Birkbeck
UNIVERSITY OF LONDON

Big Data Analytics

Session 7

Bagging and Random Forests

Pros and Cons of Decision Trees

- Pros:
  - Trees are very easy to explain to people (probably even easier than linear regression)
  - Trees can be plotted graphically
  - They work fine on both classification and regression problems

- Cons:
  - Trees don’t have the same prediction accuracy as some of the more complicated approaches that we examine in this course
  - High variance

  ➢ By aggregating many decision trees, the predictive performance of trees can be substantially improved. How?
    - using methods like bagging, random forests, and boosting

Outline

- Bagging
  - Bootstrapping
  - Bagging for Regression Trees
  - Bagging for Classification Trees
  - Out-of-Bag Error Estimation
  - Variable Importance: Relative Influence Plots

- Random Forests

Problem

- Decision trees discussed earlier suffer from high variance!
  - If we randomly split the training data into 2 parts, and fit decision trees on both parts, the results could be quite different

- We would like to have models with low variance

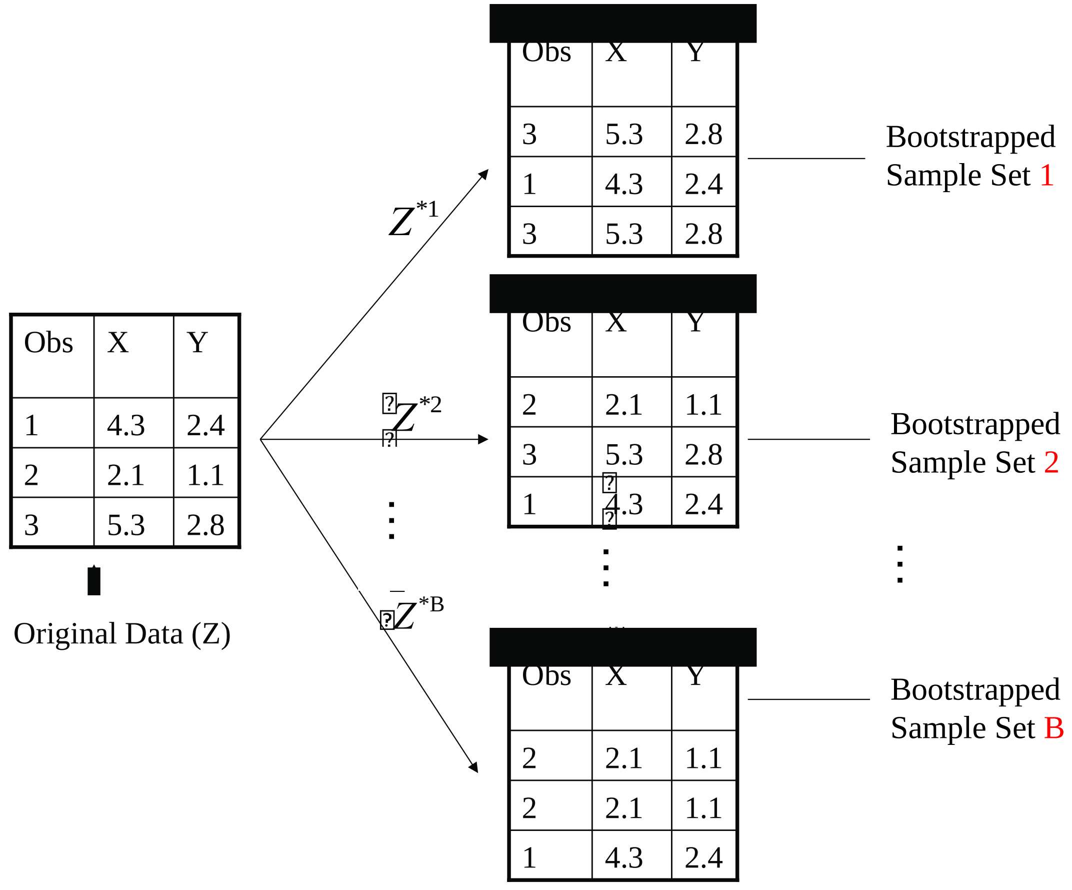
- To solve this problem, we can use bagging (***b***ootstrap ***agg***regat***ing***).

Random Sampling

- Before introducing bootstrapping, we introduce random sampling with/without replacement
  - Random sampling without replacement
    - One deliberately *avoids* choosing any member of the population more than once
    - Once a member is chosen, it cannot be chosen again
  - Random sampling with replacement
    - The population is “replaced” every time a member is chosen
    - The same member can be chosen more than once

Bootstrapping is simple!

- Resampling of the observed dataset (and of equal size to the observed dataset), each of which is obtained by random sampling with replacement from the original dataset.



Obs	X	Y
1	4.3	2.4
2	2.1	1.1
3	5.3	2.8

Original Data (Z)

Z^{*1}

Obs	X	Y
3	5.3	2.8
1	4.3	2.4
3	5.3	2.8

Bootstrapped Sample Set 1

Z^{*2}

Obs	X	Y
2	2.1	1.1
3	5.3	2.8
1	4.3	2.4

Bootstrapped Sample Set 2

⋮

Z^{*B}

Obs	X	Y
2	2.1	1.1
2	2.1	1.1
1	4.3	2.4

Bootstrapped Sample Set B

→We could have distinct “training sets” by repeatedly sampling from the original data set

→Distinct test sets are usually there to obtain a measure of variability – how the test MSE/error rate varies

What is bagging?

- Bagging is an extremely powerful idea based on two things:
  - Bootstrapping: plenty of training datasets!
  - Averaging: reduces variance!

- Why does averaging reduces variance?
  - Averaging a set of observations reduces variance.
  - Recall that given a set of n independent observations $Z_1, \ldots, Z_n$,
    - each with variance σ^2 ,
    - the variance of the mean $\overline{Z}$ of the observations is given by σ^2/n

How does bagging work?

- Generate B different bootstrapped training datasets

- Train the statistical learning method (e.g. a decision tree) on each of the B training datasets, and obtain the prediction

- For prediction:
  - Regression: average all predictions from all B trees
  - Classification: majority vote among all B trees

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Bagging for Regression Trees

- Construct B regression trees using B bootstrapped training datasets

- Average the resulting predictions

- Note: These trees are not pruned, so each individual tree has high variance but low bias

- Averaging these trees reduces variance, and thus we end up lowering both variance and bias ☺

Example: Boston Housing Data

- Apply bagging to the `Boston` data, using the `randomForest` package in R
  - Later, we will see bagging is a special case of a random forest

```
library(randomForest)
library(MASS)
set.seed(1)
train <- sample(1:nrow(Boston),nrow(Boston)/2)
set.seed(6)
bag.boston <- randomForest(medv~., data=Boston, subset=train, mtry=13,
    importance=TRUE)
```

#`importance`: Should importance of predictors be assessed?

#mtry: number of predictors sampled for splitting at each node. It indicates that all 13 predicators should be considered for each split of the tree, this indicates bagging.

#ntree=500 by default

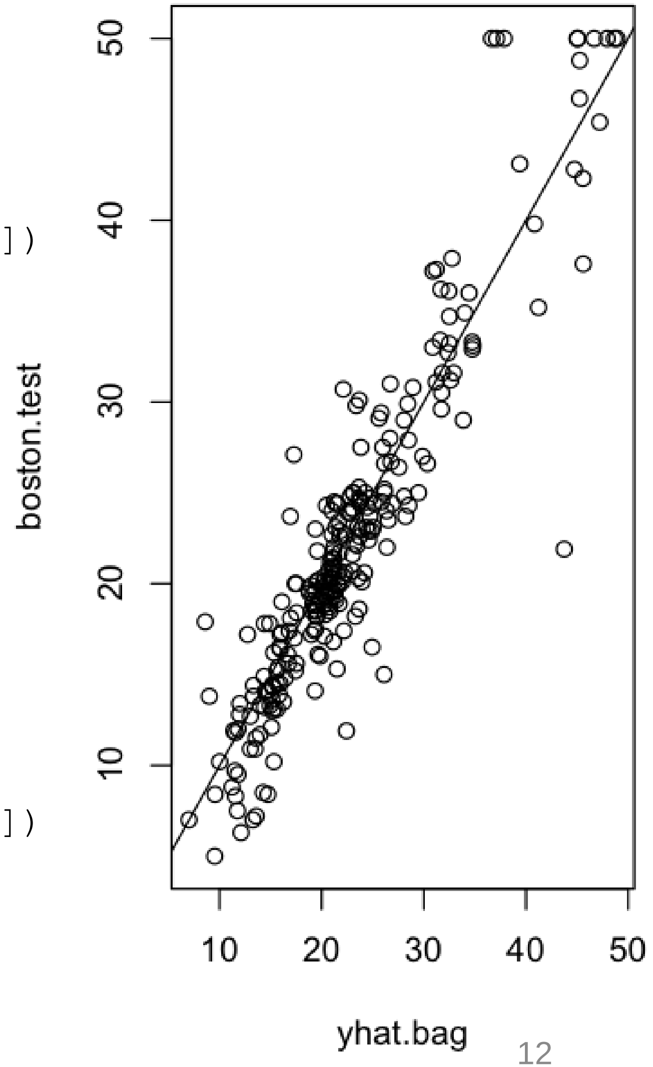
```
bag.boston
Call: randomForest(formula = medv ~ ., data = Boston, mtry = 13, importance = TRUE,
    subset = train)
               Type of random forest: regression
                     Number of trees: 500
No. of variables tried at each split: 13
          Mean of squared residuals: 10.89212
                    % Var explained: 86.81
```

Example: Boston Housing Data

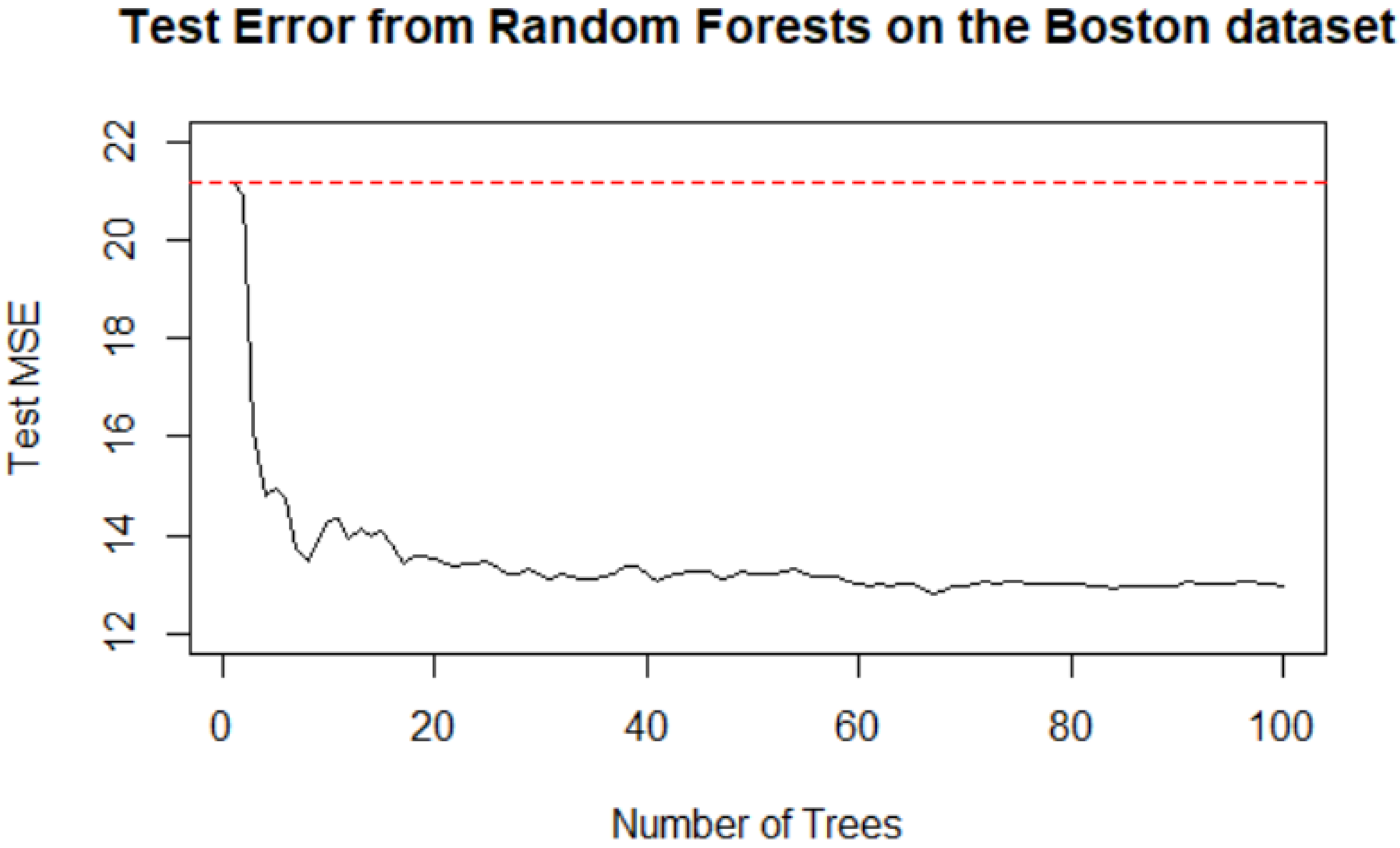
- How well does this bagged model perform on the test set?

```
yhat.bag <- predict(bag.boston,newdata=Boston[-train,])
boston.test <- Boston [-train ,"medv"]
plot(yhat.bag,boston.test)
abline(0,1)
mean((yhat.bag-boston.test)^2)
[1]13.33672 ← the test MSE asscoiated with the bagged regression tree
set.seed(6)
bag.boston <- randomForest(medv ~ ., data=Boston,
    subset=train, mtry=13, ntree=25, importance=TRUE)
    ntree=25 ← changing the number of trees grown

yhat.bag <- predict(bag.boston,newdata=Boston[-train,])
mean((yhat.bag-boston.test)^2)
[1] 14.02642 →  With less trees, the test MSE increases
```



A Comparison of Error Rates – Boston Housing Data



The red line represents the test MSE using a single tree.

The black line corresponds to the bagging test MSE.

Example: Boston Housing Data

- The code for generating the previous plot:

```
set.seed(1)
train <- sample(1:nrow(Boston), nrow(Boston)*0.5)

train.df <- Boston[train,]      # training set
test.df <- Boston[-train,]      # test set
x_train <- train.df[-14]    # the predictors (X) in the training set, the 14th column is medv
x_test <- test.df[-14]      #  train.df [-14] is the same as train.df [,-14]
                            # row is by default 1:nrow(dataframe)
y_train <- train.df$medv        #  the response in the training set
y_test <- test.df$medv          #  the response in the test set

myForest1 <- randomForest(x=x_train, y=y_train, xtest=x_test,
                          ytest=y_test, ntree=100, mtry=13)
plot(1:100, myForest1$test$mse,
     main = "Test Error from Random Forests on the Boston dataset",
     xlab = "Number of Trees", ylab = "Test MSE",
     type = "l", ylim = c(12, 22), lwd = 1)
abline(h = myForest1$test$mse[1],lty=2,col="red")  #h:the y-value(s) for
  horizontal line(s).
```

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- Random Forests

Bagging for Classification Trees

- Construct B classification trees using B bootstrapped training datasets

- For prediction, there are two approaches:
  1. Record the class that each bootstrapped data set predicts and provide an overall prediction to the most commonly occurring one (majority vote).
  2. If our classifier produces probability estimates we can just average the probabilities and then predict to the class with the highest probability.

- Both methods work well.

Example: Car Seat Data

- Apply bagging to the `Carseats` data, using the `randomForest` package in R

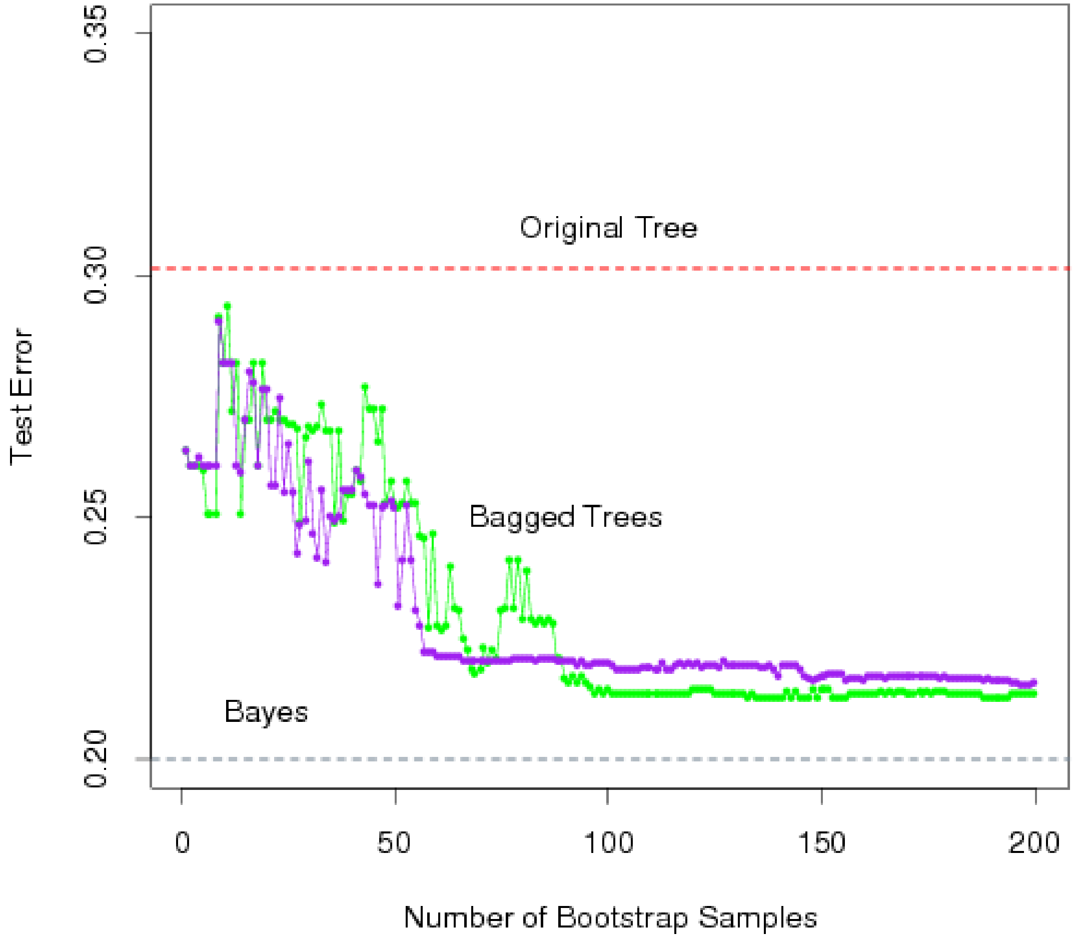
```
library(ISLR)
library(randomForest)
High <- ifelse(Carseats$Sales<=8,"No","Yes")
Carseats <- data.frame(Carseats,High) # add one column High to Carseats
set.seed(2)
train <- sample(1:nrow(Carseats), nrow(Carseats)/2)
Carseats.test <- Carseats[-train,]
High.test <- Carseats[-train, "High"]
bag.carseats <- randomForest(High~.-Sales, Carseats, subset=train, mtry=10)
yhat.carseats <- predict(bag.carseats, newdata=Carseats.test)
table(yhat.carseats,High.test)
             High.test
yhat.carseats No Yes
          No   95  17
          Yes  21  67
(21+17)/200
[1] 0.19
```

A Comparison of Error Rates

- Here the green line represents a simple majority vote approach

- The purple line corresponds to averaging the probability estimates

- Both do far better than a single tree (dashed red) and get close to the Bayes error rate (dashed grey)

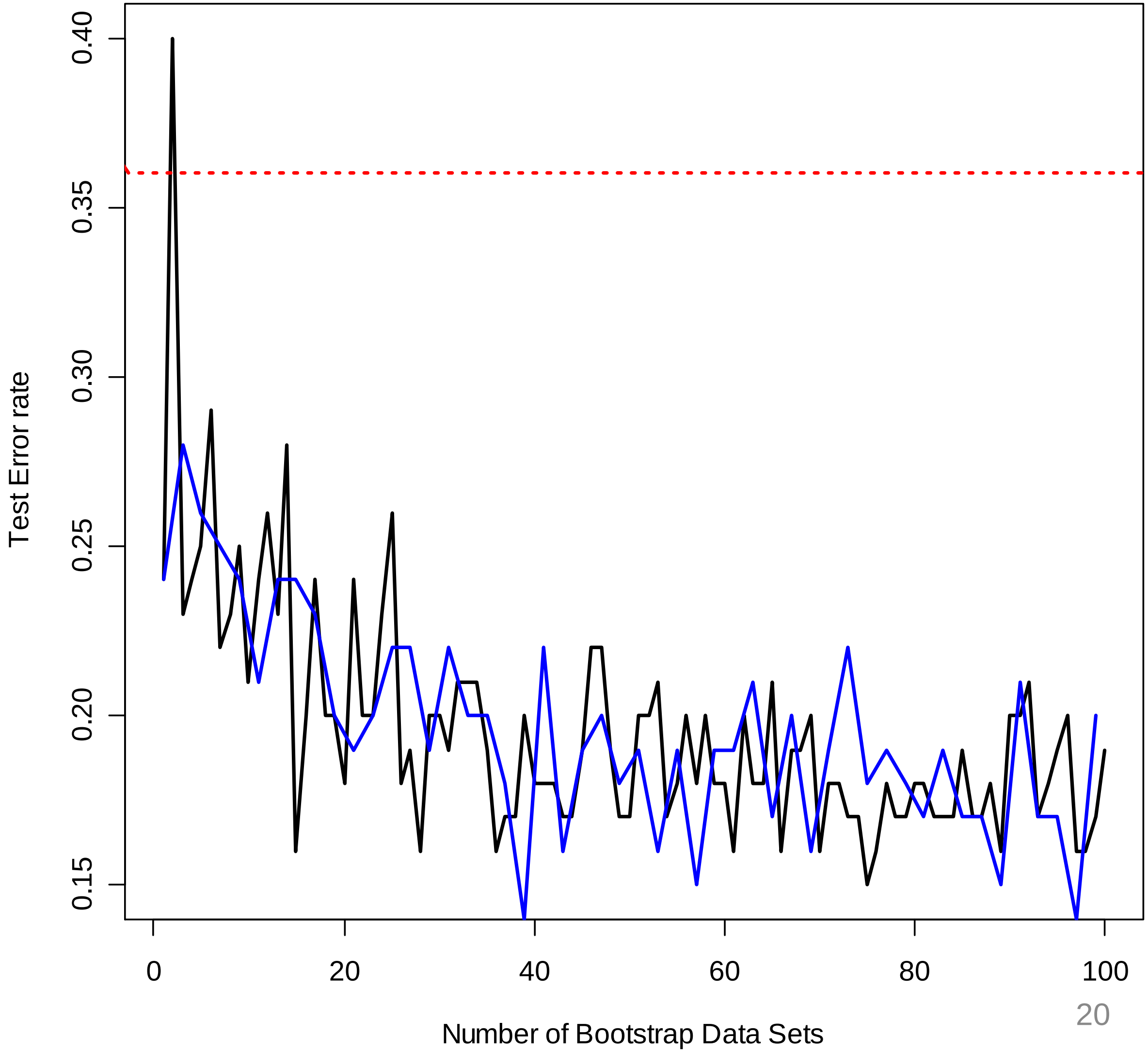


Bayes error rate is the lowest possible error rate for a given class of classifier.

Example: Car Seat Data

- The red line represents the test error rate using a single tree.

- The black line corresponds to the bagging error rate using majority vote while the blue line averages the probabilities.



Example: Car Seat Data

- Code to obtain the plot on the last slide:

```
#Prepare the dataset, training set and test set for majority vote:

library(ISLR)
library(randomForest)
data(Carseats)   #reload a fresh dataset

High <- ifelse(Carseats$Sales<=8,"No","Yes")
Carseats.mv<- data.frame(Carseats,High)  # add one column High to Carseats
Carseats.mv <- Carseats.mv[,-1] #remove the Sales column

set.seed(2)
train <- sample(400, 200)  #400 is the number of rows in Carseats/Carseats1

Carseats.mv.test <- Carseats.mv[-train,]  #test dataset
High.mv.test <- Carseats.mv[-train, 11]   #true y value for the test dataset
```

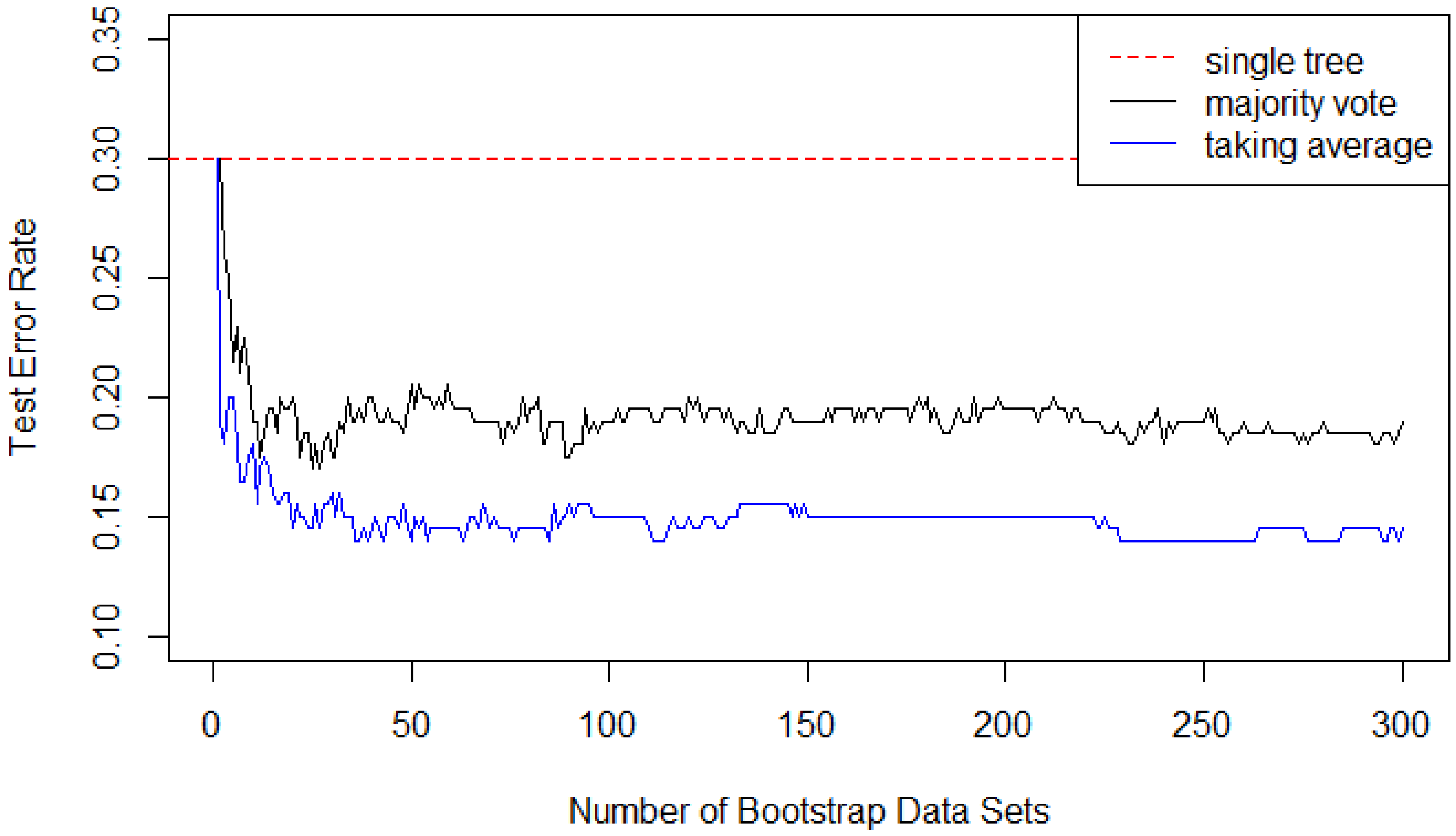
Example: Car Seat Data

```
# calculate the black line:
yhat.ter.mv <- rep(0,300)      # a vector for Test Error Rate using majority vote (by default)

for(i in 1:300){
          set.seed(4)   #randomForest() is a randomised function
          bag.carseats <- randomForest(High~., Carseats.mv, subset=train, mtry=10, ntree=i)
          yhat.carseats <- predict(bag.carseats, newdata=Carseats.mv.test)
          test.error.mv[i] <-
                    (table(yhat.carseats,High.mv.test)[1,2]+table(yhat.carseats,High.mv.test)[2,1])/200
          # or     test.error.mv[i] <-  mean(yhat.carseats!=High.mv.test)
}

#plot the black line
plot(test.error.mv, xlab="Number of Bootstrap Data Sets",
                ylab="Test Error Rate", type="l", ylim=c(0.10,0.35))

#plot the red dashed line
abline(h=test.error.mv[1],  lty=2,  col="red")
```

Example: Car Seat Data

```
#Prepare the dataset, training set and test set for averaging the probabilities:
Carseats.test <- Carseats[-train, -1]  #test dataset
High.ave.test <- High.mv.test   #true y value for the test dataset

#Calculate the blue line - in this case, we need to build a bagging for REGRESSION trees first and
discretise the result to “Yes” or “No” later.

test.error.ave <- rep(0,300)     # a vector for Test Error Rate using averaging
for(j in 1:300){
    set.seed(2)
    bag.carseats.ave <- randomForest(Sales ~ ., Carseats, subset=train, mtry=10, ntree=j)
    yhat.carseats <- predict(bag.carseats.ave, newdata=Carseats.test)
    yhat.carseats.class <- ifelse(yhat.carseats<=8, "No", "Yes")
    test.error.ave[j]<-
              (table(yhat.carseats.class,High.ave.test)[1,2]+table(yhat.carseats.class,High.ave.test)[2,1])/200
}

#plot the blue line:
lines(test.error.ave, col="blue")
```

Example: Car Seat Data



The Problem

- In the previous example, by using a for-loop, how many trees were grown in total?

- We have grown 1+2+3+4+…+300 trees!

- It's enough to grow 300 trees only.

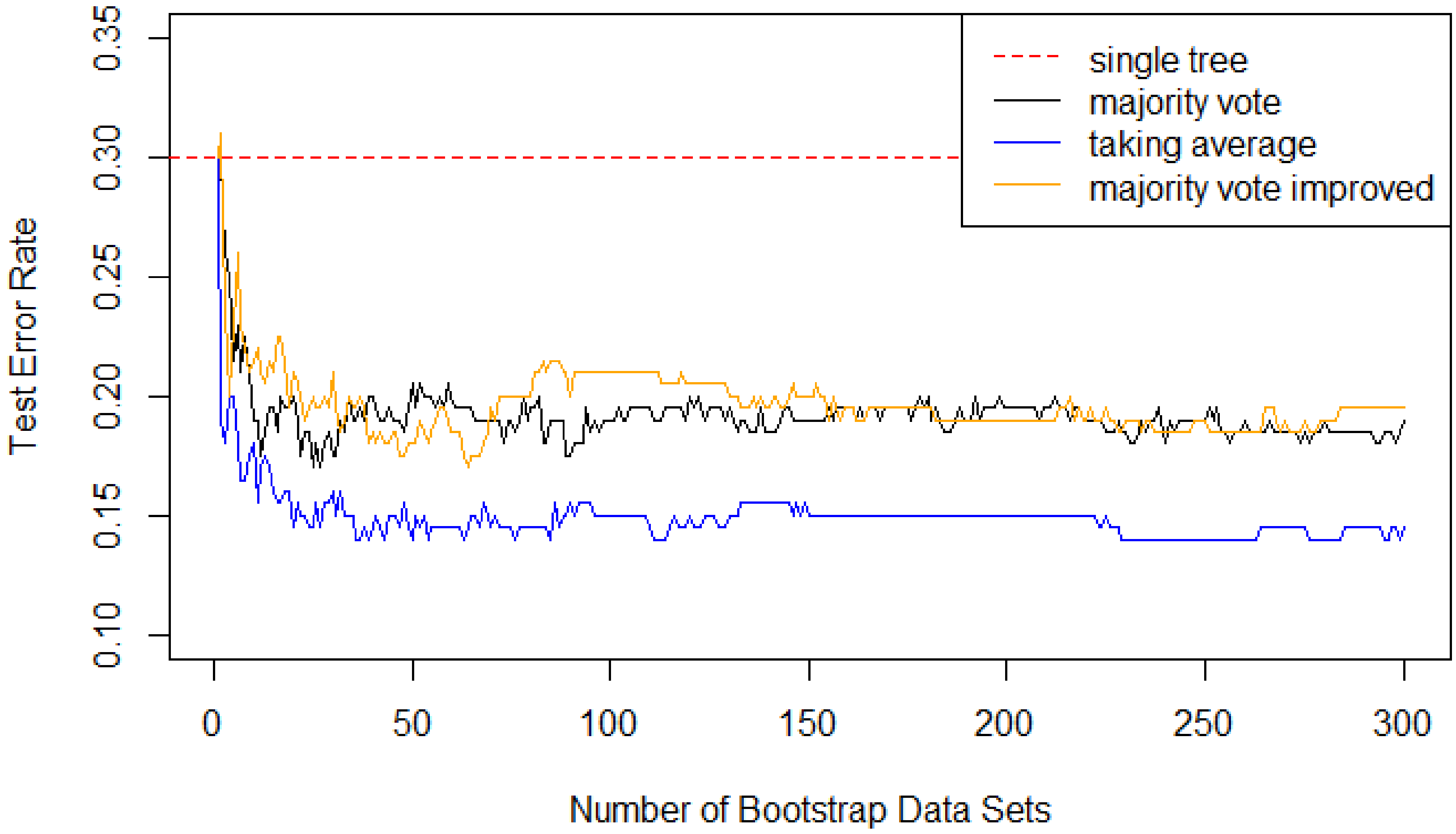
For Classification Trees

- If test set is given in randomForest() through the `xtest` and/or `ytest`, a component `test` is created.
- Assume `ntree` = 300, and `nrow`(`xtest`) = 200.
- For classification, `predicted`, `err.rate`, `confusion`, `votes` are made available.
  - `predicted`: The predicted values for the test set `xtest`. The length is 200.
  - `err.rate`: the first col. of `err.rate` is the error rate between `predicted` and `ytest`.
    - The length of `err.rate`[,1] is 300.
    - `err.rate`[j,1] means the error rate for the first j trees.
  - `confusion`: The confusion matrix for the randomForest of 300 trees.
  - `votes`: For each predicted value, it shows the percentage of votes for each category.
    - The size of `votes` is 200 rows and m categories

Improved Code

```
#prepare the datasets
data("Carseats")
High <- ifelse(Carseats$Sales<=8,"No","Yes")
set.seed(2)
train <- sample(1:nrow(Carseats), nrow(Carseats)/2)
Carseats <- data.frame(Carseats, High)

x_train <- Carseats[train,-c(1, 12)]
y_train <- Carseats[train, "High"]
x_test <- Carseats[-train,-c(1, 12)]
y_test <- Carseats[-train, "High"]

set.seed(2)  #randomForest() is a randomised function!
bag.carseats <- randomForest(x=x_train, y=y_train, xtest=x_test, ytest=y_test, ntree=300, mtry=10)

length(bag.carseats$test$err.rate[,1])    # 300 error rates, building upon incrementally

#plot the curve
lines(bag.carseats$test$err.rate[,1], col="orange")
```

Plot the New Curve



For Regression Trees

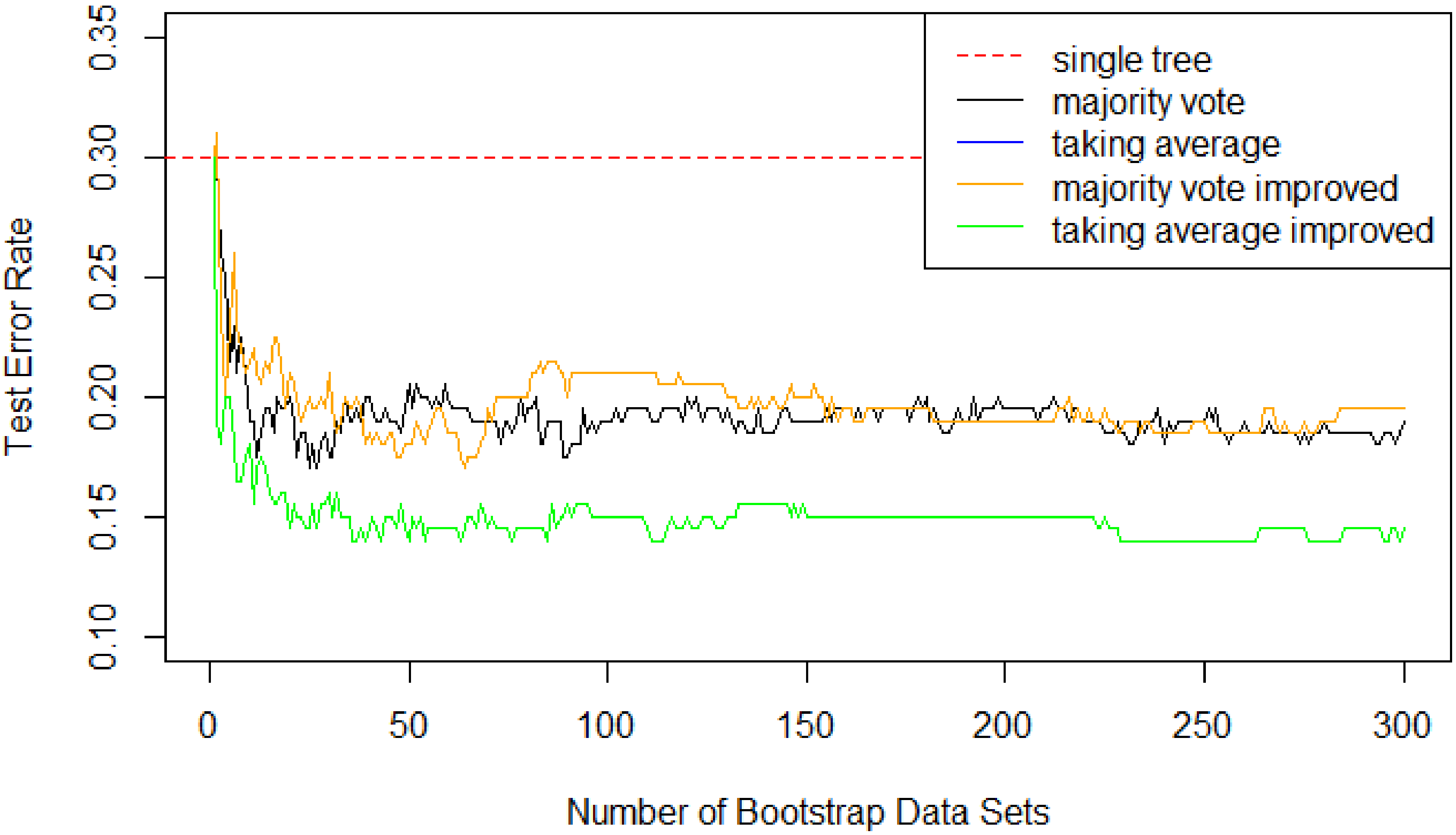
- If test set is given in randomForest() through the `xtest` and/or `ytest`, a component `test` is created.
- Assume `ntree` = 300, and `nrow`(`xtest`) = 200.
- For regression, `predicted` and `mse` are made available for the test set.
  - `predicted`: The predicted values for the test set `xtest`.
    - The length of `predicted` is 200.
    - `predicted[i]` means the predicted value for the i-th row in `xtest`
  - `mse`: The MSE between the `predicted` and `ytest`.
    - The length of `mse` is 300.
    - `mse[j]` means the MSE for the first j trees. It is grown incrementally.

For Regression Trees

```
#prepare the training and test sets
x_train.ave <- Carseats[train,-c(1, 12)]
y_train.ave <- Carseats[train, "Sales"]
x_test.ave <- Carseats[-train,-c(1, 12)]
y_test.ave <- Carseats[-train, "Sales"]
test.error.ave.imp <- rep(0,300)

for(i in 1:300){
  set.seed(2)
  bag.carseats <- randomForest(x=x_train.ave, y=y_train.ave, xtest=x_test.ave,
                                                    ytest=y_test.ave, ntree=i, mtry=10)
  yhat.High.ave <- ifelse(bag.carseats$test$predicted<=8, "No","Yes")
  test.error.ave.imp[i] <- mean(yhat.High.ave!=y_test)
   #note compare with y_test (High), not y_test_ave
}
lines(test.error.ave.imp, col="green")

legend("topright", legend = c("single tree", "majority vote", "taking average",
                 "majority vote improved", "taking average improved"),
                 col=c("red", "black", "blue", "orange","green"), lty=c(2,1,1,1,1))
```

We cannot avoid using the for-loop in this case, as the results in test cannot be used directly.

Plot the New Curve



The blue and green curve coincide!

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  - Variable Importance: Relative Influence Plots

- Random Forests

Out-of-Bag Error Estimation

- There is a very straightforward way to estimate the test error of a bagged model
  - No need to perform cross validation or the validation set approach
  - Since bootstrapping involves random selection of subsets of observations to build a training data set, the remaining non-selected part could be the testing data.
  - On average, each bagged tree makes use of around 2/3 of the observations, so we end up having 1/3 of the observations used for testing.
  - The remaining 1/3 of the observations are referred to as the out-of-bag (OOB) observations.
  - The estimated test error using the OOB observations is called the OOB error.

Out-of-Bag Error Estimation

- When the number of trees B is sufficiently large, OOB error is virtually equivalent to LOOCV error.
- The OOB approach for estimating the test error is particularly convenient when performing bagging on large data sets for which the CV would be computationally expensive.
- You may find the OOB error rate when printing the summary

```
> print(bag.carseats)
Call:
 randomForest(formula = High ~ . - Sales, data = Carseats, mtry = 10,
   subset = train)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 10

        OOB estimate of  error rate: 22%
   ……
```

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Variable Importance Measure

- Bagging typically improves the accuracy over prediction using a single tree, but it is now hard to interpret the model!
  - We have hundreds of trees, and it is no longer clear which variables are the most important to the procedure
  - Thus bagging improves prediction accuracy at the expense of interpretability
- But, we can still get an overall summary of the importance of each predictor using Relative Influence Plots

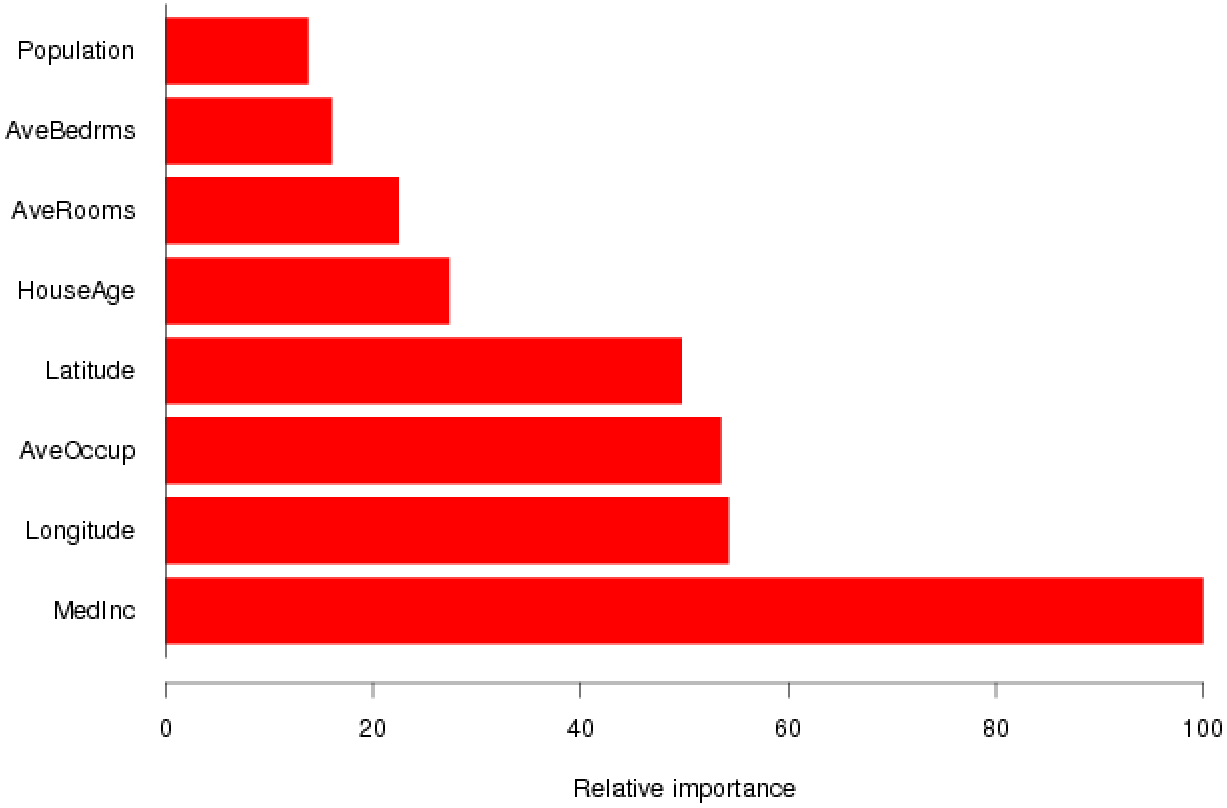
Relative Influence Plots

- How do we decide which variables are most useful in predicting the response?
  - We can compute something called relative influence plots
  - These plots give a score for each variable
  - These scores represents the decrease in MSE when splitting on a particular variable
    - A number close to zero indicates the variable is not important and could be dropped
    - The larger the score the more influence the variable has.

Example: Housing Data

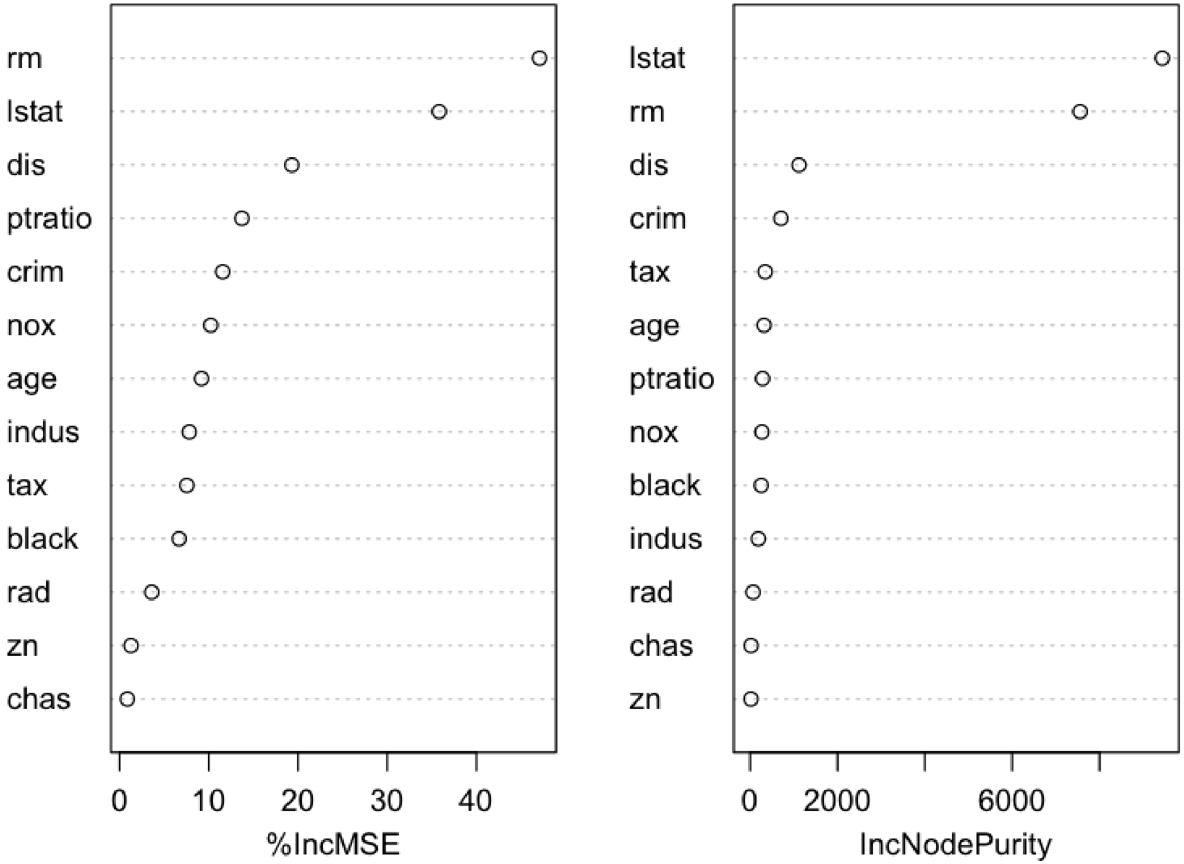
- Median Income is by far the most important variable.

- Longitude, Latitude and Average occupancy are the next most important.



Example: Boston Housing Data

```
> importance(bag.boston)
          %IncMSE IncNodePurity
crim    11.5623632    705.52039
zn       1.2742557     17.50011
indus    7.8148780    187.07632
chas     0.8714603     20.51912
nox     10.2193795    271.39076
rm      47.0763407   7555.54873
age      9.1828854    317.74911
dis     19.3127465   1117.95231
rad      3.5974754     68.49749
tax      7.5277047    344.32668
ptratio 13.7071255    285.55153
black    6.6649845    254.79199
lstat   35.8265510   9437.81585
```



```
>varImpPlot(bag.boston)   # find out how to plot in the “bar chart” style as in the previous slide
```

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Random Forests

- It is a very efficient statistical learning method

- It builds on the idea of bagging, but it provides an improvement because it de-correlates the trees

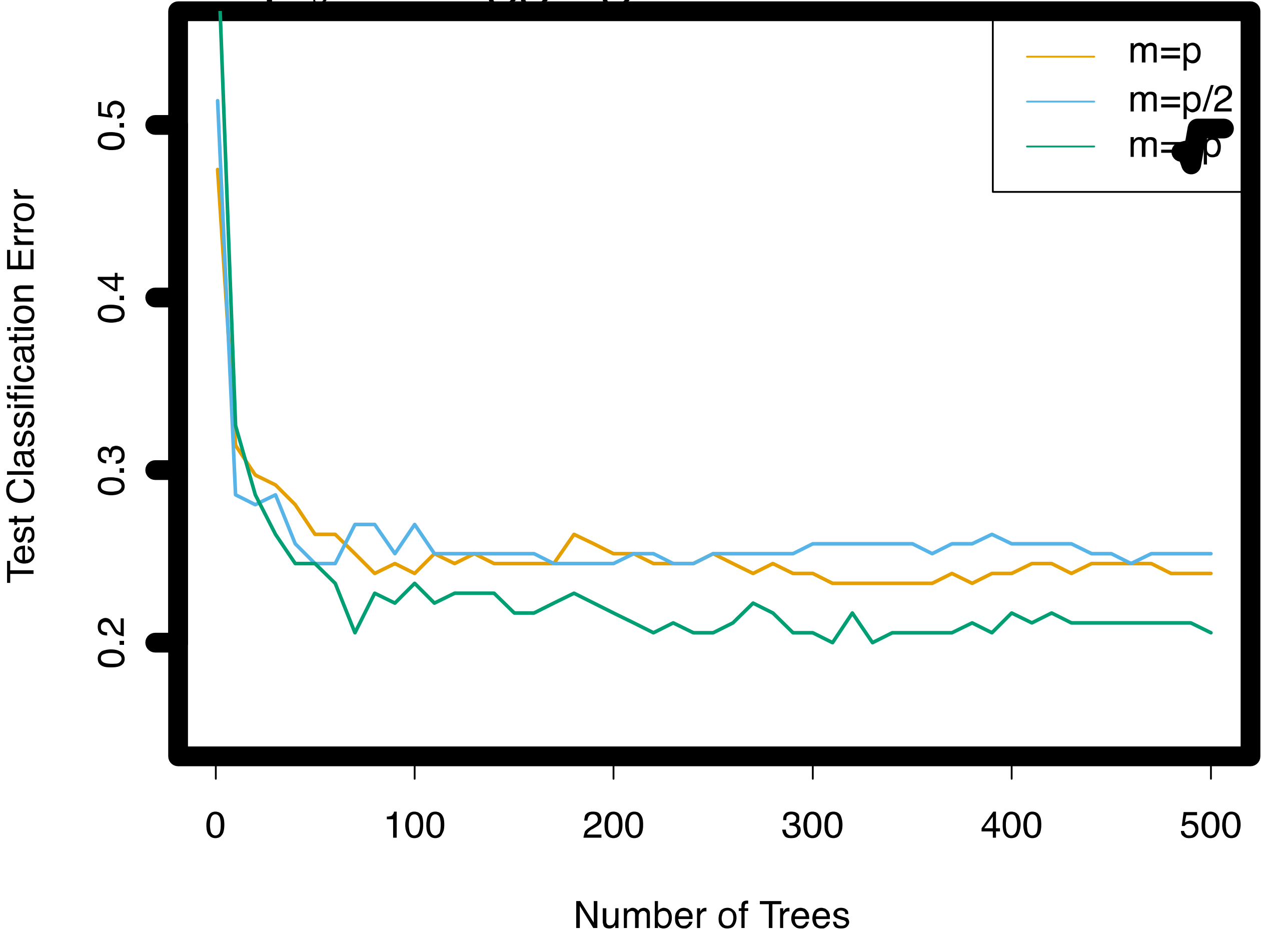
- How does it work?
  - Build a number of decision trees on bootstrapped training sample, but when building these trees, each time a split in a tree is considered, a random sample of *m* predictors is chosen as split candidates from the full set of *p* predictors (Usually m = √p (square root of p))

Why?

- Why are we considering a random sample of *m* predictors instead of all *p* predictors for splitting?
  - Suppose that we have a very strong predictor in the data set along with a number of other moderately strong predictors, then in the collection of bagged trees, most or all of them will use the very strong predictor for the first split!
  - All bagged trees will look similar. Hence all the predictions from the bagged trees will be highly correlated
  - Averaging many highly correlated quantities does not lead to a large variance reduction, and thus random forests “de-correlates” the bagged trees leading to more reduction in variance

Random Forest with Different Values of "*m*"

- Notice when random forests are built using m = p, then this amounts simply to bagging.



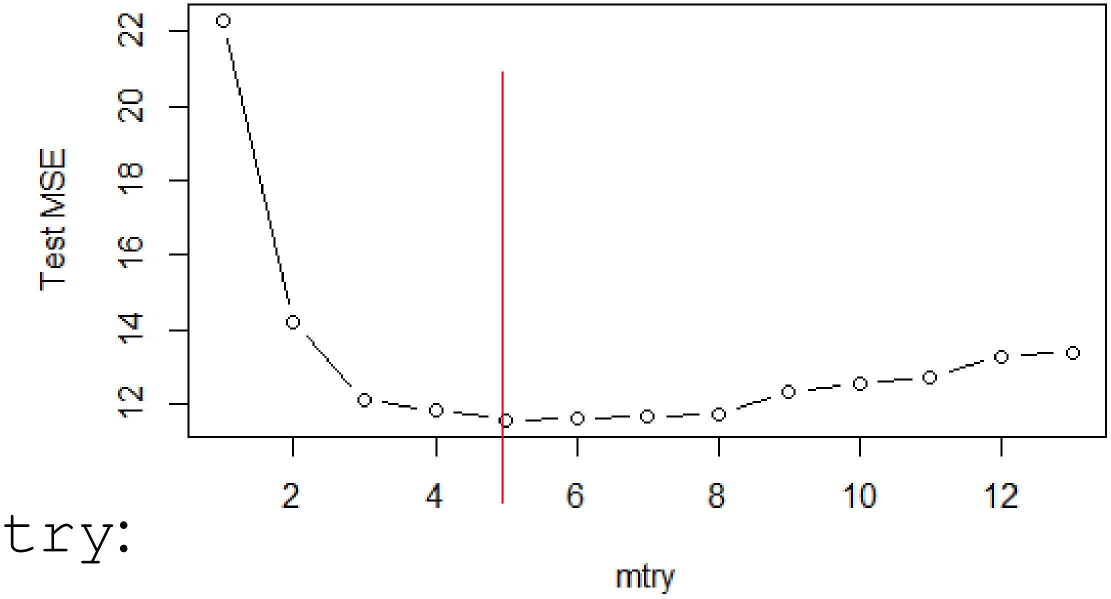
Random Forest

- Growing a random forest proceeds in exactly the same way as in bagging, except that a smaller `mtry` is used
  - By default, randomForest() uses
    - p/3 variables when building a random forest of regression trees
    - √p variables when building a random forest of classification trees

```
library(MASS)
set.seed(1)
train <- sample(nrow(Boston), nrow(Boston)/2)
set.seed(5)
rf.boston <- randomForest(medv ~ ., data=Boston,
                          subset=train, mtry=6, importance=TRUE)
yhat.rf <- predict(rf.boston,newdata=Boston[-train,])
boston.test <- Boston[-train, "medv"]
mean((yhat.rf-boston.test)^2)
```

`[1] 11.62716` ← the test set MSE, smaller than that derived from a bagged model. There is an improvement!

Random Forest



- Find the best value of `mtry`:

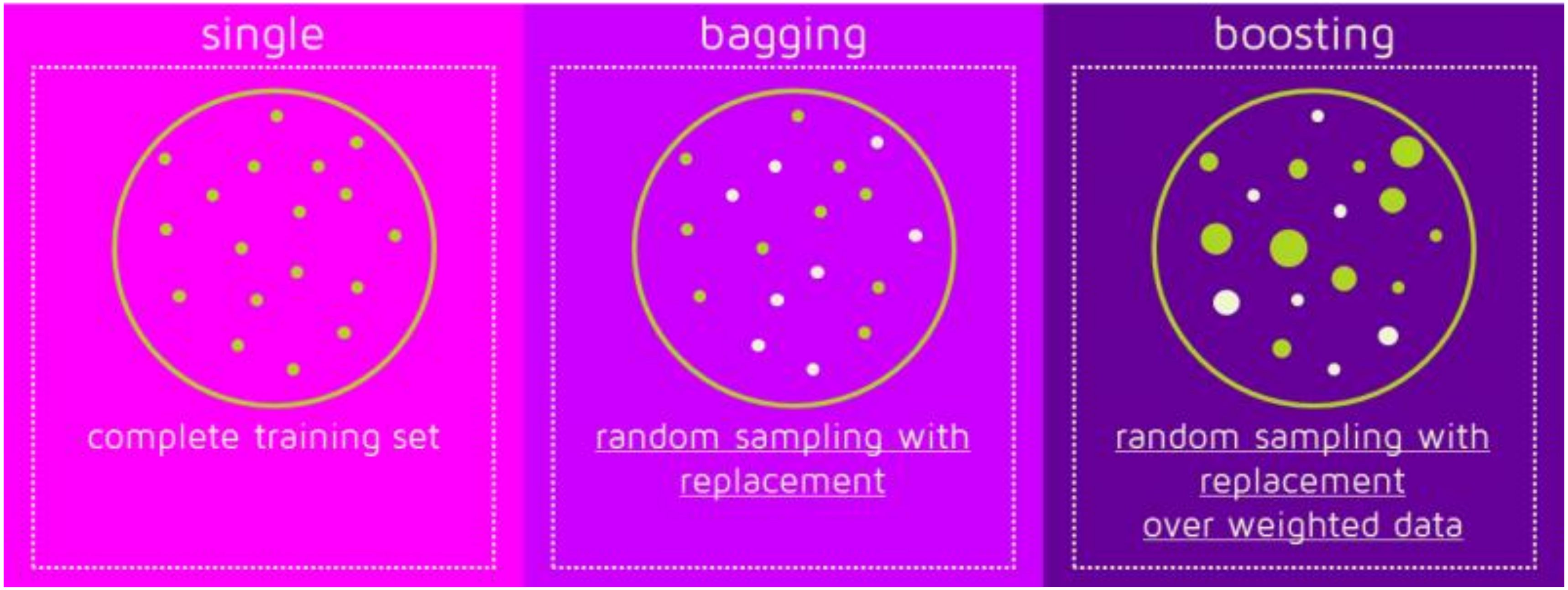
```
testMSE <- rep(0,13)
for(i in 1:13){
  set.seed(5)
  rf.boston <- randomForest(medv ~ ., data=Boston, subset=train, mtry=i,importance=TRUE)
  yhat.rf <- predict(rf.boston,newdata=Boston[-train,])
  testMSE[i] <- mean((yhat.rf-boston.test)^2)
}
plot(testMSE,type="b",xlab="mtry",ylab="Test MSE")
```

Epilogue

- An analogue
  - Decision tree: Validation set approach
    - Use only half of the training set to build a model
    - High variance
    - Decision tree is a special case of random forest
    - Validation set approach is a special case of K-fold CV
  - Bagging: LOOCV
    - A way to utilise almost all observations in the data set to train a model
    - Bagging is a special case of Random Forest
    - LOOCV is a special case of K-fold CV
  - Random Forest: K-fold CV
    - De-correlate the training sets
    - More reduction on variance

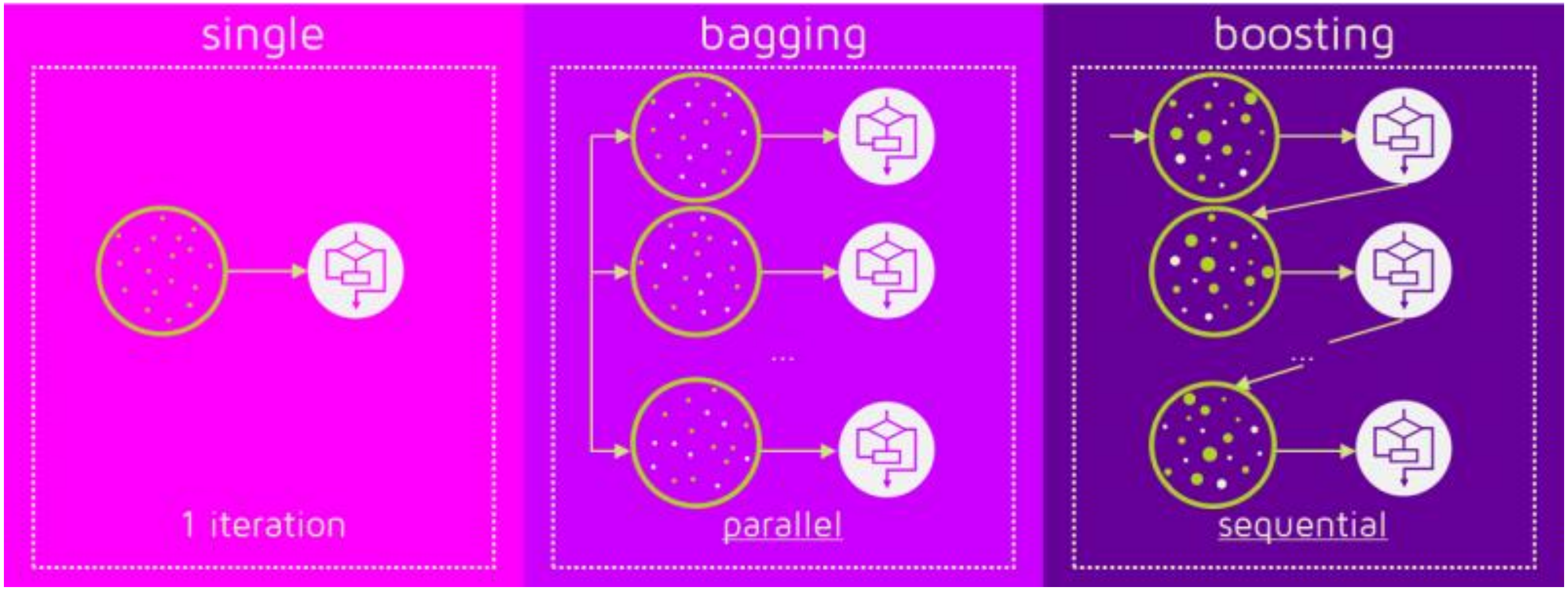
Ensemble Methods

- Ensemble methods are techniques that create multiple "weak" models and then combine them to obtain better predictive performance.


single
complete training set
bagging
random sampling with replacement
boosting
random sampling with replacement over weighted data

In Bagging, any element has the same probability to appear in a new data set.
For Boosting the observations are weighted and therefore some of them will take part in the new sets more often.

Boosting



In Boosting algorithms each classifier is trained on data, taking into account the previous classifiers' success.

After each training step, the weights are redistributed.

Misclassified data increases its weights to emphasise the most difficult cases.

In this way, subsequent learners will focus on them during their training.

https://quantdare.com/what-is-the-difference-between-bagging-and-boosting/ for more info.

LAB

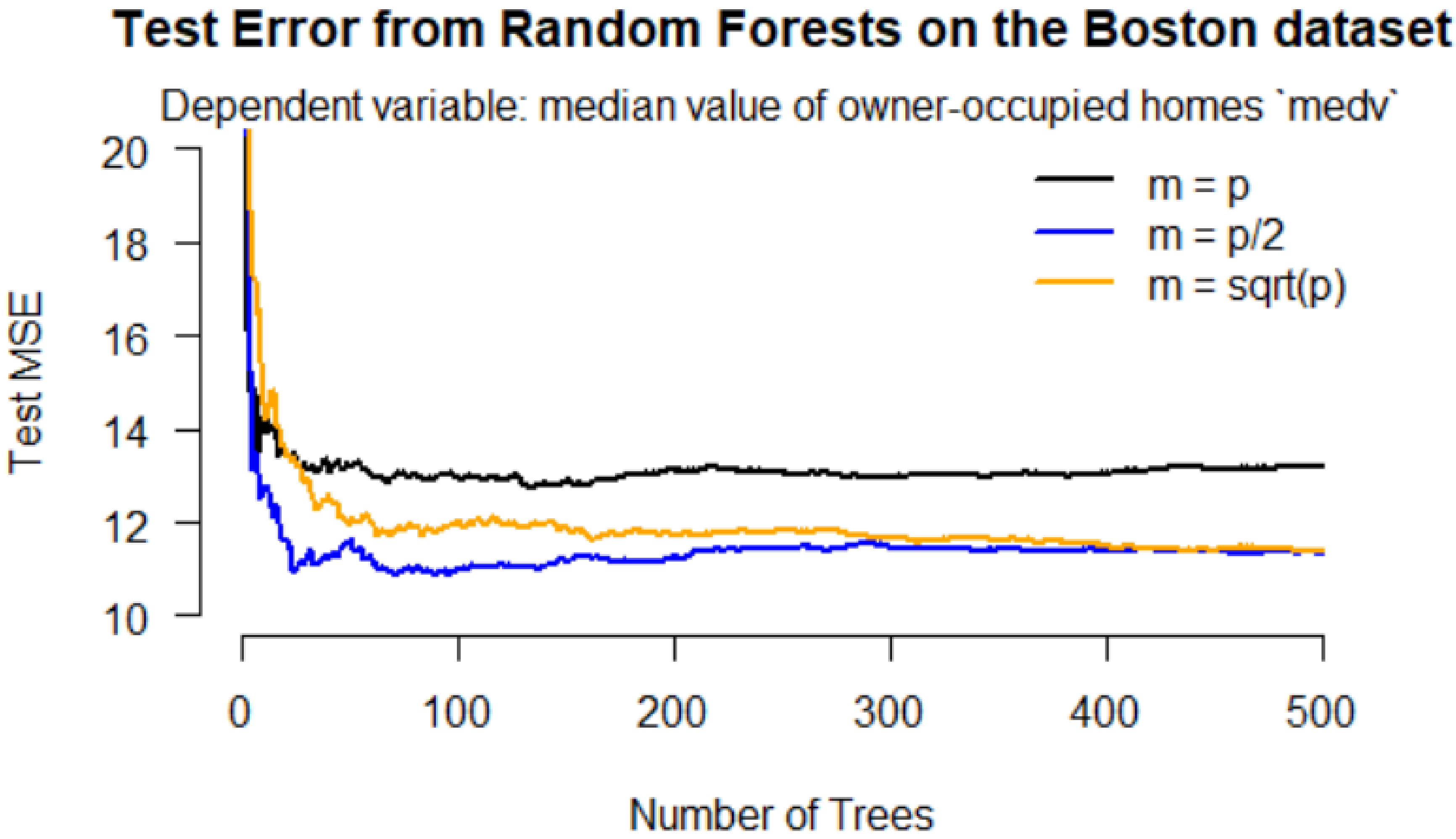
Hitters

- Explore the Hitters dataset
  - Build a bagged model and a random forest model
    - y: Salary
    - x: all the features other than Salary
  - Play with 1) set.seed 2) mtry and 3) ntree, plot
    - a graph that shows test MSE vs mtry for different seeds
    - a graph that shows test MSE vs ntree for different seeds
    - Find the best/reasonably good mtry and ntree
  - Check the importance of each predictor
  - Check the OOB error estimation
  - Compare the bagged model and RF model with the tree model
    - Compare the test MSE

A Comparison on Different mtry

```
set.seed(1)
train <- sample(1:nrow(Boston), nrow(Boston)*0.5)
train.df <- Boston[train,]
test.df <- Boston[-train,]
x_train <- train.df[-14]  #column 14 is the medv
x_test <- test.df[-14]
y_train <- train.df$medv
y_test <- test.df$medv
p <- ncol(x_train)
myForest1 <-randomForest(x=x_train, y=y_train, xtest=x_test, ytest=y_test, ntree=500, mtry=p)
myForest2 <-randomForest(x=x_train, y=y_train, xtest=x_test, ytest=y_test, ntree=500, mtry=p/2)
myForest3 <-randomForest(x=x_train, y=y_train, xtest=x_test, ytest=y_test, ntree=500, mtry=sqrt(p))
plot(1:500, myForest1$test$mse, main = "Test Error from Random Forests on the Boston dataset",
      xlab = "Number of Trees", ylab = "Test MSE",type = "l", ylim = c(10, 20), lwd = 2, las=1, bty="n")
lines(1:500, myForest2$test$mse, col = "blue", lwd = 2)
lines(1:500, myForest3$test$mse, col = "orange", lwd = 2)
legend("topright", c("m = p", "m = p/2", "m = sqrt(p)"),
col = c("black", "blue", "orange"), cex = 1, lty = 1, lwd = 2, bty = "n")
mtext("Dependent variable: median value of owner-occupied homes `medv`")
```

A Comparison on Different mtry



Summary

- If test set is given in randomForest() through the `xtest` and/or `ytest`, a component `test` is created. Assume `ntree` = 500, and nrow(`xtest`) = 200.
  - For regression, `predicted` and `mse` are made available for the test set.
    - `predicted`: The predicted values for the test set `xtest`.
      - The length of `predicted` is 200.
      - `predicted[i]` means the predicted value for the i-th row in `xtest`
    - `mse`: The MSE between the `predicted` and `ytest`.
      - The length of `mse` is 500.
      - `mse[j]` means the MSE for the first j trees. It is grown incrementally.
  - For classification, `predicted`, `err.rate`, `confusion`, `votes` are made available.
    - `predicted`: The predicted values for the test set `xtest`. The length is 200.
    - `err.rate`: the first col. of `err.rate` is the error rate between `predicted` and `ytest`.
      - The length of `err.rate`[,1] is 500. `err.rate`[j,1] means the error rate for the first j trees.
    - `confusion`: The confusion matrix for the randomForest of 500 trees.
    - `votes`: For each predicted value, it shows the percentage of votes for each category.
      - The size of `votes` is 200 rows and m categories