Tree-Based Methods

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Chapter 8

March 22, 2018

Best Machine Learning Algorithms in history?

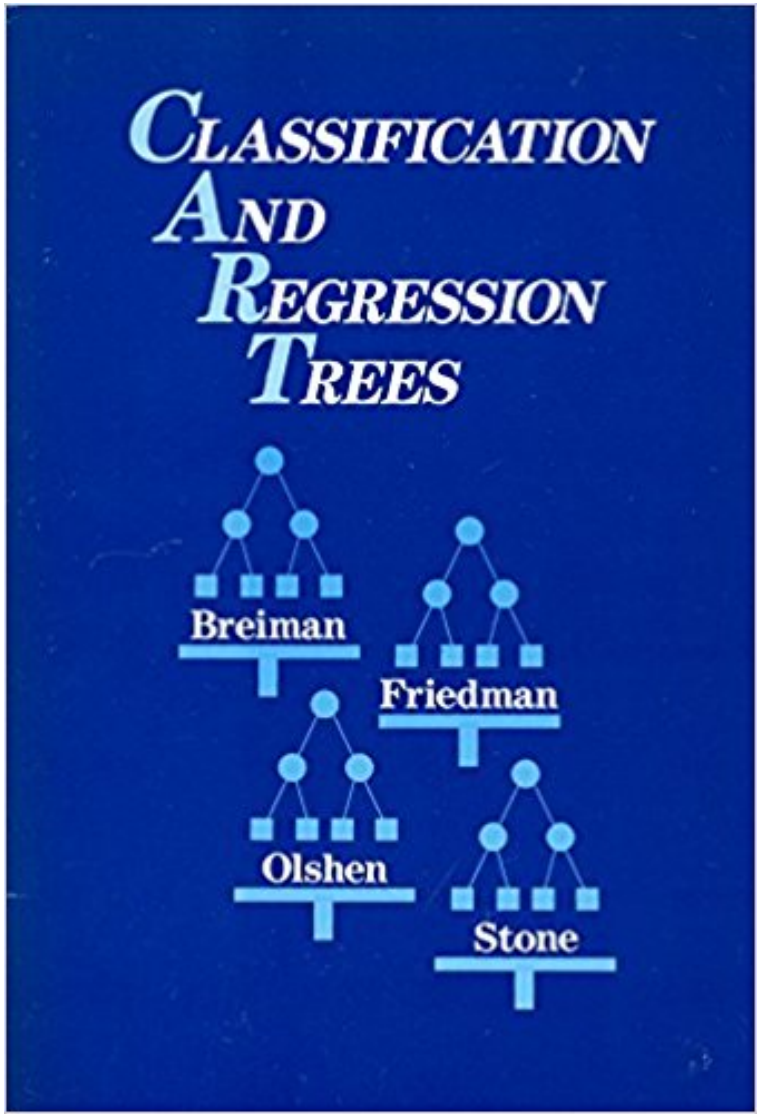
- Boosting (chapter 8): CART, adaBoost, random forests (Leo Breiman), etc.
- Support Vector Machines (chapter 9): or kernel methods (V. Vapnik), etc.
- Neural Networks (supplementary): perceptrons (1950s), deep learning (2010s), etc.

1. The basics of decision trees.

2. Bagging, random forests and boosting

About this chapter

- Decisions trees: splitting each variable sequentially, creating rectangular regions.
- Making fitting/prediction locally at each region.
- It is intuitive and easy to implement, may have good interpretation.
- Generally of lower prediction accuracy (weak learners).
- "The Boosting problem" (Kearns & Valiant): *Can a set of weak learners create a single strong learner?*
- Bagging, random forests and boosting ... make fitting/prediction based on a number of trees.
- Bagging and Boosting are general methodologies, not just limited to trees.



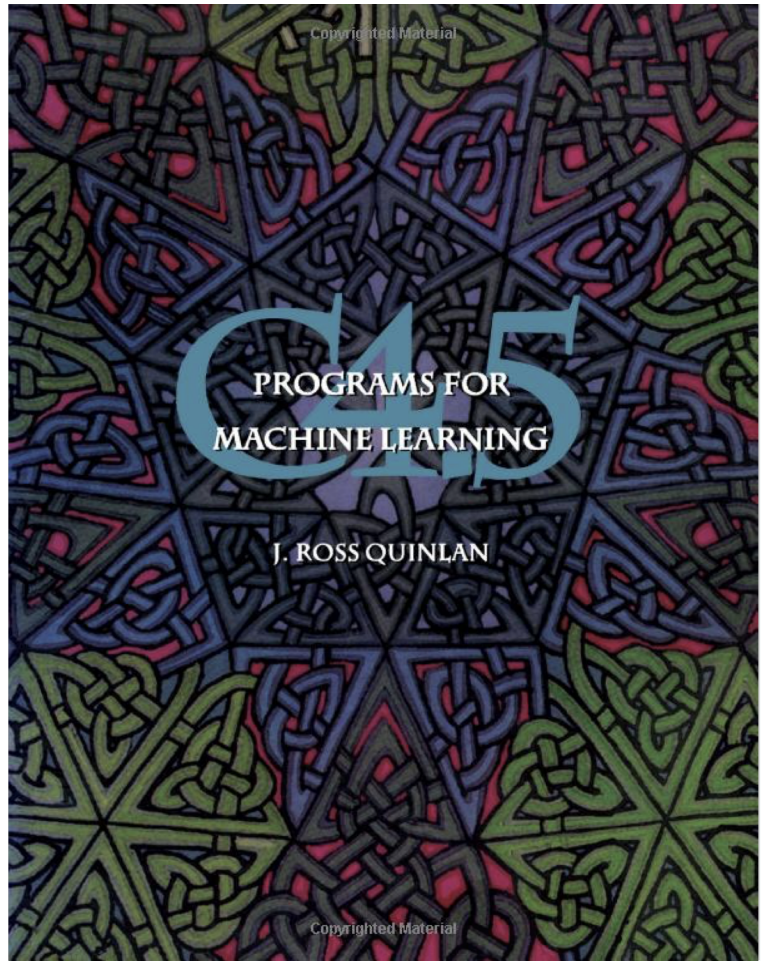


Figure: CART and C4.5

PREFACE

The tree methodology discussed in this book is a child of the computer age. Unlike many other statistical procedures which were moved from pencil and paper to calculators and then to computers, this use of trees was unthinkable before computers.

Binary trees give an interesting and often illuminating way of looking at data in classification or regression problems. They should not be used to the exclusion of other methods. We do not claim that they are always better. They do add a flexible nonparametric tool to the data analyst's arsenal.

Both practical and theoretical sides have been developed in our study of tree methods. The book reflects these two sides. The first eight chapters are largely expository and cover the use of trees as a data analysis method. These were written by Leo Breiman with the exception of Chapter 6 by Richard Olshen. Jerome Friedman developed the software and ran the examples.

Chapters 9 through 12 place trees in a more mathematical context and prove some of their fundamental properties. The first three of these chapters were written by Charles Stone and the last was jointly written by Stone and Olshen.

Trees, as well as many other powerful data analytic tools (factor analysis, nonmetric scaling, and so forth) were originated

by social scientists motivated by the need to cope with actual problems and data. Use of trees in regression dates back to the AID (Automatic Interaction Detection) program developed at the Institute for Social Research, University of Michigan, by Morgan and Sonquist in the early 1960s. The ancestor classification program is THAID, developed at the institute in the early 1970s by Morgan and Messenger. The research and developments described in this book are aimed at strengthening and extending these original methods.

Our work on trees began in 1973 when Breiman and Friedman, independently of each other, "reinvented the wheel" and began to use tree methods in classification. Later, they joined forces and were joined in turn by Stone, who contributed significantly to the methodological development. Olshen was an early user of tree methods in medical applications and contributed to their theoretical development.

Our blossoming fascination with trees and the number of ideas passing back and forth and being incorporated by Friedman into CART (Classification and Regression Trees) soon gave birth to the idea of a book on the subject. In 1980 conception occurred. While the pregnancy has been rather prolonged, we hope that the baby appears acceptably healthy to the members of our statistical community.

Figure: Historical story about CART

Regression trees

- Trees can be applied to both regression and classification.
- CART refers to classification and regression trees.
- We first consider regression trees through an example of predicting Baseball players' salaries.

The Hitters data

- Response/Outputs: Salary.
- Predictors/Inputs/Covariates:
  Years (the number of years that he has played in the major leagues)
  Hits (the number of hits that he made in the previous year).
- preparing data: remove the observations with missing data and log-transformed the Salary (preventing heavy right-skewness)

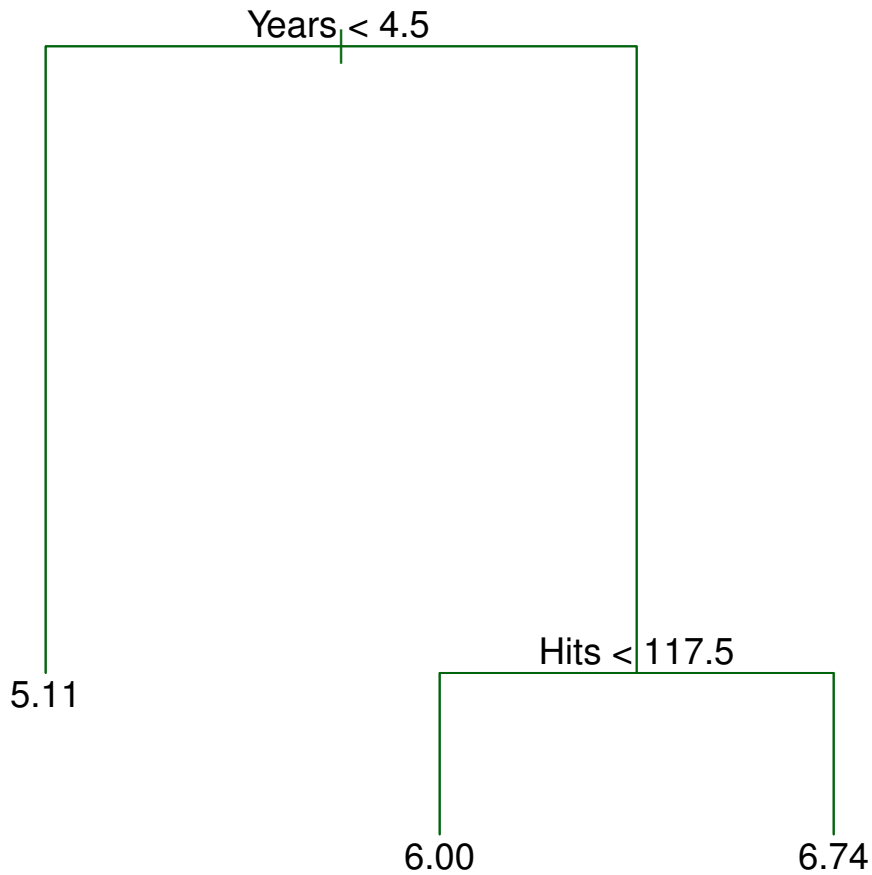


Figure: 1. Next page

Figure 1. 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 left-hand branch emanating from that split, and the right-hand branch corresponds to $X_j \geq t_k$. For instance, the split at the top of the tree results in two large branches. The left-hand branch corresponds to Years$<$ 4.5, and the right-hand branch corresponds to Years$\geq$ 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.

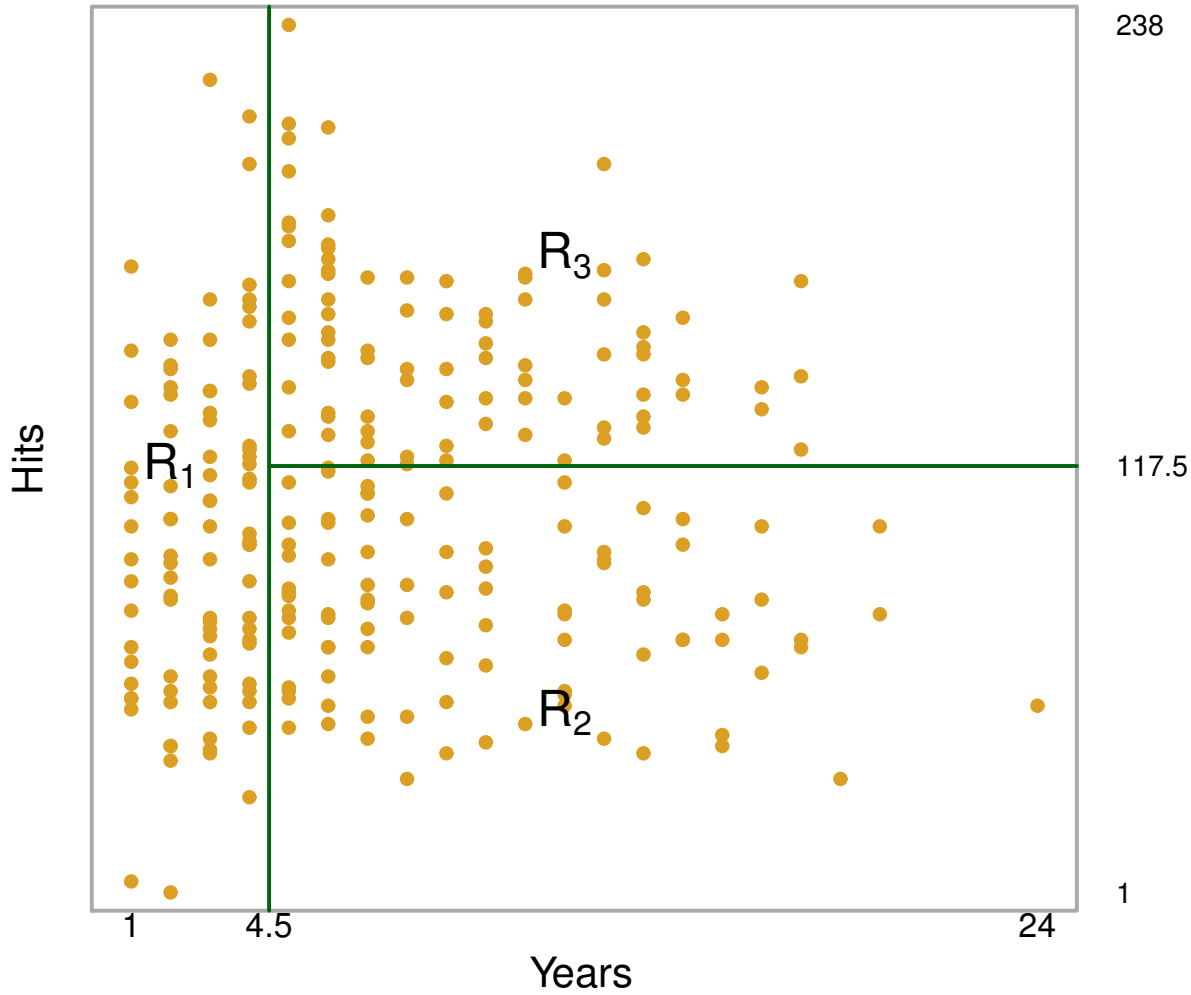


Figure: 2. The three-region partition for the Hitters data set from the regression tree illustrated in Figure 1.

Estimation/prediction

- On Regions R_1, R_2, R_3, the mean-log-salary is 5.107, and 6.74.
- Our prediction for any players in R_1, R_2 and R_3 are, respectively $1,000 \times e^{5.107} = \$165,174$, $1,000 \times e^{5.999} = \$402,834$, and $1,000 \times e^{6.740} = \$845,346$.

Estimation/prediction

- Trees involve a series of splittings of the data, each time by one variable.
- The series of actions taken place sequentially creates a tree-like results.
- As in Figure 1, the terminal nodes are the three indexed by the numbers, which represent the regions R_1, R_2 and R_3. These regions constitute he final partiation of the data.
- Terminal nodes are also called leaves.
- Each *internal node* represents a splitting,
- In Figure 1, the two internal nodes are indexed by $Y < 4.5$ and $Hits < 117.5$.
- The lines connecting nodes are called branches.
- Trees are typically drawn upside down.

Two step towards prediction

- Run the splitting according to input values sequentially, and obtain final partition of the data in regions $R_1, ..., R_J$.
- For any new observation with covariates in region R_k, we predict its response by the average of the reponses of the data points in region R_k.

How to split

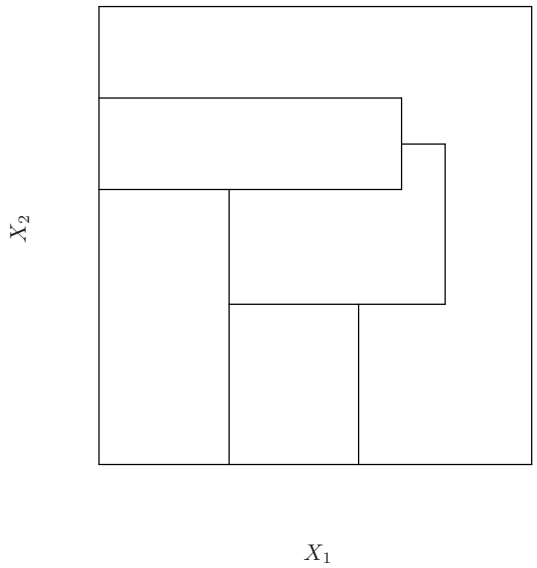
- Suppose we wish to partition a region R. In other words, we wish to separate the data in region R into two parts, day R_1 and R_2, according to one input values.
- What would be the optimal or efficient split in some sense?
- Only two flexibility in the split: 1. Choice of the input variable to split, 2. the cutpoint of the split of that chose input.
- Imagine that this is the final split of R: R_1 and R_2 would be leaves.
  And we would use the mean response of data in R_1 and R_2 to predict the response of any new/old observations.
  We wish our choice of R_1 and R_2 would be optimal in the sense of achieving miminum prediction error on the training data in region R.

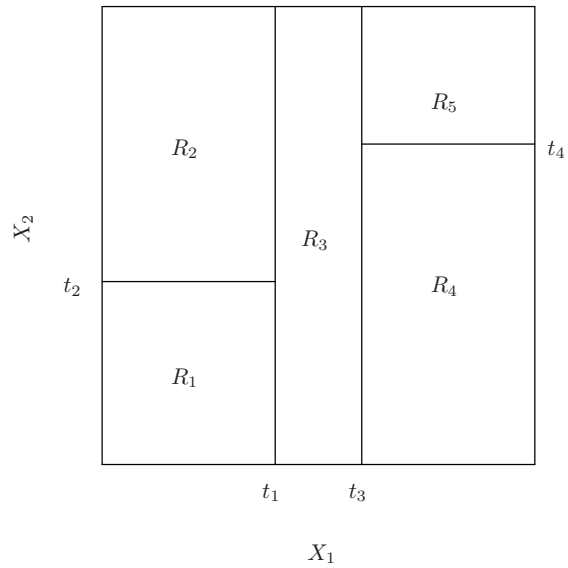
Recursive binary splitting

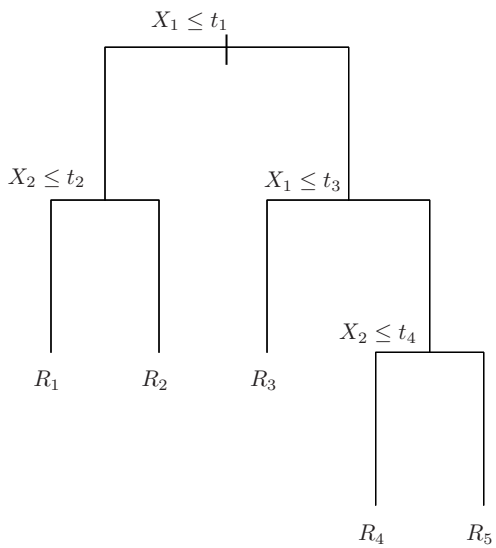
- A greedy algorithm (geedy means it is optimal at the current step): For $j = 1, ..., p$ and all real value s, let $R_1(j, s) = \{i \in R : X_j < s\}$ and $R_2(j, s) = \{i \in R : X_j \geq s\}$. And let $\hat{y}_1$ and $\hat{y}_2$ be the mean response of all observations in $R_1(j, s)$ and $R_2(j, s)$, respectively. Consider the following prediction error:

$$\text{RSS}_{new} = \sum_{i \in R_1(j,s)} (y_i - \hat{y}_1)^2 + \sum_{i \in R_2(j,s)} (y_i - \hat{y}_2)^2$$

  Choose the split which has the smallest prediction error. This split is the optimal one, denoted as R_1 and R_2.
- Continue the split till the final partition.


X_2
X_1


R_1
R_2
R_3
R_4
R_5
t_1
t_2
t_3
t_4
X_2
X_1


$X_1 \le t_1$
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R_1
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R_5

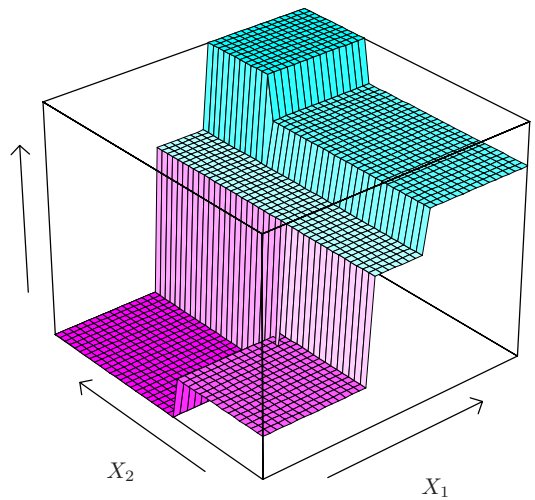

X_2
X_1

Figure 3. 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.

When to stop split

- The problem of when to stop.
- If too many steps of splitting: many leaves, too complex model, small bias but large variance, may overfit.
- If too few steps of splitting: few leaves, too simple model, large bias but small variance, may underfit.

One natural idea

- When splitting R into R_1 and R_2, consider the RSS before the split

$$\text{RSS}_{old} = \sum_{i \in R} (y_i - \hat{y})^2$$

where $\hat{y}$ is the average of the response of data in R. With the optimal split, the reduction of RSS is

$$\text{RSS}_{old} - \text{RSS}_{new}$$

- We can pre-choose a threshold, h, and decide the worthiness of the split.
- If the reduction is smaller than h, we do not do it, and stop right there; then R is one terminal node (a leave).
- If the reduction is greater than h, we make the split, and continue with next step.

One natural idea

- The idea is seemingly reasonable, but is too near-sighted.
- Only look at the effect of the current split.
- It is possible that even if the current split is not effective, the future splits could be effective and, maybe, very effective.

Tree pruning

- Grow a very large tree.
- Prune the tree back to obtain a subtree.
- Objective: find the subtree that has the best test error.
- Use cross-validation to examine the test errors for a *sequence* (parametrized by α) of subtrees during the growth/pruning, instead of all possible subtrees which is too large a model space.

Cost complexity pruning

- Let T_0 be the original (large) tree. Let T be any subtree. Use $|T_0|$ and $|T|$ to denote their numbers of teminal nodes, which represent complexity.
- Consider "Loss + Penalty":

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

  where R_m are the terminal nodes of the subtree T, and the mean response of R_m is $\hat{y}_m$; α is tuning parameter.
- Denote the minimized subtree as T_α.
- If $\alpha = 0$, no penalty the optimal tree is the original T_0.
- If $\alpha = \infty$, the tree has no split at all. The predictor is just $\bar{y}$.
- The larger the α, the more penalty for model complexity.

Cost complexity pruning

- Just like Lasso, there exists efficient computation algorithm to compute the entire sequence of T_α for all α.
- Use cross-validation to find the best α to minimize the test error.

The 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.

The algorithm

- 3. Use K-fold cross-validation to determine best α. That is, divide the training observations into K folds. For each $k = 1, ..., K$
  (a) Repeat Steps 1 and 2 on all but the kth fold of the training data.
  (b) Evaluate the mean squared prediction error on the data in the left-out k-th fold, as a function of α.
  (c) Average the results for each value of α, and pick α to minimize the average error.
- 4. Return the subtree from Step 2 that corresponds to the chosen value of α.

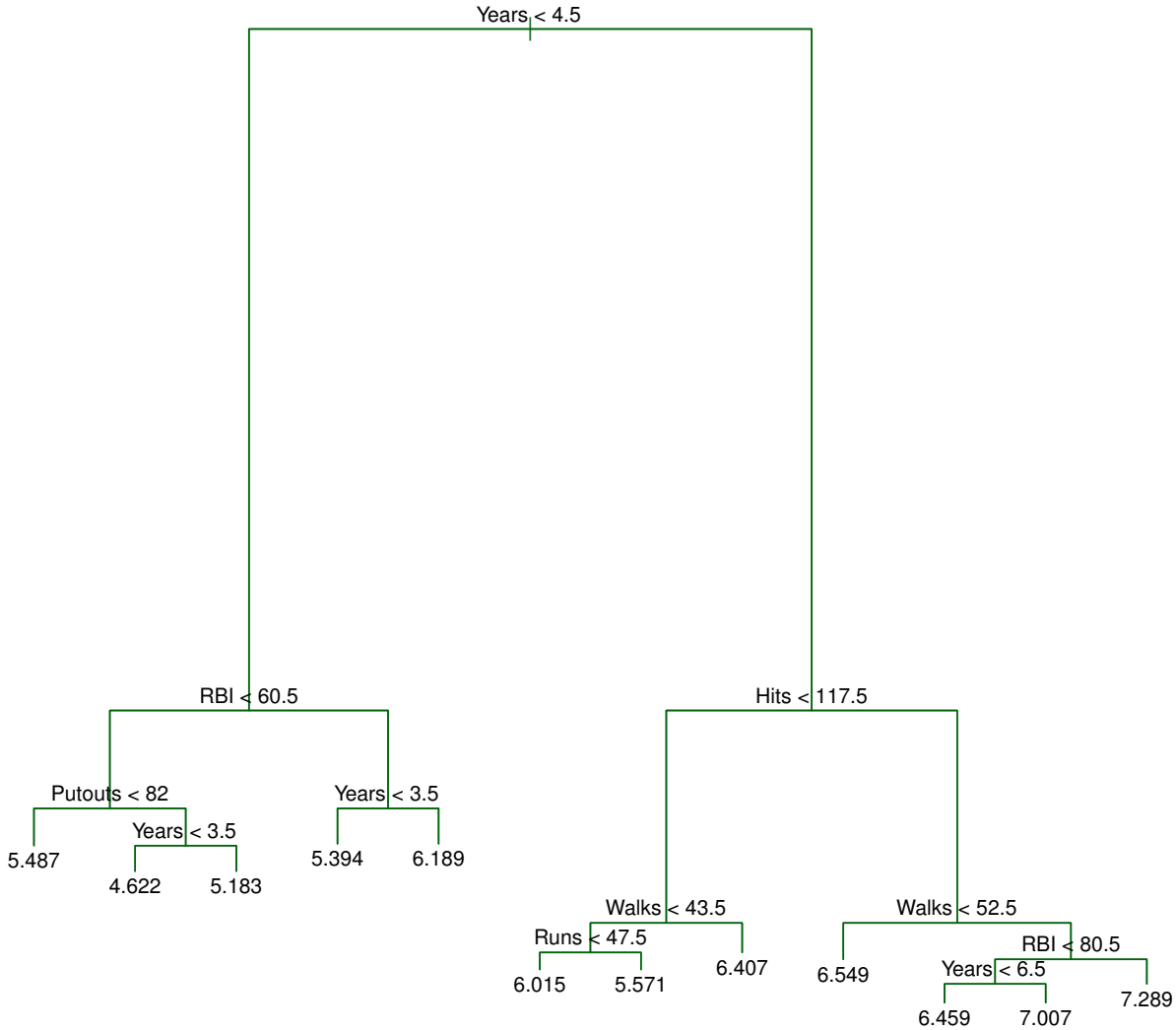


Figure: 4. Regression tree analysis for the Hitters data. The unpruned tree that results from top-down greedy splitting on the training data is shown.

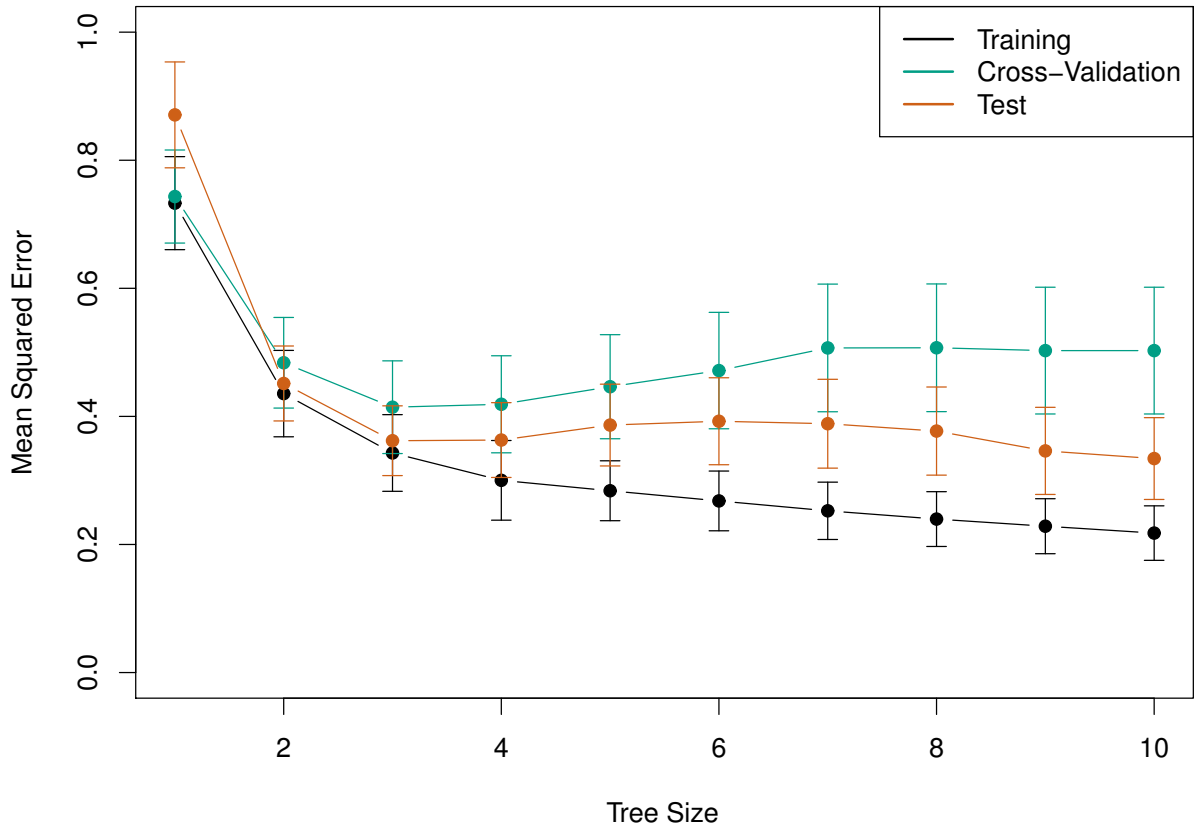


Figure: 5. Regression tree analysis for the Hitters data. The training, cross-validation, and test MSE are shown as a function of the number of terminal nodes in the pruned tree. Standard error bands are displayed. The minimum cross-validation error occurs at a tree size of three.

Classification trees

- Regression has numerical responses; and classification has qualitative responses.
- Recall that for regression trees, we chose to obtain the greatest reduction of RSS.
  RSS is using sum of squares to measure the error.
- For classification trees, one can follow the same line of procedure as that of regression trees, but using error measurements that are more appropriate for classification.

Classification error rates

- For a region R, let $\hat{p}_k$ be the percentage of observations in this region that belong to class k.
- We assign any new observation in region R as from the class with largest $\hat{p}_k$, which is the so-called *most commonly occuring class* in training data.

The impurity measure

- The classification error rate (for this region R) is

$$E = 1 - \max_k \hat{p}_k.$$

- The Gini index is

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

- The cross-entropy is

$$D = -\sum_{k=1}^{K} \hat{p}_k \log(\hat{p}_k)$$

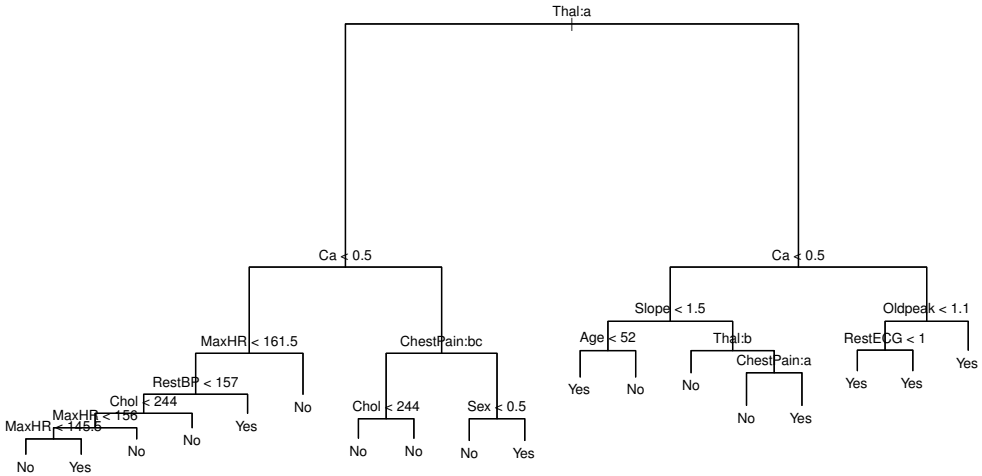
.

- Any of these three approaches might be used when pruning the tree.
- If R is nearly pure, most of the observations are from one class, then the Gini-index and cross-entropy would take smaller values than classification error rate.

$$\hat{p}_1 = [0.5, 0.25, 0.25] \Rightarrow E = 0.5, G = 0.625, D = 1.0397$$

$$\hat{p}_2 = [0.5, 0.4, 0.1] \Rightarrow E = 0.5, G = \mathbf{0.580}, D = \mathbf{0.9433}$$

- Gini-index and cross-entropy are more sensitive to node purity.
- To evaluate the quality of a particular split, the Gini-index and cross-entropy are more popularly used as error measurement criteria than classification error rate. (E can't distinguish $\hat{p}_1$ and $\hat{p}_2$ above, while G/D are more informative for $\hat{p}_2$)
- The classification error rate is preferable if only prediction accuracy of the final pruned tree is the goal.


Thal:a
Ca < 0.5
Ca < 0.5
MaxHR < 161.5
ChestPain:bc
Slope < 1.5
Oldpeak < 1.1
Age < 52
Thal:b
RestECG < 1
ChestPain:a
RestBP < 157
Chol < 244
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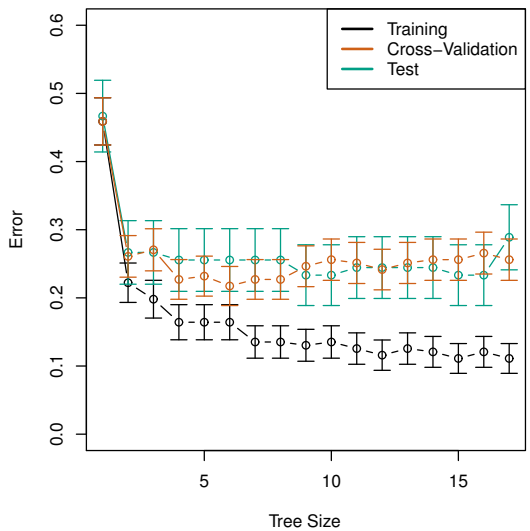
MaxHR < 145.5
No
Yes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Cross−Validation
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Error
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5
10
15

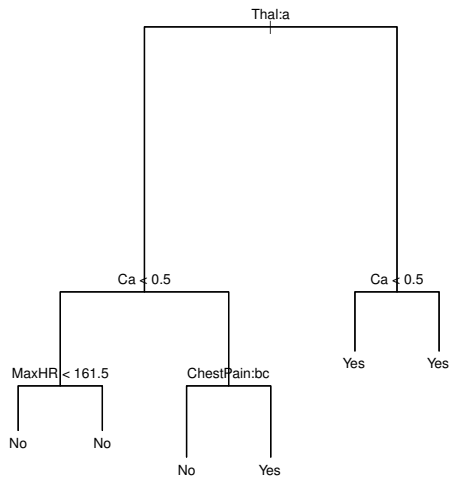
Thal:a
Ca < 0.5
Ca < 0.5
MaxHR < 161.5
ChestPain:bc
No
Yes

Figure 6. Heart data. Top: The unpruned tree. Bottom Left: Cross-validation error, training, and test error, for different sizes of the pruned tree. Bottom Right: The pruned tree corresponding to the minimal cross-validation error.

Trees vs. Linear models

- For regression model:
$$Y = f(X) + \epsilon$$
- Linear model assumes
$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$$
- Regression trees assume
$$f(X) = \sum_{m=1}^{M} c_m 1(X \in R_m)$$
where $R_1, ..., R_M$ are rectagular partitions of the input space.
- If the underlying realation is close to linear, linear model is better. Otherwise, regression trees are generally better. (Useless comments)

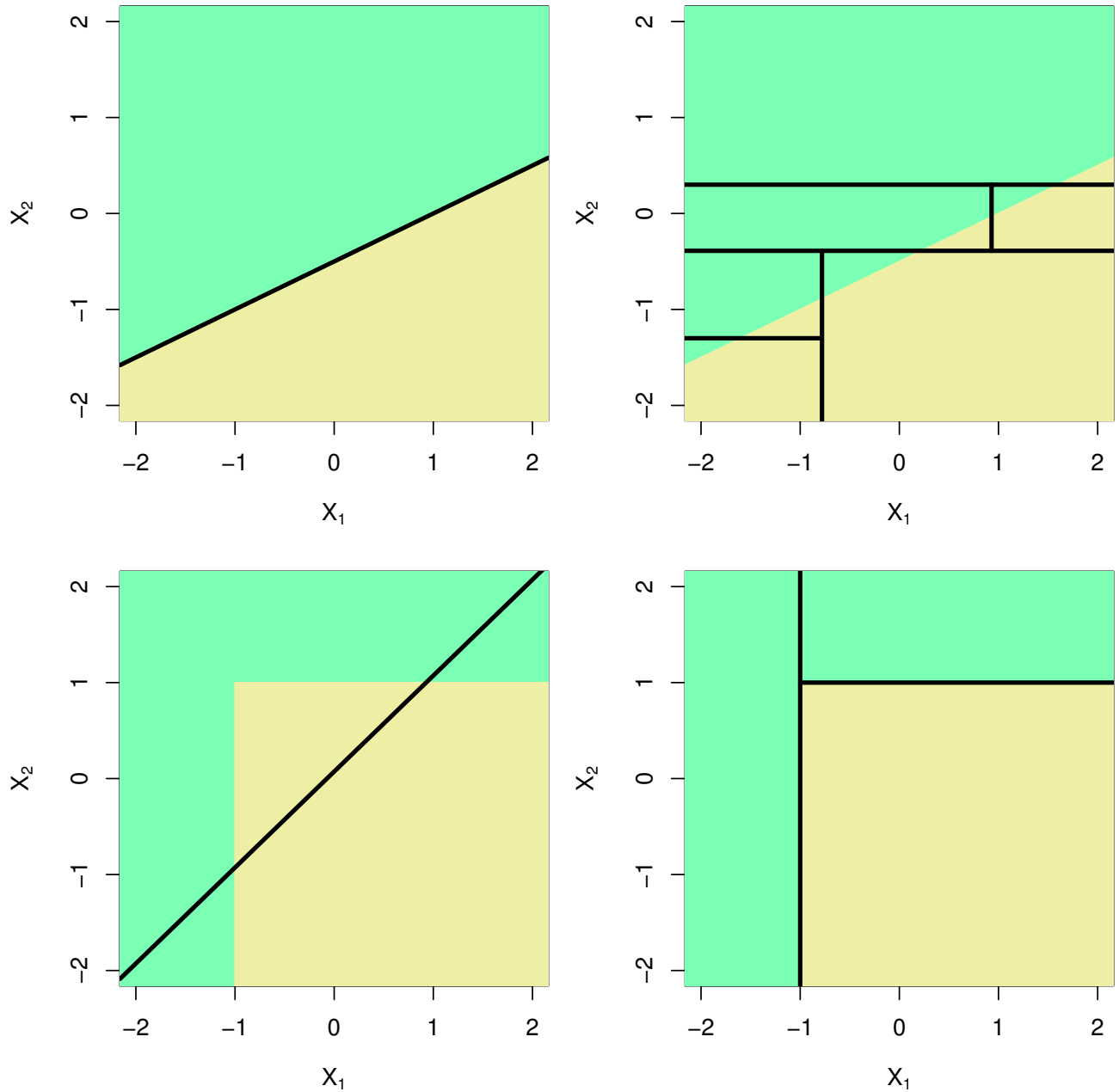
X2
X1
−2
−1
0
1
2

Figure 7. Top Row: A two-dimensional classification example in which the true decision boundary is linear, and is indicated by the shaded regions. A classical approach that assumes a linear boundary (left) will outperform a decision tree that performs splits parallel to the axes (right). Bottom Row: Here the true decision boundary is non-linear. Here a linear model is unable to capture the true decision boundary (left), whereas a decision tree is successful (right).

Advantages of Trees

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

Disadvantages of Trees

- Trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches seen in this book.
- Trees can be very non-robust. In other words, a small change in the data can cause a large change in the final estimated tree.
- However, by aggregating many decision trees, using methods like bagging, random forests, and boosting, the predictive performance of trees can be substantially improved. We introduce these concepts in the next section.

The Little Bootstrap and Other Methods for Dimensionality Selection in Regression: *X*-Fixed Prediction Error

LEO BREIMAN*

When a regression problem contains many predictor variables, it is rarely wise to try to fit the data by means of a least squares regression on all of the predictor variables. Usually, a regression equation based on a few variables will be more accurate and certainly simpler. There are various methods for picking "good" subsets of variables, and programs that do such procedures are part of every widely used statistical package. The most common methods are based on stepwise addition or deletion of variables and on "best subsets." The latter refers to a search method that, given the number of variables to be in the equation (say, five), locates that regression equation based on five variables that has the lowest residual sum of squares among all five variable equations. All of these procedures generate a sequence of regression equations, the first based on one variable, the next based on two variables, and so on. Each member of this sequence is called a submodel and the number of variables in the equation is the dimensionality of the submodel. A complex problem is determining which submodel of the generated sequence to select. Statistical packages use various *ad hoc* selection methods, including F to enter, F to delete, C_p, and t-value cutoffs. Our approach to this problem is through the criterion that a good selection procedure selects dimensionality so as to give low prediction error (PE), where the PE of a regression equation is its expected squared error over the points in the X design. Because the true PE is unknown, the use of this criteria must be based on PE estimates. We introduce a method called the *little bootstrap,* which gives almost unbiased estimates for submodel PEs and then uses these to do submodel selection. Comparison is made to C_p and other methods by analytic examples and simulations. Little bootstrap does well—C_p and, by implication, all selection methods not based on data reuse give highly biased results and poor subset selection.

KEY WORDS: Best subsets; Mallows's C_p; Subset selection; Variable selection.

1. INTRODUCTION

In a regression problem with many predictor variables, data analysts often attempt to reduce the dimensionality of the model by running a procedure such as "best subsets," stepwise forward addition of variables, or stepwise backwards deletion of variables. These dimensionality reduction methods are among the most frequently used programs in such packages as SAS, SPSS, and BMDP.

Two major difficulties with these submodel procedures are (1) selecting the dimensionality of the submodel to be used and (2) evaluating the model selected. By this is meant choosing the dimensionality to get a near-optimum balance between bias and variance, and then giving a realistic assessment of the predictive capability of the selected submodel.

In selection of dimensionality, a number of *ad hoc* methods are commonly used. In stepwise methods, use of F-to-enter, F-to-delete, and adjusted R^2 are prevalent. In "best

TECHNOMETRICS, NOVEMBER 1995, VOL. 37, NO. 4

Better Subset Regression Using the Nonnegative Garrote

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A new method, called the nonnegative (nn) garrote, is proposed for doing subset regression. It both shrinks and zeroes coefficients. In tests on real and simulated data, it produces lower prediction error than ordinary subset selection. It is also compared to ridge regression. If the regression equations generated by a procedure do not change drastically with small changes in the data, the procedure is called stable. Subset selection is unstable, ridge is very stable, and the nn-garrote is intermediate. Simulation results illustrate the effects of instability on prediction error.

KEY WORDS: Little bootstrap; Model error; Prediction; Stability.

1. INTRODUCTION

One of the most frequently used statistical procedures is subset-selection regression. That is, given data of the form $\{(y_n, x_{1n}, \ldots, x_{Mn}), n = 1, \ldots, N\}$, some of the predictor variables $x_1, \ldots, x_M$ are eliminated and the prediction equation for y is based on the remaining set of variables. The selection of the included variables uses either the best subset method or a forward/backward stepwise method. These procedures give a sequence of subsets of $\{\mathbf{x}_1, \ldots, \mathbf{x}_M\}$ of dimension $1, 2, \ldots, M$. Then some other method is used to decide which of the M subsets to use.

gave a recent overview of ridge methods. Some studies (i.e., Frank and Friedman 1993; Hoerl, Schuenemeyer, and Hoerl 1986) have shown that ridge regressions give more accurate predictions than subset regressions unless, assuming that y is of the form

$$y = \sum_k \beta_k x_k + \epsilon,$$

all but a few of the $\{\beta_k\}$ are nearly zero and the rest are large. Thus, although subset regression can improve accuracy if M is large, it is usually not as accurate as ridge.

Ridge has its own drawbacks. It gives a regression equa-

Bagging (Boostrap Aggregating)

- A general purpose procedure to reduce variance of a learning method.
- A model averaging technique.
- Decision tree is generally a high variance method. (Apply the method based on different data based on same sampling scheme would lead to very different result.)
- Average of iid random variables would have a reduced variance σ^2/n

The procedure.

- Model
$$y_i = f(x_i) + \epsilon_i, \quad i = 1, ..., n.$$
- Suppose a statistical learning method gives $\hat{f}(\cdot)$ based on the training data $(y_i, x_i), i =, 1..., n$.
- For example,
  1. Linear model: $\hat{f}(x) = \hat{\beta}_0 + \hat{\beta}^T x_i$
  2. KNN: $\hat{f}(x) = \sum_{j=1}^{J} \bar{y}_{\tilde{R}_j}$ with least distance to K-cluster partition.
  3. Decision tree: $\hat{f}(x) = \sum_{j=1}^{J} \bar{y}_{R_j}$ with rectangular partition.
  4. ...

The procedure of Bagging

- Data $(y_i, x_i), i = 1, ..., n$; and a learning method $\hat{f}$
- Draw a boostrap sample from the data, and compute a $\hat{f}_1^*$ based on this set of bootstrap sample.
- Draw another boostrap sample from the data, and compute a $\hat{f}_2^*$ based on this set of bootstrap sample.
- ....
- Repeat M times, obtain $\hat{f}_1^*, ..., \hat{f}_M^*$.
- Produce the learning method with bagging as

$$\frac{1}{M} \sum_{j=1}^{M} \hat{f}_j^*$$

The Bagging

- Bagging is general-purpose.
- It works best for high variance low bias learning methods.
- This is the case for decision trees, particularly deep trees.
- Also the case for large p.
- If the response is qualitative, we can take the majority vote (not averaging) of the predicted class based on all learning methods based on boostrap samples.

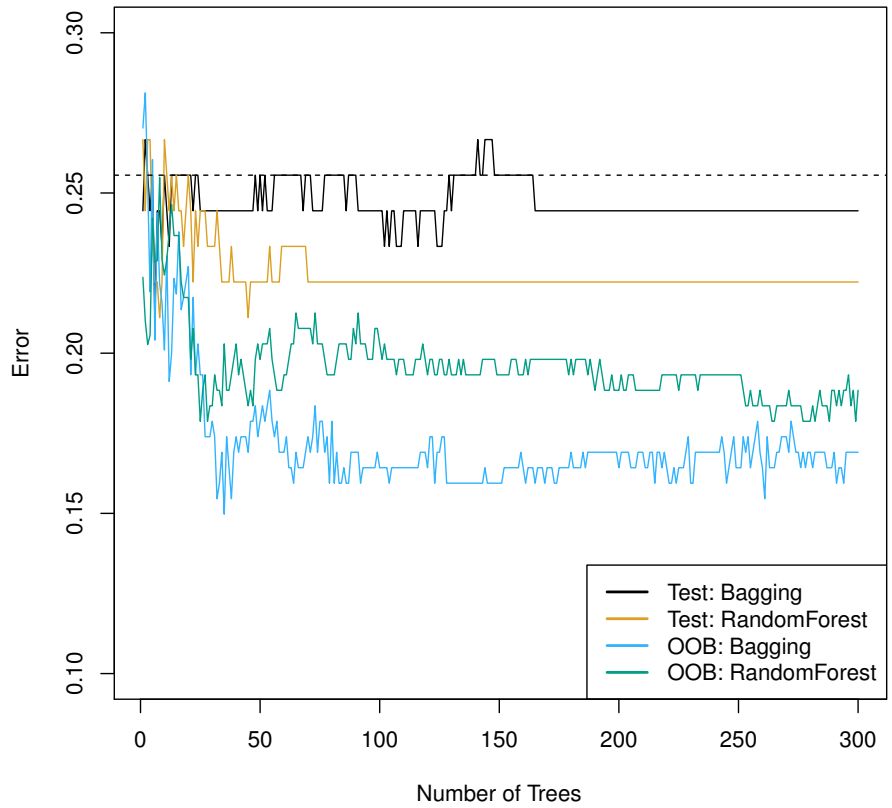

Figure: 8. Bagging and random forest results for the Heart data. The test error (black and orange) is shown as a function of B, the number of bootstrapped training sets used. Random forests were applied with $m = \sqrt{p}$. The dashed line indicates the test error resulting from a single classification tree. The green and blue traces show the OOB error, which in this case is considerably lower

Out-of-Bag (OOB) error estimation

- Estimation of test error for the bagged model.
- For each bootstrap sample, observation i is bootstrap sampled with probabilty $(1 - 1/n)^n \approx 1/e$.
- For each bootstrap sample, the number of observations not taken into this bootstrap sample is $n(1 - 1/n)^n \approx n/e$. These are referred to as out-of-bag (OOB) observations.
- For totally B bootstrap samples, about B/e times, the bootstrap sample does not contain observation i.
- The trees based on these bootstrap sample can be used to predict the response of observation i. Totally about B/e predictions.
- We average these predictions (for regression) or take majority vote (for classification) to produce the Bagged prediction for observation i, denote it as $\hat{f}^*(x_i)$.

Out-of-Bag (OOB) error estimation

- The OOB MSE is

$$\sum_{i=1}^{n}(y_i - \hat{f}^*(x_i))^2$$

- The OOB classification error is

$$\sum_{i=1}^{n} I(y_i \notin \hat{f}^*(x_i))$$

- The resulting OOB error is a valid estimate of the test error for the bagged model, since the response for each observation is predicted using only the trees that were not fit using that observation.
- It can be shown that with B sufficiently large, OOB error is virtually equivalent to leave-one-out cross-validation error.

Variable importance measures

- Bagging improves prediction accuracy at the expense of interpretability.
- An overall summary of the importance of each predictor using the RSS (for bagging regression trees) or the Gini index (for bagging classification trees).
- Bagging regression trees, we can 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.
- Bagging classification trees, we can add up the total amount that the Gini index is decreased by splits over a given predictor, averaged over all B trees.

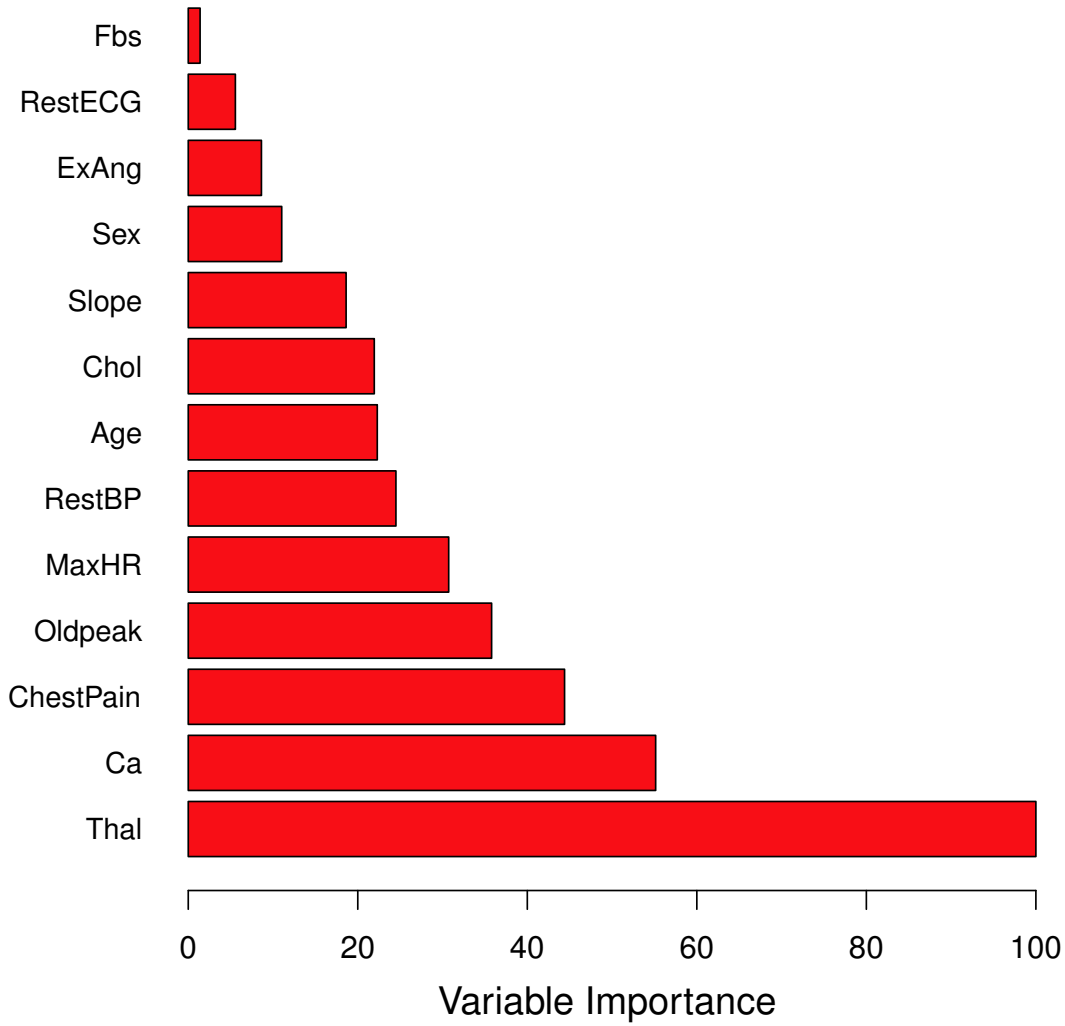

Figure: 9. A variable importance plot for the Heart data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.

Motivation of Random Forest

- An average of B i.i.d random variables, each with variance σ^2, has variance $\frac{1}{B}\sigma^2$.
- What if not independent but correlated?
- If the variables are simply i.d. (identically distributed but not necessarily independent) with positive pairwise correlation ρ, the variance of the average is

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$

- The idea of random forests is to improve the variance reduction of bagging by reducing the correlation between trees, without increasing the variance too much.

Random Forest

- Same as bagging decision trees, except ...
- When building these decision trees, each time a split in a tree is considered, a random sample of m predictors is chosen as split candidates from the full set of p predictors
- Typically $m \approx \sqrt{p}$.

Random Forest

- Every step, the split is constrained on a small number m and randomly selected inputs.
- Avoid all trees are too similar to each other.
- Too similar trees are too highly correlated, average highly correlated trees cannot achieve large amount of variance reduction.
- Extreme case: If all trees are the same, average of them is still the same one.
- Averaging uncorrelated or low-correlated trees can achieve large amount of variance reduction.
- Random forest produces less correlated trees.
- Random forest reduces to bagging if $m = p$.

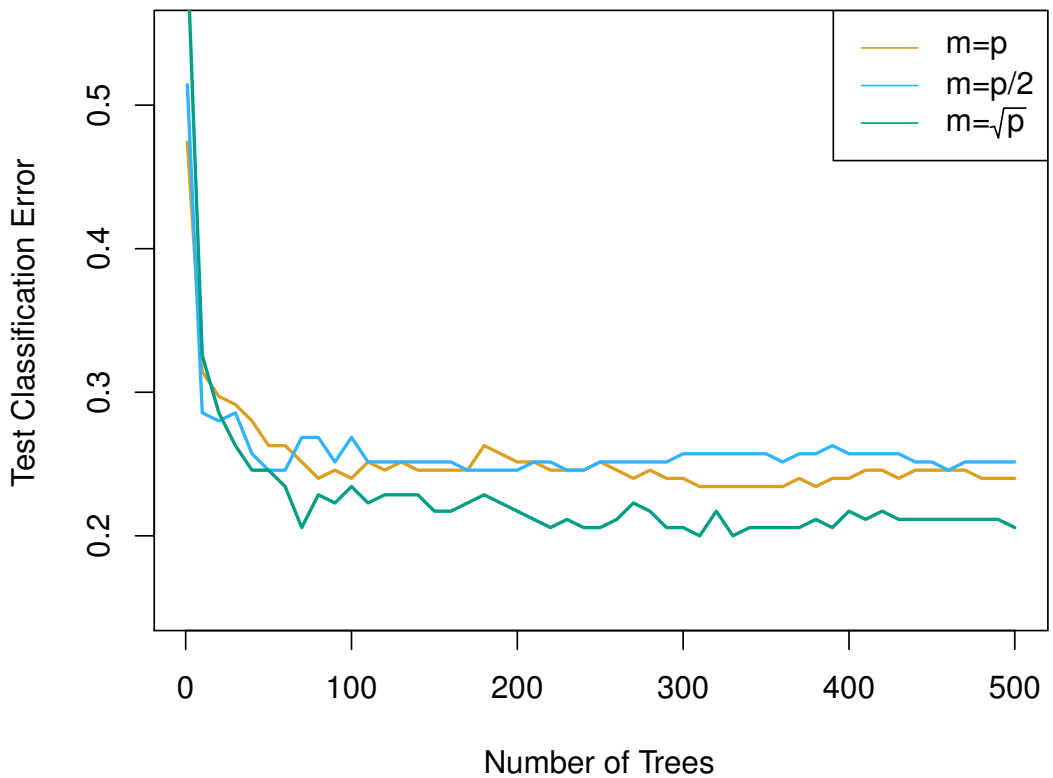

Figure: 10. Results from random forests for the 15-class gene expression data set with $p = 500$ predictors. The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m, the number of predictors available for splitting at each interior tree 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

- General purpose for improving learning methods by combining many weaker learners in attempt to produce a strong learner.
- Like bagging, boosting involves combining a large number of weaker learners.
- The weaker learners are created sequentially. (no boostrap involved).
- Bagging create large variance and possibly over-fit boostrap learners and try to reduce their variance by averaging.
- Boosting create weak learners sequentially and slowly (to avoid over-fit).

Adaboost

- 1. Initialize the data weights $\{w_n\}$ by setting $w_n^{(1)} = 1/N$ for $n = 1, \ldots, N$.
- 2. For $m = 1, \ldots, M$:
  - (a) Fit a classifier $f_m(\mathbf{x})$ to the training data by minimizing the weighted error function

$$J_m = \sum_{n=1}^{N} w_n^{(m)} \mathbb{I}(f_m(\mathbf{x}_n) \neq y_n), \tag{1}$$

where $\mathbb{I}(f_m(\mathbf{x}_n) \neq y_n)$ is the indicator function and equals 1 when $f_m(\mathbf{x}_n) \neq y_n$ and 0 otherwise.

Adaboost

- 2. (Continued)
  - (b) Evaluate the quantities

$$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} \mathbb{I}(f_m(\mathbf{x}_n) \neq y_n)}{\sum_{n=1}^{N} w_n^{(m)}} \tag{2}$$

and then use these to evaluate

$$\alpha_m = \log \left\{ \frac{1 - \epsilon_m}{\epsilon_m} \right\} \tag{3}$$

  - (c) Update the data weights

$$w_n^{(m+1)} = w_n^{(m+1)} \exp\{\alpha_m \mathbb{I}(f_m(\mathbf{x}_n) \neq y_n)\} \tag{4}$$

- 3. Make prediction by

$$F_M(\mathbf{x}) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m f_m(\mathbf{x}) \right). \tag{5}$$

Illustration of Adaboost

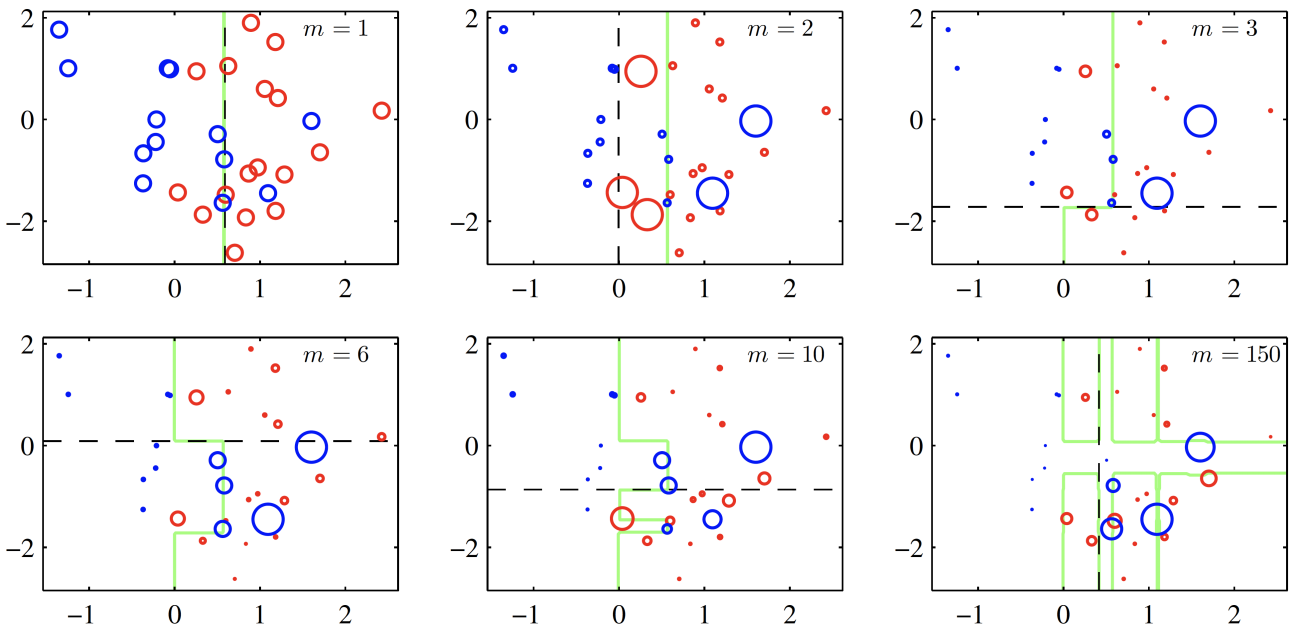

Figure: Each figure shows the number m of base learners trained so far, along with the decision boundary of the most recent base learner (dashed black line) and the combined decision boundary of the ensemble (solid green line). Each data point is depicted by a circle whose radius indicates the weight assigned to that data point when training the most recently added base learner. Thus, for instance, we see that points that are misclassified by the $m = 1$ base learner are given greater weight when training the $m = 2$ base learner. Bishop (2006).

Statistical view of Adaboost

- Consider the exponential error function

$$E = \sum_{n=1}^{N} \exp\{-y_n F_M(\mathbf{x}_n)\}, \tag{6}$$

  where $F_M(\mathbf{x}) = \frac{1}{2}\sum_{m=1}^{M} \alpha_m f_m(\mathbf{x})$ and $y_n \in \{-1, 1\}$.
- Our goal is to minimize E w.r.t. both α_m and $f_m(\mathbf{x})$.
- Instead of doing a global error function miminization, we shall suppose that the base classifiers $f_1(\mathbf{x}), \ldots, f_{m-1}(\mathbf{x})$ are fixed, as are their coefficients $\alpha_1, \ldots, \alpha_{m-1}$, and so we are minimizing only w.r.t. α_m and $f_m(\mathbf{x})$.

$$\begin{aligned} E &= \sum_{n=1}^{N} \exp\left\{-y_n F_{m-1}(\mathbf{x}_n) - \frac{1}{2} y_n \alpha_m f_m(\mathbf{x}_n)\right\} \\ &= \sum_{n=1}^{N} w_n^{(m)} \exp\{-\frac{1}{2} y_n \alpha_m f_m(\mathbf{x}_n)\} \end{aligned} \tag{7}$$

  where $w_n^{(m)} = \exp\{-y_n F_{m-1}(\mathbf{x}_n)\}$ can be viewed as constants.

- Denote $\mathcal{T}_m$ and $\mathcal{M}_m$ as the sets of correctly classifed data points by $f_m(\mathbf{x})$ and the misclassified points, respectively.
- We have

$$E = e^{-\alpha_m/2} \sum_{n\in\mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n\in\mathcal{M}_m} w_n^{(m)}$$

$$= (e^{\alpha_m/2} - e^{-\alpha_m/2}) \sum_{n-1}^{N} w_n^{(m)} \mathcal{I}(f_m(\mathbf{x}_n) \neq y_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}. \quad (8)$$

- When we minimize this w.r.t. $f_m(\mathbf{x})$, the second term is constant, and so the is equivalent to minimizing (1) because the overall multiplicative factor in front of the summation does not affect the location of the minimum.
- Similarly, minimizing w.r.t. α_m, we obtain (3) in which ϵ_m is defined by (2).

- From (7), we see that, having found α_m and $f_m(\mathbf{x})$, the weights on the data points are updated using

$$w_n^{(m+1)} = w_n^{(m)} \exp\left\{-\frac{1}{2} y_n \alpha_m f_m(\mathbf{x}_n)\right\}.$$

- Making use of the fact that

$$y_n f_m(\mathbf{x}_n) = 1 - 2\mathbb{I}(\mathbf{y}_m \neq y_n),$$

we see that the weight $w_n^{(m)}$ are updated at the next iteration using

$$w_n^{(m+1)} = w_n^m \exp(-\alpha_m/2) \exp\{\alpha_m \mathbb{I}(f_m(\mathbf{x}_n) \neq y_n)\}.$$

- Because the term $\exp(-\alpha_m/2)$ is independent of n, we see that it weights all data points by the same factor and so can be discarded. Thus we obtain (4).
- Finally, once all the base classifiers are trained, new data points are classified by evaluating the **sign** of the combined function. Because the factor of 1/2 does not affect the sign, this gives (5).

Why exponiental loss function?

- We have shown that the Adaboost algorithm minimizes the exponential loss function (6). How to justify the minimization of the exponential loss function?
- Consider the population version of the exponential loss function,

$$\mathbb{E}_{\mathbf{x},y}[\exp\{-yF(\mathbf{x})\}] = \sum_y \int \exp\{-yF(\mathbf{x})p(y|\mathbf{x})p(\mathbf{x})\}d\mathbf{x}$$

- Taking the functional derivative w.r.t. $F(\mathbf{x})$, we get

$$\frac{\partial}{\partial F(\mathbf{x})}\mathbb{E}_{\mathbf{x},y}[\exp\{-yF(\mathbf{x})\}] = -\sum_y y\exp\{-yF(\mathbf{x})\}p(y|\mathbf{x})p(\mathbf{x})$$

$$= \{\exp\{F(\mathbf{x})\}p(y=-1|\mathbf{x}) - \exp\{-F(\mathbf{x})\}p(y=1|\mathbf{x})\}p(\mathbf{x}).$$

- Setting this equal to zero and rearranging, we obtain

$$F(\mathbf{x}) = \frac{1}{2}\log\left\{\frac{p(y=1|\mathbf{x})}{p(y=-1|\mathbf{x})}\right\},$$

justifying the use of the sign function to arrive the final classification decision.

Friedman's Gradient Boost algorithm

- Initialize $\hat{F}_0(\mathbf{x})$ to be a constant, $\hat{F}_0(\mathbf{x}) = \arg\min_\rho \sum_{i=1}^N L(y_i, \rho)$.
- For m in $1, \ldots, M$ do
  1. Compute the negative gradient as the working response

$$r_i = -\frac{\partial}{\partial F_{m-1}(\mathbf{x}_i)} L(y_i, F_{m-1}(\mathbf{x}_i)) \Big|_{F_{m-1}(\mathbf{x}_i)=\hat{F}_{m-1}(\mathbf{x}_i)} \tag{9}$$

  2. Fit a regression model, $g(\mathbf{x})$, predicting r_i from the covariates $\mathbf{x}_i$.
  3. Choose a gradient descent step size as

$$\rho = \arg\min_\rho \sum_{i=1}^N L(y_i, \hat{F}_{m-1}(\mathbf{x}_i) + \rho g(\mathbf{x}_i)) \tag{10}$$

  4. Update the estimate of $F(\mathbf{x})$ as

$$\hat{F}_m(\mathbf{x}) = \hat{F}_{m-1}(\mathbf{x}) + \rho g(\mathbf{x}) \tag{11}$$

Gradient Boosting Tree

Initialize $\hat{F}_0(\mathbf{x})$ to be a constant, $\hat{F}_0(\mathbf{x}) = \arg\min_\rho \sum_{i=1}^N L(y_i, \rho)$
For m in $1, \ldots, M$ do

1. Compute the negative gradient as the working response

$$r_i = -\frac{\partial}{\partial F_{m-1}(\mathbf{x}_i)} L(y_i, F_{m-1}(\mathbf{x}_i)) \Big|_{F_{m-1}(\mathbf{x}_i)=\hat{F}_{m-1}(\mathbf{x}_i)} \tag{12}$$

2. Randomly select prop $\times N$ cases from the dataset, e.g., prop $= 0.5$.
3. Fit a regression tree with K terminal nodes, $g(\mathbf{x}) = \mathbb{E}(r|\mathbf{x})$. This tree is fit using only those randomly selected observations
4. Compute the optimal terminal node predictions, $\rho_1, \ldots, \rho_K$, as

$$\rho_k = \arg\min_\rho \sum_{\mathbf{x}_i \in S_k} L(y_i, \hat{F}_{m-1}(\mathbf{x}_i) + \rho) \tag{13}$$

   where S_k is the set of $\mathbf{x}$s that define terminal node k. Again this step uses only the randomly selected observations.
5. Update $\hat{F}_m(\mathbf{x})$ as

$$\hat{F}_m(\mathbf{x}) = \hat{F}_{m-1}(\mathbf{x}) + \lambda \rho_{k(\mathbf{x})} \tag{14}$$

   where $k(\mathbf{x})$ indicates the index of the terminal node into which an observation with features $\mathbf{x}$ would fall.

Tuning parameters for boosting trees

- The number of trees M. Large M leads to overfit. (not a tuning parameter for bagging)
- The learning rate λ.
- The number d in splits in each tree (the size of each tree). Often $d = 1$ works well, in which case each tree is a *stump*, consisting of a single split

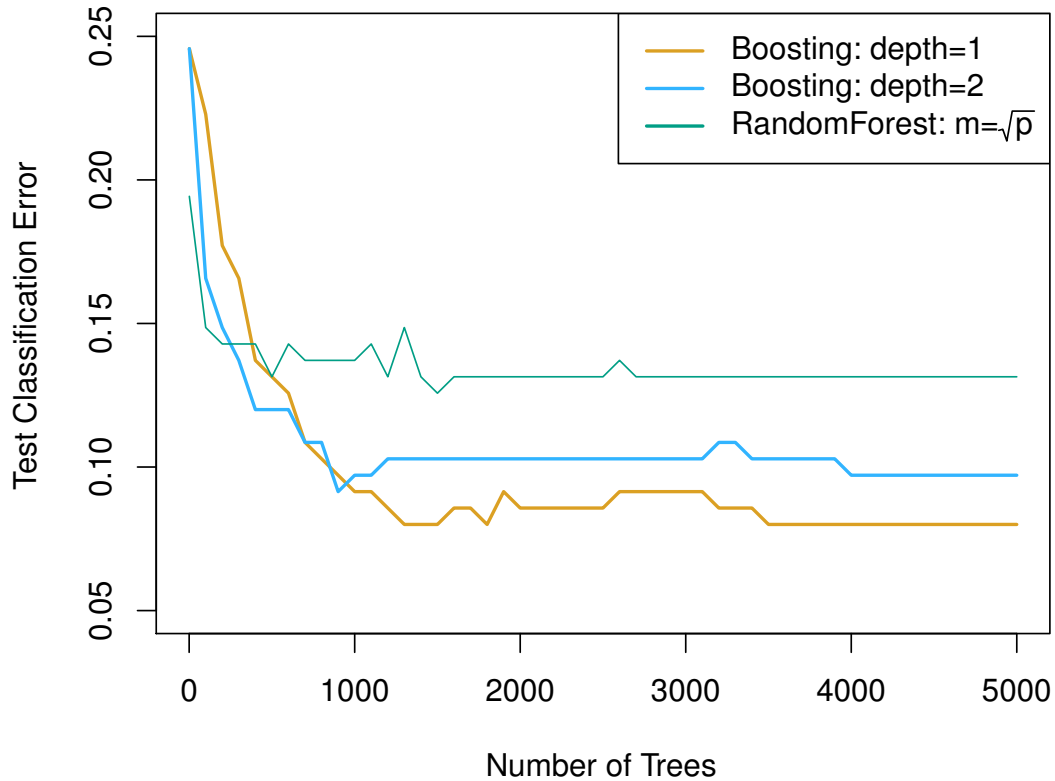

Figure: 8.11. Results from performing boosting and random forests on the 15-class gene expression data set in order to predict cancer versus normal. The test error is displayed as a function of the number of trees. For the two boosted models, $\lambda = 0.01$. Depth-1 trees slightly outperform depth-2 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%.

Forward Stagewise linear regression

Consider a set of fixed basis functions $\{T_k\}_{k=1,\ldots,K}$.

- Initialze $\check{\alpha}_k = 0, k = 1, \ldots, K$. Set $\epsilon > 0$ to some small constant, and M large.
- For $m = 1$ to M:
  - (a) $(\beta^*, k^*) = \arg\min_{\beta,k} \sum_{i=1}^N \left(y_i - \sum_{l=1}^K \check{\alpha}_l T_l(\mathbf{x}_i) - \beta T_k(\mathbf{x}_i) \right)$
  - (b) $\check{\alpha}_{k^*} \leftarrow \check{\alpha}_{k^*} + \epsilon \cdot \text{sign}(\beta^*)$.
- Output $F_M(\mathbf{x}) = \sum_{k=1}^K \check{\alpha}_k T_k(\mathbf{x})$.

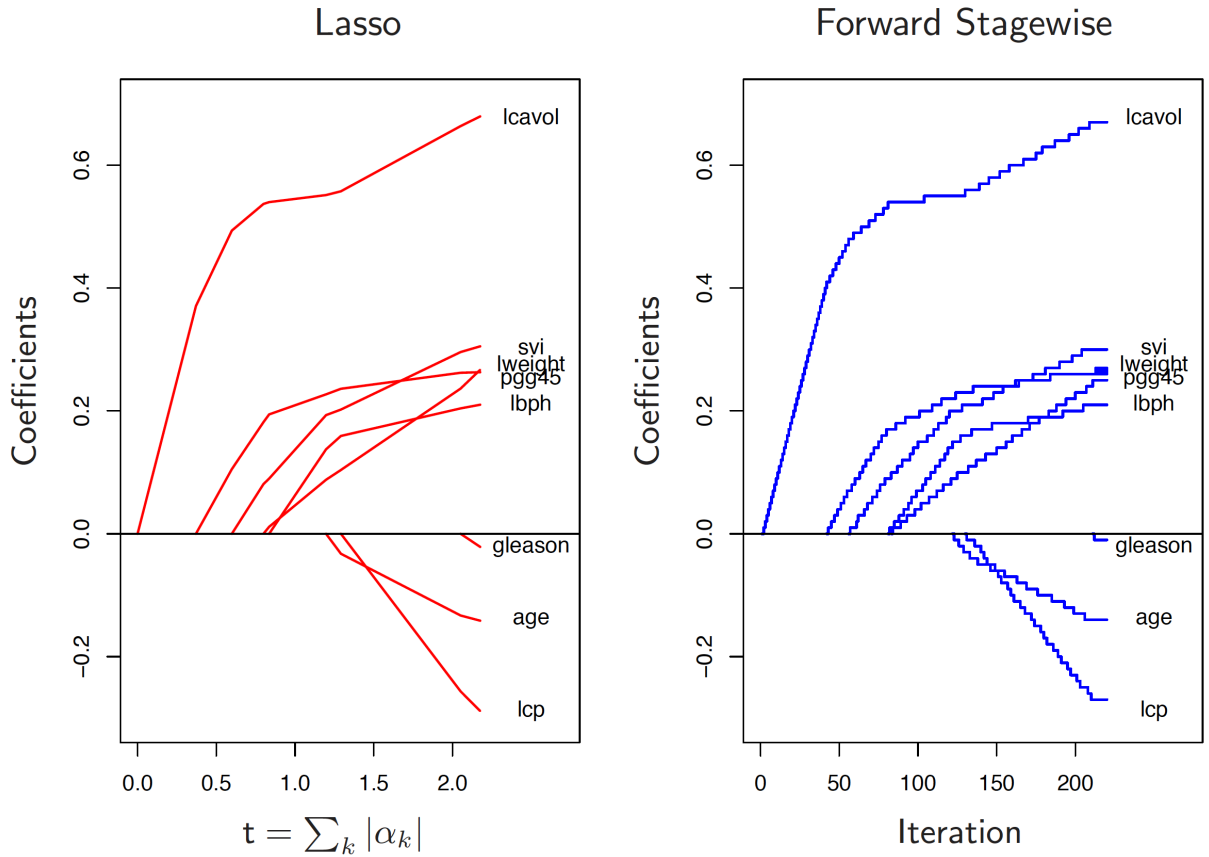

Figure: Profiles of estimated coefficients from linear regression, for the prostate data. The left panel shows the results from the Lasso, for different values of the bound parameter $t = \sum_k |\alpha_k|$. The right panel shows the results of the forward stagewise linear regression, using $M = 220$ consecutive steps of size $\epsilon = 0.01$.

Summary: Statistical view of boosting methods

Boosting methods have three important properties that contribute to their success:

- they fit an additive model in a flexible set of basis functions.
- they use a suitable loss function for the fitting process.
- they regularize by forward stagewise fitting; with shrinkage this mimics an L_1 (Lasso) penalty on the weights.