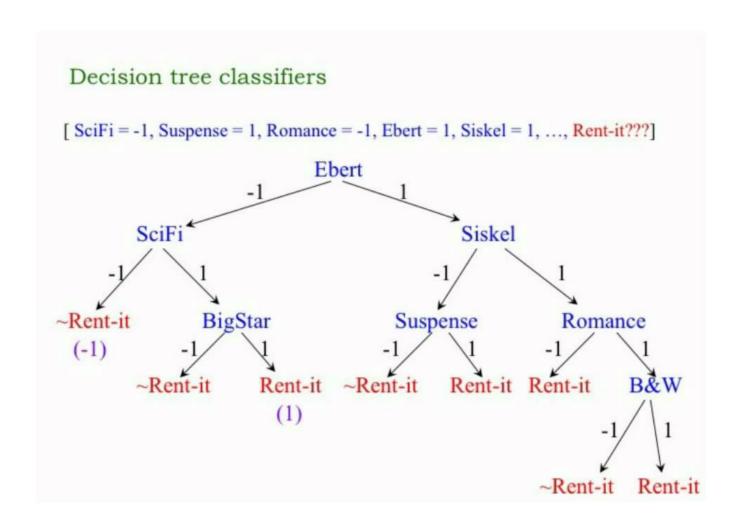
Introduction to Statistical Learning

INF 552, Machine Learning for Data Informatics

University of Southern California

M. R. Rajati, PhD

Tree-Based Methods



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 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.

Pros and Cons

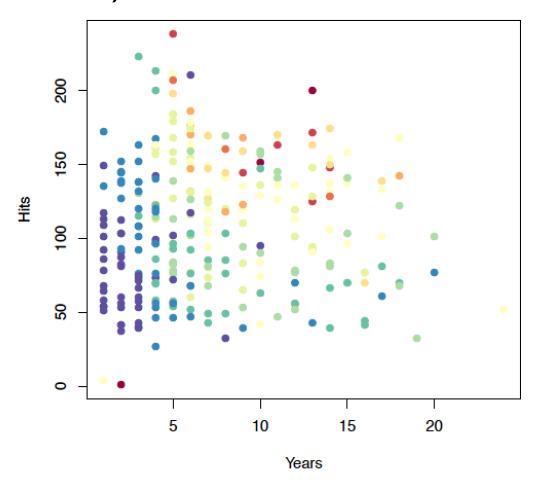
- Hence we also discuss bagging, random forests, and boosting. These methods grow multiple trees which are then combined to yield a single consensus prediction.
- Combining a large number of trees can often result in dramatic improvements in prediction accuracy, at the expense of some loss of interpretation.

The Basics of Decision Trees

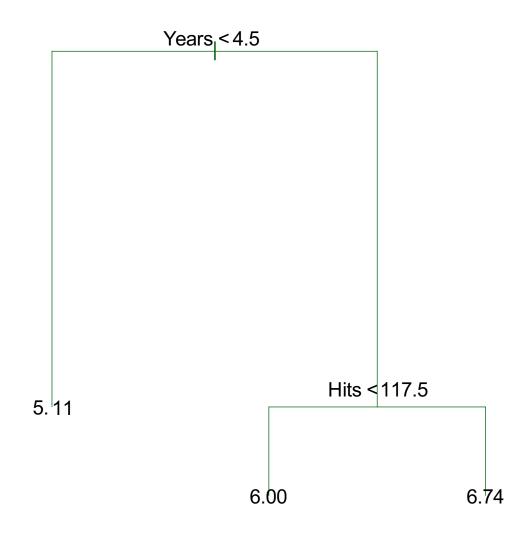
- Decision trees can be applied to both regression and classification problems.
- We first consider regression problems, and then move on to classification.

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



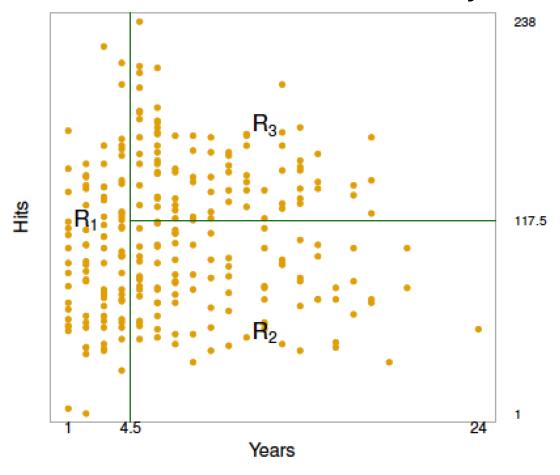
 For the Hitters data, a regression tree for predicting the log salary of a baseball player, based on the number of years that he has played in the major leagues and the number of hits that he made in the previous year.

 At a given internal node, the label (of the form $X_i < t_k$) indicates the left-hand branch emanating from that split, and the right-hand branch corresponds to X_i $\geq t_k$. 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: R₁ ={X | Years < 4.5}, R₂ ={X | Years ≥ 4.5, Hits < 117.5}, and R₃ ={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.

Terminology for Trees

- 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.

Interpretation of Results

 For players with an experience of 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.

Interpretation of Results

 Surely an over-simplification, but compared to a regression model, it is easy to display, interpret and explain

- 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 .

 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.

- Unfortunately, it is computationally infeasible to consider every possible partition of the feature space into J boxes.
- For this reason, we take a topdown, 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

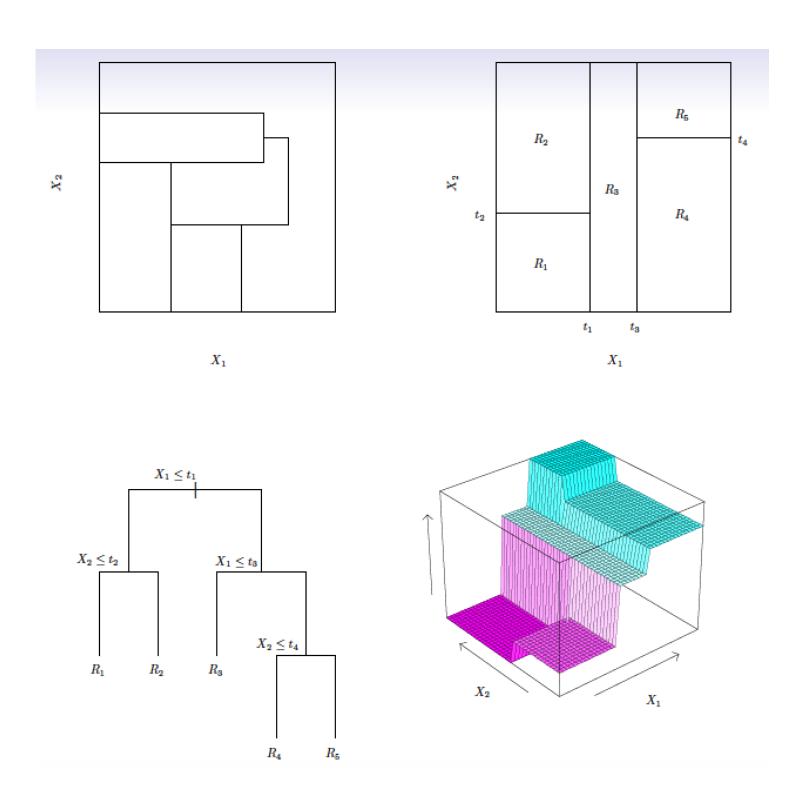
- We first select the predictor X_j and the cutpoint s such that splitting the predictor space into the regions $\{X|X_j < s\}$ and $\{X|X_j \ge s\}$ leads to the greatest possible reduction in RSS.
- Next, we repeat the process, looking for the best predictor and best cutpoint in order to split the data further so as to minimize the RSS within each of the resulting regions.

Details— Continued

- 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 in the next slide.



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.

Pruning a tree

 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.

Pruning a tree

 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.

Pruning a tree— continued

- A better strategy is to grow a very large tree T₀, 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

Pruning a tree— continued

• We consider a sequence of trees indexed by a nonnegative tuning parameter α . For each value of α there corresponds a subtree $T \subseteq T_0$ such that

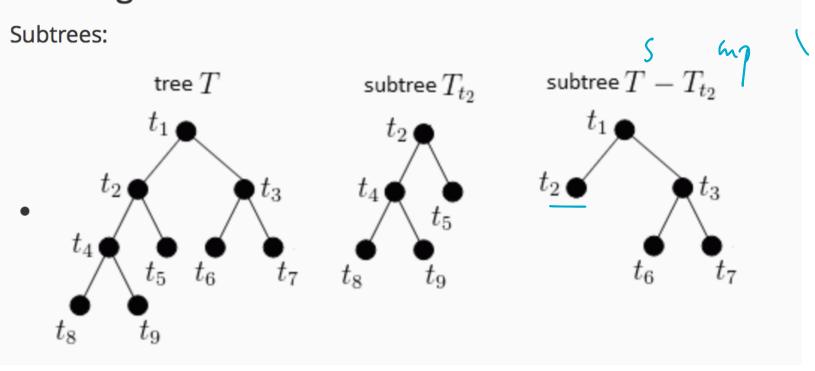
$$\sum_{m=1}^{|T|} \sum_{i: x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T| \qquad \emptyset$$

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}_{Rm} is the mean of the training observations in R_m .

Pruning a tree— continued

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

Pruning Subtrees



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 .

Summary: tree algorithm

3. Use K-fold cross-validation to choose α . For each

$$k = 1, ..., K$$
:

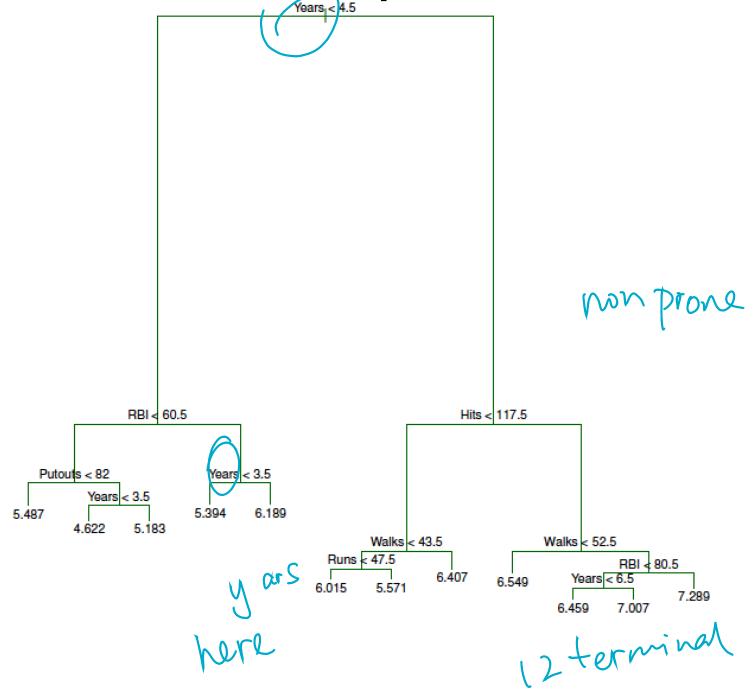
- 3.1Repeat Steps 1 and 2 on the $\frac{K-1}{K}$ th fraction of the training data, excluding the kth fold.
- 3.2Evaluate the mean squared prediction error on the data in the left-out *k*th fold, as a function of *α*.

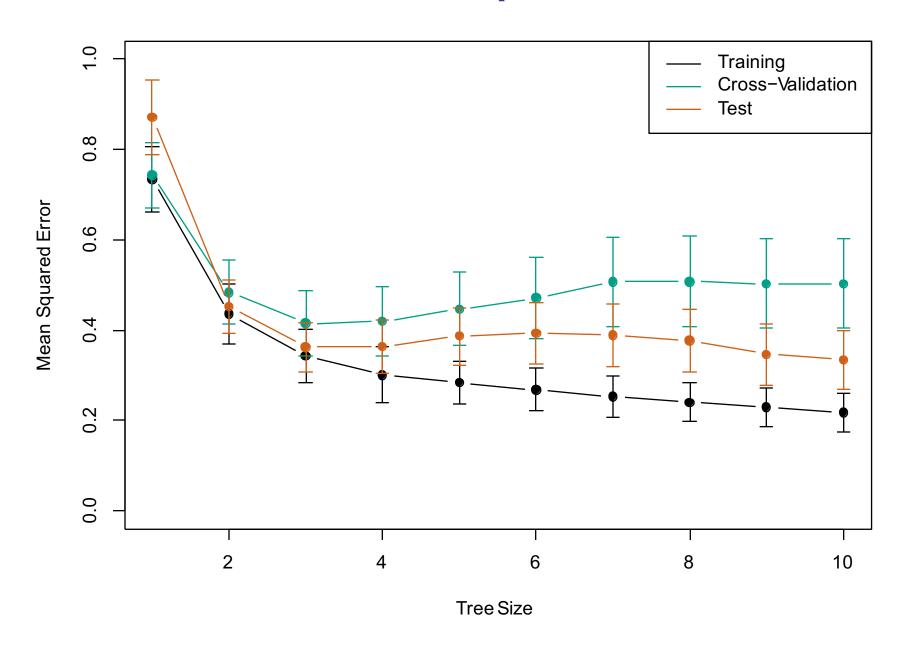
Average the results, and pick α to minimize the average error.

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

• First, we randomly divided the data set in half, yielding 132 observations in the training set and 131 observations in the test set.

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





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.

 Lecision trees are suitable for catogorical

 predictors can easily used for multiclass

 problems

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

Details of classification trees

 A natural alternative to RSS is the classification error rate, which is simply the fraction of the training observations in that region that do not belong to the most common class:

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

Example

A simple example:

egr

Details of classification trees

- Here 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 treegrowing, 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 p^*_{mk} 's are close to zero or one.

Gini index and Deviance

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

- 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 Tree Algorithm in this case is called ID3

Gini index and Deviance

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

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

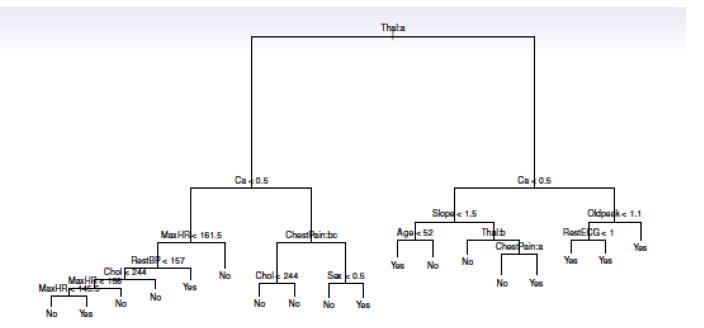
- The tree algorithm in this case is called C4.5
- It turns out that the Gini index and the cross-entropy are very similar numerically.

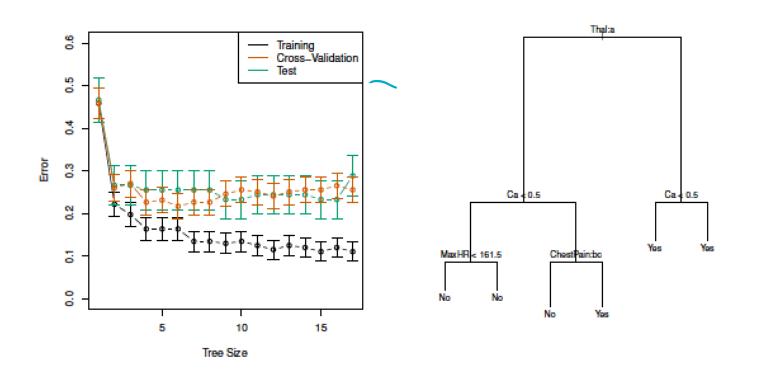
Example: heart data

- 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.

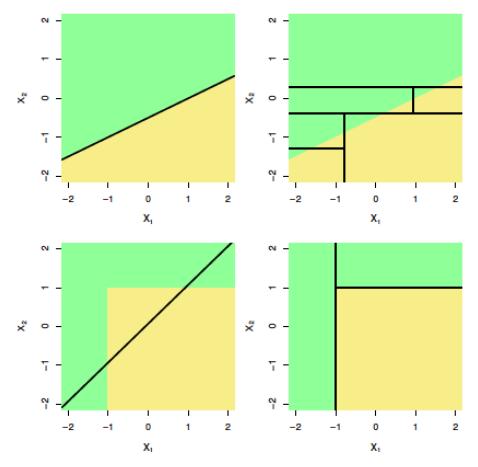
Example: heart data

- 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.





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.

Advantages and Disadvantages of Trees

- 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.

Advantages and Disadvantages of Trees

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

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

Bagging

aggregation of weak (earners

 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.

Bagging

- Recall that given a set of n independent observations Z_1, \ldots, Z_n , each with variance σ^2 , the variance of the mean 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 *b*th bootstrapped training set in order to get *f****b*(*x*), the prediction at a point *x*. We then average all the predictions to obtain

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

This is called *bagging*.

Bagging classification trees

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

Out-of-Bag Error Estimation

- 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 twothirds of the observations.

Out-of-Bag Error Estimation

 The remaining one-third of the observations not used to fit a given bagged tree are called the *out-of-bag* (OOB) observations.

Out-of-Bag Error Estimation

- 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 LOO cross-validation error for bagging, if B is large.

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.

Random Forests

 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

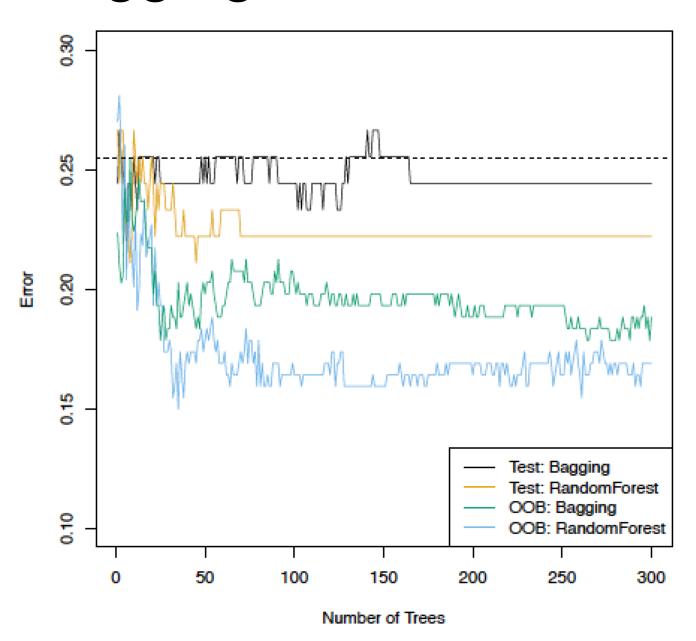
use only one of those m predictors.

equivalently, for each tree, we only allow a set of an predictors

Random Forests

 A fresh selection of m predictors is taken at each split, and typically we choose $m \approx p_{\text{predictors}}^{1/2}$ —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).

Bagging the heart data



Details of previous figure

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 used.
- Random forests were applied with $m = p^{1/2}$.
- 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

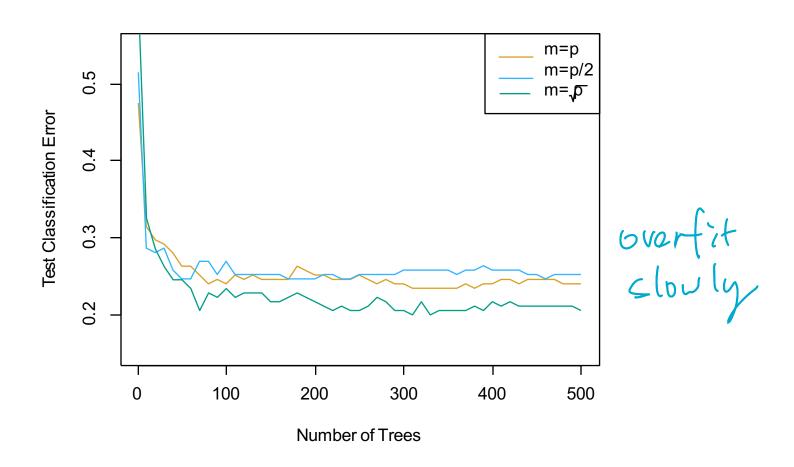
 We applied random forests to a high-dimensional biological data set consisting of expression measurements of 4,718 genes measured on tissue samples from 349 patients.

 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.

Details of previous figure

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.

Boosting

 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.

Boosting

- 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, ..., B, repeat:
 - 1. Fit a tree \hat{f}^b with d splits (d+1 terminal nodes) to the training data (X, r).
 - 2. Update f by adding in a shrunken version of the new tree:

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

3. Update the residuals,

$$r_i \leftarrow r_i - \lambda f^b(x_i)$$
.

Boosting algorithm for regression trees

Output the boosted model,

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

 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.

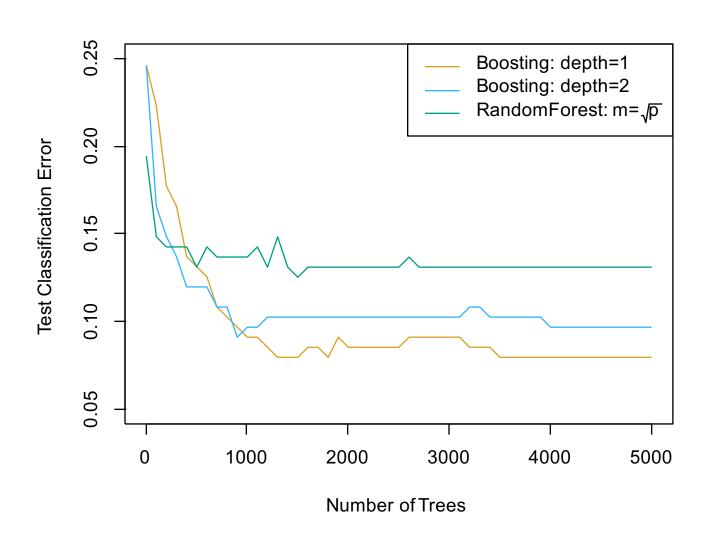
 Each of these trees can be rather small, with just a few terminal nodes, determined by the parameter d in the algorithm.

• By fitting small trees to the residuals, we slowly improve *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, nor do we in the text book.
- More details in Elements of Statistical Learning, chapter 10 or Appendix.
- 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*.

Details of previous figure

- 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

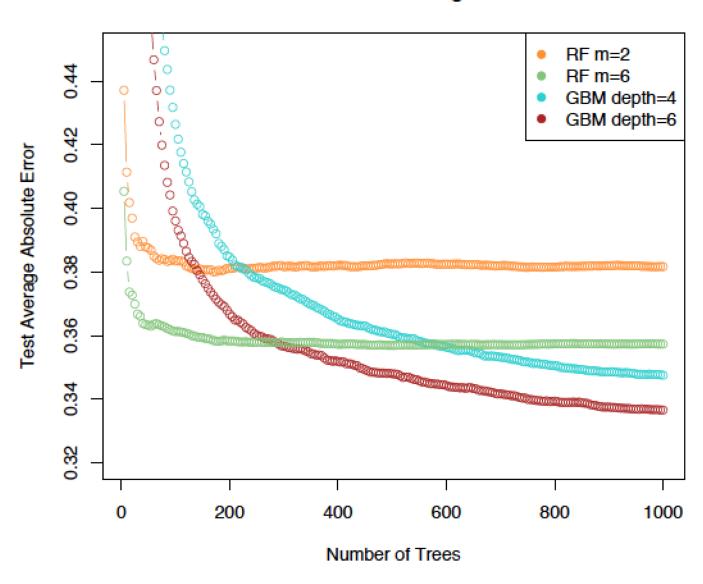
- 1. The *number of trees B*. Unlike bagging and random forests, boosting can overfit if *B* is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select *B*.
- 2. The *shrinkage parameter* λ , a small positive number. This controls the rate at which boosting 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.

Tuning parameters for boosting

3. The *number of splits d* in each tree, which controls the complexity of the boosted ensemble. Often d = 1works 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.

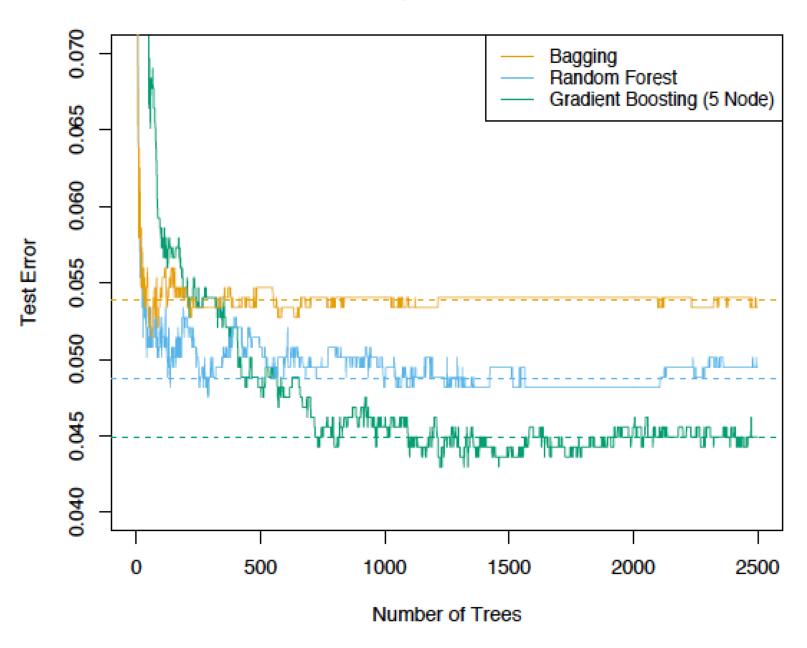
Another regression example

California Housing Data



Another classification example

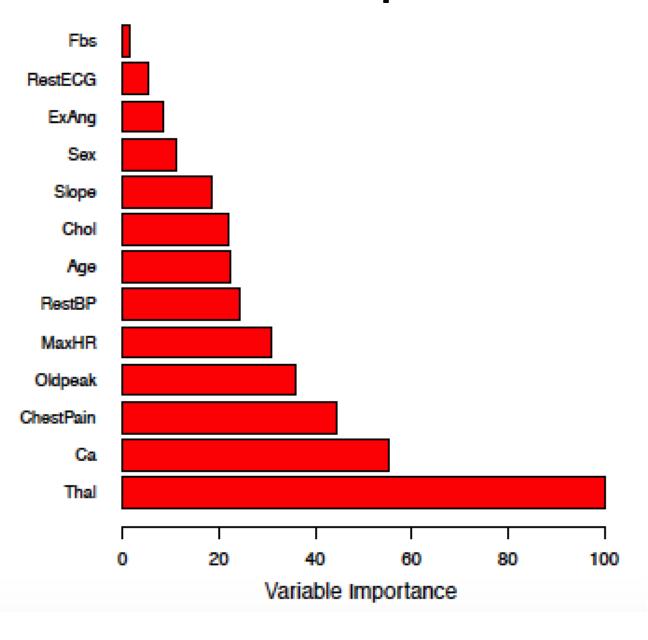
Spam Data



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 measure



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

Summary

- 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-theart methods for supervised learning.
 However their results can be difficult to interpret.

Boosting (Appendix) Boosting for Classification Boosting iteratively learns weak classifiers; a weak classifier is one whose error rate is only slightly better than random guessing.

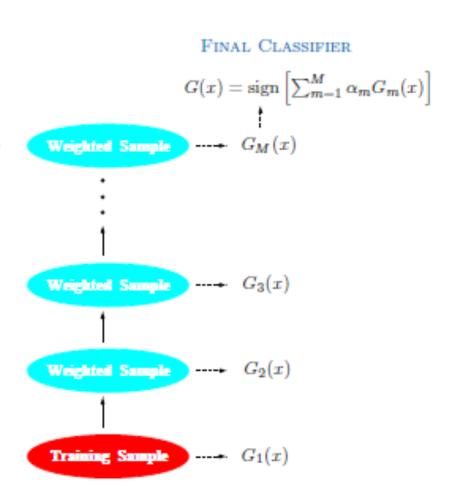
Boosting (Appendix) Boosting for Classification

The purpose of boosting is to sequentially apply the weak classification algorithm to repeatedly modified versions of the data, thereby producing a sequence of weak classifiers.

The predictions from all of them are then combined through a weighted majority vote to produce the final prediction.

Boosting for Classification (cont'd)

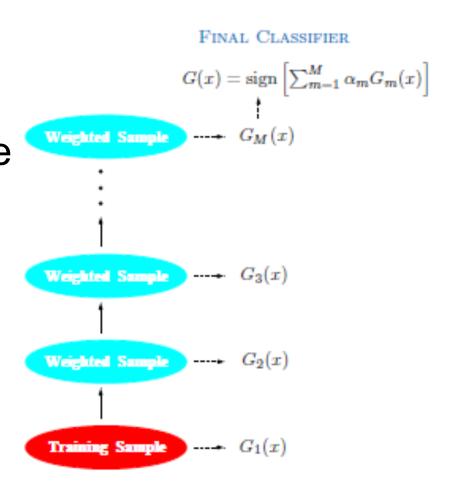
Thus, the final result is the weighted sum of the results of weak classifiers.



Boosting for Classification (cont'd)

The alphas in the final classifie are computed by the boosting algorithm, which weight the contribution to give higher influence to more accurate classifiers in the sequence.

Weights are modified at each boosting step!



Up-weight data that are difficult; incorrectly classified in the previous round. **Down-weight data** that are easy; correctly classified in the previous round.

Here are some commonly used loss functions, gradients, population minimizers, and algorithms to minimize the loss:

Name	Loss	Derivative	f^*	Algorithm
Squared error	$\frac{1}{2}(y_i - f(\mathbf{x}_i))^2$	$y_i - f(\mathbf{x}_i)$	$\mathbb{E}\left[y \mathbf{x}_i\right]$	L2Boosting
Absolute error	$ y_i - f(\mathbf{x}_i) $	$\operatorname{sgn}(y_i - f(\mathbf{x}_i))$	$median(y \mathbf{x}_i)$	Gradient boosting
Exponential loss	$\exp(-\tilde{y}_i f(\mathbf{x}_i))$	$-\tilde{y}_i \exp(-\tilde{y}_i f(\mathbf{x}_i))$	$\frac{1}{2}\log\frac{\pi_i}{1-\pi_i}$	AdaBoost
Logloss	$\log(1 + e^{-\tilde{y}_i f_i})$	$y_i - \pi_i$	$\frac{1}{2}\log\frac{\pi_i}{1-\pi_i}$	LogitBoost

Boosting (cont.) There are many different boosting algorithms for classification:

AdaBoost, LPBoost, BrownBoost, LogitBoost, Gradient Boosting, etc.

Example of Boosting Algorithm (AdaBoost):

Algorithm 10.1 AdaBoost.M1.

- Initialize the observation weights w_i = 1/N, i = 1, 2, ..., N.
- For m = 1 to M:
 - (a) Fit a classifier G_m(x) to the training data using weights w_t.
 - (b) Compute

$$\operatorname{err}_{m} = \frac{\sum_{i=1}^{N} w_{i} I(y_{i} \neq G_{m}(x_{i}))}{\sum_{i=1}^{N} w_{i}}.$$

- (c) Compute α_m = log((1 − err_m)/err_m).
- (d) Set w_i ← w_i · exp[α_m · I(y_i ≠ G_m(x_i))], i = 1, 2, . . . , N.
- 3. Output $G(x) = \text{sign} \left[\sum_{m=1}^{M} \alpha_m G_m(x) \right]$.

Boosting is remarkably resistant to overfitting, and it is fast and simple.

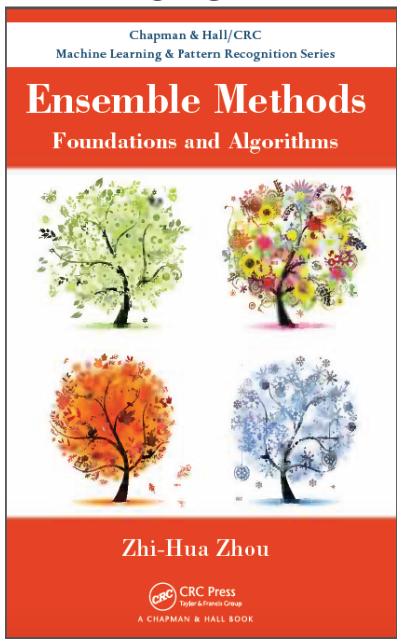
In fact, it can often continue to improve even when the training error has gone to zero.

It improves the performance of many kinds of machine learning algorithms.

Boosting does not work when:

Not enough data, base learner is too
weak or too strong, and/or
susceptible to noisy data.

More



Monographs on Statistics and Applied Probability 57

An Introduction to the Bootstrap

Bradley Efron Robert J. Tibshirani



More

