MA5832: Data Mining & Machine Learning

Collaborate Week 3: Tree Based Methods

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Housekeeping

- Collaborates = Thursdays 6-7:30pm

For my Collaborate Sessions, you can get the slides & R code for each week on Github:

https://github.com/MarthaCooper/MA8532

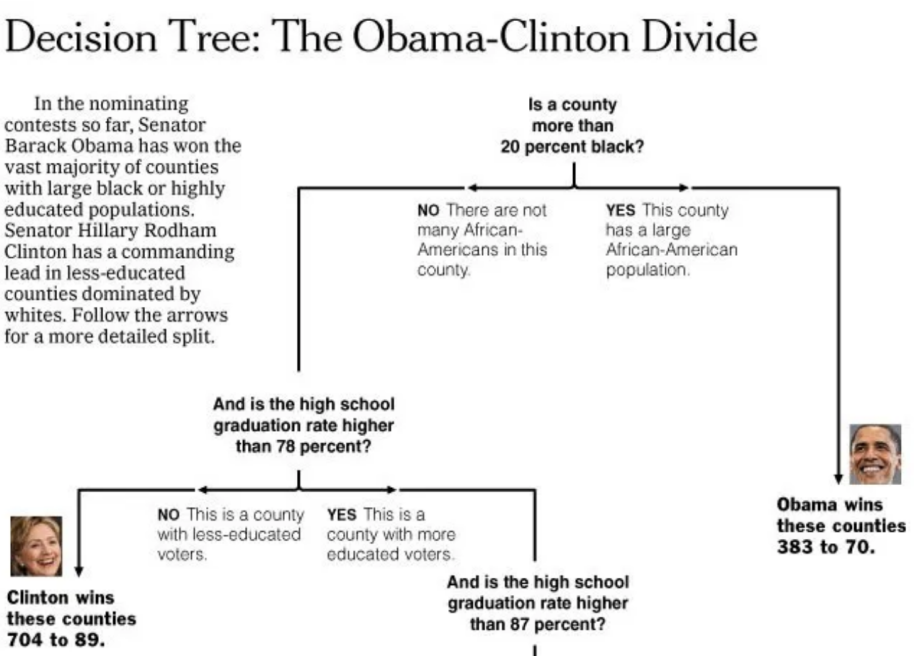
Today's Goals

- Regression Trees
- Decision Trees
- Bagging
- Random Forest
- Boosting

Tree Based Methods

Tree Based Methods

- Split samples into groups
- Test homogeneity or purity of each group
- Split again



New York Times

Jeff Leek's Practical Machine Learning

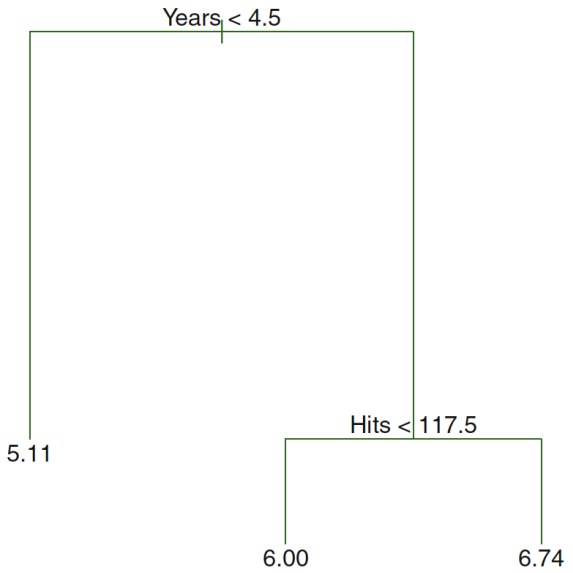
Tree Based Methods

- CART = classification & regression trees
- Stratifying or segmenting predictor spare into a number of simple regions
- The set of splitting rules used to segment predictor space can be summarized as a *tree* or dendrogram.
- Trees are simple and easy to interpret, but have poor predictive accuracy.
- Bagging, Random Forest and Boosting are all approaches that combine multiple trees together to yield a consensus prediction. This improves predictive accuracy at the cost of interpretation.

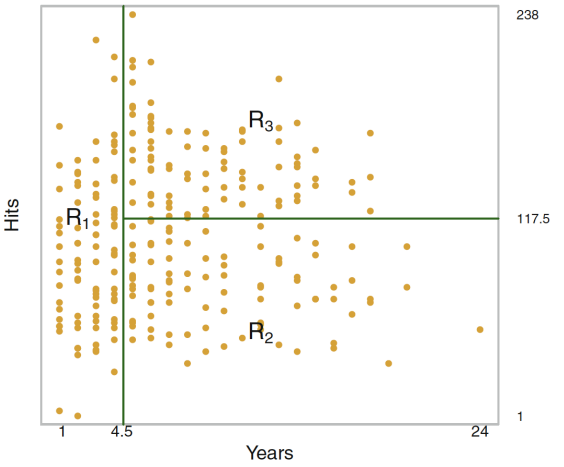
Regression Trees

- Predicting a continuous response
- Predicting baseball player's salaries using the number of years playing major league baseball and the number of hits made in the previous year.

Regression Tree



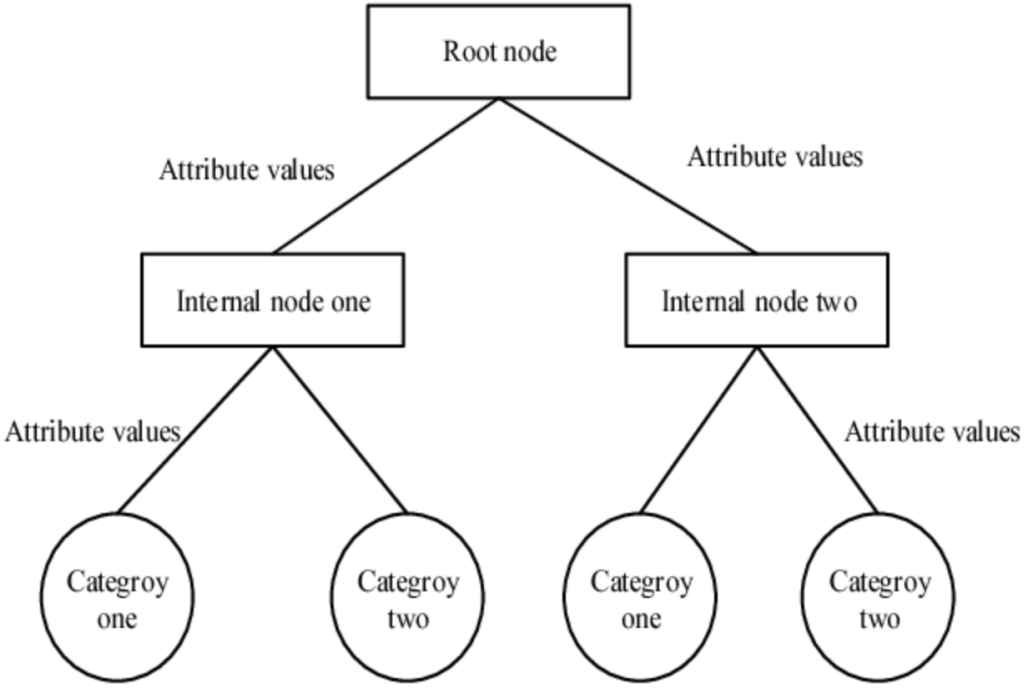
Three-region partition



Predicted salaries are given by the mean value for players in each region.

Tree terminology

- Root node: no incoming edge, zero or more outgoing edges
- Internal node: one incoming edge, two (or more) outgoing edges
- Leaf or Terminal node: each leaf node is assigned a class label, contain a response variable, y
- Parent and Child nodes: If a node is split, we refer to that node as a parent node, and the resulting nodes are called child nodes.
- Branches: Segments that connect the nodes.



Building a regression tree

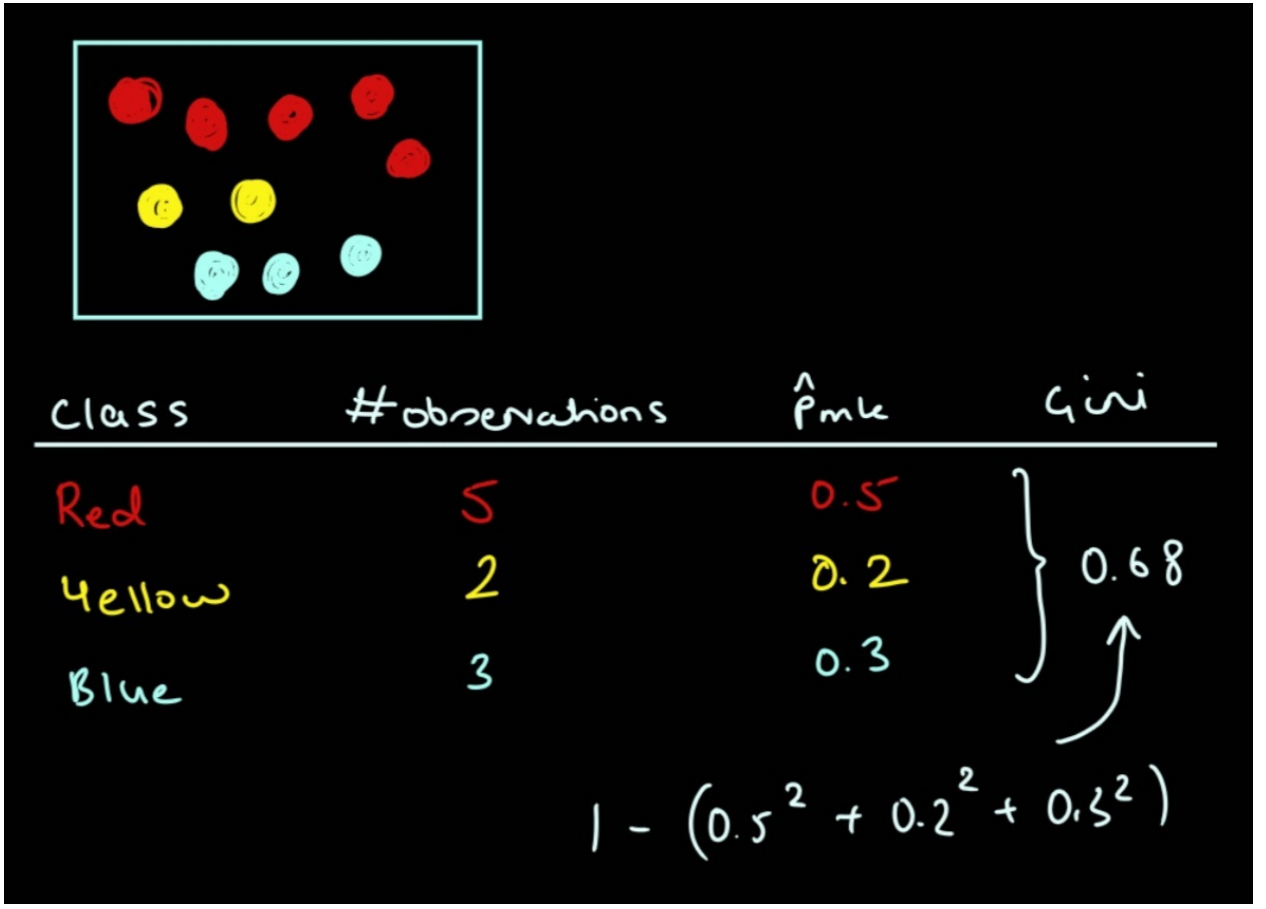
1. Divide the predictor space into j distinct and non-overlapping regions $R_1, R_2, \ldots, R_j$
2. For every observation in region R_j we make the same prediction - the mean on the response values for training observations

- Regions $R_1, R_2, \ldots, R_j$ are high-dimensional rectangles or *boxes*
- Loss function: $\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$
- where $\hat{y}_{R_j}$ is the mean response for observation in the jth region.
- Greedy algorithm - looks for best split at each step.

Classification Trees

- Predicting a qualitative response
- Different loss functions to measure class impurity or at each node, m
- Gini Index: $1 - \sum_{k=1}^{K} (\hat{p}_{mk})^2$
- Cross entropy: $- \sum_{k=1}^{K} \hat{p}_{mk} log \hat{p}_{mk}$
- where $\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$, or the proportion of observations in the mth region that are from the kth class

An example


Class
#observations
$\hat{p}_{mk}$
Gini
Red
5
0.5
Yellow
2
0.2
Blue
3
0.3
0.68
$1 - (0.5^2 + 0.2^2 + 0.3^2)$

Regression Trees in R

```r
library(ggplot2) #for plotting
library(caret) #for trees
library(rattle)

data(iris) #get data
head(iris) #view data
table(iris$Species) #groups to classify
set.seed(6)
test_index <- createDataPartition(iris$Species, p = 0.3, list = F)
training <- iris[-test_index, ] #training and test splits
testing <- iris[test_index, ]
set.seed(6)
fit1 <- train(Species ~., method = "rpart", data = training) #fit model
fancyRpartPlot(fit1$finalModel) #plot
preds <-predict(fit1, newdata = testing) #make predictions
table(preds, testing$Species) #compare preds
```

CART Summary

- Non-linear models
- Easy to interpret
- High variance - sensitive to small changes in training data and not very accurate at making predictions

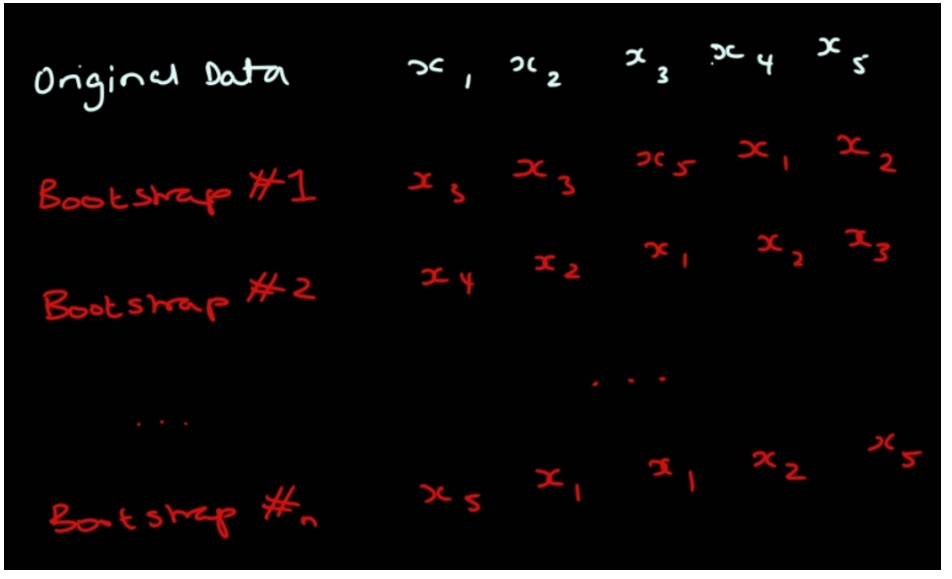
Bagging, Random Forest and Boosting

- Making more powerful prediction models

Bagging

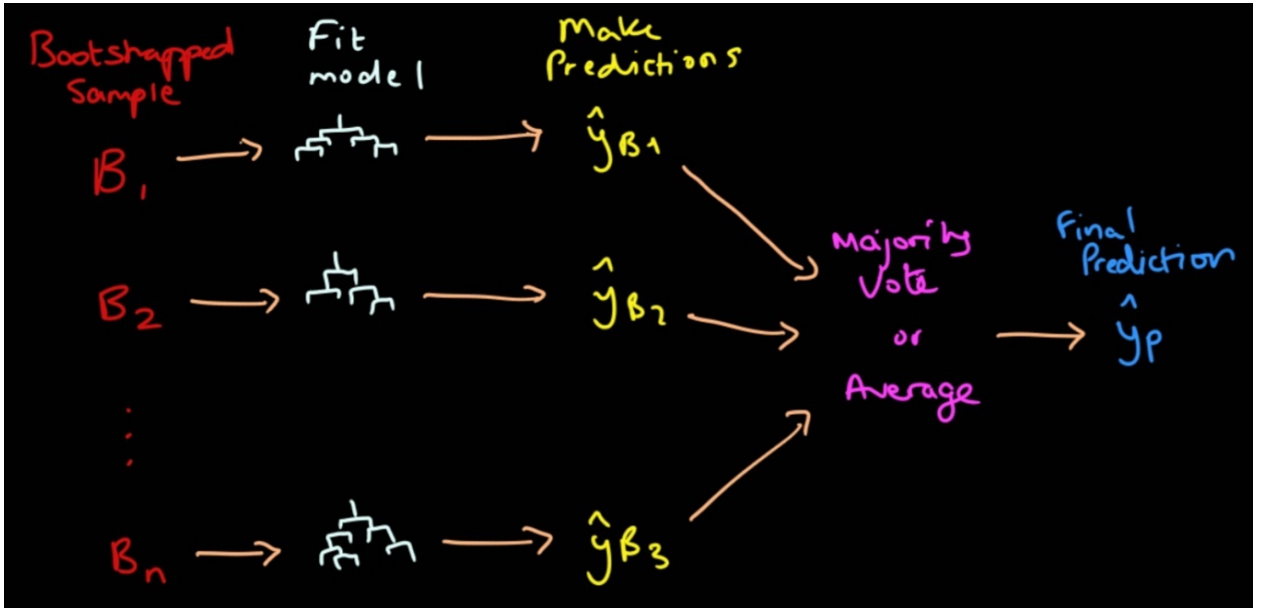
Bootstrap Aggregation = Bagging

1. *Bootstrap* the samples = draw many random samples with replacement
2. Refit the model (note: *any* model) to the bootstrapped samples and aggregate the results between all models.



Bagging Tree

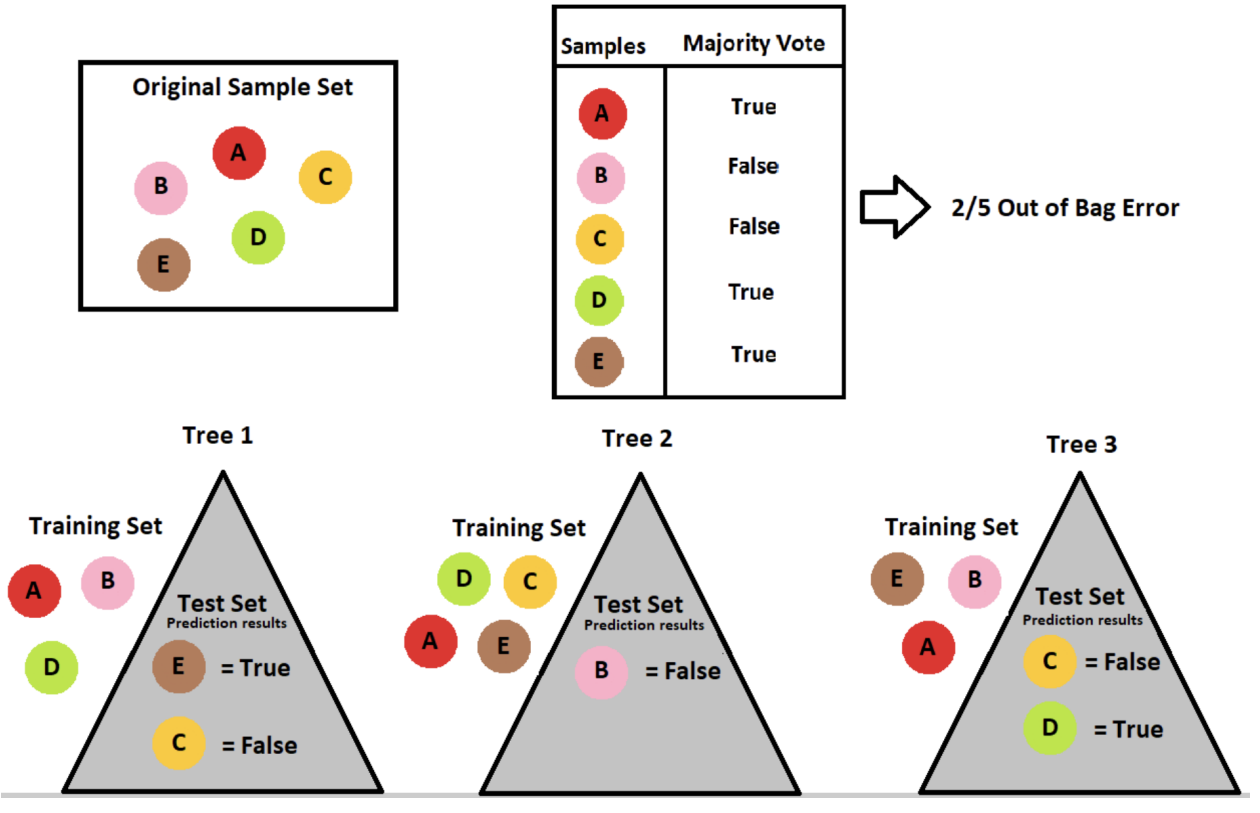
- Bagging can improve the accuracy of unstable models that tend to overfit



Out-of-Bag Error Estimation

- Estimating the error of a bagged model
- Each bagged tree uses ~2/3rd of the training data
- The remaining ~1/3rd are called *Out-of-Bag* observations
- We can predict the response for the ith observation using each of the trees for with that sample was *OOB*
- We then take the majority vote/ average result to get a prediction for that sample.
- Compile results to get overall estimate of OOB error.

Out-of-Bag Error Estimation



OOB Error

Bagging in R

```
set.seed(6)
fit2 <- ipred::bagging(Species~., data = training, coob = T, nbagg = 10)
preds <<- predict(fit2, testing)
table(preds, testing$Species)
```

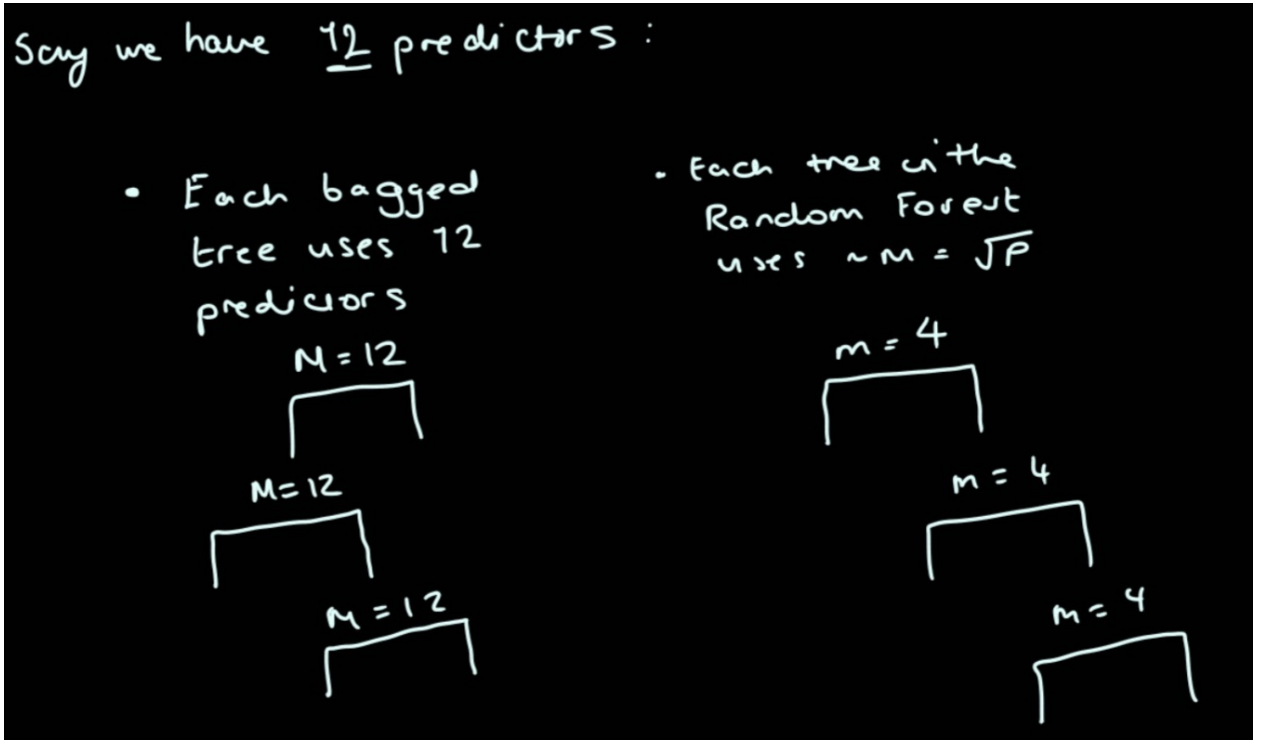
Random Forests

- Similar to bagging trees
- At each split, a random sample of m predictors is chosen as split candidates from the full set of P predictions
- We can select a value of m to start (e.g. $\sqrt{P}$), and tune by cross-validation
- Why?

Random Forests

- Similar to bagging trees
- At each split, a random sample of m predictors is chosen as split candidates from the full set of P predictions
- We can select a value of m to start (e.g. $\sqrt{P}$), and tune by cross-validation
- Why? *Decorrelates* the trees

Random Forests



Random forest in R

```
tc <- trainControl(method = "repeatedcv", number = 10, repeats  = 3) #se
tg <- expand.grid(mtry = seq(2,ncol(training)-2,1)) #set up tunegrid
set.seed(6)
fit3 <- train(Species ~., method = "rf", data = training, trControl = tc
fit3$finalModel
randomForest::getTree(fit3$finalModel, k = 3) #get individual trees
preds <- predict(fit3, testing) #make predictions
table(preds, testing$Species) #compare predictions
plot(varImp(fit3, scale = F)) #variable importance
```

Boosting

Note: *not just for trees*, but we will focus on trees here

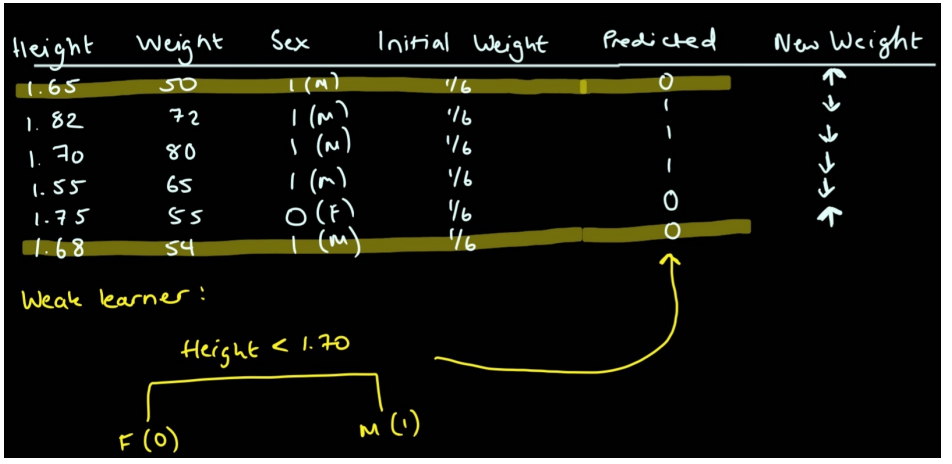
- Combine weak learners to create strong learners. A weak learning is a classifier that performs poorly, but is still better than a random guess.
- Weak the weak learners and add them up
- Sequential - each tree is grown using information from the previous tree. This is an iterative process , where samples in the training set are re-weighted at each iteration, so that the second iteration can correct errors from the model in the first iteration. Trees are added until the training set is predicted perfectly

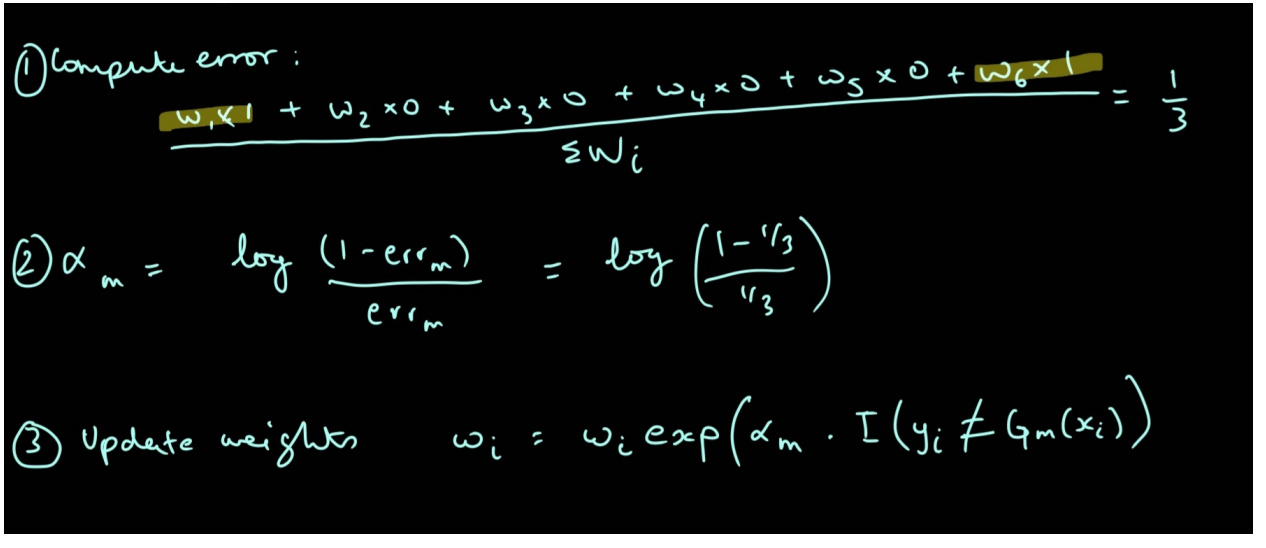
e.g. AdaBoost & Gradient Boosting

Adaboost for Decision Trees

1. Combine weak learners (small trees or stumps) to create strong learners.
2. Each individual tree is weighted based on how well it classifies samples
3. Each sequential tree learns from the previous tree's mistake by adjusting the weight of samples. If the observation is misclassified by the previous tree, the weight of the observation increases; conversely, the weight decreases if correctly classified. The updated weights are then used in the next iteration for tree fitting.

Adaboost for Decision Trees





Gradient boosting

Algorithm 8.2 *Boosting for Regression Trees*

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   (a) Fit a tree $\hat{f}^b$ with d splits ($d+1$ terminal nodes) to the training data (X, r).
   (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:

$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \tag{8.10}$$

   (c) Update the residuals,

$$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \tag{8.11}$$

3. Output the boosted model,

$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x). \tag{8.12}$$

Boosting in R

- gbm
- xgboost

Homework to try this in R...

Extra reading

- Chapter 8 ISLR
- Chapters 9.2 & 10 ESL
- StatQuest!

References

- Chapter 8 ISLR
- Jeff Leek's Practical Machine Learning

Slides

- xaringhan, xaringanthemer, remark.js, knitr, R Markdown