Classification And Regression Trees : A Practical Guide for Describing a Dataset

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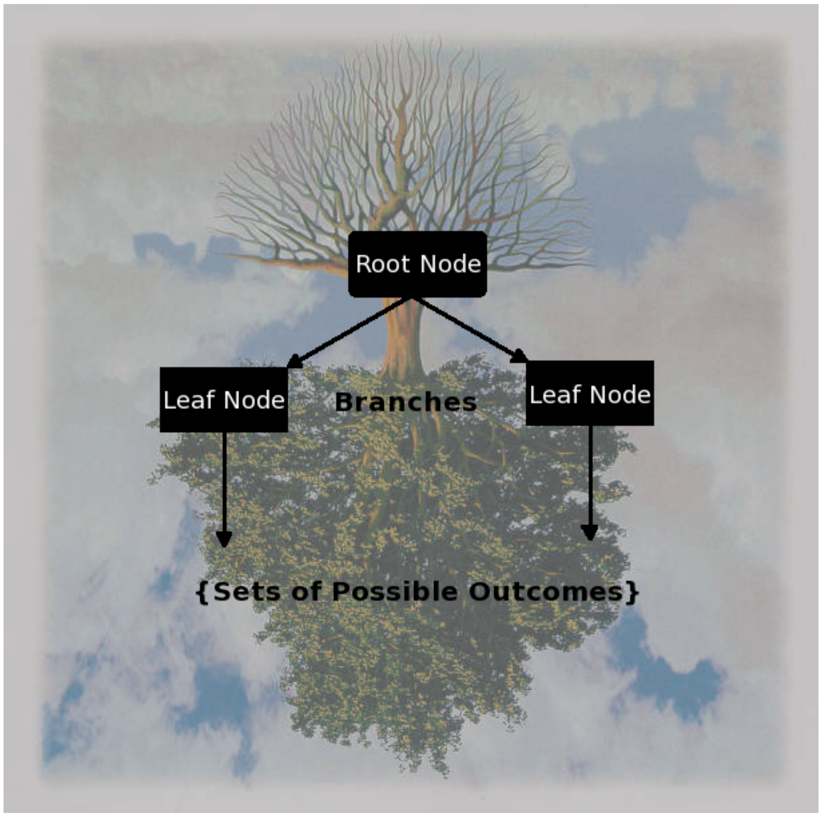
What is a Tree?

… ?

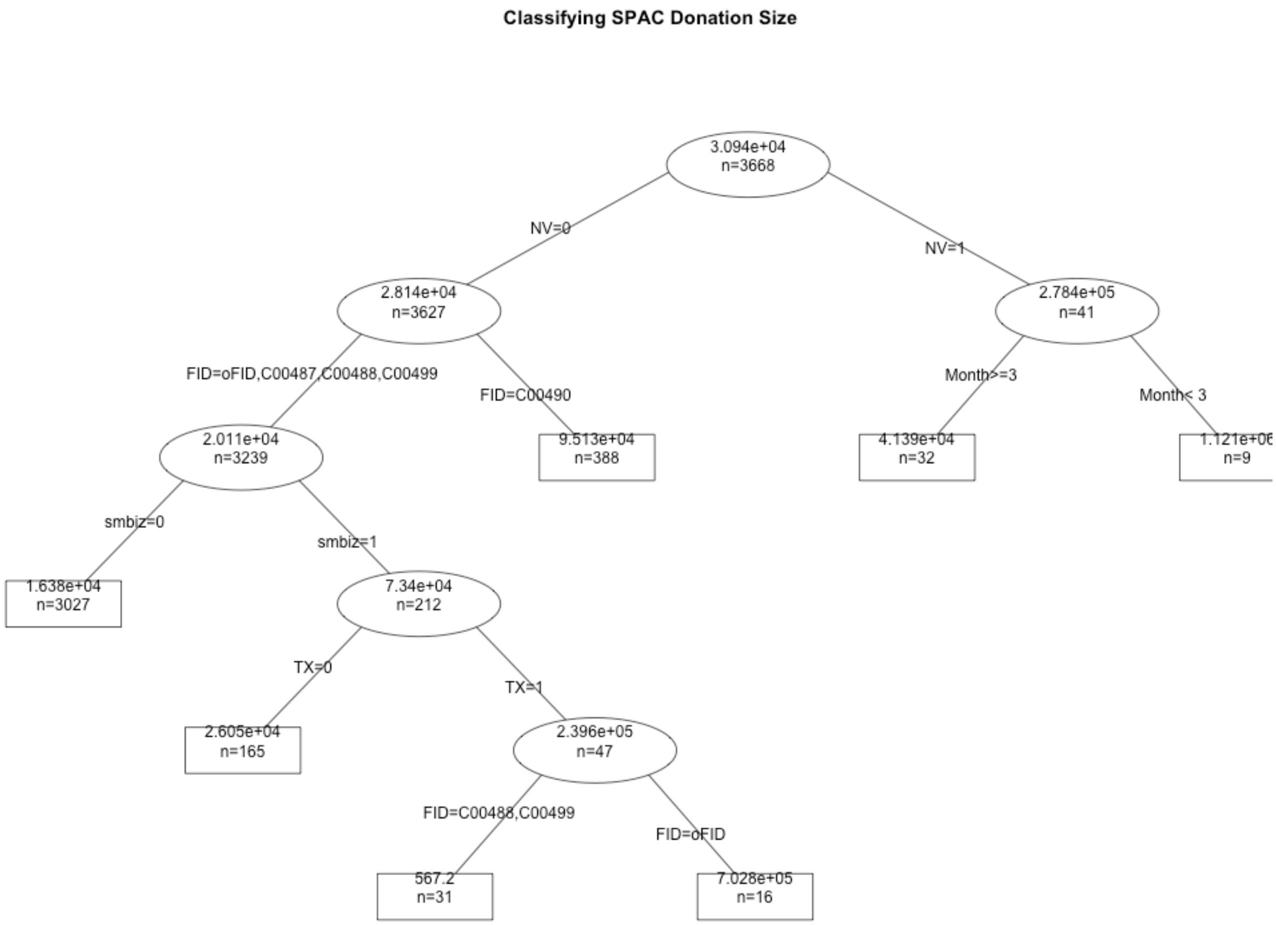
What is a Tree?

… ?!

What is a (binary) Decision Tree?



What is a (binary) Decision Tree? Example



- The data is all donations to SPACs in excess of $200, by early 2012, from fec.gov

The Structural Model

- $F(x) = \sum_{i=1}^{M} c_m I(x \in R_m)$

- $\{R_m\}_1^M$ are subregions of the input variable space, and x is a vector of input variables.
  - *Examples:* $\{x_9 < 15.2\}$, $\{9 <= x_{300} < 786 \; \& \; color = red\}$
- c_m are the estimated values of the outcome (y) in region R_m

- CART tries to minimize
  - $e(T) = \sum_{i=1}^{N} \left[y_i - \sum_{m=1}^{M} c_m I(x \in R_m) \right]^2$
  - *with respect to* c_m *and* R_m

Some Important Facts about CART

1. The R_m regions are disjoint and rectangular

    - *giving a piecewise constant approximation to the true* $F(x)$

2. CART doesn't find the "best" regions exactly

    - *uses recursive partitioning, or a greedy stepwise descent*

3. Both simplifications are to simplify a combinatorally hard problem and make it solvable in reasonable time.

    - *also allows for natural representations of regions as a binary decision tree*

How do we run it?

```
# install the package to R
install.packages("rpart", repos = "http://cran.us.r-project.org")
```

```
##
## The downloaded binary packages are in
##  /var/folders/0m/xzr0fktj78sgl36y77z34djr0000gn/T//RtmpPUlWHm/downloaded_packages
```

```
# load the library
library(rpart)

# load the dataset
load("spac.Rdata")

spac.tree = rpart(Donation ~ ., data = spac.data, cp = 10^(-6))

#### the function arguments:

# 1) formula, of the form: outcome ~ predictors

# note: outcome ~ . is 'use all other variables in data'

# 2) data: a data.frame object, or any matrix which has variables as
# columns and observations as rows

# 3) cp: used to choose depth of the tree, we'll manually prune the tree
# later and hence set the threshold very low (more on this later)

# The commands, print() and summary() will be useful to look at the tree.
# But first, lets see how big the created tree was

# The object spac.tree is a list with a number of entires that can be
# accessed via the $ symbol.  A list is like a hash table.

# To see the entries in a list, use names()
names(spac.tree)
```

```
##  [1] "frame"               "where"               "call"
##  [4] "terms"               "cptable"             "method"
##  [7] "parms"               "control"             "functions"
## [10] "numresp"             "splits"              "csplit"
## [13] "variable.importance" "y"                   "ordered"
```

```
# Within spac.tree the cptable will tell us a little about the size of the
# tree
spac.tree$cptable[1:10, ]
```

```
##          CP nsplit rel error xerror   xstd
## 1  0.037317      0    1.0000  1.000 0.3477
## 2  0.016462      2    0.9254  1.078 0.3493
## 3  0.003617      6    0.8595  1.068 0.3300
## 4  0.002751      8    0.8523  1.051 0.3171
## 5  0.001581      9    0.8495  1.050 0.3170
## 6  0.001516     17    0.8369  1.064 0.3170
## 7  0.001470     21    0.8305  1.064 0.3170
## 8  0.001454     27    0.8217  1.066 0.3170
## 9  0.001432     29    0.8188  1.066 0.3170
## 10 0.001020     32    0.8145  1.069 0.3170
```

```
# ...

spac.tree$cptable[dim(spac.tree$cptable)[1] - 9:0, ]
```

```
##           CP nsplit rel error xerror   xstd
## 84 1.901e-06    169    0.7951  1.067 0.3133
```

```
## 85 1.725e-06    170    0.7951  1.067 0.3133
## 86 1.584e-06    171    0.7951  1.067 0.3133
## 87 1.188e-06    172    0.7951  1.067 0.3133
## 88 1.177e-06    173    0.7951  1.067 0.3133
## 89 1.156e-06    174    0.7951  1.067 0.3133
## 90 1.135e-06    175    0.7951  1.067 0.3133
## 91 1.129e-06    177    0.7951  1.067 0.3133
## 92 1.061e-06    179    0.7951  1.067 0.3133
## 93 1.000e-06    181    0.7951  1.067 0.3133
```

```
# that's a lot of splits! I'm going to prune the tree to 9 splits

cp9 = which(spac.tree$cptable[, 2] == 9)

spac.tree9 = prune(spac.tree, spac.tree$cptable[cp9, 1])

# now lets look at the tree with print() and summary()

print(spac.tree9)
```

```
## n= 3668
##
## node), split, n, deviance, yval
##       * denotes terminal node
##
##  1) root 3668 1.438e+14   30940.0
##    2) NV=0 3627 9.400e+13   28140.0
##      4) FID=otherFID,C00487470,C00488403,C00499335 3239 8.088e+13   20110.0
##        8) smbiz=0 3027 2.897e+13   16380.0
##         16) blank=0 2467 1.580e+13   10930.0 *
##         17) blank=1 560 1.278e+13   40370.0 *
##        9) smbiz=1 212 5.126e+13   73400.0
##         18) TX=0 165 1.867e+12   26050.0 *
##         19) TX=1 47 4.772e+13  239600.0
##           38) FID=C00488403,C00499335 31 5.142e+06     567.2 *
##           39) FID=otherFID 16 4.252e+13  702800.0 *
##      5) FID=C00490045 388 1.117e+13   95130.0
##       10) NY=0 345 6.533e+12   82900.0 *
##       11) NY=1 43 4.176e+12  193300.0
##         22) Day< 27.5 35 2.033e+12  138000.0 *
##         23) Day>=27.5 8 1.568e+12  435000.0 *
##    3) NV=1 41 4.723e+13  278400.0
##      6) Month>=3 32 3.476e+11   41390.0 *
##      7) Month< 3 9 3.869e+13 1121000.0 *
```

```
summary(spac.tree9)
```

```
## Call:
## rpart(formula = Donation ~ ., data = spac.data, cp = 10^(-6))
##   n= 3668
##
##          CP nsplit rel error xerror   xstd
## 1 0.037317      0    1.0000  1.000 0.3477
## 2 0.016462      2    0.9254  1.078 0.3493
## 3 0.003617      6    0.8595  1.068 0.3300
## 4 0.002751      8    0.8523  1.051 0.3171
## 5 0.001581      9    0.8495  1.050 0.3170
##
## Variable importance
##   Month     FID      NV      TX    tech     oil  doctor writing   smbiz
##      35      28       9       6       3       3       3       3       2
##     Day      NY   blank     biz
##       2       2       1       1
##
## Node number 1: 3668 observations,    complexity param=0.03732
##   mean=3.094e+04, MSE=3.919e+10
##   left son=2 (3627 obs) right son=3 (41 obs)
##   Primary splits:
##       NV      splits as  LR,       improve=0.017660, (0 missing)
##       FID     splits as  LRLLL,    improve=0.012390, (0 missing)
##       Month   < 5.5  to the right, improve=0.005567, (0 missing)
```

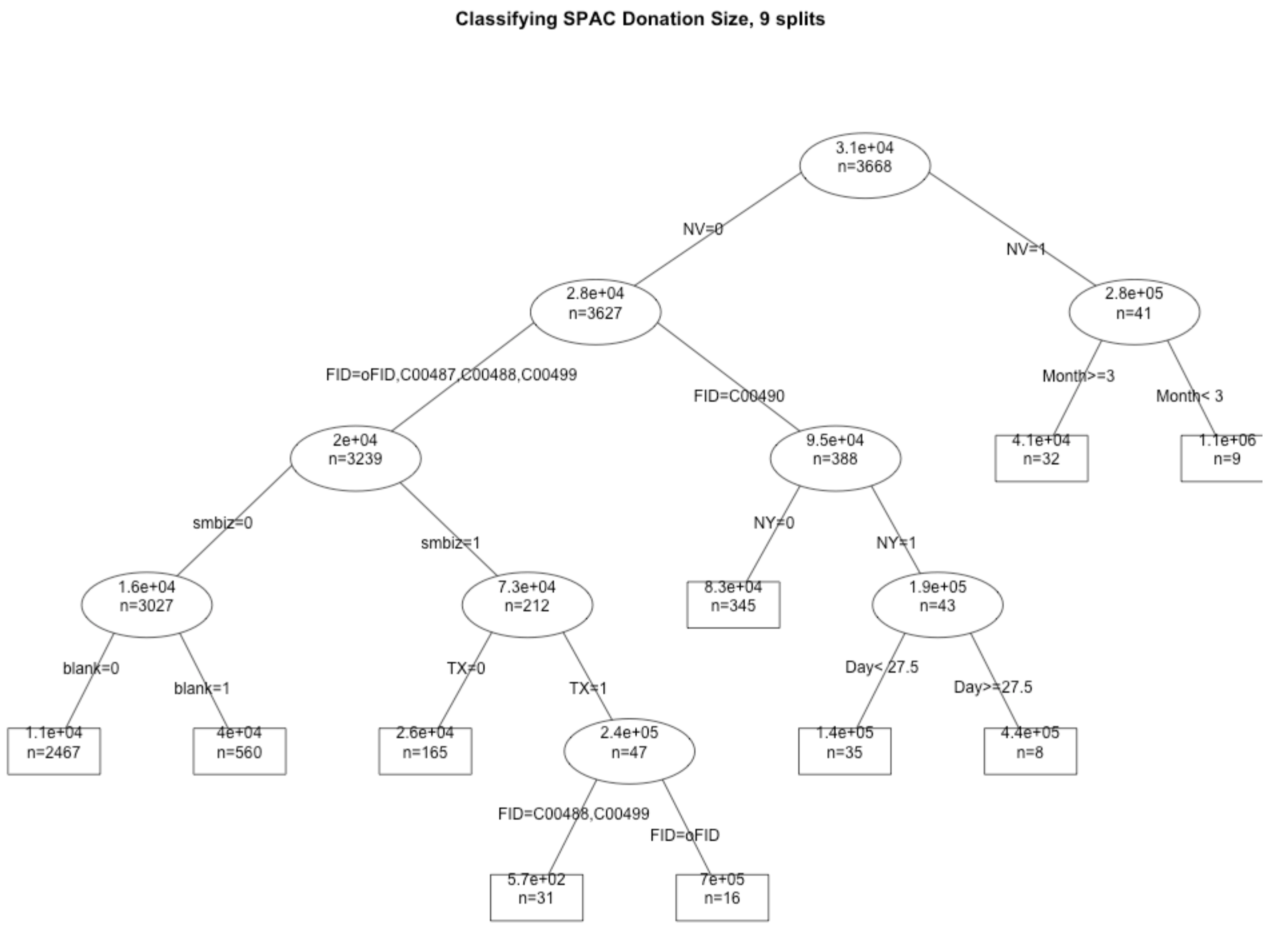
```
##       smbiz   splits as  LR,       improve=0.004716, (0 missing)
##       retired splits as  RL,       improve=0.003653, (0 missing)
##
## Node number 2: 3627 observations,    complexity param=0.01646
##   mean=2.814e+04, MSE=2.592e+10
##   left son=4 (3239 obs) right son=5 (388 obs)
##   Primary splits:
##       FID     splits as  LRLLL,    improve=0.020740, (0 missing)
##       smbiz   splits as  LR,       improve=0.008136, (0 missing)
##       money   splits as  LR,       improve=0.004718, (0 missing)
##       retired splits as  RL,       improve=0.004439, (0 missing)
##       Month   < 6.5  to the right, improve=0.004148, (0 missing)
##   Surrogate splits:
##       UT      splits as  LR, agree=0.897, adj=0.036, (0 split)
##       leisure splits as  LR, agree=0.893, adj=0.003, (0 split)
##
## Node number 3: 41 observations,    complexity param=0.03732
##   mean=2.784e+05, MSE=1.152e+12
##   left son=6 (32 obs) right son=7 (9 obs)
##   Primary splits:
##       Month        < 3    to the right, improve=0.17340, (0 missing)
##       Day          < 7.5  to the right, improve=0.02769, (0 missing)
##       manage       splits as  LR,       improve=0.02717, (0 missing)
##       FID          splits as  RL--L,    improve=0.02251, (0 missing)
##       professional splits as  RL,       improve=0.01382, (0 missing)
##   Surrogate splits:
##       doctor  splits as  LR, agree=0.805, adj=0.111, (0 split)
##       tech    splits as  LR, agree=0.805, adj=0.111, (0 split)
##       oil     splits as  LR, agree=0.805, adj=0.111, (0 split)
##       writing splits as  LR, agree=0.805, adj=0.111, (0 split)
##
## Node number 4: 3239 observations,    complexity param=0.01646
##   mean=2.011e+04, MSE=2.497e+10
##   left son=8 (3027 obs) right son=9 (212 obs)
##   Primary splits:
##       smbiz   splits as  LR,    improve=0.007964, (0 missing)
##       FID     splits as  R-LLL, improve=0.005066, (0 missing)
##       blank   splits as  LR,    improve=0.003437, (0 missing)
##       TX      splits as  LR,    improve=0.002374, (0 missing)
##       retired splits as  RL,    improve=0.002351, (0 missing)
##
## Node number 5: 388 observations,    complexity param=0.003617
##   mean=9.513e+04, MSE=2.88e+10
##   left son=10 (345 obs) right son=11 (43 obs)
##   Primary splits:
##       NY      splits as  LR,       improve=0.041680, (0 missing)
##       Day     < 27.5 to the left,  improve=0.028980, (0 missing)
##       CA      splits as  RL,       improve=0.023540, (0 missing)
##       retired splits as  RL,       improve=0.011260, (0 missing)
##       Month   < 1.5  to the left,  improve=0.007873, (0 missing)
##   Surrogate splits:
##       community splits as  LR, agree=0.892, adj=0.023, (0 split)
##
## Node number 6: 32 observations
##   mean=4.139e+04, MSE=1.086e+10
##
## Node number 7: 9 observations
##   mean=1.121e+06, MSE=4.299e+12
##
## Node number 8: 3027 observations,    complexity param=0.002751
##   mean=1.638e+04, MSE=9.572e+09
##   left son=16 (2467 obs) right son=17 (560 obs)
##   Primary splits:
##       blank   splits as  LR,       improve=0.013650, (0 missing)
##       FID     splits as  R-LLL,    improve=0.007902, (0 missing)
##       DC      splits as  LR,       improve=0.007561, (0 missing)
##       retired splits as  RL,       improve=0.003920, (0 missing)
##       Day     < 14.5 to the left,  improve=0.002814, (0 missing)
##   Surrogate splits:
##       DC splits as  LR, agree=0.870, adj=0.300, (0 split)
##       ZZ splits as  LR, agree=0.815, adj=0.002, (0 split)
##
## Node number 9: 212 observations,    complexity param=0.01646
##   mean=7.34e+04, MSE=2.418e+11
```

```
##   left son=18 (165 obs) right son=19 (47 obs)
##   Primary splits:
##       TX           splits as  LR,       improve=0.032550, (0 missing)
##       Month        < 1.5  to the right, improve=0.017010, (0 missing)
##       FID          splits as  R-LLL,    improve=0.009249, (0 missing)
##       Day          < 28.5 to the left,  improve=0.007682, (0 missing)
##       professional splits as  RL,       improve=0.002284, (0 missing)
##   Surrogate splits:
##       FID   splits as  L-LRL, agree=0.892, adj=0.511, (0 split)
##       teach splits as  LR,    agree=0.783, adj=0.021, (0 split)
##       oil   splits as  LR,    agree=0.783, adj=0.021, (0 split)
##
## Node number 10: 345 observations
##   mean=8.29e+04, MSE=1.894e+10
##
## Node number 11: 43 observations,    complexity param=0.003617
##   mean=1.933e+05, MSE=9.711e+10
##   left son=22 (35 obs) right son=23 (8 obs)
##   Primary splits:
##       Day          < 27.5 to the left,  improve=0.137500, (0 missing)
##       Month        < 5    to the right, improve=0.062300, (0 missing)
##       money        splits as  LR,       improve=0.012980, (0 missing)
##       professional splits as  RL,       improve=0.010520, (0 missing)
##       manage       splits as  LR,       improve=0.009981, (0 missing)
##   Surrogate splits:
##       tech splits as  LR, agree=0.837, adj=0.125, (0 split)
##
## Node number 16: 2467 observations
##   mean=1.093e+04, MSE=6.405e+09
##
## Node number 17: 560 observations
##   mean=4.037e+04, MSE=2.282e+10
##
## Node number 18: 165 observations
##   mean=2.605e+04, MSE=1.131e+10
##
## Node number 19: 47 observations,    complexity param=0.01646
##   mean=2.396e+05, MSE=1.015e+12
##   left son=38 (31 obs) right son=39 (16 obs)
##   Primary splits:
##       FID    splits as  R--LL,    improve=0.109000, (0 missing)
##       Day    < 28.5 to the left,  improve=0.043090, (0 missing)
##       Month  < 5    to the right, improve=0.038900, (0 missing)
##       manage splits as  RL,       improve=0.005604, (0 missing)
##   Surrogate splits:
##       Month < 3.5  to the right, agree=0.787, adj=0.375, (0 split)
##       biz   splits as  LR,       agree=0.681, adj=0.063, (0 split)
##
## Node number 22: 35 observations
##   mean=1.38e+05, MSE=5.809e+10
##
## Node number 23: 8 observations
##   mean=4.35e+05, MSE=1.961e+11
##
## Node number 38: 31 observations
##   mean=567.2, MSE=1.659e+05
##
## Node number 39: 16 observations
##   mean=7.028e+05, MSE=2.658e+12
##
```

```
# finally, lets get a graphical representation of the tree, and save to a
# png file
png("spactree9.png", width = 1200, height = 800)
post(spac.tree9, file = "", title. = "Classifying SPAC Donation Size, 9 splits",
    bp = 18)
dev.off()
```

```
## pdf
##   2
```

How do we run it? The graphical representation.



What about exporting the results?

```
# will use a combination of list entries: frame, splits, and csplit

spac.tree9$frame[1:5, ]
```

```
##       var    n   wt       dev  yval complexity ncompete nsurrogate
## 1      NV 3668 3668 1.438e+14 30936   0.037317        4          0
## 2     FID 3627 3627 9.400e+13 28138   0.016462        4          2
## 4   smbiz 3239 3239 8.088e+13 20113   0.016462        4          0
## 8   blank 3027 3027 2.897e+13 16381   0.002751        4          2
## 16 <leaf> 2467 2467 1.580e+13 10935   0.001581        0          0
```

```
####

# frame is a matrix with 1 row per node of the tree

# row name corresponds to a unique node index

# var - name of the variable used in the split, or <leaf>

# n - number of observations reaching the node

# yval - the fitted outcome value at the node

####

spac.tree9$splits[1:5, ]
```

```
##         count ncat  improve index adj
## NV       3668    2 0.017664   1.0   0
## FID      3668    5 0.012395   2.0   0
## Month    3668    1 0.005567   5.5   0
## smbiz    3668    2 0.004716   3.0   0
## retired  3668    2 0.003653   4.0   0
```

```
# splits characterizes the splits making the regions Rm

# row name is the variable being split

# count - the number of observations coming into the split

# ncat - number of categories of categorical variable, or 1 if the
# variable is numeric

# improve - the improvement in the objective using the split

# index - either the row number of the csplit matrix (for categorical
# variables), or the value of the optimal split (for numeric variables)

spac.tree9$csplit[1:5, ]
```

```
##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1    3    2    2    2
## [2,]    1    3    1    1    1
## [3,]    1    3    2    2    2
## [4,]    3    1    2    2    2
## [5,]    1    3    1    1    1
```

```
# has 1 row for each split on a categorical variable

# the row number corresponds to index in spac.tree11$split above

# each column is an ordered level of a categorical variable, up to the max
# levels of any categorical var

# an entry of 1 - that level goes left in the split

# 3 - that level goes right in the split
```

```
# 2 - that level is not included in the split
```

What about exporting the results?

- To recreate a decision tree, you would at least extract the following columns of information:
  - *`rownames(spac.tree9$splits)`*
  - *`spac.tree9$splits[,"count"]`, `spac.tree9$splits[,"index"]` and `spac.tree9$splits[,"ncat"]`*
  - *`spac.tree9$frame[,"var"]`, `spac.tree9$[,"n"]` and `spac.tree9$frame[,"yval"]`*
  - *`spac.tree9$csplit` corresponding to the rows given by `"index"` where `"ncat" > 2` in `"splits"`*
- The order of splits in `"frame"` are depth first, and left branch first
- Match between `"frame"` and `"splits"` by variable name and number of observations
  - *since a variable can be split multiple times, and frame also includes competing and surrogate splits*

Automatic Way to Select Tree Size

- Can calculate contribution of split to decreasing objective $e(T)$ by
- $e_m = \frac{1}{N} \sum_{x_i \in R_m} (y_i - \bar{y}_m)^2$
- $Imp_m = e_m - e_{ml} - e_{mr}$
- If $Imp_m \geq cp$ then accept the split, otherwise make m a terminal node
  - *$cp > 0$ is a tuning parameter, giving tree sizes as in "cptable"*
  - *Actually a little trickier because the rule is applied in inverse order of depth*
- Solves the problem:

$$\min_T \left[e(T) + cp|T| \right]$$

- *where $|T|$ is the number of terminal nodes of the tree*

Automatic Way to Select Tree Size

- The entry `"cptable"` gives tree statistics for each cp
- `"rel error"` is the ratio of the objective, $e(T)$, to that of a single root tree
  - *This is **always** decreasing with* cp
- `"xerror"` is the average of 10 fold cross validation error
  - *i.e. leave out 1/10th of the dataset,*
    - train a size n tree on the other 9/10ths,
    - and compute $e(T)$ on the left out part
  - *this is more useful for prediction, and not as useful to us for describing a dataset*
  - *can be thought of as a measure of **pervasiveness***
- Could consider a criteria that penalizes large trees
  - *Not unreasonable:* $N \times (relerror) + 2|T|$

Automatic Way to Select Tree Size

```
which.min(spac.tree$cptable[, 4])
```

```
## 1
## 1
```

```
# gives a value of 1, meaning none of the splits are 'pervasize'

# but using the criteria above, penalizing large trees
cpstat = dim(spac.data)[1] * spac.tree$cptable[, 3] + 2 * (spac.tree$cptable[,
    2] + 1)

round(spac.tree$cptable[which.min(cpstat), ], 3)
```

```
##        CP    nsplit rel error    xerror      xstd
##     0.001    39.000     0.808     1.064     0.313
```

```
# suggests a tree size with 39 splits
```

Advantages of Trees

1. **Fast** computations
2. **Invariant** under monotone transformations of variables
    - *Scaling doesn't matter!*
    - *Immune to outliers in x*
3. **Resistence** to irrelevant variables, so can throw lots of variables into it
4. **One tuning parameter** (tree size, or cp)
5. **Interpretable** model representation
6. **Handles missing data** by keeping track of surrogate, or highly correlated, backup splits at every node
7. Extends to **categorical outcomes** easily

Disadvantages of Trees

1. **Accuracy**

   - $F(x)$ *may not be piecewise constant (but decent overall approximation)*
   - *Data Fragmentation (ok, if you have lots of data)*
   - $F(x)$ *must involve high order interactions*

2. **Variance**

   - *Each subsequent split depends on the previous ones, so an error in a higher split is propogated down.*
   - *Small change in dataset can cause big change in tree*
     - If you only have a random sample of a population, this can be a problem.
     - Not as much of an issue if you're *describing* a dataset

CART libraries outside of R: weka

- weka 3: Data mining software in JAVA
- http://www.cs.waikato.ac.nz/ml/weka/
- Relevent class `weka.classifiers.trees.J48`
- Simple command line syntax
  - *`java weka.classifiers.trees.J48 -t data/weather.arff -i`*
- ARFF is *Attribute-Relation File Format* and data format for weka
  - *`weka.core.converters` package contains converters for usual data files*
- Also call classes directly

```
import weka.core.Instances;
import weka.classifiers.Evaluation;
import weka.classifiers.trees.J48;
…
Instances train = … // from somewhere
Instances test = … // from somewhere //
train classifier Classifier cls = new J48();
cls.buildClassifier(train);
// evaluate classifier and print some statistics
Evaluation eval = new Evaluation(train);
eval.evaluateModel(cls, test);
System.out.println(eval.toSummaryString("", false));
```

- `weka.gui.treevisualizer.TreeVisualizer` class to vizualize trees

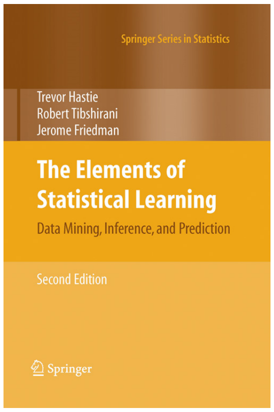
CART libraries outside of R: orange

- orange: Data mining through visual programming programming or Python scripting.
- http://orange.biolab.si/
- has proprietary tab-deliminated data format
  - *Can import from csv, but is not very robust*
  - *More info: /Orange.data.formats/*
- Relevant function: `Orange.regression.tree.TreeLearner(...)`
- Vizualizing trees: Orange renders trees in dot - plain text graph description langauge readable by both human and computer
  - *`tree.dot(file_name="0.dot", node_shape="ellipse", leaf_shape="box")`*

CART libraries outside of R: opencv

- opencv: (Open Source Computer Vision) is a library of programming functions for real time computer vision, in C++
- http://opencv.willowgarage.com/wiki/
- Uses n-dimensional array class `Mat` to store and operate on data
  - *core_basic_structures.html#mat*
- `CvDTree` class is an honest representation of CART algorithm
  - *ml_decision_trees.html*
  - *`mushroom.cpp` example file demonstrates how to use decision trees*

References

- Elements of Statistical Learning. 2009. New York. Springer. xxii, 745 p. : ill. ; 24 cm.
  - 

- Jerome Friedman's 315b course notes

Two solutions to Disadvantages (extra slides)

1. Boosted Trees, aka Forests, MART

    - $F(x) = \sum_{k=1}^{K} a_k f(x\ ;\ c_m^k, R_m^k)$
    - *Now each $f()$ is a tree, and $F()$ is a linear combination of trees*
    - *Each tree can model an additive effect, or many low order interactions*
    - *Variance of a combination of identically distributed objects is lower than any individual*
    - *Disadvantage: loses decision tree interpretability unless K is small*

2. Random Forests

    - *Similar to boosted trees, but now random subsets of the data are used for each tree*
    - *Simpler to fit than boosted trees*
    - *Accuracy is usually somewhere in between a single tree and boosted trees*

How are Boosted Trees Interpreted? (extra slides)

- Relative Importance
  - $Imp_l^2 = Avg\left[\sum_{m=1}^{M} Imp_m \, I(var(m) = l)\right]$
  - *Average overall improvement of objective by variable* l

- Partial Dependence
  - $pd(x_l) = E_{notl}\left[F(x_l, x_{notl})\right]$
  - *Predicted outcome using* x_l*, after averaging out the others*