Advanced Computational Econometrics: Machine Learning

Chapter 5: Tree-based and ensemble methods

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Spring 2023

Tree-based methods

- Here we describe tree-based methods for regression and classification.
- These involve recursively segmenting the predictor space into a number of simple regions.
- Since the set of splitting rules used to segment the predictor space can be summarized in a tree, these types of approaches are known as tree-based methods.

Tree-based methods

- Tree-based methods are simple and useful for interpretation.
- However they typically are not competitive with the best supervised learning approaches in terms of prediction accuracy.
- Hence we also discuss two methods for combining several trees:
  - Bagging and
  - Random forests.

  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 interpretability.

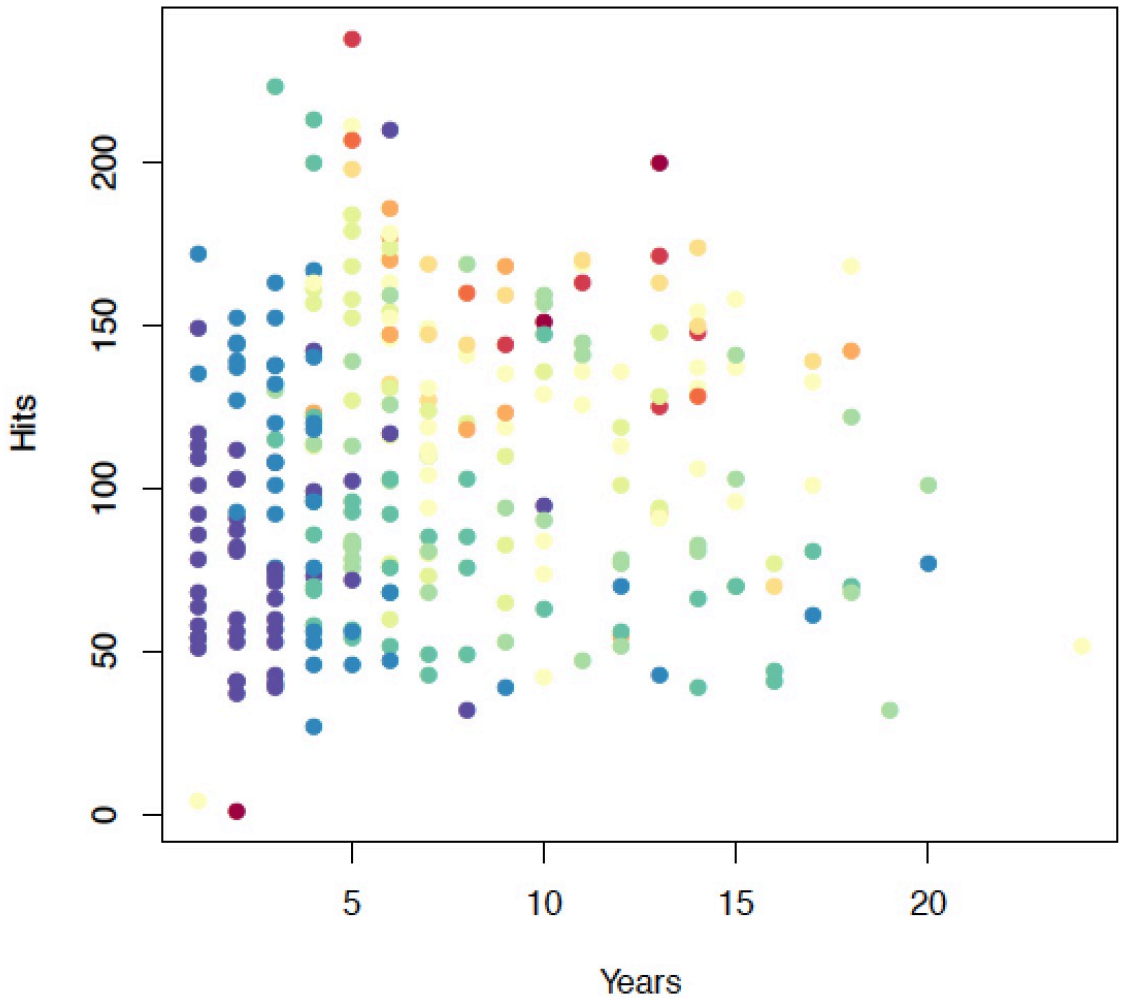
Regression and classification trees

- The tree-based approach can be applied to both regression and classification problems.
- We first consider regression trees, and then move on to classification/decision trees.

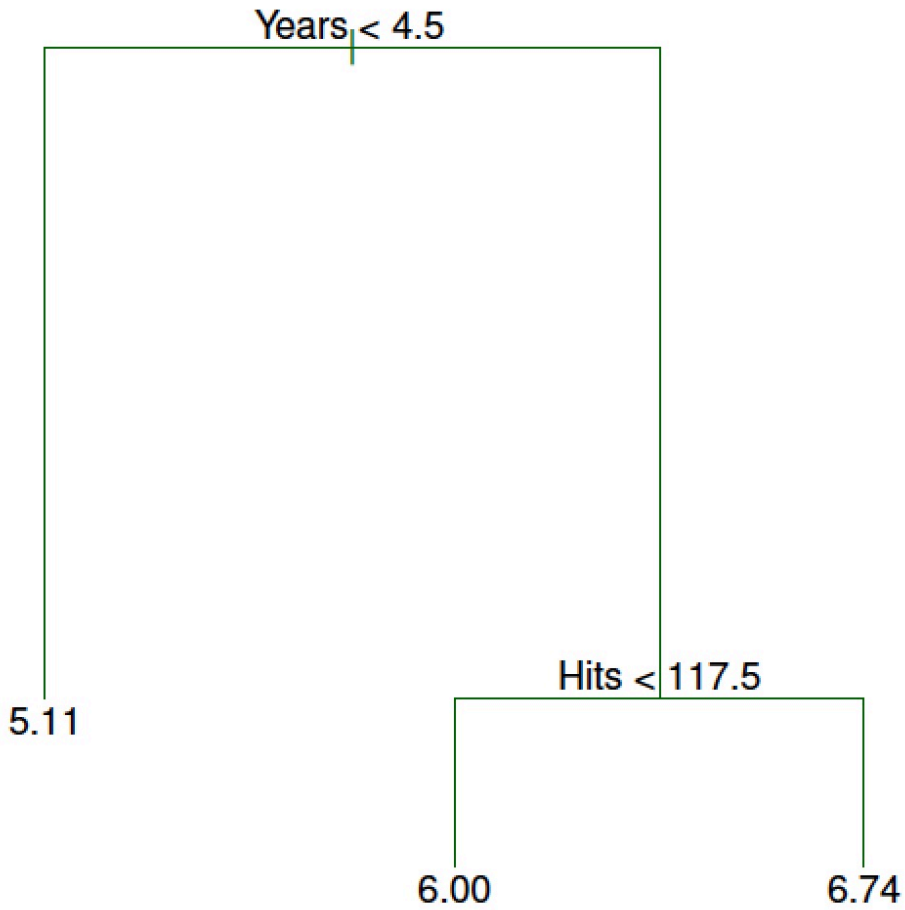
Overview

Baseball salary data

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



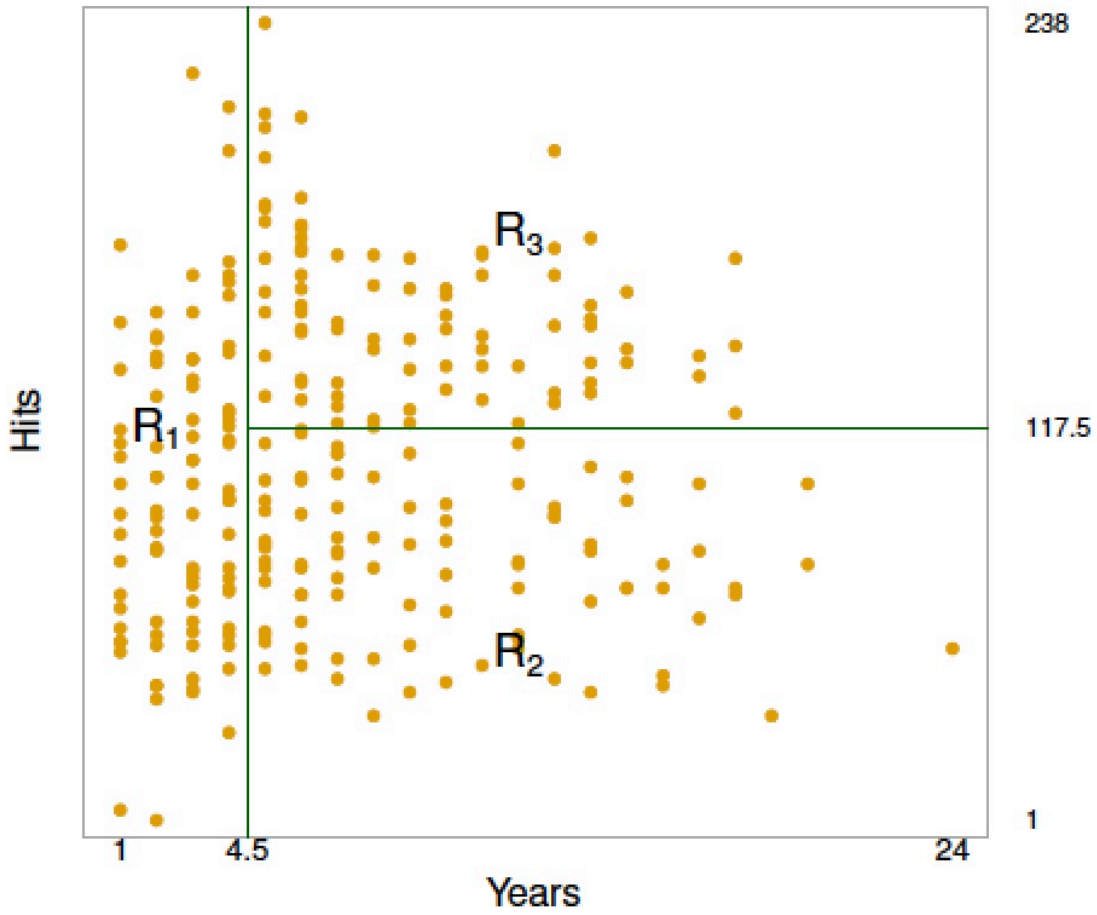
Regression tree for these data



- At a given internal node, the label (of the form $X_j < s$) indicates the left-hand branch emanating from the split, and the right-hand branch corresponds to $X_j \geq s$.
- 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.

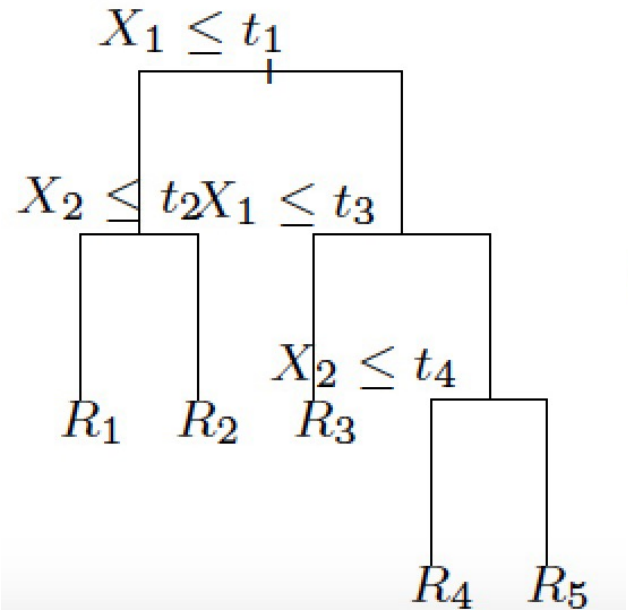
Results

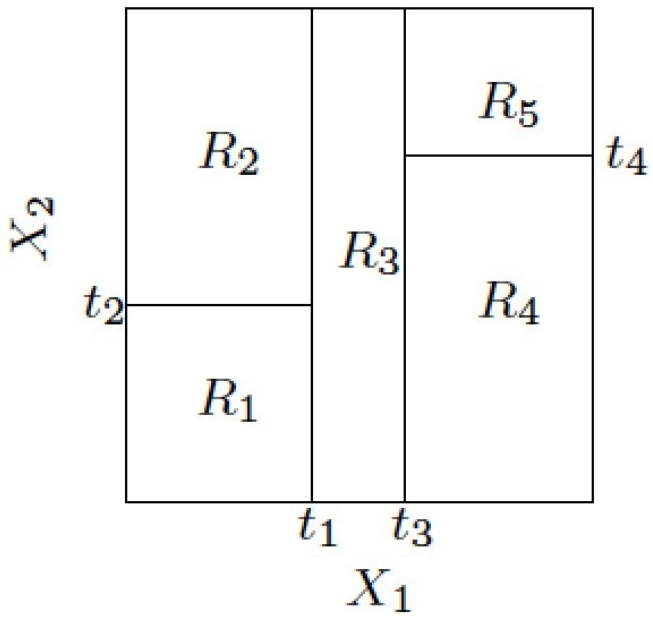
Overall, the tree stratifies or segments the players into 3 regions of predictor space: $R_1 = \{X : Years < 4.5\}$, $R_2 = \{X : Years \geq 4.5, Hits < 117.5\}$, and $R_3 = \{X : Years \geq 4.5, Hits \geq 117.5\}$.

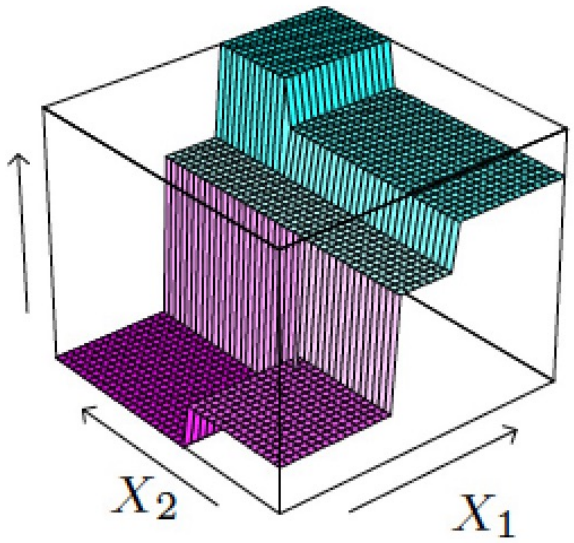


Predictions

- 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.
- The prediction function is, thus, stepwise constant.







Overview

Overview

Growing a regression tree

- We now turn to the question of how to grow a regression tree.
- Our training set consists of p predictors and a response, for each of n observations: that is, $\{(x_i, y_i)\}_{i=1}^n$, with $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$.
- The algorithm needs to automatically decide on
  1. The splitting variables and split points
  2. What topology (shape) the tree should have.

Predicted response in a given region

- Suppose first that we have a partition into M regions $R_1, R_2, \ldots, R_M$, and we model the response as a constant c_m in each region:

$$f(x) = \sum_{m=1}^{M} c_m \, I(x \in R_m)$$

- If we adopt as our criterion minimization of the RSS error, we have

$$\text{RSS}(c_1, \ldots, c_M) = \sum_{i=1}^{n} (y_i - f(x_i))^2 = \sum_{m=1}^{M} \sum_{\{i : x_i \in R_m\}} (y_i - c_m)^2$$

The LS estimate of c_m is, thus, the average of y_i in region R_m:

$$\widehat{c}_m = \text{Ave}\left\{ y_i : x_i \in R_m \right\}.$$

Finding the best partition

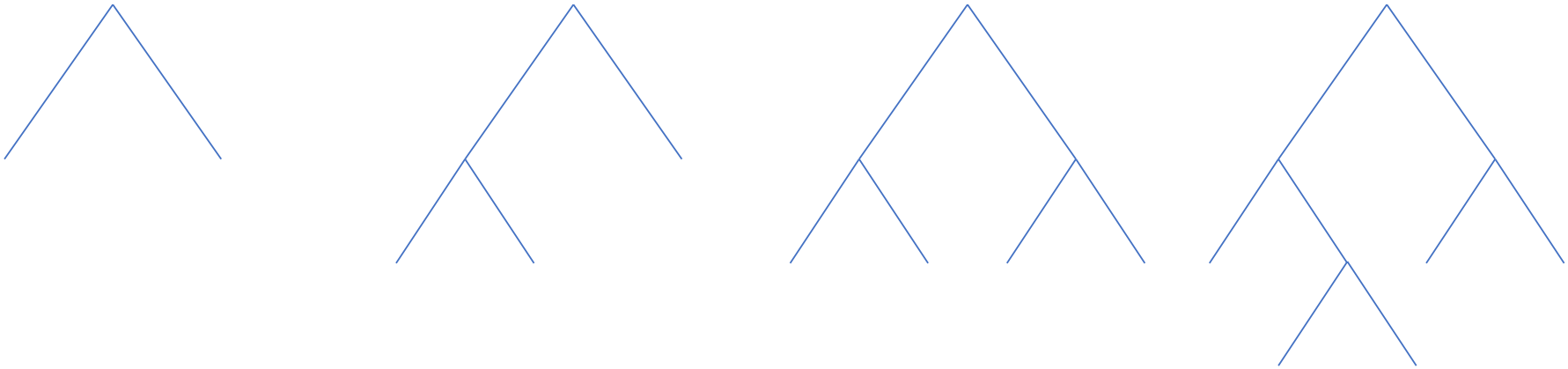
- The best partition in M regions, according to the RSS error, is defined as the solution of the following optimization problem:

$$\min_{R_1,\ldots,R_M} \sum_{m=1}^{M} \sum_{\{i:x_i \in R_m\}} (y_i - \widehat{c}_m)^2$$

- Solving this problem exactly in computationally infeasible. We use a heuristic algorithm that finds only an approximate solution.

Top-down, greedy approach

- We start at the top of the tree and successively split the predictor space; each split is indicated via two new branches further down on the tree.
- 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.



Selecting a splitting variable and split point

- Starting with all of the data, consider a splitting variable X_j and split point s, and define the pair of half-spaces

$$R_1(j,s) = \{X : X_j \leq s\} \text{ and } R_2(j,s) = \{X : X_j > s\}$$

- Then we seek the splitting variable X_j and split point s that solve

$$\min_{j,s} \left[\sum_{x_i \in R_1(j,s)} (y_i - \widehat{c}_1(j,s))^2 + \sum_{x_i \in R_2(j,s)} (y_i - \widehat{c}_2(j,s))^2 \right]$$

with

$$\widehat{c}_1(j,s) = \text{Ave}\{y_i : x_i \in R_1(j,s)\} \text{ and } \widehat{c}_2(j,s) = \text{Ave}\{y_i : x_i \in R_2(j,s)\}$$

- For each splitting variable, the determination of the split point s can be done very quickly and hence by scanning through all of the predictors, determination of the best pair (j,s) is feasible.

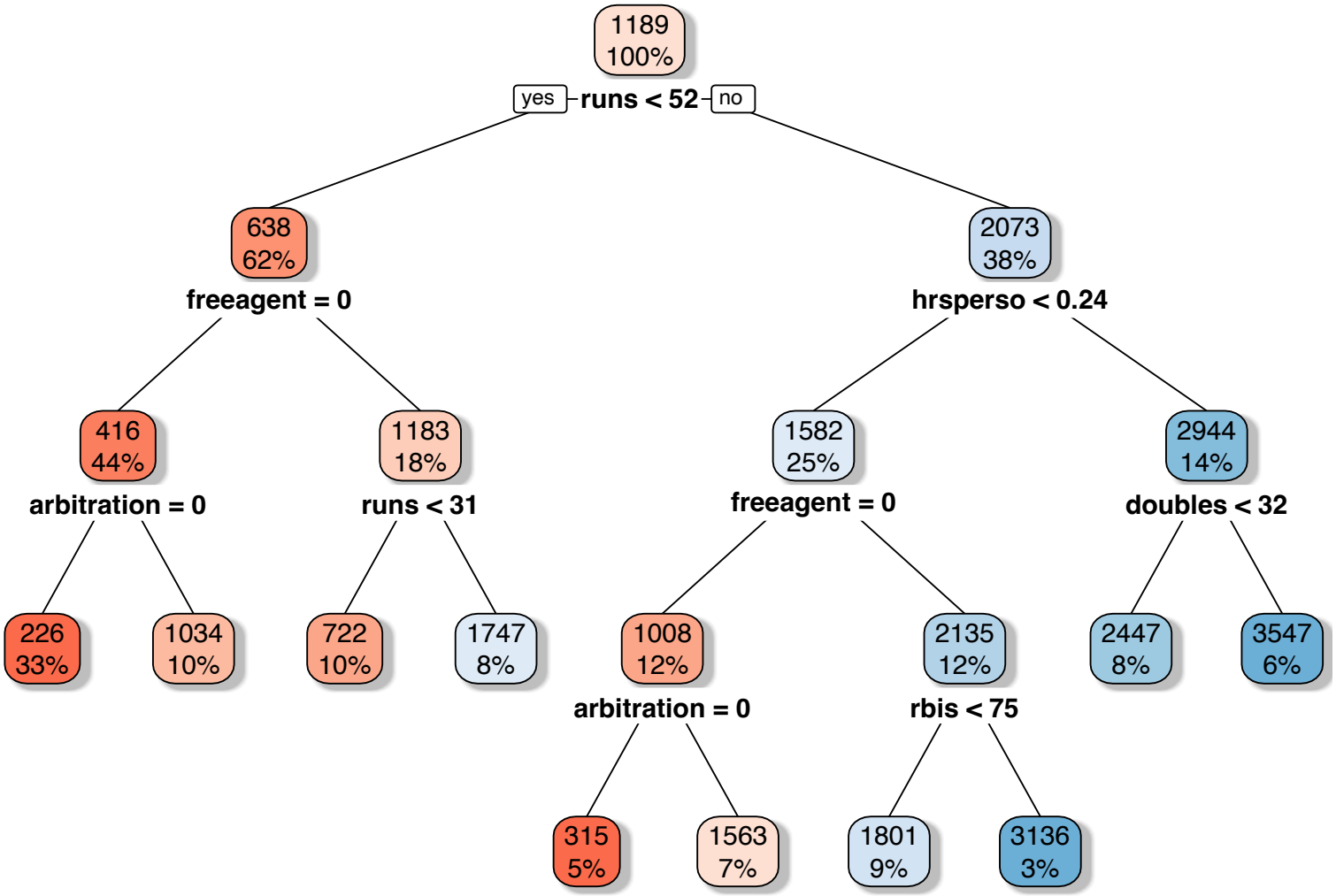
Recursive building process

- Having found the best split, we partition the data into the two resulting regions and repeat the splitting process on each of the two regions.
- Then this process is repeated on all of the resulting regions.
- How large should we grow the tree? Clearly a very large tree has a large variance and might overfit the data, while a small tree has a large bias and might not capture the important structure. (More on this later).

Regression trees in R

```
library(rpart)
baseball <- read.table("baseball.dat",header=TRUE)
n<-nrow(baseball)

train = sample(n, 2*n/3)
fit<-rpart(salary~.,data=baseball,subset=train,method="anova")

library(rpart.plot)
rpart.plot(fit, box.palette="RdBu", shadow.col="gray",
fallen.leaves=FALSE)
```

Regression trees in R



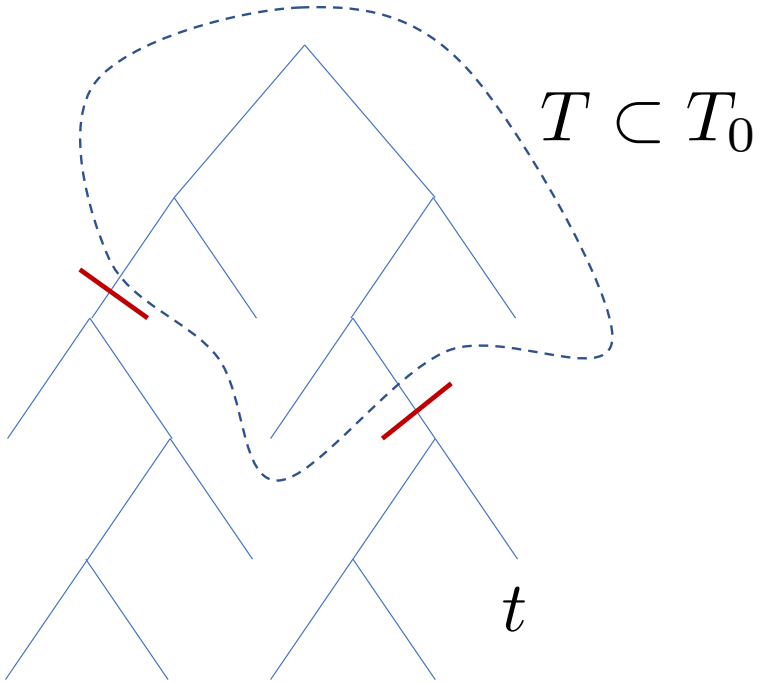
Overview

Tuning the model's complexity

- Tree size is a tuning parameter governing the model's complexity, and the optimal tree size should be adaptively chosen from the data.
- One approach would be to split tree nodes only if the decrease in sum-of-squares due to the split exceeds some threshold. This strategy is too short-sighted, however, since a seemingly worthless split might lead to a very good split below it.
- The preferred strategy is to grow a large tree T_0, stopping the splitting process only when some minimum node size (say 5) is reached. Then this large tree is pruned using cost-complexity pruning.

Notations

- We define a subtree $T \subset T_0$ to be any tree that can be obtained by pruning T_0, that is, collapsing any number of its internal nodes.
- We index terminal nodes by t, with node t representing region R_t.



Cost-complexity criterion

- Let $\widetilde{T}$ denote the set of terminal nodes in T. Let

$$n_t = \#\{x_i \in R_t\}, \quad \widehat{c}_t = \frac{1}{n_t} \sum_{x_i \in R_t} y_i,$$

$$\text{RSS}(T) = \sum_{t \in \widetilde{T}} \sum_{x_i \in R_t} (y_i - \widehat{c}_t)^2$$

- We define the cost-complexity criterion as

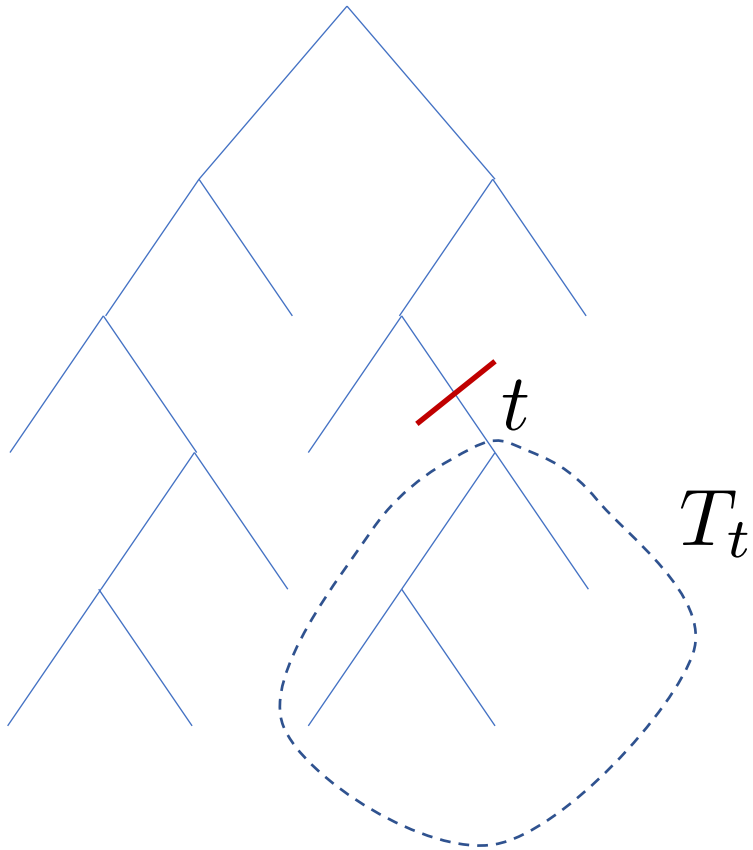
$$\boxed{C_\lambda(T) = \text{RSS}(T) + \lambda |\widetilde{T}|}$$

Cost-complexity pruning

- The idea is to find, for each λ, the subtree $T(\lambda) \subseteq T_0$ that minimizes $C_\lambda(T)$.
- The tuning parameter $\lambda \geq 0$ governs the tradeoff between tree size and its goodness of fit to the data. Larger values of λ result in smaller trees $T(\lambda)$.
- For $\lambda = 0$, the solution is the full tree T_0.
- Questions:
  1. For given λ, how to find a tree that minimizes $C_\lambda(T)$?
  2. How to choose λ?

Weakest link

- We start from the full tree T_0.
- For any internal node t, let T_t be the branch of T with root t.



Weakest link (continued)

- If we prune T_t, the cost-complexity criterion becomes smaller if

$$\text{RSS}(t) + \lambda < \text{RSS}(T_t) + \lambda|\widetilde{T}_t| \Leftrightarrow \lambda > \frac{\text{RSS}(t) - \text{RSS}(T_t)}{|\widetilde{T}_t| - 1} = g_0(t)$$

- The weakest link t_0 in T_0 is the node such that $g_0(t_0) = \min_t g_0(t)$. Let $\lambda_1 = g_0(t_0)$.
- Meaning: if we increase λ starting from 0, t_0 is the first node t such that pruning T_t improves the cost-complexity criterion.
- Let $T_1 = T_0 - T_{t_0}$. We again find the weakest link t_1 in T_1, etc.

Sequence of optimal trees

- By iterating the above process until the tree is reduced to the root node t_{root}, we get a decreasing sequence of trees

$$T_0 \supset T_1 \supset \ldots \supset t_{root},$$

  and an increasing sequence of λ values, $0 = \lambda_0 < \lambda_1 < \lambda_2 < \ldots$.
- We can show that, for all $k \geq 0$ and all $\lambda \in [\lambda_k, \lambda_{k+1})$, the optimum tree $T(\lambda)$ is equal to T_k.

Choosing λ

- If we have a lot of data, it is easy to estimate the sum-of-squares error of each subtree in the sequence $T_0 \supset T_1 \supset \ldots \supset t_{root}$ using a validation set. We choose the tree T_k with minimum validation error.
- Otherwise, we use cross-validation.

Cross-validation

- Using the whole training set, we get a sequence of trees, $T_0 \supset T_1 \supset \ldots \supset t_{root}$, where T_k is the best tree for $\lambda_k \leq \lambda < \lambda_{k+1}$.
- For $k = 0, 1, 2, \ldots$, set $\beta_k = \sqrt{\lambda_k \lambda_{k+1}}$
- Assume we use K-fold cross validation: we partition the training data in K subsets of approximately equal size.
- We construct K sequences of trees by leaving each of K subsets out and building the trees using the $K - 1$ remaining subsets. Let $T_0^{(r)} \supset T_1^{(r)} \supset \ldots \supset t_{root}^{(r)}$ be the sequence of trees obtained by leaving subset r out.
- Compute the cross-validated error $\text{RSS}_{cv}(T_k)$ by averaging the errors of trees $T^{(r)}(\beta_k)$, $r = 1, \ldots, K$.
- Select the tree T_k corresponding to the minimum cross-validated error.

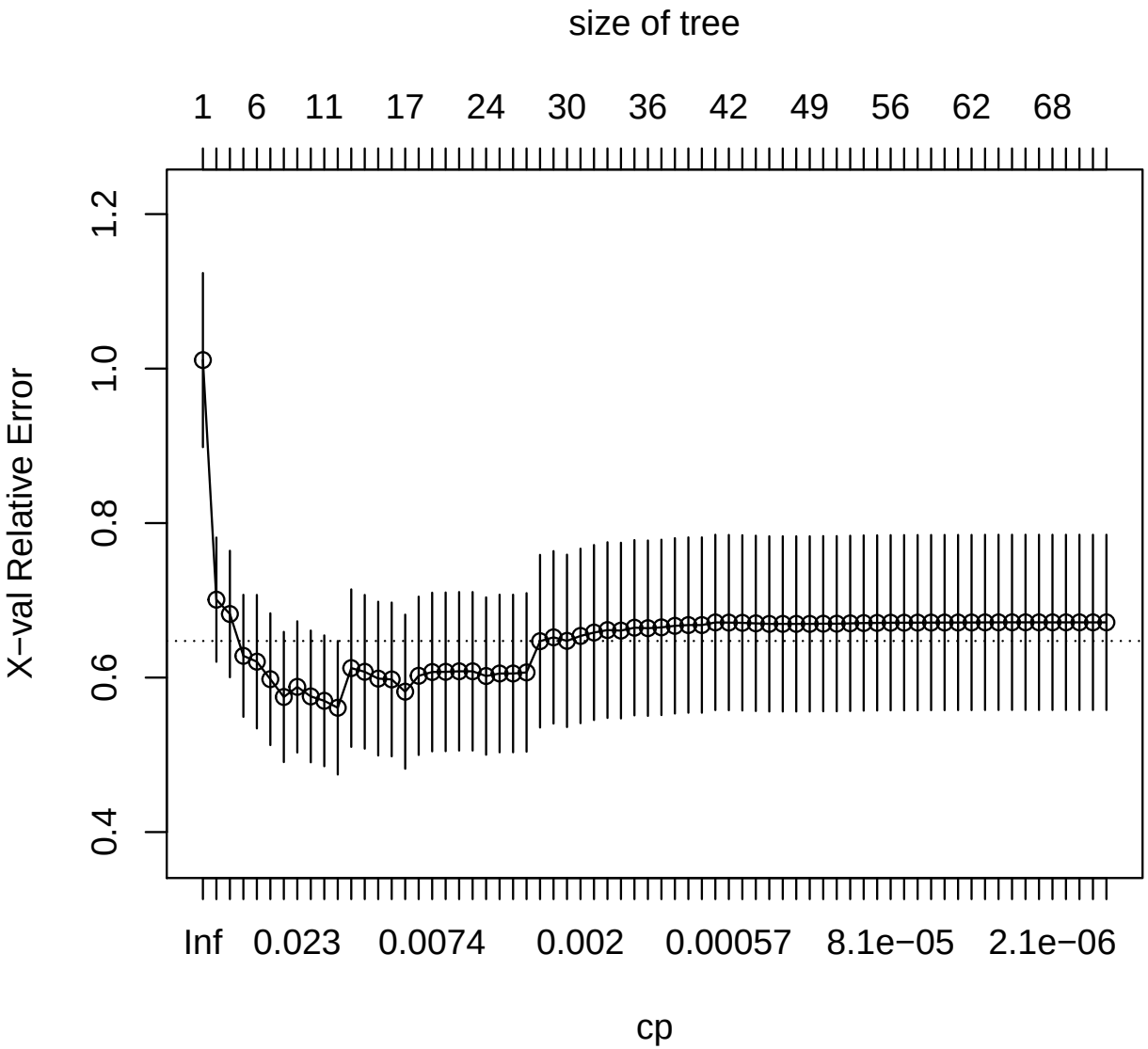
Pruning a regression tree in R

```
fit<-rpart(salary~.,data=baseball,subset=train,method="anova",
control = rpart.control(xval = 10, minbucket = 2,))

printcp(fit)
plotcp(fit)
```

Pruning a regression tree in R

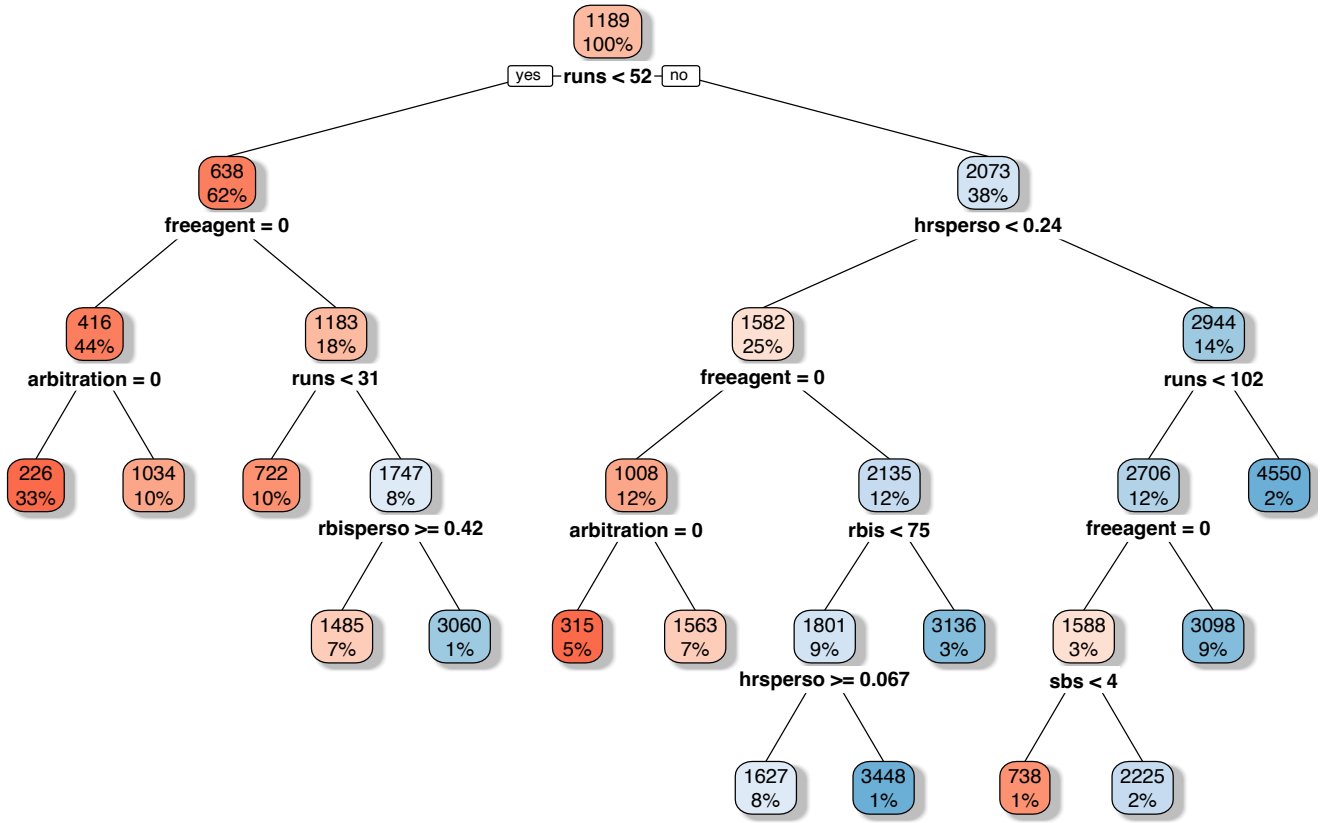
```
> printcp(fit)

Regression tree:
rpart(formula = salary ~ ., data = baseball, subset = train,
    method = "anova", control = rpart.control(xval = 10, minbucket = 2,
        cp = 0))

Variables actually used in tree construction:
 [1] arbitration  average      doubles      errors       freeagent    hits         hitspererror hitsperso    homeruns
[10] hrspererror  hrsperso     obp          obppererror  rbis         rbisperso    runs         runspererror runsperso
[19] sbs          sos          soserrors    triples      walks        walksperso

Root node error: 313437738/224 = 1399276

n= 224

           CP nsplit rel error  xerror     xstd
1  3.4783e-01      0  1.000000 1.00344 0.117517
2  1.1739e-01      1  0.652167 0.76437 0.092597
3  5.5625e-02      2  0.534779 0.70021 0.090761
4  5.3391e-02      3  0.479154 0.68278 0.094417
5  3.7790e-02      4  0.425763 0.63239 0.087908
6  3.7702e-02      5  0.387973 0.58561 0.084022
7  3.6599e-02      6  0.350271 0.58153 0.082973
8  3.3189e-02      7  0.313672 0.58220 0.083858
9  3.3163e-02      8  0.280483 0.57446 0.083812
10 2.9877e-02      9  0.247320 0.54956 0.082977
11 1.9796e-02     10  0.217443 0.46989 0.071235
12 1.9137e-02     11  0.197647 0.46028 0.070273
13 1.2088e-02     12  0.178510 0.45846 0.071254
14 1.1084e-02     13  0.166422 0.47282 0.069678
15 1.0561e-02     15  0.144254 0.47282 0.069678
16 8.7022e-03     16  0.133693 0.48546 0.071218
17 8.6945e-03     17  0.124991 0.49028 0.071321
```

Pruning a regression tree in R



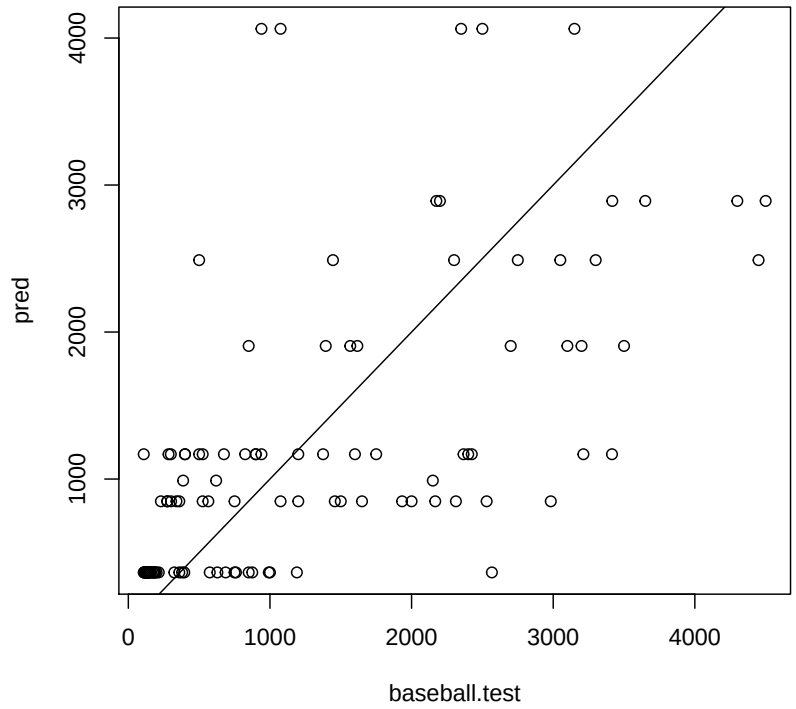
Pruning a regression tree in R

```
pruned_tree<-prune(fit,cp=1.2088e-02)
rpart.plot(pruned_tree, box.palette="RdBu", shadow.col="gray",
fallen.leaves=FALSE)
```



Prediction with a regression tree in R

```
yhat=predict(pruned_tree,newdata=baseball[-train,])
baseball.test=baseball[-train,"salary"]
plot(baseball.test,pred,xlab='observed',ylab='predicted')
abline(0,1,col="red")
```



Overview

Classification trees

- If the response is a categorical variable (factor) taking c values indexed by $1, 2, \ldots, c$, we have a classification problem.
- The only changes needed in the tree-growing algorithm concern the criteria for splitting nodes and pruning the tree.
- In classification, each split will aim at obtaining nodes as "pure" as possible (a node is pure if it contains observations from only one class). For that, we need to define a suitable impurity measure.

Notations

- In a node t, let

$$\widehat{p}_{tk} = \frac{1}{n_t} \sum_{x_i \in R_t} I(y_i = k)$$

  be the proportion of class k observations in node t.
- We have $\sum_{k=1}^{c} \widehat{p}_{tk} = 1$.
- We classify the observations in node t to the majority class in that node:

$$k(t) = \arg\max_k \widehat{p}_{tk},$$

Impurity measures

- Different measures Q_t of node impurity include the following:

  Misclassification error:

$$Q_t^{\text{mis}} = \frac{1}{n_t} \sum_{x_i \in R_t} I(y_i \neq k(t)) = 1 - \widehat{p}_{tk(t)}$$

  Gini index:

$$Q_t^{\text{Gini}} = \sum_{k=1}^{c} \widehat{p}_{tk}(1 - \widehat{p}_{tk})$$

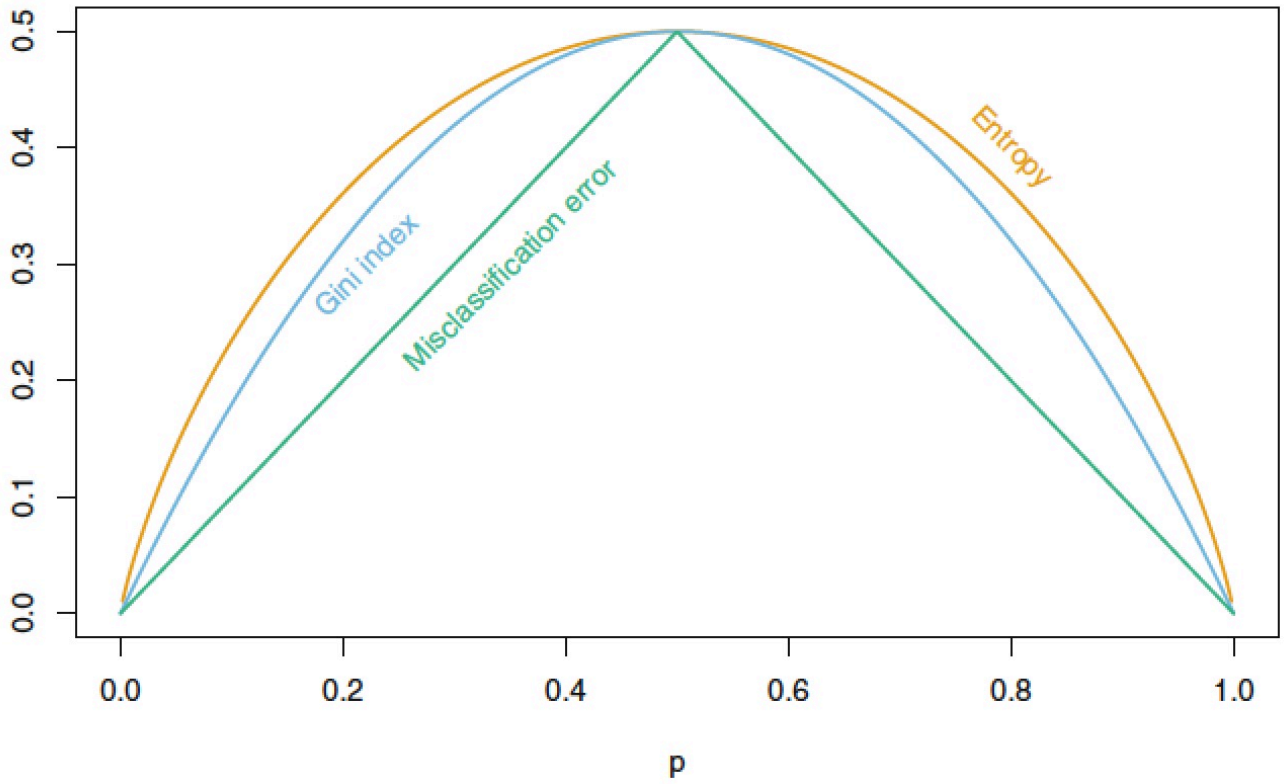
  Entropy:

$$Q_t^{\text{ent}} = -\sum_{k=1}^{c} \widehat{p}_{tk} \log \widehat{p}_{tk}$$

- All three criteria are equal to 0 when $\widehat{p}_{tk} = 1$ for some k, and are maximum when $\widehat{p}_{tk} = 1/c$ for all k.

Comparison between impurity measures

- Plot as a function of the proportion p of one class in the case $c = 2$:



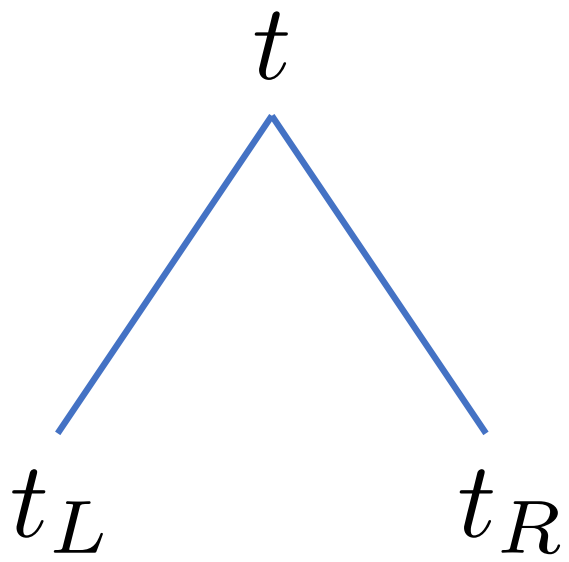
- All three are similar, but entropy and the Gini index are differentiable, and hence more amenable to numerical optimization.

Comparison between impurity measures

- In addition, entropy and the Gini index are more sensitive to changes in the node probabilities than the misclassification rate.
- For example, in a two-class problem with 400 observations in each class (denote this by (400, 400)), suppose one split created nodes (300, 100) and (100, 300), while the other created nodes (200, 400) and (200, 0).
- Both splits produce a misclassification rate of 0.25, but the second split produces a pure node and is probably preferable. Both the Gini index and entropy are lower for the second split. For this reason, either the Gini index or entropy should be used when growing the tree.
- To guide cost-complexity pruning, any of the three measures can be used, but typically we use the misclassification rate.

Selecting the best split

- Consider a node t with size n_t with impurity Q_t.
- For some variable j and split point s, we split t in two nodes, t_L and t_R, with sizes n_{t_L} and n_{t_R}, and with impurities Q_{t_L} and Q_{t_R}.



Selecting the best split

- The average decrease of impurity is

$$\Delta(j, s) = Q_t - \left(\frac{n_{t_L}}{n_t} Q_{t_L} + \frac{n_{t_R}}{n_t} Q_{t_R} \right)$$

- If Q_t is the entropy, then $\Delta(j, s)$ is interpreted as an information gain.
- We select at each step the splitting variable j and the split point s that maximizes $\Delta(j, s)$ or, equivalently, that minimizes the average impurity

$$\frac{n_{t_L}}{n_t} Q_{t_L} + \frac{n_{t_R}}{n_t} Q_{t_R}$$

Categorical predictors

- When splitting a predictor having q possible unordered values, there are $2^{q-1} - 1$ possible partitions of the q values into two groups.
- All the dichotomies can be explored for small q, but the computations become prohibitive for large q.
- In the 2-class case, this computation simplifies. We order the predictor levels according to the proportion falling in class 1. Then we split this predictor as if it were an ordered predictor. One can show this gives the optimal split, in terms of entropy or Gini index, among all possible $2^{q-1} - 1$ splits.
- The partitioning algorithm tends to favor categorical predictors with many levels q; the number of partitions grows exponentially in q, and the more choices we have, the more likely we can find a good one for the data at hand. This can lead to severe overfitting if q is large, and such variables should be avoided.

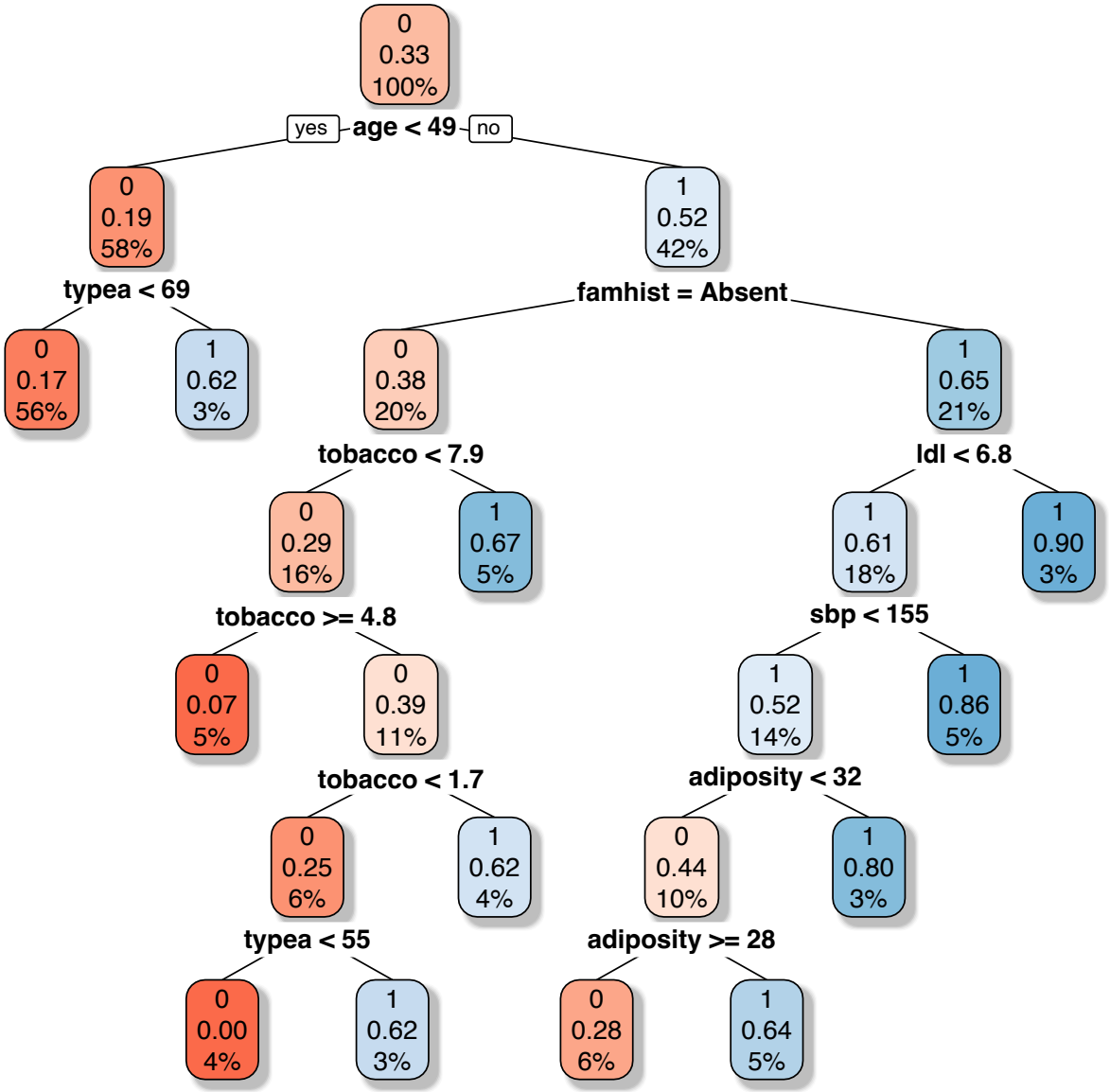
Example: Heart data

- A retrospective sample of males in a coronary heart disease (CHD) high-risk region of the Western Cape, South Africa.
- There are roughly two controls per positive case of CHD.
- Variables:
  - sbp: systolic blood pressure
  - tobacco: cumulative tobacco (kg)
  - ldl: low density lipoprotein cholesterol
  - adiposity
  - famhist: family history of heart disease (Present, Absent)
  - typea: type-A behavior
  - obesity
  - alcohol: current alcohol consumption
  - age: age at onset
  - chd: response, coronary heart disease

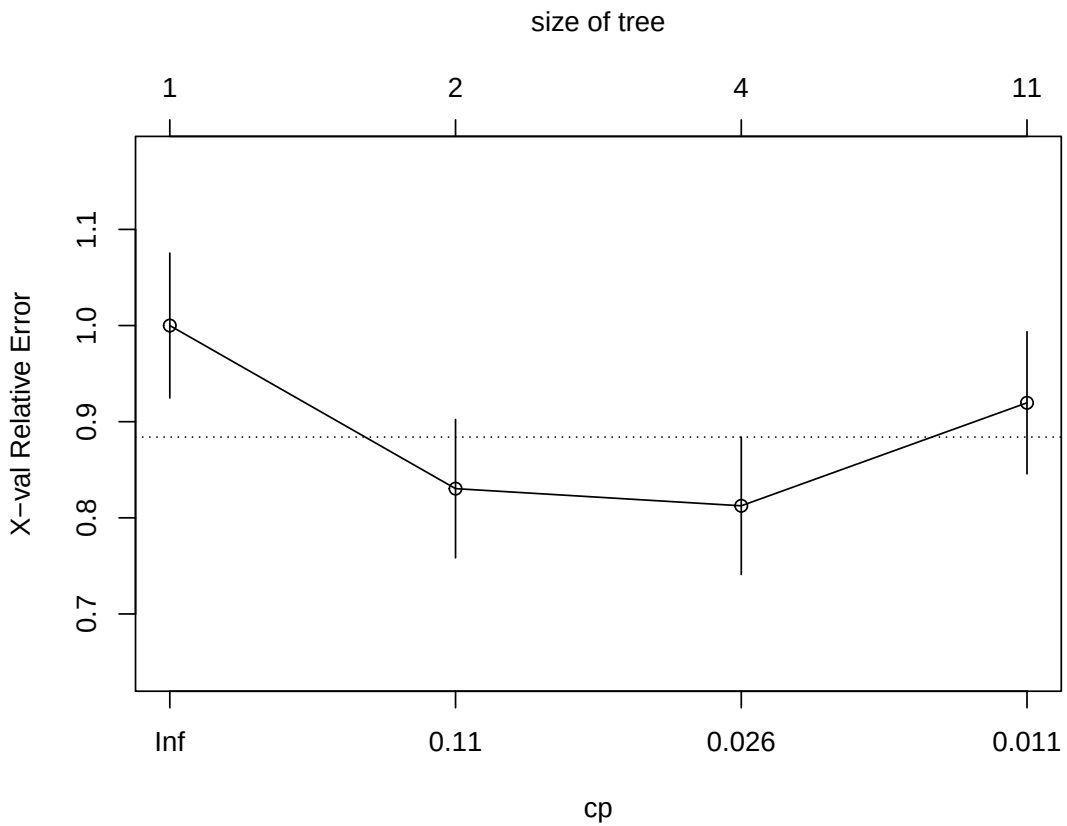
Tree growing in R

```
heart<-read.table(file = "SAheart.data",sep=",",header=T,
          row.names=1)
n<-nrow(heart)

train = sample(n, 2*n/3)
fit <- rpart(chd ~ ., data = heart, method="class",
          subset=train, parms = list(split = 'gini'))
rpart.plot(fit, box.palette="RdBu", shadow.col="gray",
          fallen.leaves=FALSE)

plotcp(fit)
```

Tree


0
0.33
100%
yes
age < 49
no
0
0.19
58%
1
0.52
42%
typea < 69
famhist = Absent
0
0.17
56%
1
0.62
3%
0
0.38
20%
1
0.65
21%
tobacco < 7.9
ldl < 6.8
0
0.29
16%
1
0.67
5%
1
0.61
18%
1
0.90
3%
tobacco >= 4.8
sbp < 155
0
0.07
5%
0
0.39
11%
1
0.52
14%
1
0.86
5%
tobacco < 1.7
adiposity < 32
0
0.25
6%
1
0.62
4%
0
0.44
10%
1
0.80
3%
typea < 55
adiposity >= 28
0
0.00
4%
1
0.62
3%
0
0.28
6%
1
0.64
5%

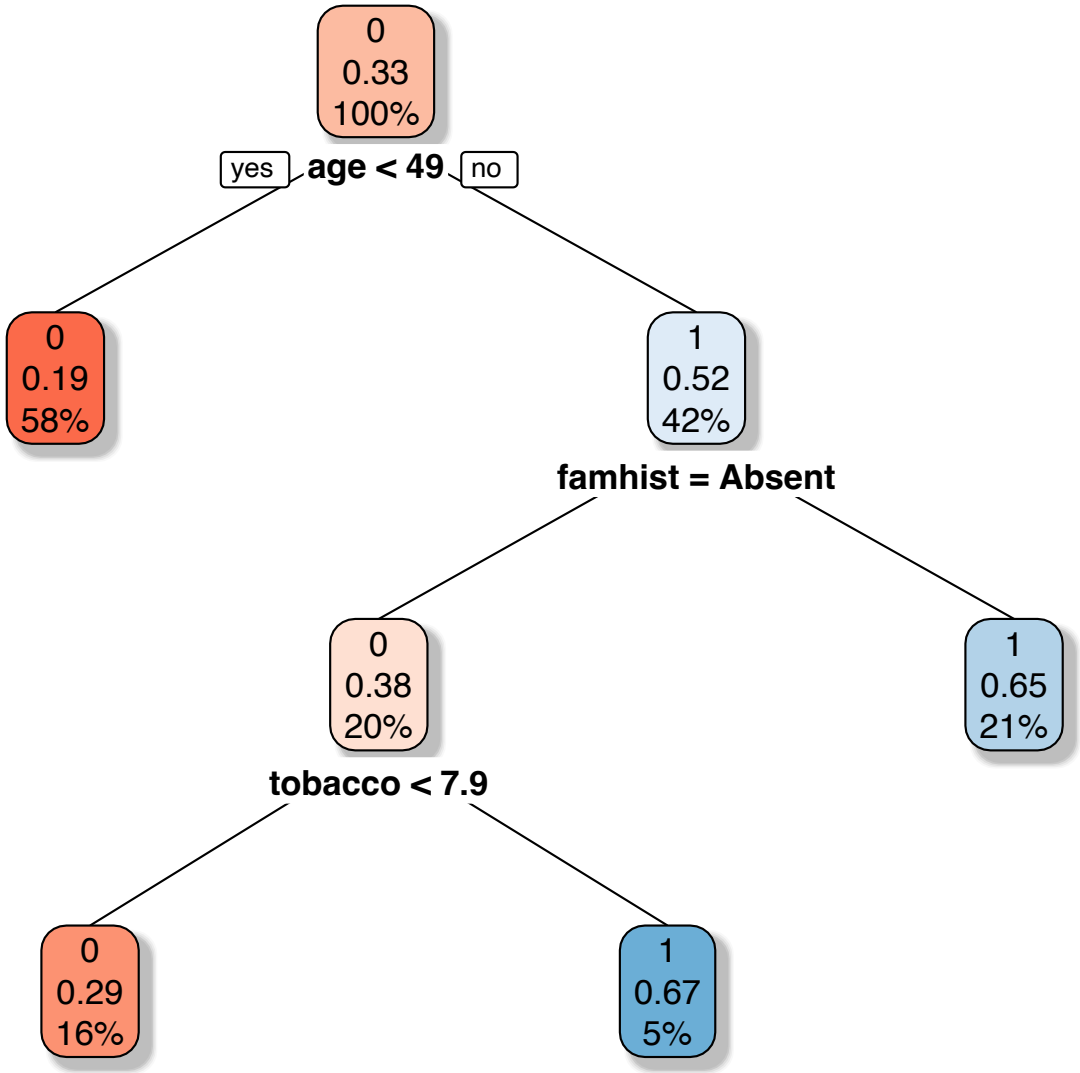
Cross-validation error



Pruning

```
pruned_tree<-prune(fit,cp=0.026)
rpart.plot(pruned_tree, box.palette="RdBu", shadow.col="gray",
           fallen.leaves=FALSE)
```

Pruned tree


0
0.33
100%
yes
age < 49
no
0
0.19
58%
1
0.52
42%
famhist = Absent
0
0.38
20%
1
0.65
21%
tobacco < 7.9
0
0.29
16%
1
0.67
5%

Test error rate estimation

```
yhat=predict(pruned_tree,newdata=heart[-train,],type='class')
y.test=heart[-train,"chd"]
table(y.test,yhat)
err<-1-mean(y.test==yhat)
```

- Confusion matrix:

	prediction	
true class	0	1
0	82	13
1	28	31

- Test error rate: 0.27

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.
- Unfortunately, trees generally do not have the same level of predictive accuracy as some of the other modern regression and classification approaches.
- However, by aggregating many decision trees, the predictive performance of trees can be substantially improved.
- We will see two combination methods, both based on the same resampling technique: the bootstrap.

Overview

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The bootstrap

- The bootstrap is a flexible and powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- For example, it can provide an estimate of the standard error of an estimator, or a confidence interval for a parameter.

A simple problem

- Let $X \sim F_\theta$ be a random variable whose distribution depends on a parameter θ.
- Assume that we have an iid sample $X_1, \ldots, X_n$ and an estimator $\widehat{\theta}(X_1, \ldots, X_n)$ of θ.
- How to estimate the standard error $\text{se}(\widehat{\theta})$ of $\widehat{\theta}$?
- In simple cases a closed-form expression of $\text{se}(\widehat{\theta})$ can be derived, but most of the times it cannot.

Ideal solution

If we could draw a large number N of datasets from the same distribution, we could compute the corresponding realizations of $\widehat{\theta}$:

$$x_1^{(1)}, \ldots, x_n^{(1)} \longrightarrow \widehat{\theta}^{(1)}$$
$$\vdots$$
$$x_1^{(N)}, \ldots, x_n^{(N)} \longrightarrow \widehat{\theta}^{(N)}$$

and estimate $\text{se}(\widehat{\theta})$ by the empirical standard deviation:

$$\widehat{\text{se}}(\widehat{\theta}) = \sqrt{\frac{1}{N}\sum_{r=1}^{N}(\widehat{\theta}^{(r)} - \overline{\widehat{\theta}})^2} \xrightarrow{P} \text{se}(\widehat{\theta})$$

Real life solution

- In real life, we only have one realization $x_1, \ldots, x_n$ of the sample and we do not know the true distribution.
- The bootstrap idea is to replace the true distribution by the empirical distribution, with a mass $1/n$ on each observation x_i.
- To draw a bootstrap dataset $x_1^*, \ldots, x_n^*$, we randomly draw n observations from $x_1, \ldots, x_n$ with replacement.
- For instance, if $n = 5$, the sample is $(0.5, 1.2, -0.3, 0.8, -1.4)$ and $\widehat{\theta}$ is the mean, we have the following $B = 3$ bootstrap samples and corresponding values of $\widehat{\theta}^*$:

$$
\begin{aligned}
(-0.30, 0.50, 0.50, 0.80, -0.30) &\longrightarrow 0.24 \\
(0.8, -0.3, 0.5, 0.8, -0.3) &\longrightarrow 0.3 \\
(1.20, 1.20, 0.80, 0.80, 1.20) &\longrightarrow 1.04
\end{aligned}
$$

Bootstrap estimation of the standard error

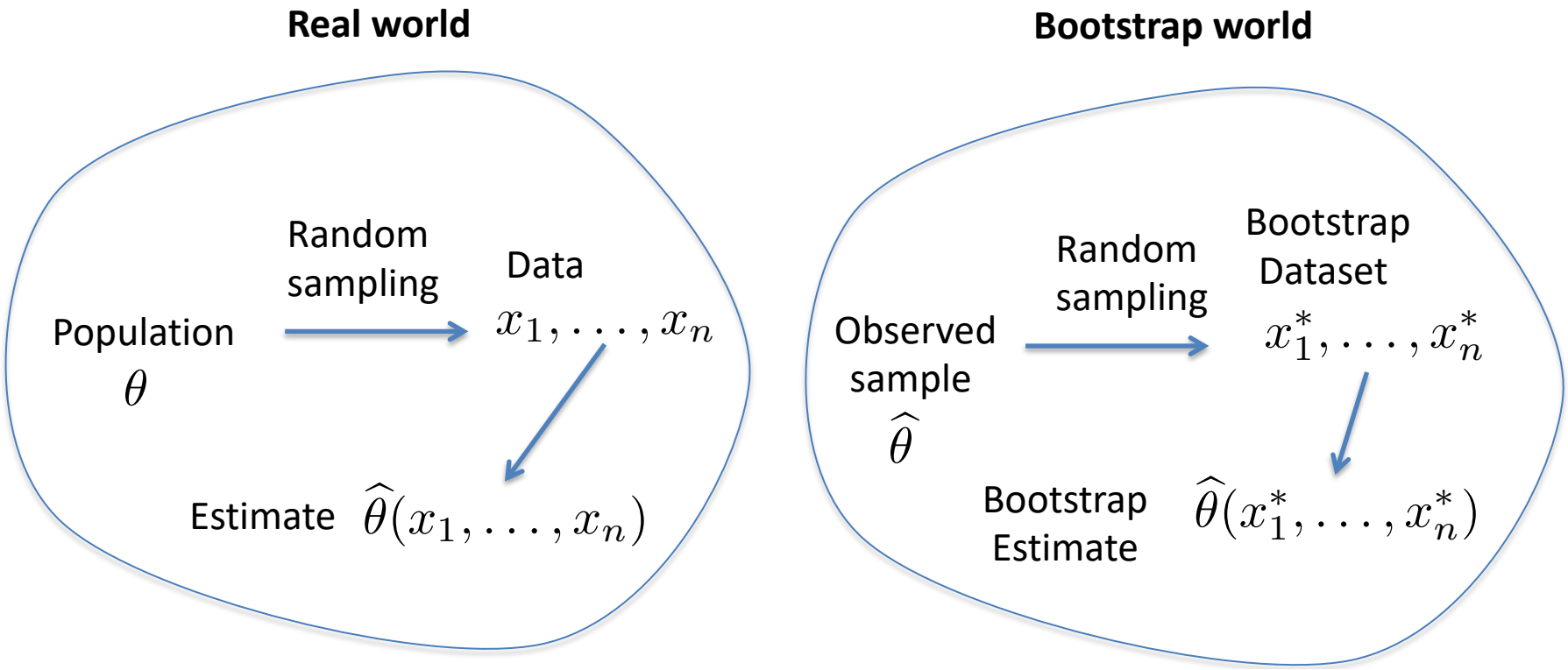
- To estimate the standard error using the bootstrap, we generate B bootstrap datasets $x_1^{*b}, \ldots, x_n^{*b}$, $b = 1, \ldots, B$ and we compute the corresponding estimates $\widehat{\theta}^{*b} = \widehat{\theta}(x_1^{*b}, \ldots, x_n^{*b})$, $b = 1, \ldots, B$.
- The bootstrap estimate of standard error is then

$$\widehat{\text{se}}_B(\widehat{\theta}) = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}(\widehat{\theta}^{*(b)} - \overline{\widehat{\theta}^*})^2}.$$

with

$$\overline{\widehat{\theta}^*} = \frac{1}{B}\sum_{b=1}^{B}\widehat{\theta}^{*(b)}$$

General picture of the bootstrap



Overview

Bagging

- Bootstrap aggregation, or bagging, is a general-purpose procedure for reducing the variance of a statistical learning method; we introduce it here because it is particularly useful and frequently used in the context of decision trees.
- Recall that given a set of n independent observations $X_1, \ldots, X_n$, each with variance σ^2, the variance of the mean $\overline{X}$ 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 and we train B decision trees, one from each bootstrap dataset.
- For regression problems, we then average all the predictions to obtain

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

where $\widehat{f}^{*b}(x)$ is the prediction at x for the b-th tree.

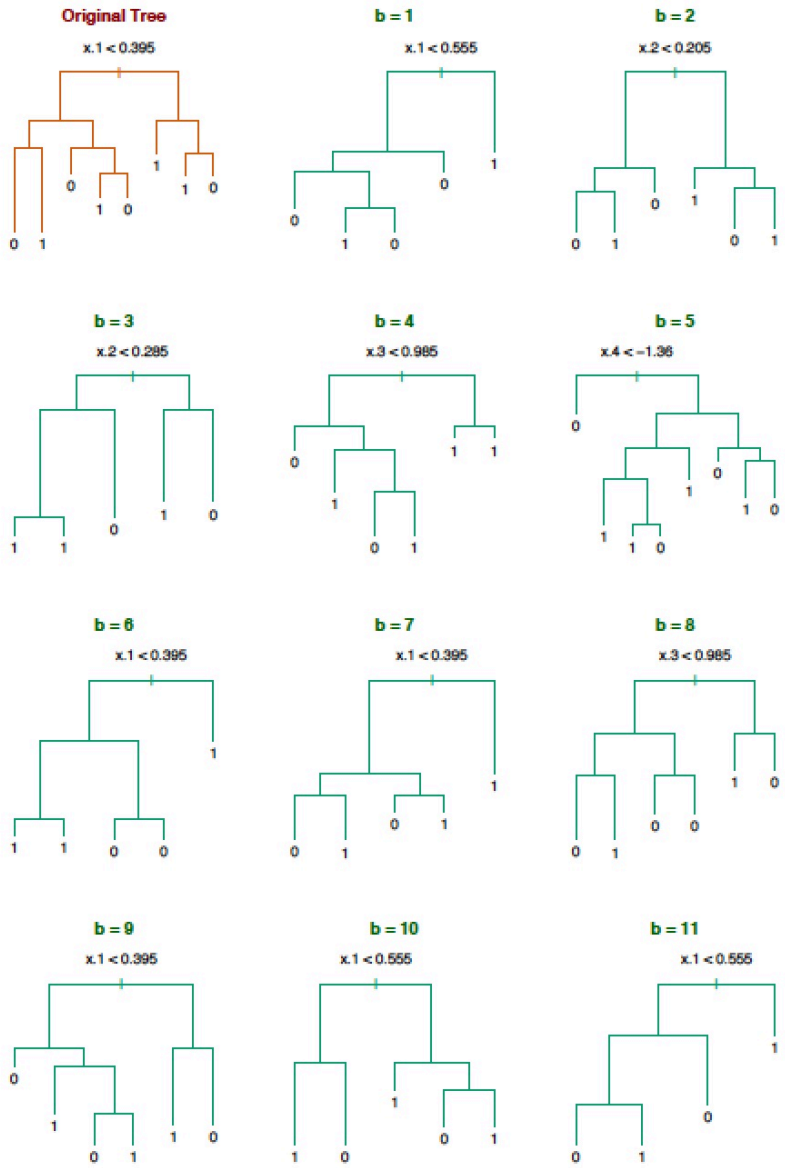
Bagging classification trees

- The above prescription 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 majority class among the B predictions.
- If we are interested in the posterior class probabilities, we can rather average the class proportions in the terminal nodes.

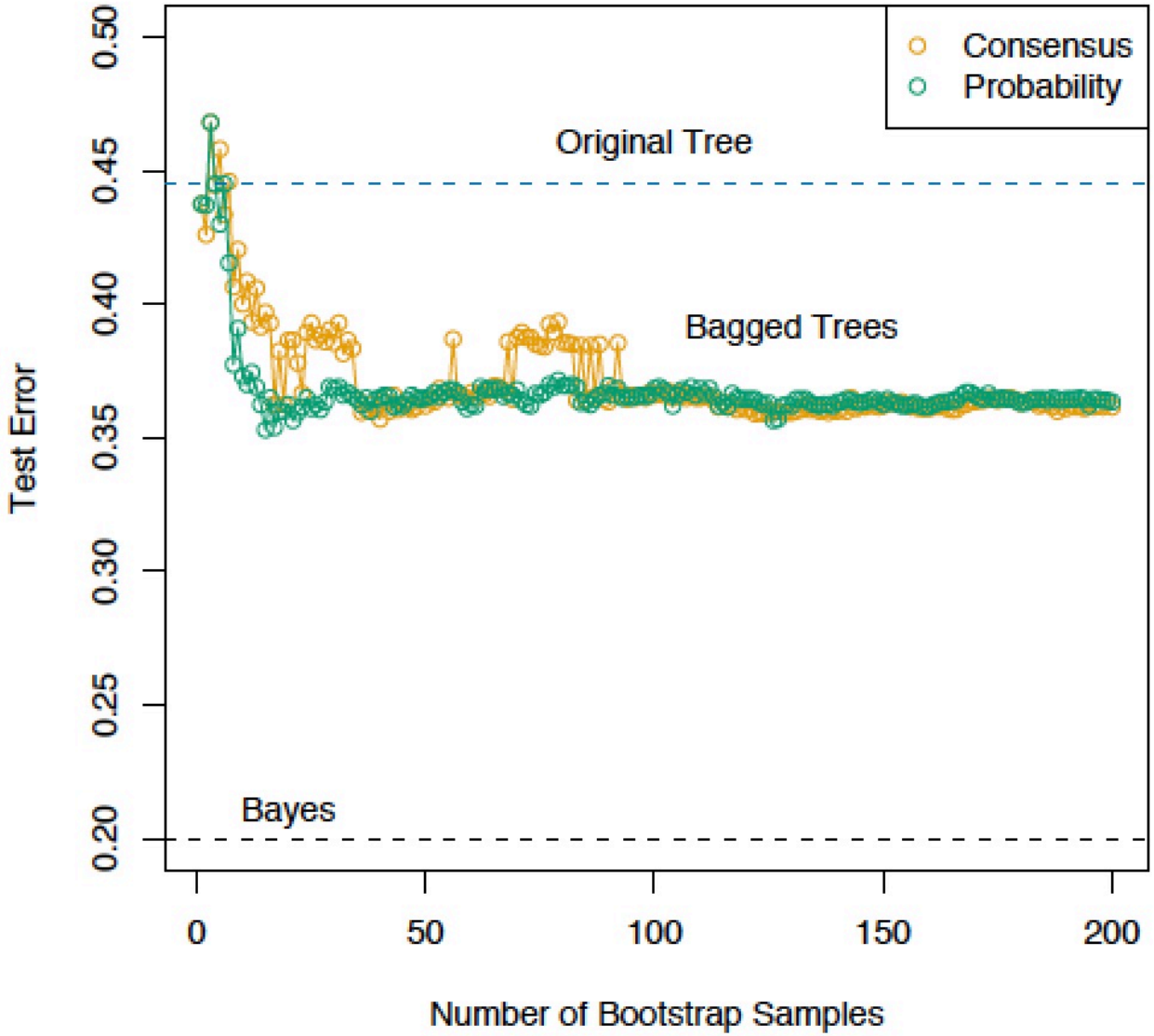
Example

- We generated a sample of size $n = 30$, with two classes and $p = 5$ predictors, each having a standard Gaussian distribution with pairwise correlation 0.95.
- The response Y was generated according to $\mathbb{P}(Y = 1 \mid x_1 \leq 0.5) = 0.2$, $\mathbb{P}(Y = 1 \mid x_1 > 0.5) = 0.8$. The Bayes error is 0.2.
- A test sample of size 2000 was also generated from the same population.
- We fit classification trees to the training sample and to each of $B = 200$ bootstrap samples. No pruning was used.

Bagged decision trees



Error curves



Out-of-Bag Error Estimation

- It is a straightforward way to estimate the test error of a bagged model.
- Recall that the key to bagging is that trees are repeatedly fit to bootstrapped subsets of the observations. One can show that on average, each bagged tree makes use of around two-thirds of the observations.
- The remaining one-third of the observations not used to fit a given bagged tree are referred to as the out-of-bag (OOB) observations.
- We can predict the response for the i-th observation using all trees in which that observation was OOB. This will yield around $B/3$ predictions for the i-th observation, which we average.

Overview

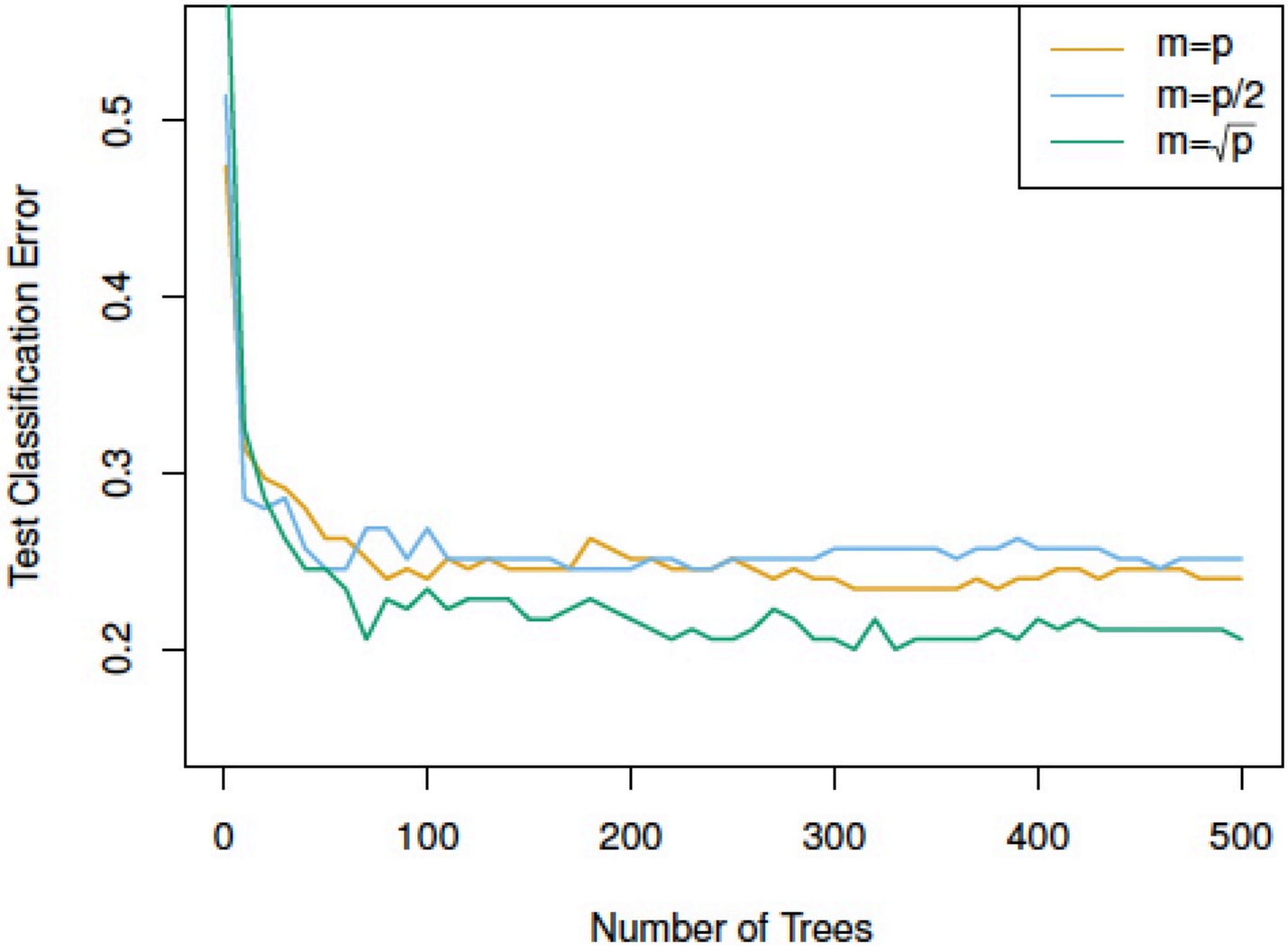
Random Forests

- Random forests provide an improvement over bagged trees by way of a small tweak that decorrelates the trees. This reduces the variance when we average the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, a random selection of m predictors is chosen as split candidates from the full set of p predictors. The split is allowed to use only one of those m predictors.
- A fresh selection of m predictors is taken at each split, and typically we choose $m \approx \sqrt{p}$ for classification, $m \approx p/2$ for regression.
- When $m = p$, random forests boil down to bagging.

Example: gene expression data

- We applied random forests to a high-dimensional biological data set consisting of expression measurements of 500 genes measured on tissue samples from 349 patients.
- Each of the patient samples belongs to one of $c = 15$ classes: either normal or one of 14 different types of cancer.
- We randomly divided the observations into a training set 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



Variable importance

- Bagging improves prediction accuracy at the expense of interpretability.
- Although the collection of bagged trees is much more difficult to interpret than a single tree, one can obtain an overall summary of the importance of each predictor.
- There are, at least, two ways to measure the importance of a variable.

Variable importance measures

Mean decrease in accuracy: For each tree, the prediction error on the OOB portion of the data is recorded (error rate for classification, MSE for regression). Then the same is done after randomly permuting (i.e., randomly shuffling the values of) each predictor variable. The differences between the two are then averaged over all trees.

Mean decrease in node impurity: total decrease in node impurities from splitting on the variable, averaged over all trees. For classification, the node impurity is measured by the Gini index. For regression, it is measured by RSS.

Bagging in R

```
library(randomForest)
p<-ncol(heart)-1
bag.heart=randomForest(as.factor(chd) ~.,data=heart,subset=train,
            mtry=p)
yhat1=predict(bag.heart,newdata=heart[-train,],type="response")
table(y.test,yhat1)
1-mean(y.test==yhat1)
```

- Confusion matrix:

	prediction	
true class	1	2
1	81	13
2	38	22

- Test error rate: 0.33

Random forests in R

```
library(randomForest)
RF.heart=randomForest(as.factor(chd) ~.,data=heart,subset=train,
            mtry=3,importance=TRUE)
yhat2=predict(RF.heart,newdata=heart[-train,],type="response")
table(y.test,yhat2)
1-mean(y.test==yhat2)
varImpPlot(RF.heart)
```

- Confusion matrix:

	prediction	
true class	1	2
1	84	10
2	36	24

- Test error rate: 0.30

Variable importance plot