Predicting with trees

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Key ideas

- Iteratively split variables into groups
- Evaluate "homogeneity" within each group
- Split again if necessary

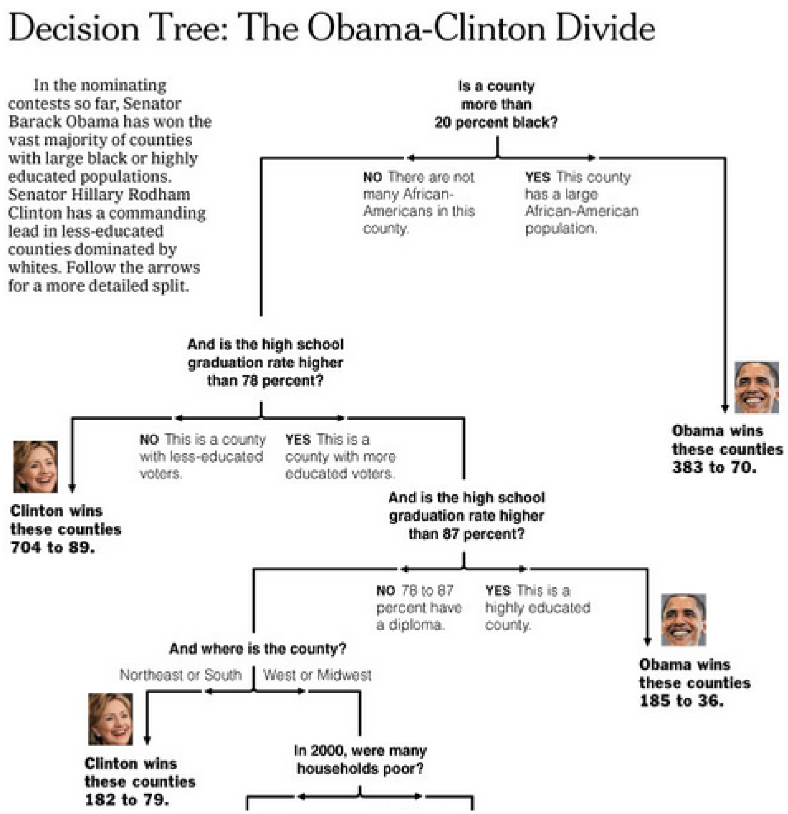
Pros:

- Easy to interpret
- Better performance in nonlinear settings

Cons:

- Without pruning/cross-validation can lead to overfitting
- Harder to estimate uncertainty
- Results may be variable

Example Tree



http://graphics8.nytimes.com/images/2008/04/16/us/0416-nat-subOBAMA.jpg

Basic algorithm

1. Start with all variables in one group
2. Find the variable/split that best separates the outcomes
3. Divide the data into two groups ("leaves") on that split ("node")
4. Within each split, find the best variable/split that separates the outcomes
5. Continue until the groups are too small or sufficiently "pure"

Measures of impurity

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \ in \ Leaf \ m} 1(y_i = k)$$

Misclassification Error:

$$1 - \hat{p}_{mk(m)}; k(m) = \mathrm{most; common; k}$$

- 0 = perfect purity
- 0.5 = no purity

Gini index:

$$\sum_{k \neq k'} \hat{p}_{mk} \times \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) = 1 - \sum_{k=1}^{K} p_{mk}^2$$

- 0 = perfect purity
- 0.5 = no purity

http://en.wikipedia.org/wiki/Decision_tree_learning

Measures of impurity

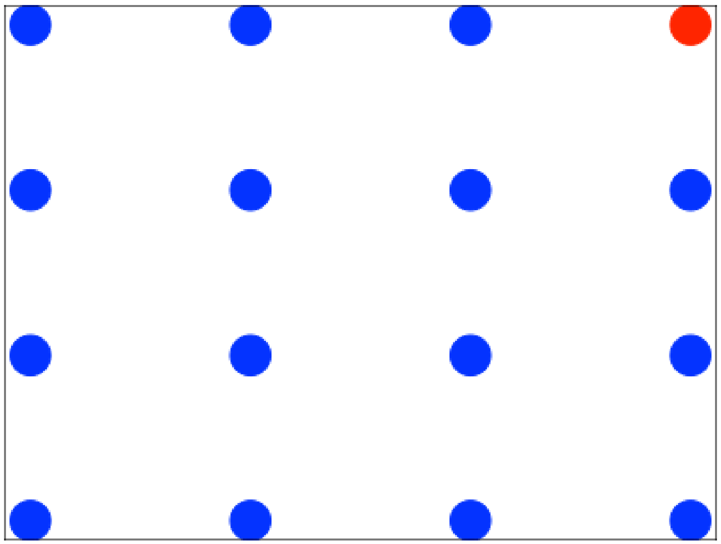
Deviance/information gain:

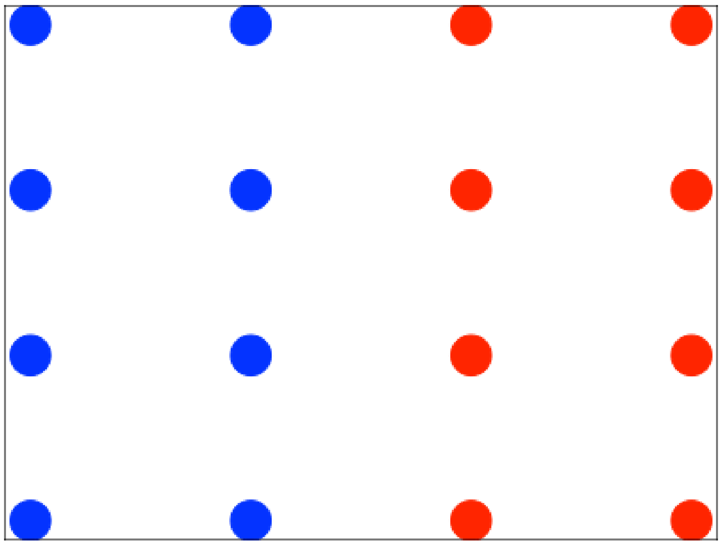
$$-\sum_{k=1}^{K} \hat{p}_{mk} \log_2 \hat{p}_{mk}$$

- 0 = perfect purity
- 1 = no purity

http://en.wikipedia.org/wiki/Decision_tree_learning

Measures of impurity





- **Misclassification:** $1/16 = 0.06$
- **Gini:** $1 - [(1/16)^2 + (15/16)^2] = 0.12$
- **Information:** $-[1/16 \times log2(1/16) + 15/16 \times log2(15/16)] = 0.34$

- **Misclassification:** $8/16 = 0.5$
- **Gini:** $1 - [(8/16)^2 + (8/16)^2] = 0.5$
- **Information:** $-[1/16 \times log2(1/16) + 15/16 \times log2(15/16)] = 1$

Example: Iris Data

```
data(iris); library(ggplot2)
names(iris)
```

```
[1] "Sepal.Length" "Sepal.Width"  "Petal.Length" "Petal.Width"  "Species"
```

```
table(iris$Species)
```

```

    setosa versicolor  virginica 
        50         50         50 
```

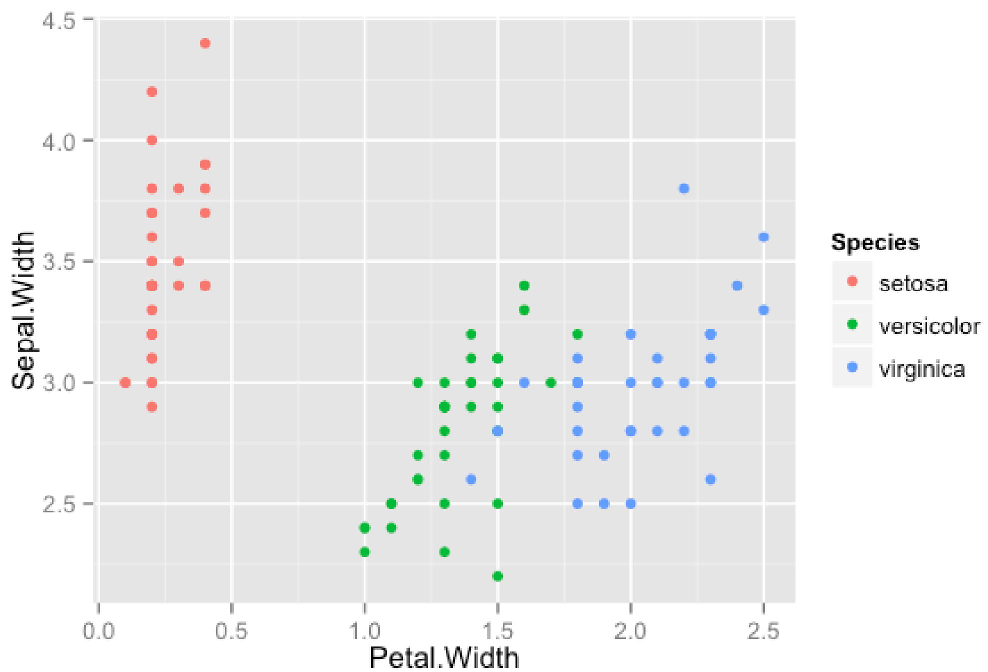
Create training and test sets

```
inTrain <- createDataPartition(y=iris$Species,
                              p=0.7, list=FALSE)
training <- iris[inTrain,]
testing <- iris[-inTrain,]
dim(training); dim(testing)
```

```
[1] 45  5
```

Iris petal widths/sepal width

```
qplot(Petal.Width,Sepal.Width,colour=Species,data=training)
```



Iris petal widths/sepal width

```
library(caret)
modFit <- train(Species ~ .,method="rpart",data=training)
print(modFit$finalModel)
```

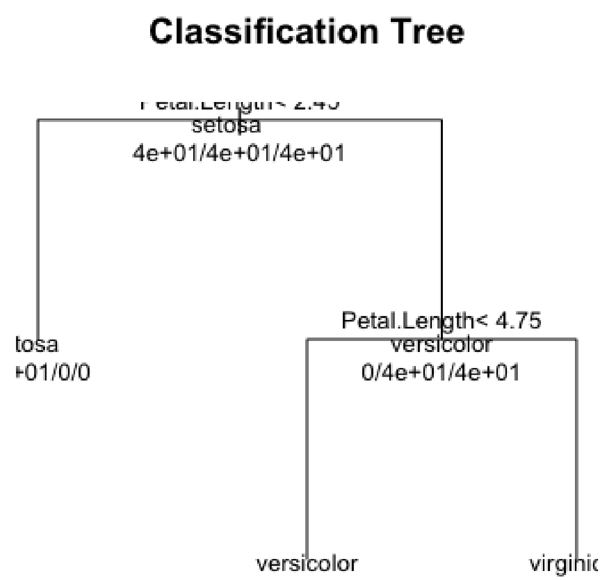
```
n= 105

node), split, n, loss, yval, (yprob)
      * denotes terminal node

1) root 105 70 setosa (0.3333 0.3333 0.3333)
  2) Petal.Length< 2.45 35  0 setosa (1.0000 0.0000 0.0000) *
  3) Petal.Length>=2.45 70 35 versicolor (0.0000 0.5000 0.5000)
    6) Petal.Length< 4.75 31  0 versicolor (0.0000 1.0000 0.0000) *
    7) Petal.Length>=4.75 39  4 virginica (0.0000 0.1026 0.8974) *
```

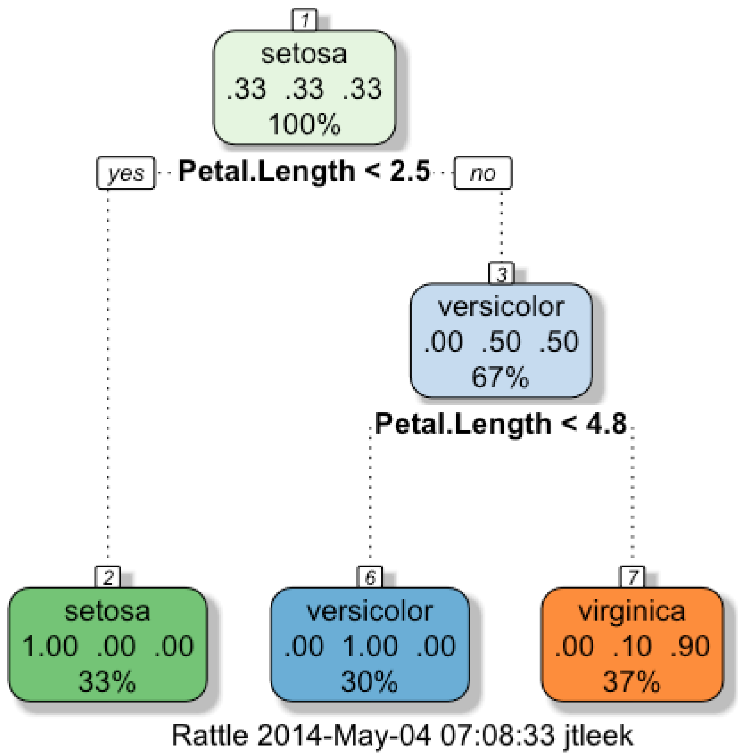
Plot tree

```r
plot(modFit$finalModel, uniform=TRUE,
      main="Classification Tree")
text(modFit$finalModel, use.n=TRUE, all=TRUE, cex=.8)
```



Prettier plots

```
library(rattle)
fancyRpartPlot(modFit$finalModel)
```



Predicting new values

```
predict(modFit,newdata=testing)
```

```
 [1] setosa     setosa     setosa     setosa     setosa     setosa     setosa     setosa    
 [9] setosa     setosa     setosa     setosa     setosa     setosa     setosa     versicolor
[17] versicolor versicolor versicolor versicolor versicolor versicolor versicolor versicolor
[25] virginica  versicolor virginica  versicolor versicolor versicolor virginica  virginica 
[33] virginica  versicolor virginica  virginica  virginica  virginica  virginica  virginica 
[41] virginica  virginica  virginica  virginica  virginica 
Levels: setosa versicolor virginica
```

Notes and further resources

- Classification trees are non-linear models
  - They use interactions between variables
  - Data transformations may be less important (monotone transformations)
  - Trees can also be used for regression problems (continuous outcome)
- Note that there are multiple tree building options in R both in the caret package - party, rpart and out of the caret package - tree
- Introduction to statistical learning
- Elements of Statistical Learning
- Classification and regression trees