Predicting with trees

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Key ideas

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

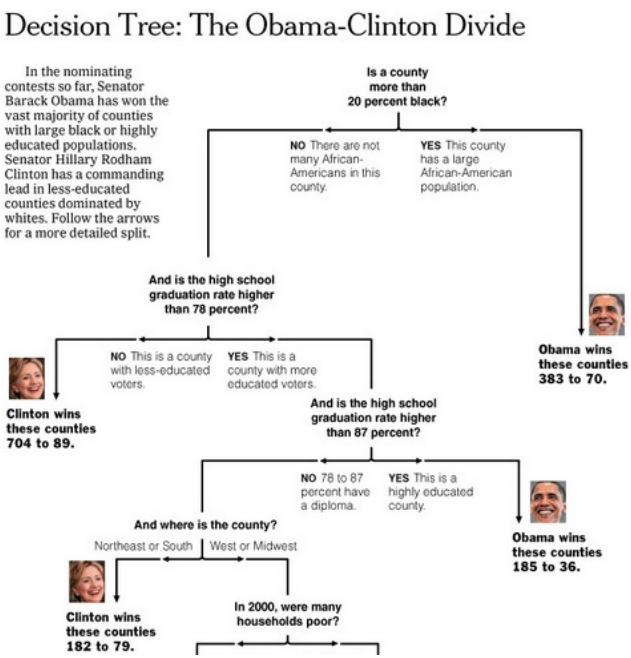
Pros:

- 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

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

Misclassification Error:

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

- 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

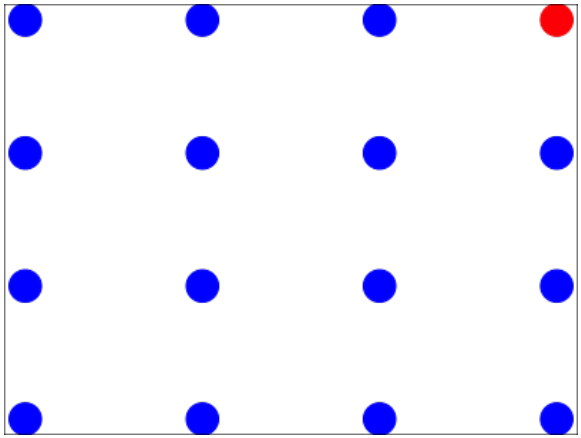
Deviance/information gain:

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

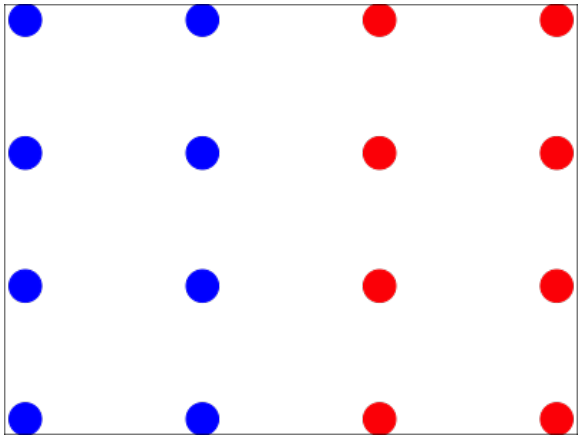
- 0 = perfect purity
- 1 = no purity

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
```

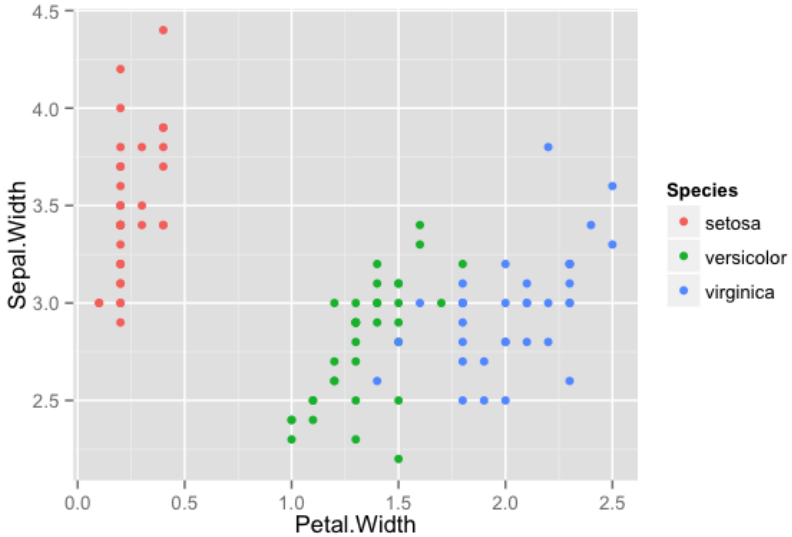
Create training and test sets

```
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)
```

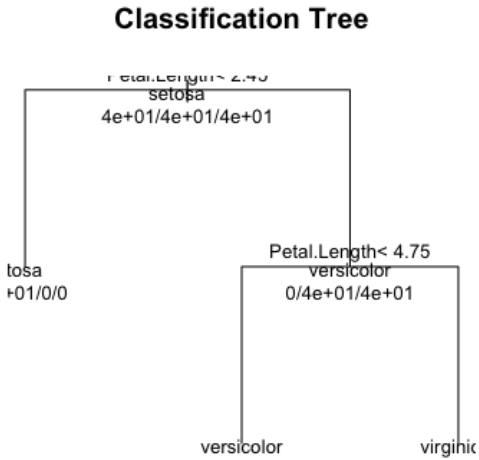
```
n= 105

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) *
```

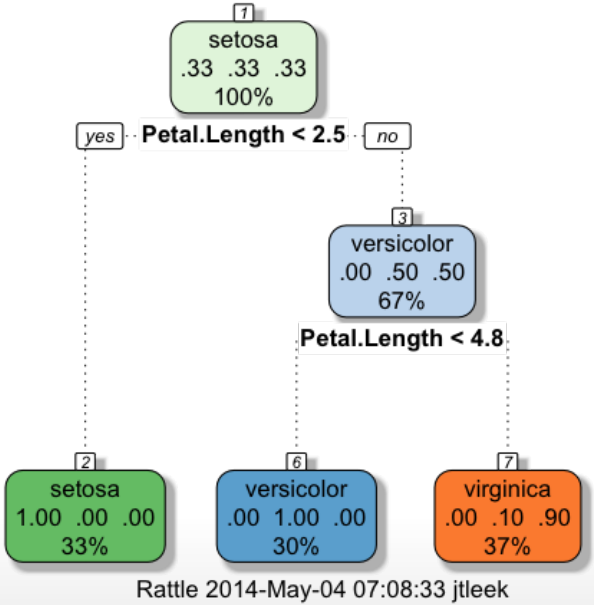
Plot tree

```
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

Bagging

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Bootstrap aggregating (bagging)

Basic idea:

1. Resample cases and recalculate predictions
2. Average or majority vote

Notes:

- Similar bias
- Reduced variance
- More useful for non-linear functions

Ozone data

```
library(ElemStatLearn); data(ozone,package="ElemStatLearn")
ozone <- ozone[order(ozone$ozone),]
head(ozone)
```

```
    ozone radiation temperature wind
17      1         8          59  9.7
19      4        25          61  9.7
14      6        78          57 18.4
45      7        48          80 14.3
106     7        49          69 10.3
7       8        19          61 20.1
```

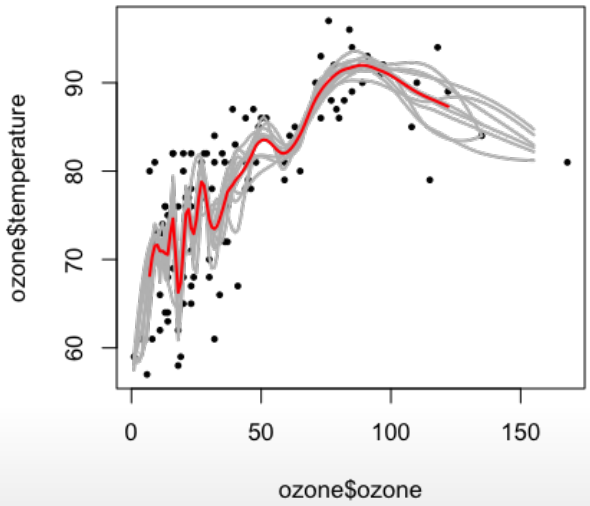
http://en.wikipedia.org/wiki/Bootstrap_aggregating

Bagged loess

```
ll <- matrix(NA,nrow=10,ncol=155)
for(i in 1:10){
  ss <- sample(1:dim(ozone)[1],replace=T)
  ozone0 <- ozone[ss,]; ozone0 <- ozone0[order(ozone0$ozone),]
  loess0 <- loess(temperature ~ ozone,data=ozone0,span=0.2)
  ll[i,] <- predict(loess0,newdata=data.frame(ozone=1:155))
}
```

Bagged loess

```
plot(ozone$ozone,ozone$temperature,pch=19,cex=0.5)
for(i in 1:10){lines(1:155,ll[i,],col="grey",lwd=2)}
lines(1:155,apply(ll,2,mean),col="red",lwd=2)
```



Bagging in caret

- Some models perform bagging for you, in `train` function consider `method` options
  - `bagEarth`
  - `treebag`
  - `bagFDA`
- Alternatively you can bag any model you choose using the `bag` function

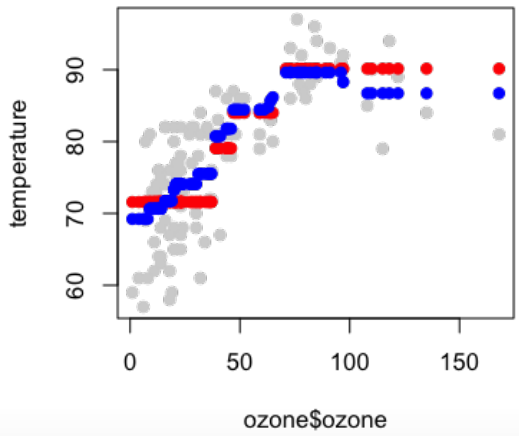
More bagging in caret

```
predictors = data.frame(ozone=ozone$ozone)
temperature = ozone$temperature
treebag <- bag(predictors, temperature, B = 10,
               bagControl = bagControl(fit = ctreeBag$fit,
                                       predict = ctreeBag$pred,
                                       aggregate = ctreeBag$aggregate))
```

http://www.inside-r.org/packages/cran/caret/docs/nbBag

Example of custom bagging (continued)

```
plot(ozone$ozone,temperature,col='lightgrey',pch=19)
points(ozone$ozone,predict(treebag$fits[[1]]$fit,predictors),pch=19,col="red")
points(ozone$ozone,predict(treebag,predictors),pch=19,col="blue")
```



Parts of bagging

```
ctreeBag$fit
```

```
function (x, y, ...)
{
    library(party)
    data <- as.data.frame(x)
    data$y <- y
    ctree(y ~ ., data = data)
}
<environment: namespace:caret>
```

Parts of bagging

```
ctreeBag$pred
```

```
function (object, x)
{
    obsLevels <- levels(object@data@get("response")[, 1])
    if (!is.null(obsLevels)) {
        rawProbs <- treeresponse(object, x)
        probMatrix <- matrix(unlist(rawProbs), ncol = length(obsLevels),
            byrow = TRUE)
        out <- data.frame(probMatrix)
        colnames(out) <- obsLevels
        rownames(out) <- NULL
    }
    else out <- unlist(treeresponse(object, x))
    out
}
<environment: namespace:caret>
```

Parts of bagging

```
ctreeBag$aggregate
```

```
function (x, type = "class")
{
    if (is.matrix(x[[1]]) | is.data.frame(x[[1]])) {
        pooled <- x[[1]] & NA
        classes <- colnames(pooled)
        for (i in 1:ncol(pooled)) {
            tmp <- lapply(x, function(y, col) y[, col], col = i)
            tmp <- do.call("rbind", tmp)
            pooled[, i] <- apply(tmp, 2, median)
        }
        if (type == "class") {
            out <- factor(classes[apply(pooled, 1, which.max)],
                levels = classes)
        }
        else out <- as.data.frame(pooled)
    }
    else {
        x <- matrix(unlist(x), ncol = length(x))
```

Notes and further resources

Notes:

- Bagging is most useful for nonlinear models
- Often used with trees - an extension is random forests
- Several models use bagging in caret's *train* function

Further resources:

- Bagging
- Bagging and boosting
- Elements of Statistical Learning

Random forests

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Random forests

1. Bootstrap samples
2. At each split, bootstrap variables
3. Grow multiple trees and vote

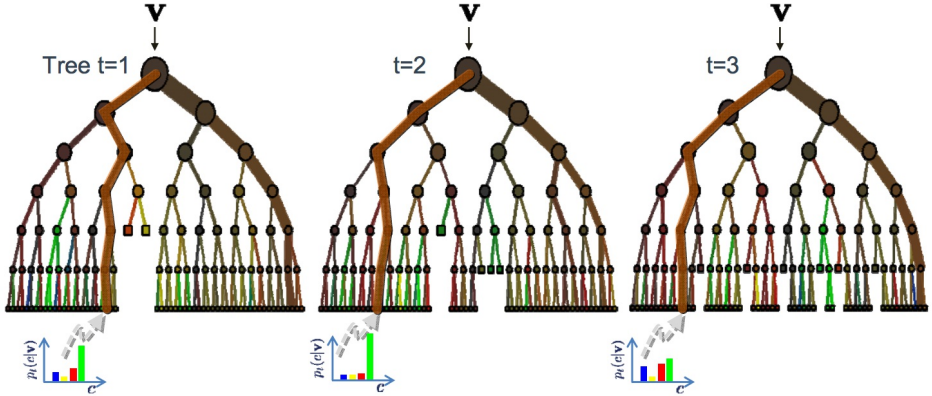
Pros:

1. Accuracy

Cons:

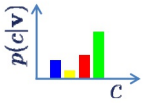
1. Speed
2. Interpretability
3. Overfitting

Random forests



The ensemble model

Forest output probability $p(c|\mathbf{v}) = \frac{1}{T}\sum_{t}^{T} p_t(c|\mathbf{v})$



http://www.robots.ox.ac.uk/~az/lectures/ml/lect5.pdf

Iris data

```
data(iris); library(ggplot2)
inTrain <- createDataPartition(y=iris$Species,
                               p=0.7, list=FALSE)
training <- iris[inTrain,]
testing <- iris[-inTrain,]
```

Random forests

```
library(caret)
modFit <- train(Species~ .,data=training,method="rf",prox=TRUE)
modFit
```

```
105 samples
  4 predictors
  3 classes: 'setosa', 'versicolor', 'virginica'

No pre-processing
Resampling: Bootstrap (25 reps)

Summary of sample sizes: 105, 105, 105, 105, 105, 105, ...

Resampling results across tuning parameters:

  mtry  Accuracy  Kappa  Accuracy SD  Kappa SD
  2     0.9       0.9    0.03         0.04
  3     0.9       0.9    0.03         0.05
  4     0.9       0.9    0.03         0.05
```

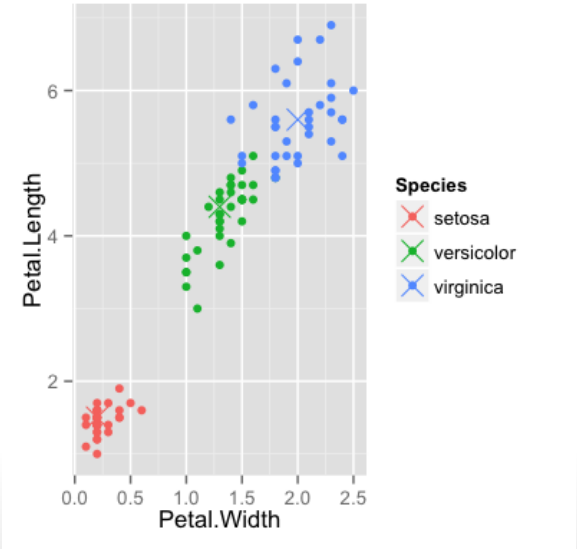
Getting a single tree

```
getTree(modFit$finalModel,k=2)
```

```
   left daughter right daughter split var split point status prediction
1              2              3         4        0.70      1          0
2              0              0         0        0.00     -1          1
3              4              5         4        1.70      1          0
4              6              7         3        4.95      1          0
5              8              9         3        4.85      1          0
6              0              0         0        0.00     -1          2
7             10             11         4        1.55      1          0
8             12             13         1        5.95      1          0
9              0              0         0        0.00     -1          3
10             0              0         0        0.00     -1          3
11             0              0         0        0.00     -1          2
12             0              0         0        0.00     -1          2
13             0              0         0        0.00     -1          3
```

Class "centers"

```
irisP <- classCenter(training[,c(3,4)], training$Species, modFit$finalModel$prox)
irisP <- as.data.frame(irisP); irisP$Species <- rownames(irisP)
p <- qplot(Petal.Width, Petal.Length, col=Species,data=training)
p + geom_point(aes(x=Petal.Width,y=Petal.Length,col=Species),size=5,shape=4,data=irisP)
```



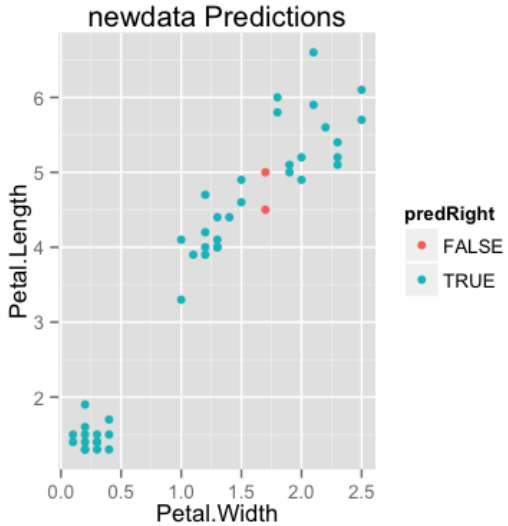
Predicting new values

```
pred <- predict(modFit,testing); testing$predRight <- pred==testing$Species
table(pred,testing$Species)
```

```
pred         setosa versicolor virginica
  setosa         15          0         0
  versicolor      0         14         1
  virginica       0          1        14
```

Predicting new values

```
qplot(Petal.Width,Petal.Length,colour=predRight,data=testing,main="newdata Predictions")
```



Notes and further resources

Notes:

- Random forests are usually one of the two top performing algorithms along with boosting in prediction contests.
- Random forests are difficult to interpret but often very accurate.
- Care should be taken to avoid overfitting (see rfcv funtion)

Further resources:

- Random forests
- Random forest Wikipedia
- Elements of Statistical Learning

Boosting

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Basic idea

1. Take lots of (possibly) weak predictors
2. Weight them and add them up
3. Get a stronger predictor

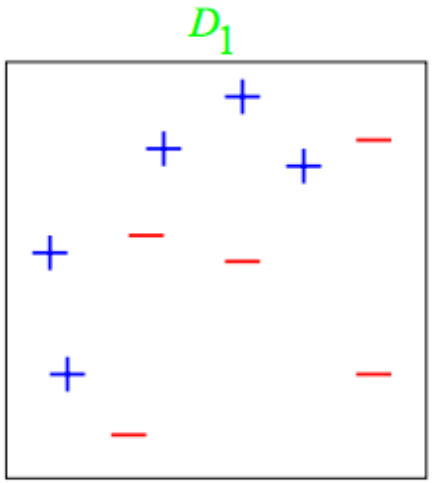
Basic idea behind boosting

1. Start with a set of classifiers $h_1, \ldots, h_k$
   - Examples: All possible trees, all possible regression models, all possible cutoffs.
2. Create a classifier that combines classification functions: $f(x) = \text{sgn}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$.
   - Goal is to minimize error (on training set)
   - Iterative, select one h at each step
   - Calculate weights based on errors
   - Upweight missed classifications and select next h

Adaboost on Wikipedia

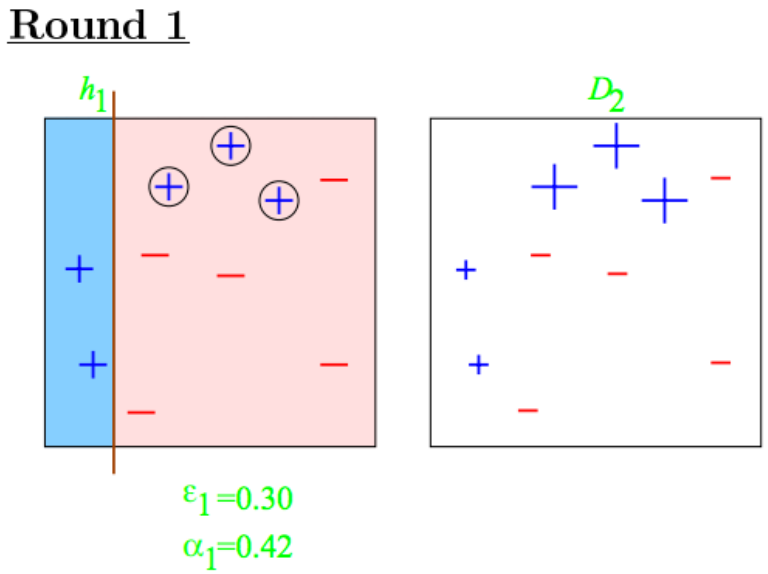
http://webee.technion.ac.il/people/rmeir/BoostingTutorial.pdf

Simple example



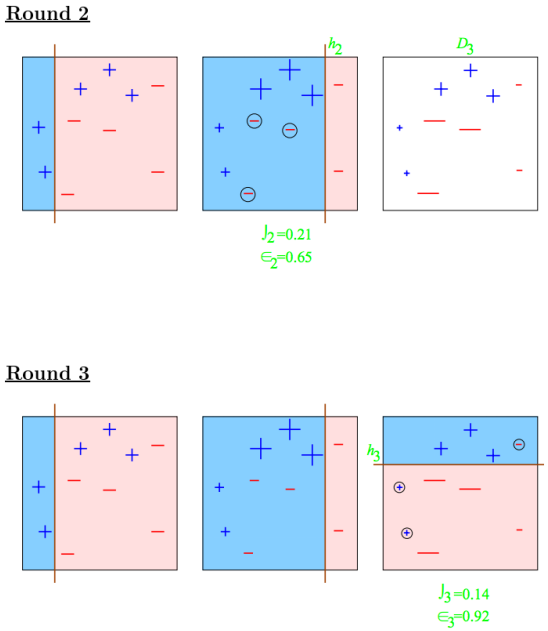
http://webee.technion.ac.il/people/rmeir/BoostingTutorial.pdf

Round 1: adaboost



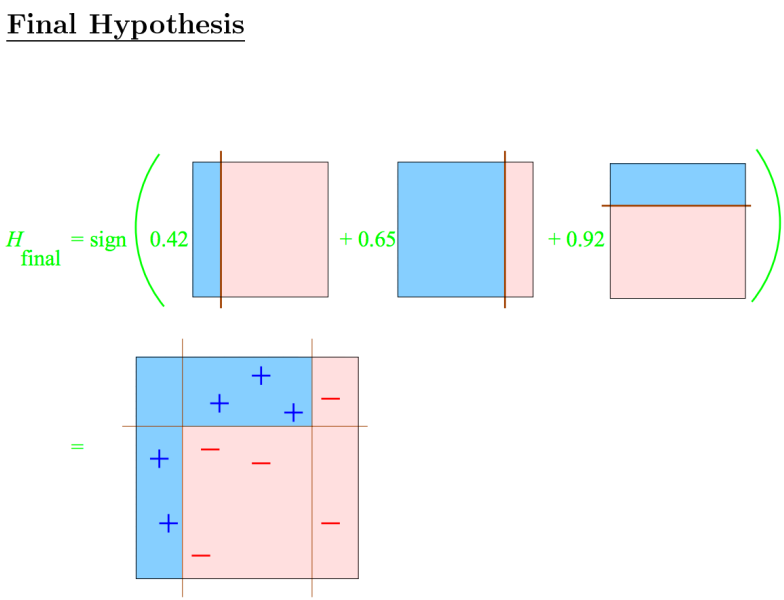
http://webee.technion.ac.il/people/rmeir/BoostingTutorial.pdf

Round 2 & 3



http://webee.technion.ac.il/people/rmeir/BoostingTutorial.pdf

Completed classifier



http://webee.technion.ac.il/people/rmeir/BoostingTutorial.pdf

Boosting in R

- Boosting can be used with any subset of classifiers
- One large subclass is gradient boosting
- R has multiple boosting libraries. Differences include the choice of basic classification functions and combination rules.
  - gbm - boosting with trees.
  - mboost - model based boosting
  - ada - statistical boosting based on additive logistic regression
  - gamBoost for boosting generalized additive models
- Most of these are available in the caret package

Wage example

```
library(ISLR); data(Wage); library(ggplot2); library(caret);
Wage <- subset(Wage,select=-c(logwage))
inTrain <- createDataPartition(y=Wage$wage,
                               p=0.7, list=FALSE)
training <- Wage[inTrain,]; testing <- Wage[-inTrain,]
```

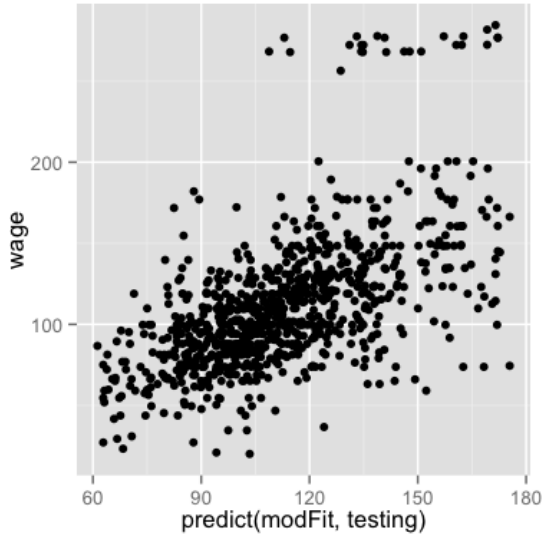
Fit the model

```
modFit <- train(wage ~ ., method="gbm",data=training,verbose=FALSE)
print(modFit)
```

```
2102 samples
  10 predictors

No pre-processing
Resampling: Bootstrap (25 reps)

Summary of sample sizes: 2102, 2102, 2102, 2102, 2102, 2102, ...

Resampling results across tuning parameters:

  interaction.depth  n.trees  RMSE  Rsquared  RMSE SD  Rsquared SD
  1                  50       30    0.3       1        0.02
  1                  100      30    0.3       1        0.02
  1                  200      30    0.3       1        0.02
  2                  50       30    0.3       1        0.02
  2                  100      30    0.3       1        0.02
  2                  200      30    0.3       1        0.02
```

Plot the results

```
qplot(predict(modFit,testing),wage,data=testing)
```



Notes and further reading

- A couple of nice tutorials for boosting
  - Freund and Shapire - http://www.cc.gatech.edu/~thad/6601-gradAI-fall2013/boosting.pdf
  - Ron Meir- http://webee.technion.ac.il/people/rmeir/BoostingTutorial.pdf
- Boosting, random forests, and model ensembling are the most common tools that win Kaggle and other prediction contests.
  - http://www.netflixprize.com/assets/GrandPrize2009_BPC_BigChaos.pdf
  - https://kaggle2.blob.core.windows.net/wiki-files/327/09ccf652-8c1c-4a3d-b979-ce2369c985e4/Willem%20Mestrom%20-%20Milestone%201%20Description%20V2%202.pdf

Model based prediction

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Basic idea

1. Assume the data follow a probabilistic model
2. Use Bayes' theorem to identify optimal classifiers

Pros:

- Can take advantage of structure of the data
- May be computationally convenient
- Are reasonably accurate on real problems

Cons:

- Make additional assumptions about the data
- When the model is incorrect you may get reduced accuracy

Model based approach

1. Our goal is to build parametric model for conditional distribution $P(Y = k|X = x)$
2. A typical approach is to apply Bayes theorem:

$$Pr(Y = k|X = x) = \frac{Pr(X = x|Y = k)Pr(Y = k)}{\sum_{\ell=1}^{K} Pr(X = x|Y = \ell)Pr(Y = \ell)}$$

$$Pr(Y = k|X = x) = \frac{f_k(x)\pi_k}{\sum_{\ell=1}^{K} f_\ell(x)\pi_\ell}$$

3. Typically prior probabilities π_k are set in advance.
4. A common choice for $f_k(x) = \frac{1}{\sigma_k\sqrt{2\pi}} e^{-\frac{(x-\mu_k)^2}{\sigma_k^2}}$, a Gaussian distribution
5. Estimate the parameters (μ_k, σ_k^2) from the data.
6. Classify to the class with the highest value of $P(Y = k|X = x)$

Classifying using the model

A range of models use this approach

- Linear discriminant analysis assumes $f_k(x)$ is multivariate Gaussian with same covariances
- Quadratic discrimant analysis assumes $f_k(x)$ is multivariate Gaussian with different covariances
- Model based prediction assumes more complicated versions for the covariance matrix
- Naive Bayes assumes independence between features for model building

http://statweb.stanford.edu/~tibs/ElemStatLearn/

Why linear discriminant analysis?

$$\log \frac{\Pr(Y = k|X = x)}{\Pr(Y = j|X = x)}$$

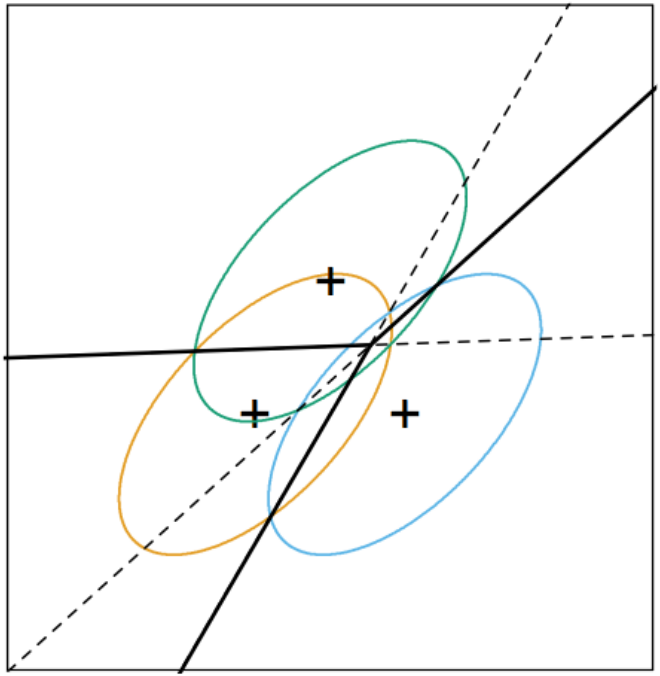
$$= \log \frac{f_k(x)}{f_j(x)} + \log \frac{\pi_k}{\pi_j}$$

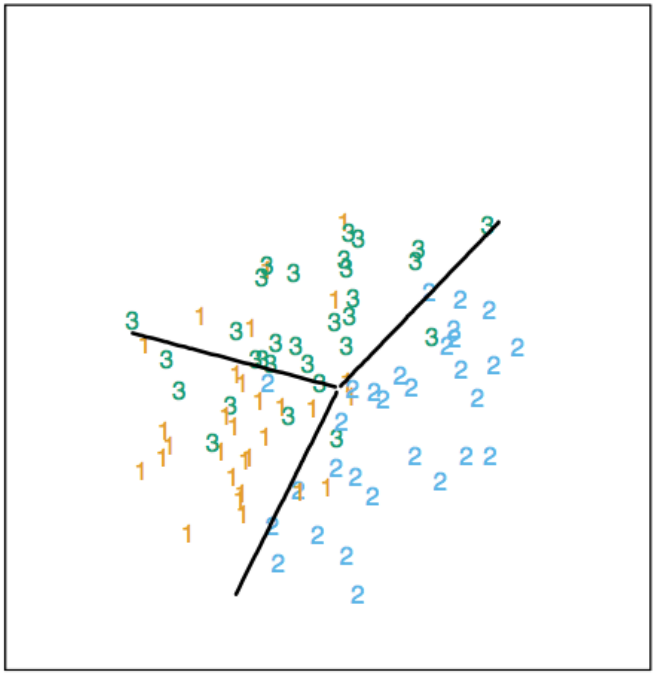
$$= \log \frac{\pi_k}{\pi_j} - \frac{1}{2}(\mu_k + \mu_j)^T \Sigma^{-1}(\mu_k + \mu_j)$$

$$+ x^T \Sigma^{-1}(\mu_k - \mu_j)$$

http://statweb.stanford.edu/~tibs/ElemStatLearn/

Decision boundaries





Discriminant function

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k \Sigma^{-1} \mu_k + \log(\mu_k)$$

- Decide on class based on $\hat{Y}(x) = \text{argmax}_k \delta_k(x)$
- We usually estimate parameters with maximum likelihood

Naive Bayes

Suppose we have many predictors, we would want to model: $P(Y = k|X_1, \ldots, X_m)$

We could use Bayes Theorem to get:

$$P(Y = k|X_1, \ldots, X_m) = \frac{\pi_k P(X_1, \ldots, X_m|Y = k)}{\sum_{\ell=1}^{K} P(X_1, \ldots, X_m|Y = k)\pi_\ell}$$

$$\propto \pi_k P(X_1, \ldots, X_m|Y = k)$$

This can be written:

$$P(X_1, \ldots, X_m, Y = k) = \pi_k P(X_1|Y = k)P(X_2, \ldots, X_m|X_1, Y = k)$$

$$= \pi_k P(X_1|Y = k)P(X_2|X_1, Y = k)P(X_3, \ldots, X_m|X_1, X_2, Y = k)$$

$$= \pi_k P(X_1|Y = k)P(X_2|X_1, Y = k) \ldots P(X_m|X_1 \ldots, X_{m-1}, Y = k)$$

We could make an assumption to write this:

$$\approx \pi_k P(X_1|Y = k)P(X_2|Y = k) \ldots P(X_m|, Y = k)$$

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
```

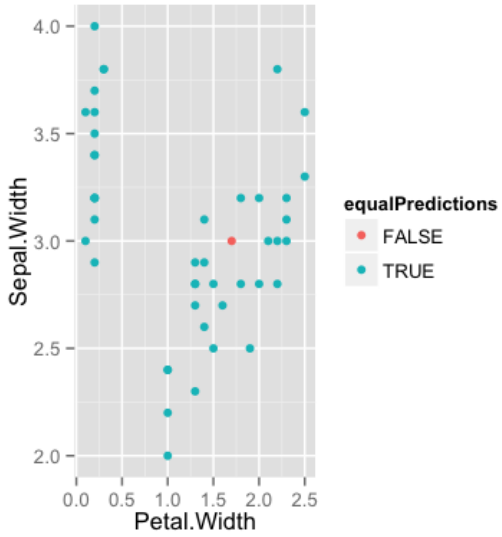
Build predictions

```
modlda = train(Species ~ .,data=training,method="lda")
modnb = train(Species ~ ., data=training,method="nb")
plda = predict(modlda,testing); pnb = predict(modnb,testing)
table(plda,pnb)
```

```
            pnb
plda         setosa versicolor virginica
  setosa         15          0         0
  versicolor      0         13         1
  virginica       0          0        16
```

Comparison of results

```
equalPredictions = (plda==pnb)
qplot(Petal.Width,Sepal.Width,colour=equalPredictions,data=testing)
```



Notes and further reading

- Introduction to statistical learning
- Elements of Statistical Learning
- Model based clustering
- Linear Discriminant Analysis
- Quadratic Discriminant Analysis