

Lecture 21:

Tree Base Methods

Big Data and Machine Learning for Applied Economics
Econ 4676

Ignacio Sarmiento-Barbieri

Universidad de los Andes

October 27, 2020

Recap

- ▶ Classification:
 - ▶ KNN
 - ▶ Logit
 - ▶ Linear Discriminant Analysis
 - ▶ Misclassification Rates: ROC curve

Agenda

- 1 Motivation
- 2 Trees
 - Regression Trees
 - Classification Trees
- 3 Advantages and disadvantages of trees
 - Trees vs. Linear Models
 - Advantages and disadvantages of trees
- 4 CART Demo
 - CART Demo: Regression
 - CART Demo: Classification
- 5 Review & Next Steps
- 6 Further Readings

Motivation

- ▶ I'm going to change slightly the approach
- ▶ Inspired by Leo Breiman:

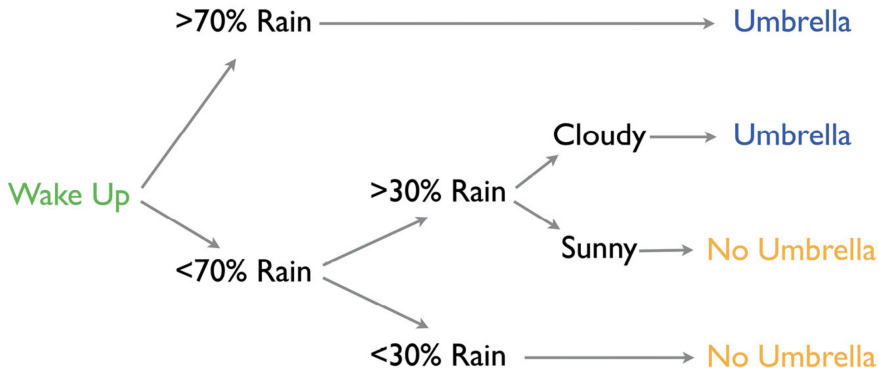
"There are two cultures in the use of statistical modeling to reach conclusions from data. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown." Breiman [2001b], p199.

"The statistical community has been committed to the almost exclusive use of data models. This commitment has led to irrelevant theory, questionable conclusions, and has kept statisticians from working on a large range of interesting current problems. Algorithmic modeling, both in theory and practice, has developed rapidly in fields outside statistics. It can be used both on large complex data sets and as a more accurate and informative alternative to data modeling on smaller data sets. If our goal as a field is to use data to solve problems, then we need to move away from exclusive dependence on data models and adopt a more diverse set of tools." Breiman [2001b], p199.

Motivation

- ▶ End goal is to model $y = f(x) + \epsilon$ for predictive power
 - ▶ Thus far we have imposed a lot of structure to the problem
 - ▶ Linear
 - ▶ Spatial
 - ▶ Logit
- ▶ Regression trees, and their extension random forests are very popular and effective methods
- ▶ They are very flexibly at regression functions in settings where out-of-sample predictive power is important.

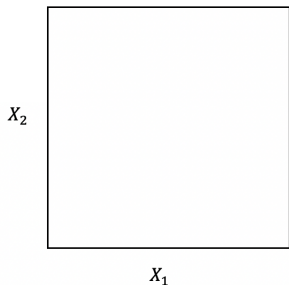
Motivation



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

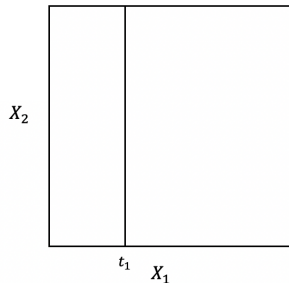
$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (1)$$



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

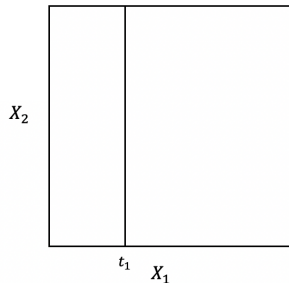
$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (2)$$



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

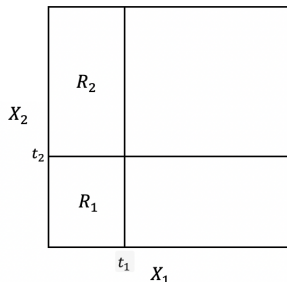
$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (3)$$



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

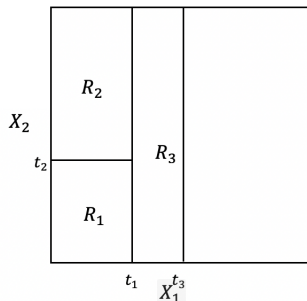
$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (4)$$



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

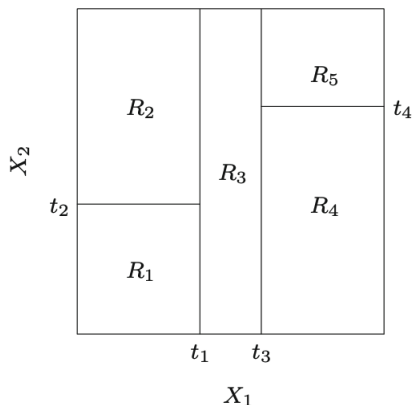
$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (5)$$



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

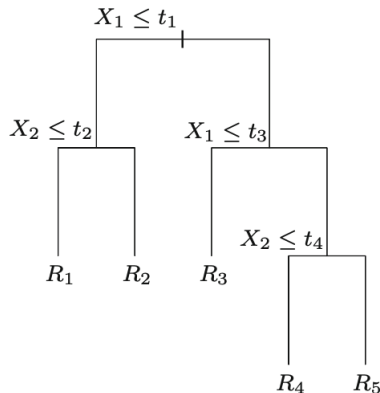
$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (6)$$



Trees: Background

- 1 Tree-based methods partition the feature space into a set of rectangles,
- 2 fit a simple model (like a constant) in each one.

$$f(x) = \sum_{m=1}^M c_m I(x \in R_m) \quad (7)$$



Regression Trees

- ▶ We have data Y $n \times 1$ and X $n \times p$
- ▶ Some definitions
 - ▶ j is the partition variable and s is the partition point
 - ▶ Define the following half-planes

$$R_1(j, s) = \{X | X_j \leq s\} \ \& \ R_2(j, s) = \{X | X_j \geq s\} \quad (8)$$

- ▶ Problem then boils down to searching the partition variable X_j and the partition point s such that

$$\min_{j,s} \left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y - c_2)^2 \right] \quad (9)$$

Regression Trees

- ▶ For each partition variable, and partition point, the internal minimization is the mean of each region

$$\hat{c}_m = \frac{1}{n_m} \sum (y_i | x_i \in R_m) \quad (10)$$

- ▶ Process is repeated inside each region.
- ▶ If the final tree has M regions then

$$\hat{f}(x) = \sum_{m=1}^M \hat{c}_m I(x \in R_m) \quad (11)$$

Regression Trees

- ▶ We grew our Tree, now how do we stop?
- ▶ A tree too big, overfits the data (like a dummy for each observation)
- ▶ A smaller tree, with fewer splits (fewer regions R_1, \dots, R_j) might lead to lower variance and better interpretation at the cost of a little bias
- ▶ One solution: Pruning
 - ▶ Grow a very large tree T_0
 - ▶ Prune it to get a *subtree*
 - ▶ How do we determine the best way to prune the tree? → lowest test error using cross-validation

Regression Trees

- ▶ Draw back, estimate the CV error for every possible subtree would be too much (too many possible subtrees)
- ▶ Solution: *Cost complexity pruning (weakest link pruning)*
 - ▶ We index the trees with T .
 - ▶ A subtree $T \in T_0$ is a tree obtained by collapsing the terminal nodes of another tree (cutting branches).
 - ▶ $[T]$ = number of terminal nodes of tree T

Regression Trees

- ▶ Cost complexity of tree T

$$C_{\alpha}(T) = \sum_{m=1}^{[T]} n_m Q_m(T) + \alpha [T] \quad (12)$$

- ▶ where $Q_m(T) = \frac{1}{n_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$ for regression trees
- ▶ $Q_m(T)$ penalizes heterogeneity (impurity) within each region, and the second term the number of regions.
- ▶ Objective: for a given α , find the optimal pruning that minimizes $C_{\alpha}(T)$

Regression Trees

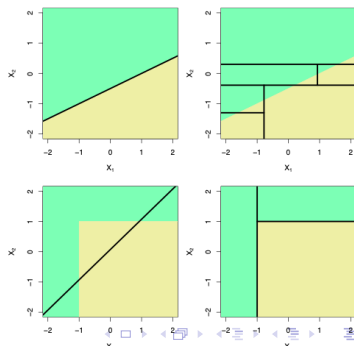
- ▶ Search mechanism for T_α (optimal pruning given α).
 - ▶ Result: for each α there is a unique subtree T_α that minimizes $C_\alpha(T)$.
 - ▶ Weakest link: successively eliminate the branches that produce the minimum increase in $\sum_{m=1}^{[T]} Q_m(T)$
 - ▶ Idea: to remove branches is to collapse, this increases the variance, ergo, we collapse the least necessary partition.
 - ▶ This eventually collapses at the initial node, but goes through a succession of trees, from the largest to the smallest, through the weakest link pruning process.
 - ▶ Breiman et al. (1984): T_α belongs to this sequence.
 - ▶ Narrow your search to this succession of subtrees.
 - ▶ Choice of α : cross validation.

Classification Trees

- ▶ A classification tree is very similar to a regression tree except that we try to make a prediction for a categorical rather than continuous Y .
- ▶ For each region (or node) we predict the most common category among the training data within that region.
- ▶ The tree is grown (i.e. the splits are chosen) in exactly the same way as with a regression tree except that minimizing MSE no longer makes sense.
- ▶ There are several possible different criteria to use
 - ▶ Misclassification error: $\frac{1}{n_m} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \max_k(\hat{p}_{mk})$
 - ▶ Gini Index: $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^K \hat{p}_{mk}(1 - \hat{p}_{mk})$
 - ▶ Cross entropy or deviance: $-\sum_{k=1}^K \hat{p}_{mk} \log(\hat{p}_{mk})$

Trees vs. Linear Models

- ▶ Which model is better?
 - ▶ If the relationship between the predictors and response is linear, then classical linear models such as linear regression would outperform regression trees
 - ▶ On the other hand, if the relationship between the predictors is non-linear, then decision trees would outperform classical approaches
- ▶ Top row: the true decision boundary is linear
 - ▶ Left: linear model (good)
 - ▶ Right: decision tree
- ▶ Bottom row: the true decision boundary is non-linear
 - ▶ Left: linear model
 - ▶ Right: decision tree (good)



Advantages and disadvantages of trees

► Pros:

- Trees are very easy to explain to people (probably even easier than linear regression)
- Trees can be plotted graphically, and are easily interpreted even by non-expert. More important variables at the top
- They work fine on both classification and regression problems

► Cons:

- Trees are not very accurate or robust (Bagging, random forests y boosting to the rescue)
- If the structure is lineal, CART doesn't work well

CART Demo: Regression

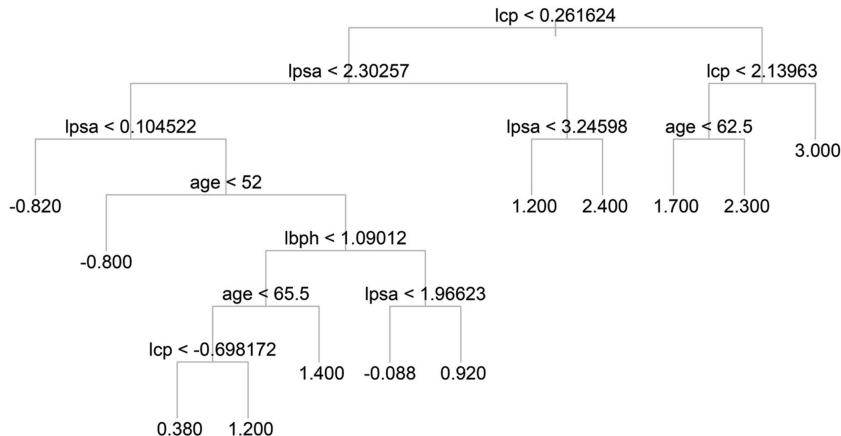
```
library("tree")
```

```
prostate <- read.csv("prostate.csv")  
str(prostate)
```

```
## 'data.frame':  97 obs. of  6 variables:  
## $ lcavol : num  -0.58 -0.994 -0.511 -1.204 0.751 ...  
## $ age : int  50 58 74 58 62 50 64 58 47 63 ...  
## $ lbph : num  -1.39 -1.39 -1.39 -1.39 -1.39 ...  
## $ lcp : num  -1.39 -1.39 -1.39 -1.39 -1.39 ...  
## $ gleason: int  6 6 7 6 6 6 6 6 6 6 ...  
## $ lpsa : num  -0.431 -0.163 -0.163 -0.163 0.372 ...
```

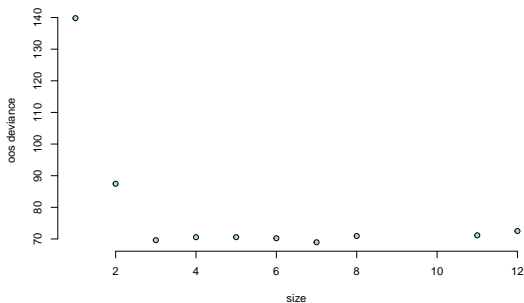
CART Demo: Regression

```
pstree <- tree(lcavol ~ ., data=prostate, mincut=1)
par(mfrow=c(1,1))
plot(pstree, col=8)
text(pstree, digits=2)
```



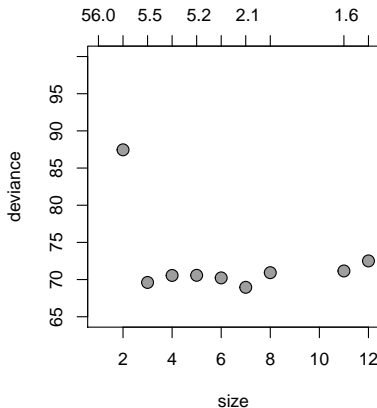
CART Demo: Regression

```
## Use cross-validation to prune the tree  
cvpst <- cv.tree(pstree, K=10)  
par(mai=c(.8,.8,0.1,0.1))  
plot(cvpst$size, cvpst$dev, xlab="size", ylab="oos deviance", pch=21, bg="lightblue")
```



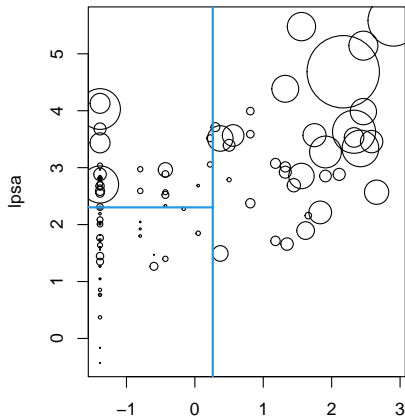
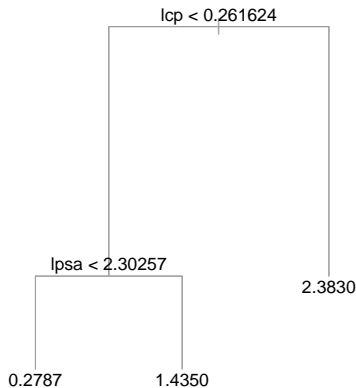
CART Demo: Regression

```
par(mfrow=c(1,2))  
## note across the top is 'average number of observations per leaf';  
plot(cvpst, pch=21, bg=8, type="p", cex=1.5, ylim=c(65,100))  
pstcut <- prune.tree(pstree, best=3)
```



CART Demo: Regression

```
par(mai=c(.8,.8,0.2,0.2), mfrow=c(1,2))  
plot(pstcut, col=8)  
text(pstcut)  
plot(prostate[,c("lcp", "lpsa")], cex=exp(prostate$lca)*.2)  
abline(v=.261624, col=4, lwd=2)  
lines(x=c(-2,.261624), y=c(2.30257,2.30267), col=4, lwd=2)
```



CART Demo: Classification

```
## read in the NBC show characteristics
nbc <- read.csv("nbc_showdetails.csv")
## lets look at the show demographics for predicting genre
demos <- read.csv("nbc_demographics.csv", row.names=1)
demos$genre <- as.factor(nbc$Genre)
head(demos[,c(11:17)])
```

```
##                               WIRED.CABLE.W.PAY WIRED.CABLE.W.O.PAY
## Living with Ed                      36.4929                      43.6019
## Monarch Cove                       31.2500                      39.5395
## Top Chef                           42.8806                      34.1528
## Iron Chef America                  44.3794                      29.9661
## Trading Spaces: All Stars          46.4945                      34.5018
## Lisa Williams: Life Among the Dead 36.7206                      35.3349
##
##                               DBS.OWNER BROADCAST.ONLY VIDEO.GAME.OWNER
## Living with Ed                      20.2607                      0.000      66.4692
## Monarch Cove                       29.0132                      0.000      54.7368
## Top Chef                           23.2329                      0.041      50.5019
## Iron Chef America                  25.7776                      0.000      56.9295
## Trading Spaces: All Stars          19.1882                      0.000      49.4465
## Lisa Williams: Life Among the Dead 28.6374                      0.000      51.7321
##
##                               DVD.OWNER VCR.OWNER
## Living with Ed                      98.4597      90.4028
## Monarch Cove                       94.2105      74.1447
## Top Chef                           92.2557      78.0783
## Iron Chef America                  94.2408      83.6464
## Trading Spaces: All Stars          90.2214      81.1808
## Lisa Williams: Life Among the Dead 94.2263      84.9885
```

CART Demo: Classification

```
## tree fit; it knows to fit a classification tree since genre is a factor.
```

```
genretree <- tree(genre ~ . , data=demos, mincut=1)
```

```
genretree
```

```
## node), split, n, deviance, yval, (yprob)
```

```
##      * denotes terminal node
```

```
##
```

```
## 1) root 40 75.800 Drama/Adventure ( 0.47500 0.42500 0.10000 )
```

```
## 2) WIRED.CABLE.W.O.PAY < 28.6651 22 33.420 Drama/Adventure ( 0.72727 0.09091 0.18182 )
```

```
## 4) VCR.OWNER < 83.749 5 6.730 Situation Comedy ( 0.00000 0.40000 0.60000 ) *
```

```
## 5) VCR.OWNER > 83.749 17 7.606 Drama/Adventure ( 0.94118 0.00000 0.05882 )
```

```
## 10) TERRITORY.EAST.CENTRAL < 16.4555 16 0.000 Drama/Adventure ( 1.00000 0.00000 0.00000 ) *
```

```
## 11) TERRITORY.EAST.CENTRAL > 16.4555 1 0.000 Situation Comedy ( 0.00000 0.00000 1.00000 ) *
```

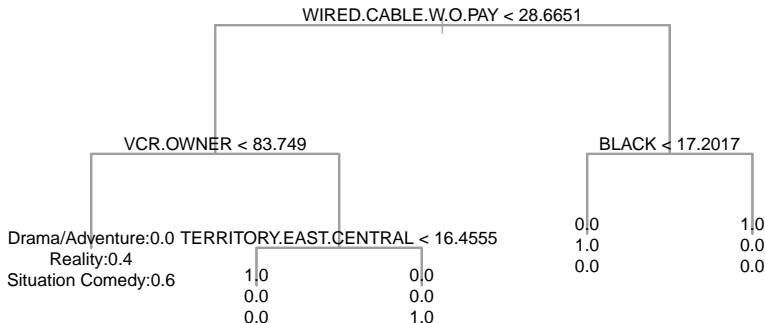
```
## 3) WIRED.CABLE.W.O.PAY > 28.6651 18 16.220 Reality ( 0.16667 0.83333 0.00000 )
```

```
## 6) BLACK < 17.2017 15 0.000 Reality ( 0.00000 1.00000 0.00000 ) *
```

```
## 7) BLACK > 17.2017 3 0.000 Drama/Adventure ( 1.00000 0.00000 0.00000 ) *
```

CART Demo: Classification

```
## tree plot  
plot(genretree, col=8, lwd=2)  
## print the predictive probabilities  
text(genretree, label="yprob")
```



CART Demo: Classification

```
## example of prediction (type="class" to get max prob classifcations back)
genrepred <- predict(genretree, newdata=demos, type="class")
genrepred
```

```
## [1] Reality      Drama/Adventure Reality      Reality
## [5] Reality      Reality      Reality      Reality
## [9] Reality      Reality      Reality      Reality
## [13] Reality      Drama/Adventure Drama/Adventure Drama/Adventure
## [17] Drama/Adventure Drama/Adventure Situation Comedy Drama/Adventure
## [21] Drama/Adventure Drama/Adventure Situation Comedy Situation Comedy
## [25] Situation Comedy Drama/Adventure Reality      Drama/Adventure
## [29] Drama/Adventure Drama/Adventure Reality      Drama/Adventure
## [33] Situation Comedy Drama/Adventure Situation Comedy Drama/Adventure
## [37] Reality      Drama/Adventure Drama/Adventure Drama/Adventure
## Levels: Drama/Adventure Reality Situation Comedy
```

Review & Next Steps

- ▶ Trees
- ▶ Regression Trees
- ▶ Classification Trees
- ▶ Advantages and disadvantages of trees
- ▶ CART Demo

- ▶ Next class: more on trees

- ▶ Questions? Questions about software?

Further Readings

- ▶ Athey, S., & Imbens, G. W. (2019). Machine learning methods that economists should know about. *Annual Review of Economics*, 11, 685-725.
- ▶ Leo Breiman. Statistical modeling: The two cultures (with comments and a rejoinder by the author). *Statistical Science*, 16(3):199–231, 2001b.
- ▶ Friedman, J., Hastie, T., & Tibshirani, R. (2001). The elements of statistical learning (Vol. 1, No. 10). New York: Springer series in statistics.
- ▶ James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An introduction to statistical learning (Vol. 112, p. 18). New York: springer.
- ▶ Taddy, M. (2019). Business data science: Combining machine learning and economics to optimize, automate, and accelerate business decisions. McGraw Hill Professional.