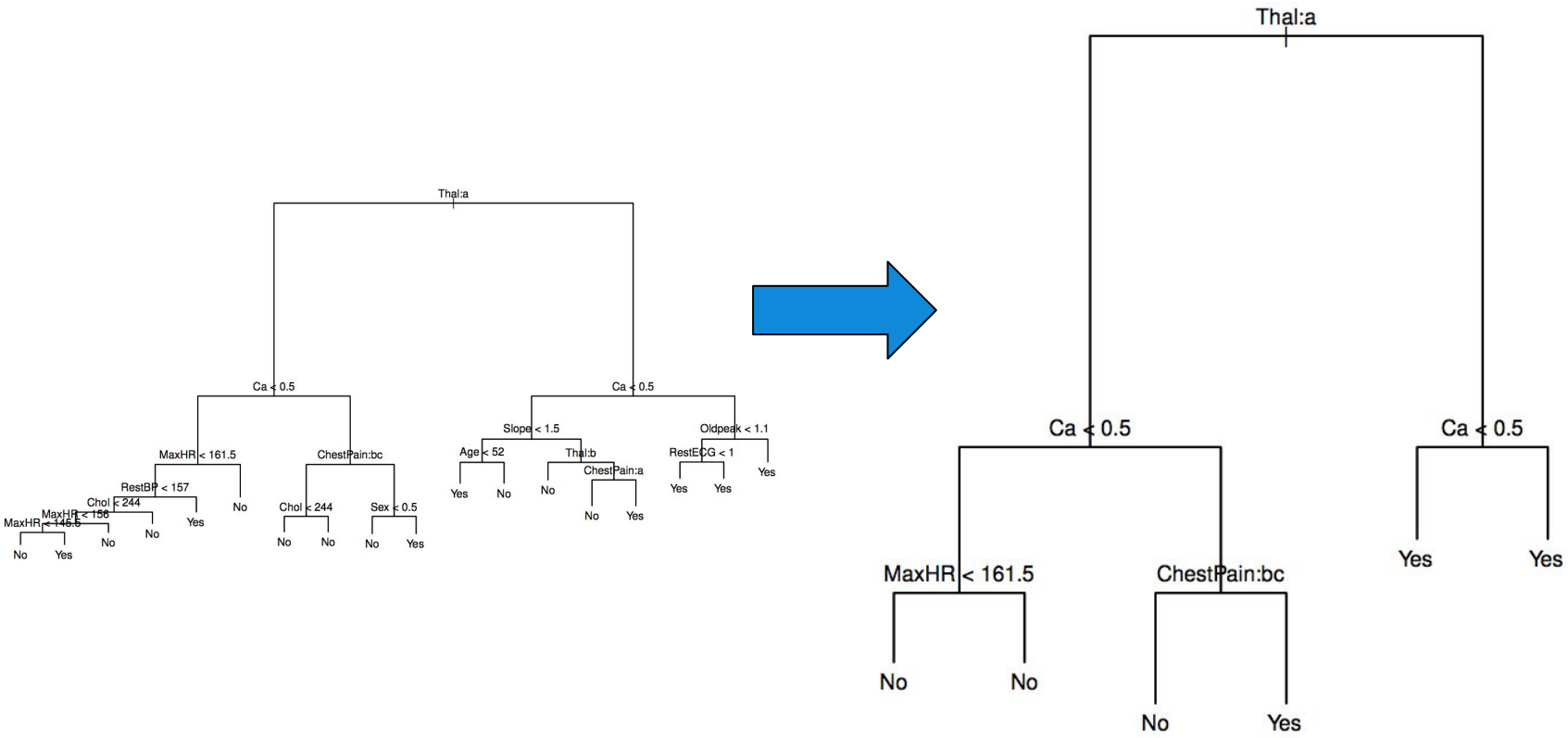
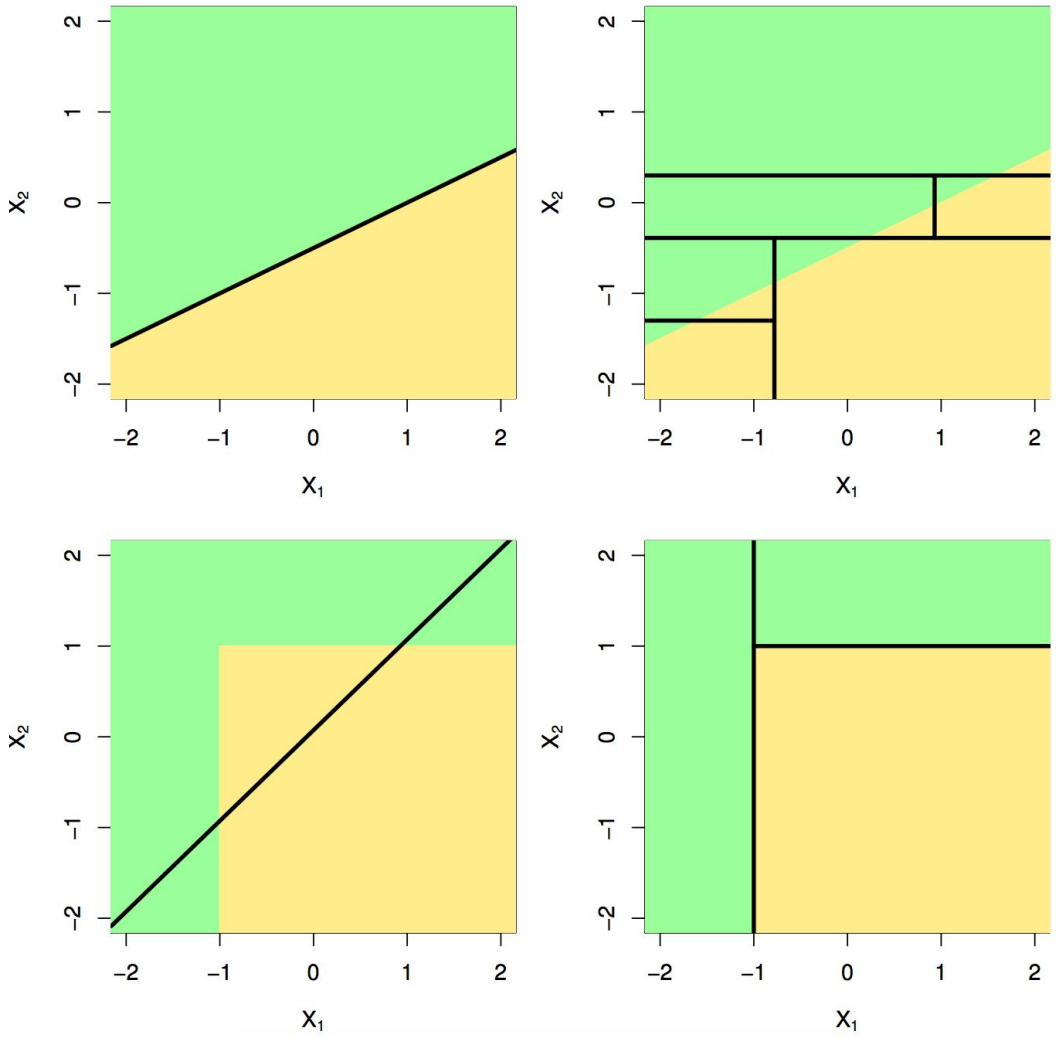


Classification Trees

- It is interesting to note that some splits yield terminal nodes that have the same predicted value.
  - Why was this split performed at all in the first place?

- Such duplicate splits are recorded by the classification tree because they lead to increased node purity.
  - Having an increased sense of node purity yields an increased sense of certainty pertaining to the response value corresponding to each terminal node.

Advantages & Disadvantages of Decision Trees



Advantages & Disadvantages of Decision Trees

- Without a heavy mathematical background, it is easy to interpret a decision tree (especially if it is small); linear regression requires the understanding of an equation.
- Decision trees can graphically depict a higher dimensionality easier than linear regression and still be interpreted by a novice.
- The process can easily adapt to qualitative predictors without the need to create and interpret dummy variables.
- Decision trees are often believed to reflect a more "human" decision-making process as compared to other machine learning methods.

Advantages & Disadvantages of Decision Trees

- While relatively non-complex among other supervised learning procedures, as a trade-off their predictive accuracy tends to be lower and thus not as competitive.

- What if we could combine the benefits of multiple trees in order to yield an overall prediction? Taking the penalty of decreased interpretative value, could this potentially increase our predictive accuracy?
  - Bagging
  - Random Forests
  - Boosting

PART 2

Bagging

Variance & Bootstrap Aggregation

- One of the biggest drawbacks of decision trees is that they suffer from high variance:
  - If we randomly split our data into two different parts and fit independent decision trees, the results are likely to be quite different.

- **B**ootstrap **agg**regation (i.e., bagging) is a procedure that aids in the reduction of variance for a statistical learning method; it is frequently used alongside trees.
  - Recall that given a set of n independent observations $X_1, X_2, \ldots, X_n$, each themselves drawn from a distribution with variance σ^2, the mean of these observations as a group would be given by σ^2/n.
  - Averaging the set of observations reduces the overall variance.

- Why is this not practical in the general sense? We typically do not have access to multiple training sets.

Bagging by Bootstrapping

- What if we could create multiple pseudo-training sets? We can do so by bootstrapping:
  - Take repeated samples of the same size from the single overall training dataset. Treat these different sets of data as pseudo-training sets.

- By bootstrapping, we create B different training datasets. The method is trained on the b^{th} bootstrapped training set in order to get predictions for each observation. We can then average all predictions (or take the majority vote) to obtain the bagged estimate:

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

- Why is this a clever idea for trees?

Bagging by Bootstrapping

- Recall that previously we tried to reduce variance by the process of pruning our large trees.
  - While pruning reduces the variance of the overall tree model upon repeated builds with different datasets, we induce bias because the trees are much simpler.

- The idea of bagging averts the pruning methodology but still gets its benefits:
  - Instead of pruning back our trees, create very large trees in the first place. These large trees will tend to have low bias, but high variance.
  - Retain the low bias, but get rid of the high variance by averaging across many trees.

Out of Bag Error Estimation

- How do we estimate the test error of a bagged model?

- Recall that in the bagging process, decision trees are fit to bootstrapped subsets of the overall available observations.
  - Observations that are used to fit the tree are said to be "in the bag."
  - Observations that are not used to fit the tree are said to be "out of bag."

- We can first predict the response for a given observation using each of the trees in which that observation was out of bag, and then average the results.
  - The averaged predictions are used to calculate the out of bag error estimate.
  - When the number of bootstrapped samples is large, this is essentially the same as leave-one-out cross-validation error for bagging.

PART 3

Random Forests

Benefits of Random Forests

- It can be shown that the variance of the mean of a sample increases as observations are correlated with one another.
  - In other words, correlated observations are not as effective at reducing the uncertainty of the mean as uncorrelated, independent observations.

- If we could generate trees that are not correlated with one another, we could improve upon the bagging procedure.

- Random forests help us by decorrelating our trees.
  - As expected, this results in a reduction in variance once we average the trees.

The Random Forest Procedure

- Similar to bagging, we first build various decision trees on bootstrapped training samples, but we split internal nodes in a special way.

- Each time a split is considered within the construction of a decision tree, only a random subset of m of the overall p predictors are allowed to be candidates.
  - In other words, only the m predictors have the possibility to be chosen as the splitting factor.

- At every split, a new subset of predictors is randomly selected.
  - Typically, $m \approx \sqrt{p}$ is a sufficient rule for subset selection.
  - What happens if we choose $m = p$?

The Random Forest Procedure

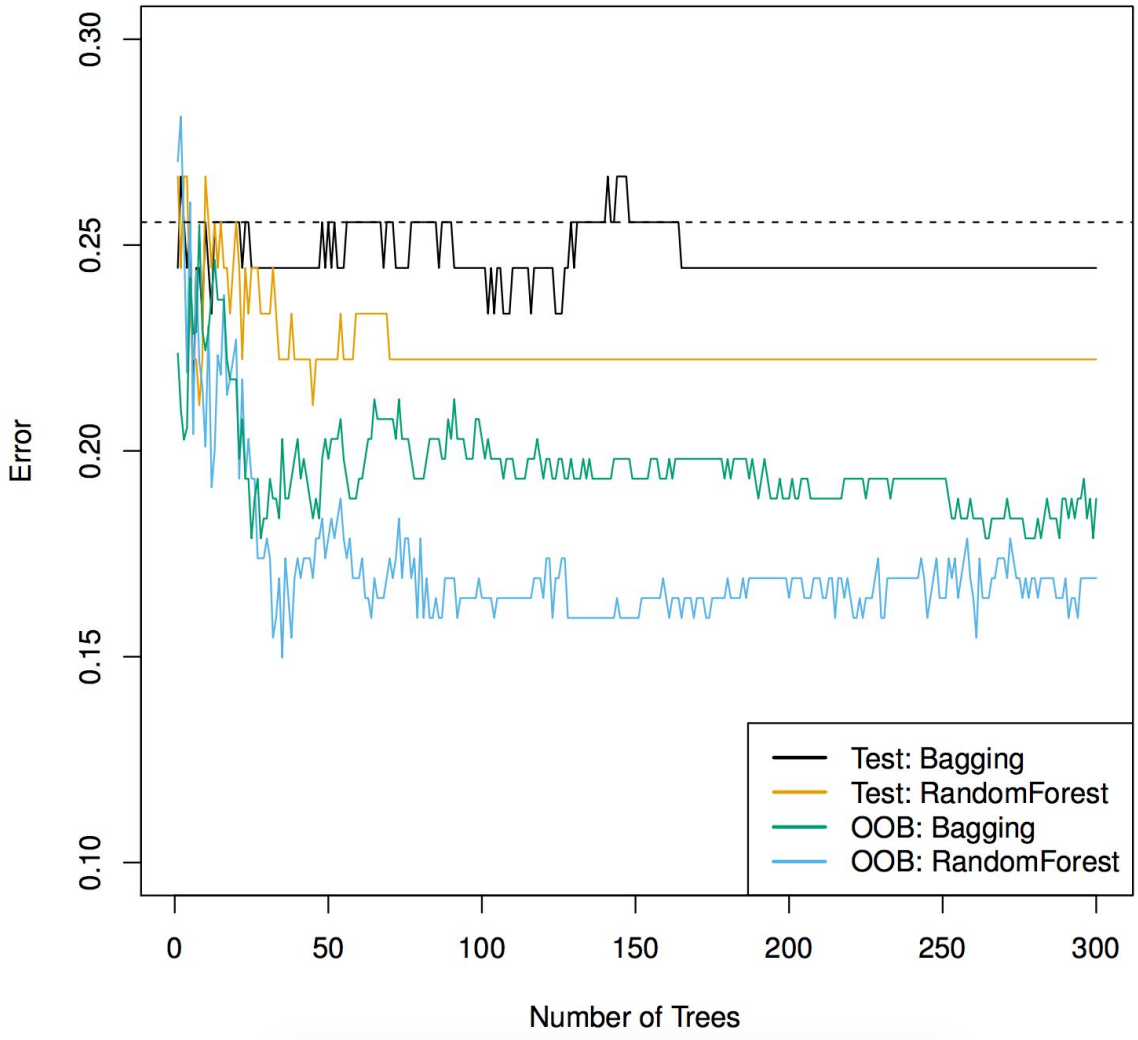
- Although it seems crazy to throw away most predictor variables at each of the splits, why does this end up helping in the long run?
  - The random forest procedure forces the decision tree building process to use different predictors to split at different times.

- Should a good predictor be left out of consideration for some splits, it still has many chances to be considered in the construction of other splits.
  - The same idea goes for predictors surfacing in trees as a whole.

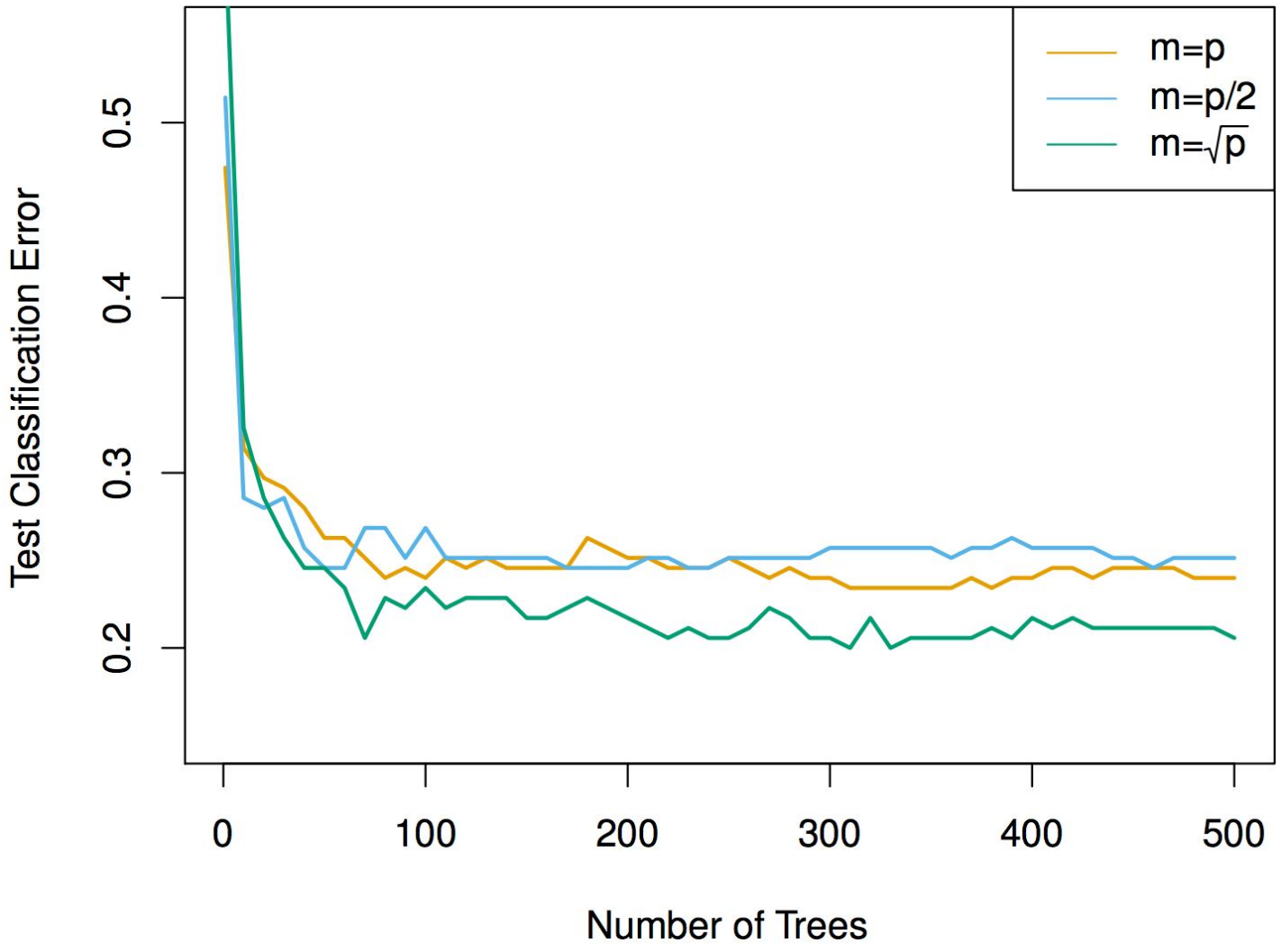
- Even if we used the same training sample, using the random forest procedure would likely yield different trees.

- We can't overfit by adding more trees! The variance just ends up decreasing!

Bagging & Random Forests



Bagging & Random Forests



PART 4

Boosting

Boosting Decision Trees

- Recall that the bagging procedure involves:
  - Creating multiple pseudo-training data sets using bootstrapped sampling.
  - Fitting separate, independent decision trees to each of the bootstrapped training data sets.
  - Combining all of the separate trees by averaging in order to create a single predictive model.

- The boosting procedure works in a similar way, except that the decision trees are generated in a sequential manner:
  - Each tree is generated using information from previously grown trees; the addition of a new tree improves upon the performance of the previous trees.
  - The trees are now dependent upon one another.

The Boosting Algorithm

- The boosting algorithm is as follows:
  1. For each i in the training data, set: $\hat{f}(x) = 0, r_i = y_i$
  2. For b = 1, 2, ... , B:
     a. Fit a tree with d splits (d + 1 terminal nodes) to the training data (X, r).
     b. Update f by adding in a shrunken version of the new tree:

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

     c. Update the residuals:

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

  3. Output the boosted model:

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

Details of Boosting

- Whereas creating a single large decision tree can amount to severe overfitting to our training data, the boosting approach tends to slowly learn our data.

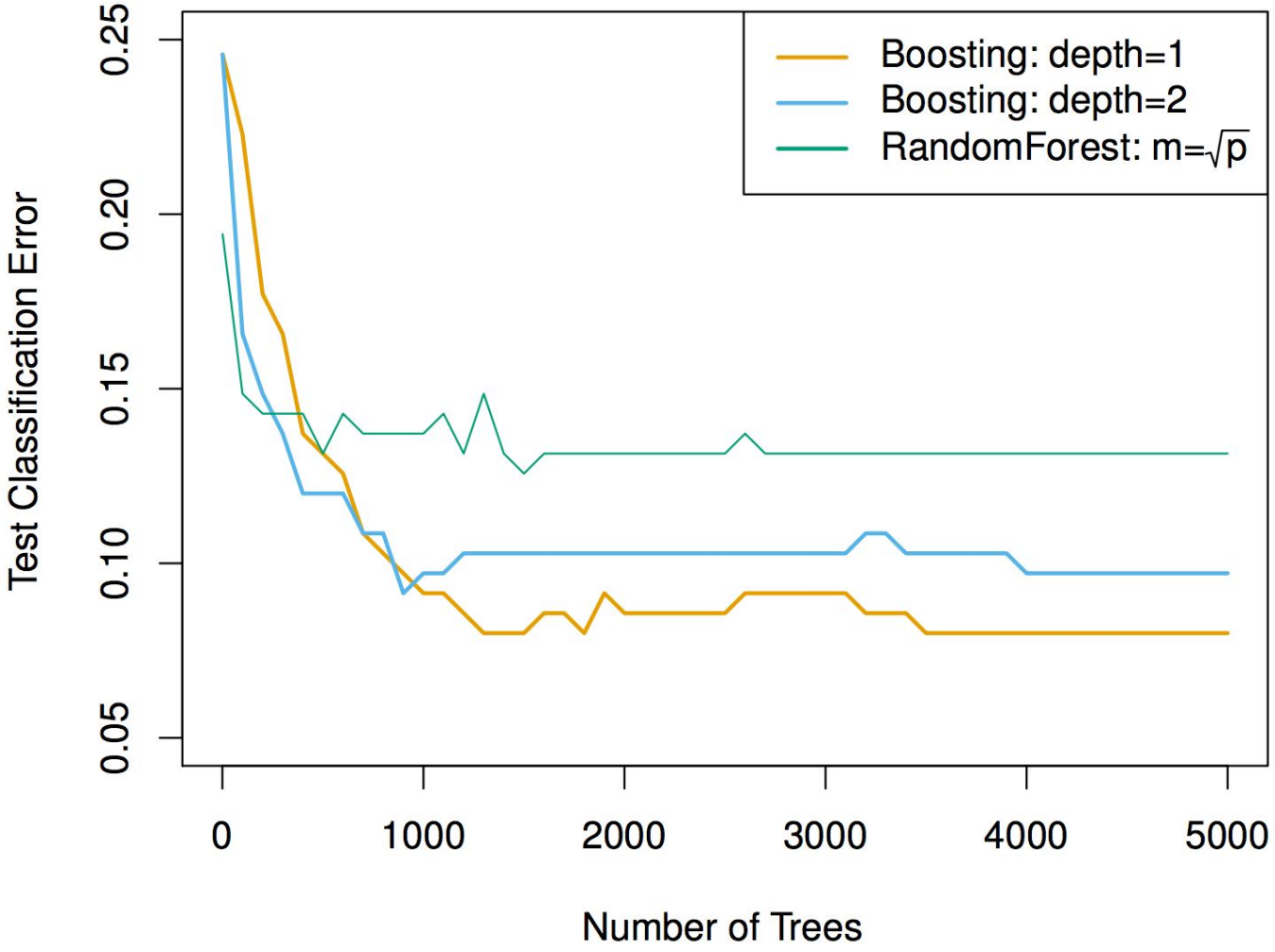
- Given a current decision tree model, we fit a new decision tree to the residuals of the current decision tree.
  - The new decision tree (based on the residuals) is then added to the current decision tree, and the residuals are updated.

- We limit the number of terminal nodes in order to sequentially fit small trees.
  - By fitting small trees to the residuals, we slowly improve the overall model in areas where it does not perform well.
  - The shrinkage parameter λ is taken to be quite small, and slows the process down even further to avoid overfitting.

Tuning Parameters for Boosting

- Boosting requires three tuning parameters:
  1. The number of trees B.
     a. Unlike in bagging and random forests, boosting can overfit if B is large (although very slowly). Use cross-validation to select B.
  2. The shrinkage parameter λ, a small positive number.
     a. This controls the rate at which boosting learns. Typical values are around 0.01 to 0.001. Note that a very small λ may require using a large value of B.
  3. The number of splits d in each tree.
     a. This controls the complexity of the boosted ensemble. Typically using stumps (single splits where $d = 1$) is sufficient and results in an additive model. The tree depth corresponds to the interaction order of the boosted model since d splits can involve (at most) d distinct variables.

Boosting & Random Forests



PART 5

Variable Importance

Variable Importance

- For bagged and random forest trees, we can record the total amount that a given criterion is decreased over all splits relevant to a given predictor, averaged over all B trees.
  - For regression trees, we can use the reduction in the RSS.
  - For classification trees, we can use the reduction in the Gini index.

- In both the regression and classification setting, we can do this for each predictor of our original dataset.
  - A relatively large value indicates a notable drop in the RSS or Gini index, and thus a better fit to the data; corresponding variables are relatively important predictors.

- This allows us to gain a qualitative understanding of the variables in our dataset.

PART 5

Review

Review

- Part 1: Decision Trees
  - What are Tree Based Methods?
  - Regression Trees: Visually
  - How to Interpret a Decision Tree
  - Regression Trees: Mathematically
  - Recursive Binary Splitting
    - Mathematically
    - Visually
  - When do we Stop Splitting?
  - Tree Pruning
  - Cost Complexity Tree Pruning
  - Building a Regression Tree
  - Classification Trees
    - The Gini Index
  - Advantages & Disadvantages of Decision Trees
- Part 2: Bagging
  - Variance & Bootstrap Aggregation
  - Bagging by Bootstrapping
  - Out of Bag Error Estimation
- Part 3: Random Forests
  - Benefits of Random Forests
  - The Random Forest Procedure
  - Bagging & Random Forests
- Part 4: Boosting
  - Boosting Decision Trees
  - The Boosting Algorithm
  - Details of Boosting
  - Tuning Parameters for Boosting
  - Boosting & Random Forests
- Part 5: Variable Importance