Lecture 21:
Tree Base Methods

Big Data and Machine Learning for Applied Economics
Econ 4676

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Recap

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

Agenda

Motivation

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

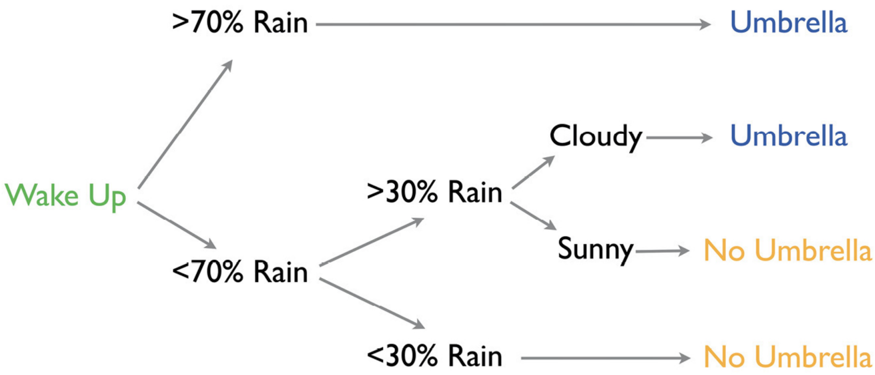
"There are two cultures in the use of statistical modeling to reach conclusions from data. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown." Breiman [2001b], p199.

"The statistical community has been committed to the almost exclusive use of data models. This commitment has led to irrelevant theory, questionable con- clusions, and has kept statisticians from working on a large range of interesting current problems. Algorithmic modeling, both in theory and practice, has devel- oped 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

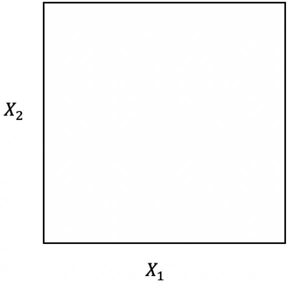


>70% Rain
Umbrella
Cloudy
Umbrella
Wake Up
>30% Rain
Sunny
No Umbrella
<70% Rain
<30% Rain
No Umbrella

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.

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



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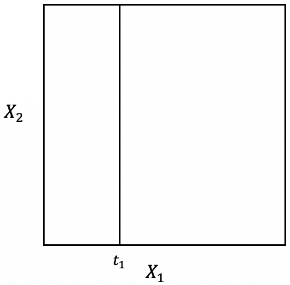
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m) \quad (2)$$



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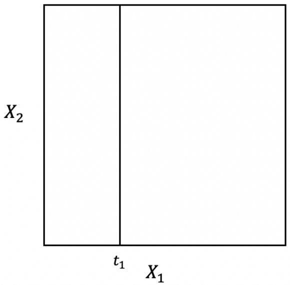
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m) \tag{3}$$



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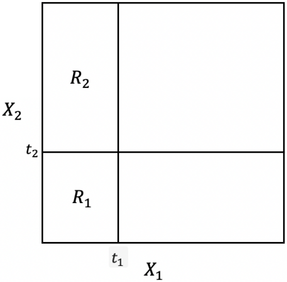
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m) \tag{4}$$



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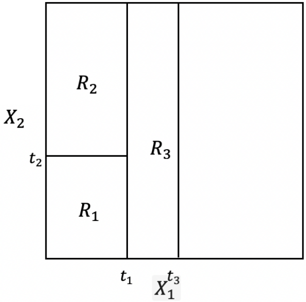
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m) \tag{5}$$



Trees: Background

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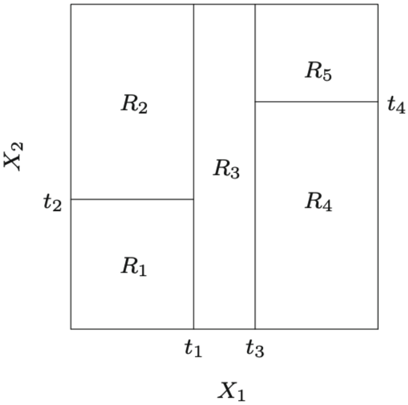
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m) \tag{6}$$



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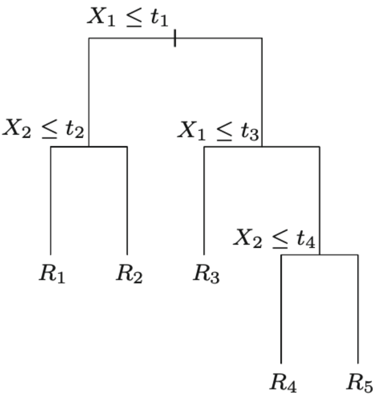
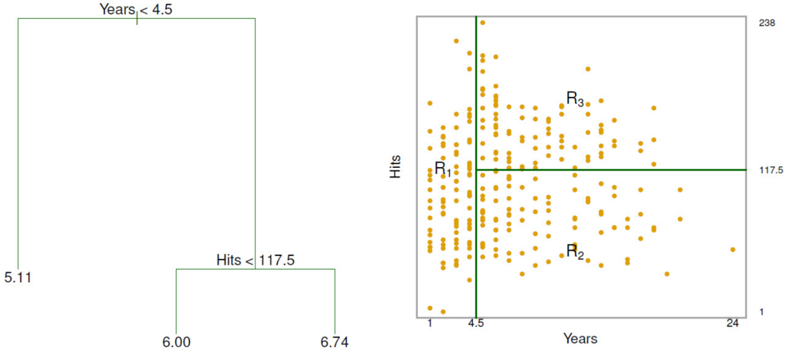
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m) \tag{7}$$



Trees: Background



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

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

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

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

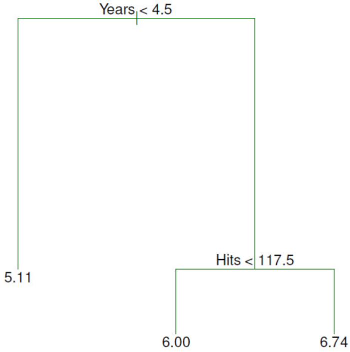
Regression Trees

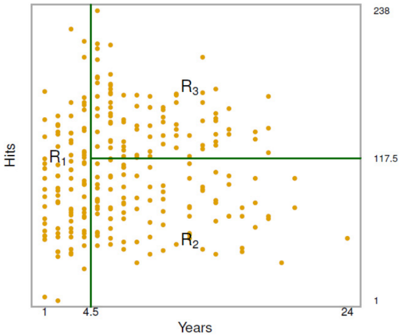
- For each partition variable, and partition point, the internal minimization is the mean of each region

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

- Process is repeated inside each region.

Regression Trees





Regression Trees

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

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

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

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

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 $R_1, \ldots, R_j$) might lead to lower variance and better interpretation at the cost of a little bias
- 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? $\rightarrow$ lowest test error using cross-validation

Regression Trees

- Draw back, estimate the CV error for every possible subtree would be too much (two 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

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

  - 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 Cα (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.

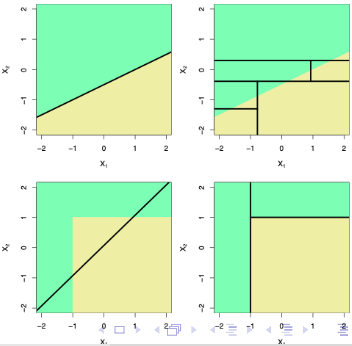
Classification Trees

- 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
  - Misclasification 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

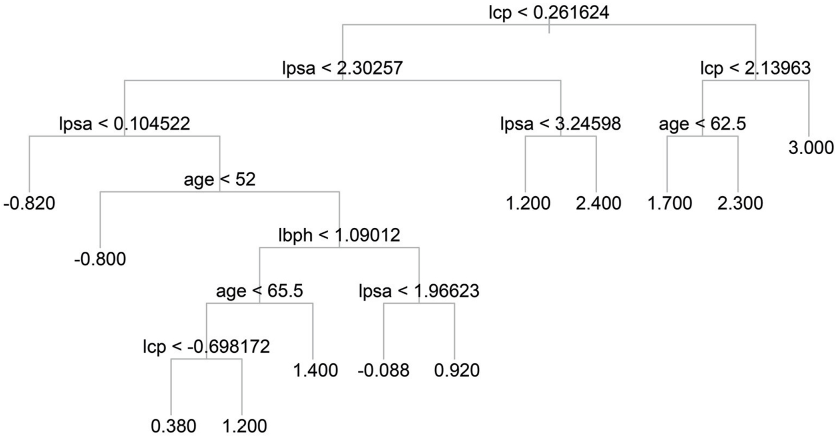
```r
library("tree")

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 ...
```

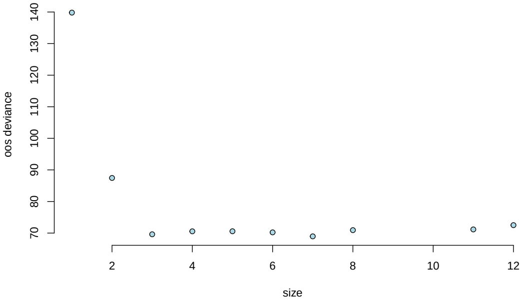
CART Demo: Regression

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



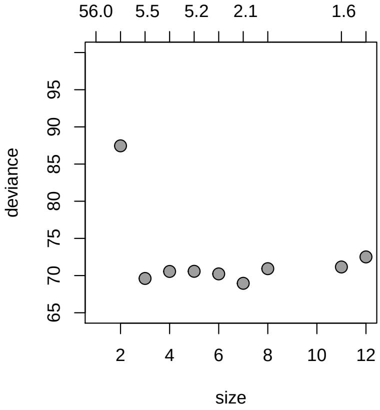
CART Demo: Regression

```r
## 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
```



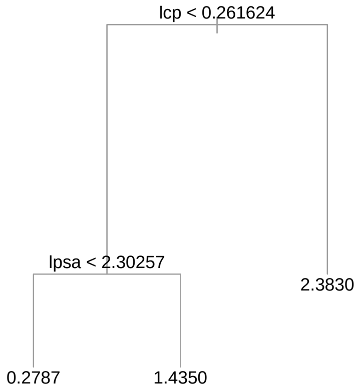
CART Demo: Regression

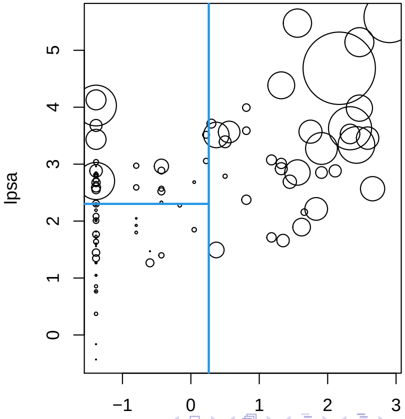
```
par(mfrow=c(1,2))
## note across the top is 'average number of observations per leaf';
plot(cvpst, pch=21, bg=8, type="p", cex=1.5, ylim=c(65,100))
pstcut <- prune.tree(pstree, best=3)
```



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

```r
## 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
```

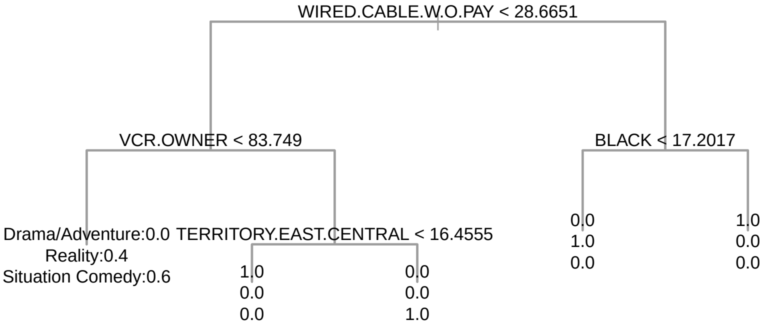
CART Demo: Classification

```r
## 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

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



CART Demo: Classification

```r
## example of prediction (type="class"  to get max prob classifications 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.