STA 5936: Homework 2

Due January 23rd, 11:59pm

In this problem we use the abalone dataset available on Canvas. The dataset is about predicting the age of the abalone from its physical measurements. Use the first 7 variables as predictors and the 8-th as the response. Obtain all results using 10-fold cross-validation, which is computed as follows:

1. Generate a random permutation of the data. Use this random permutation to split the data into 10 disjoint subsets of almost equal size (417 or 418 observations each).

2. For each fold $i \in \{1, \ldots, 10\}$, train the model on all data except subset i and test it on subset i, obtaining test error εi.

3. Obtain the final test error as the average of the 10 test errors εi obtained above. Here the errors εi could be the MSE, or the R2. Report results for the following models:

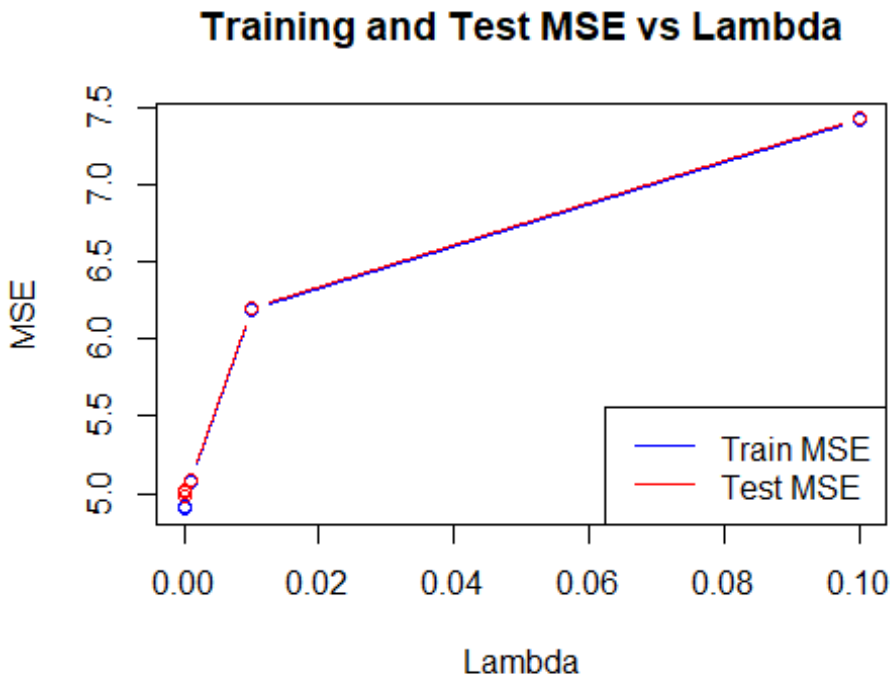
    a) Null model. Report the average train and test MSE of the null model that always predicts training $\bar{y}$ (average training y). (1 point)

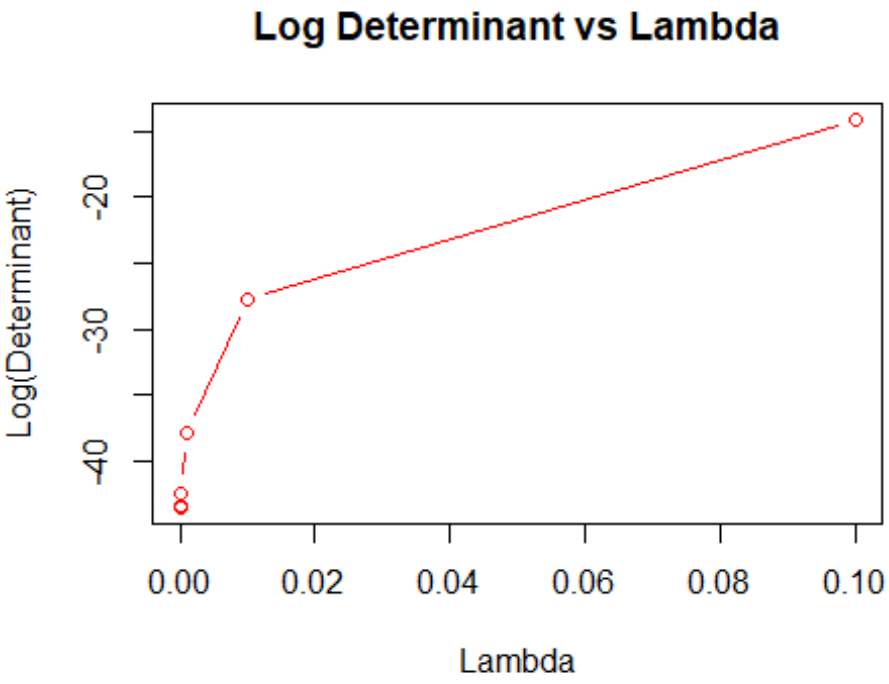
        a) **Average Training MSE (Null Model):** 10.39242
        b) **Average Test MSE (Null Model):** 10.40003

    b) OLS regression computed analytically by solving the following normal equations: $(1\ N\ X^T X + \lambda I_p)\beta = 1\ N\ X^T Y$ where $\lambda \in \{0, 10{-}5, 10{-}4, 10{-}3, 10{-}2, 10{-}1\}$ and N is the number of observations in X. Report in a table the average training and test R2 and MSE, as well as their standard deviations obtained from the 10 folds. On the same graph, plot the average average training and test MSE vs λ as two separate curves. Also plot the average value of the logarithm of the determinant of $1\ N\ X^T X + \lambda I_p$ (average obtained from the 10 folds) vs λ. (3 points)

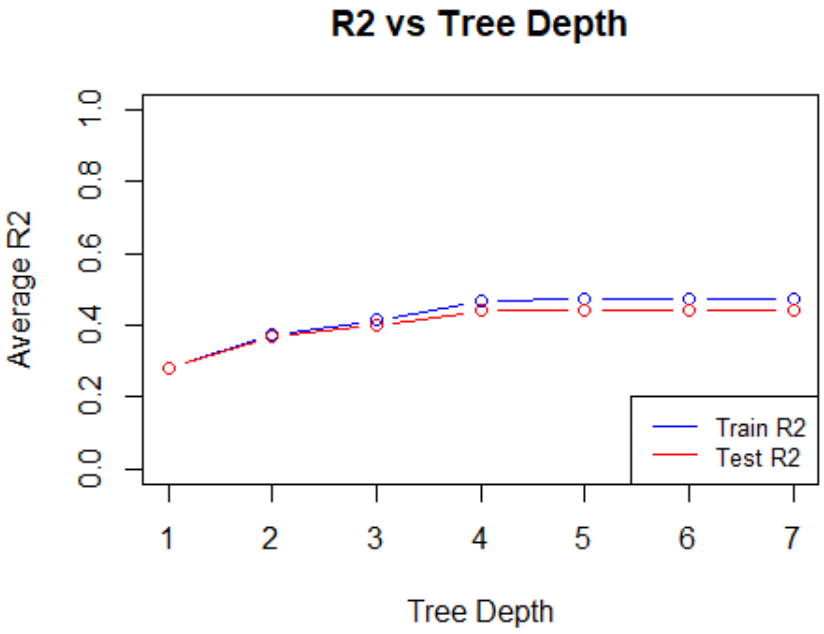
        - **Graphs and Table on pages 2 and 3**

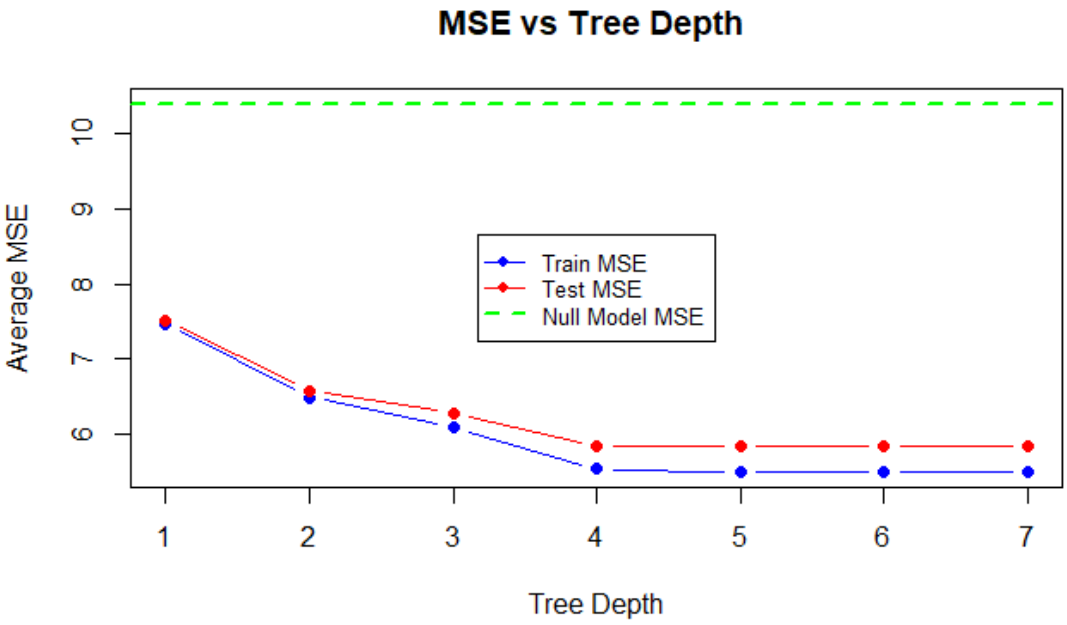
Lambda	Train R2 avg	Test R2 avg	Train MSE avg	Test MSE avg	Train MSE std	Test MSE std
0e+0	0.5280324	0.5216713	4.904990	5.016222	0.0738030 5	0.8108113
1e-05	0.5280203	0.5221116	4.905133	5.009041	0.0737674 4	0.7887751
1e-04	0.5273338	0.5241585	4.913411	4.977585	0.0718274 8	0.6703977
1e-03	0.5154296	0.5162472	5.071642	5.091793	0.0602401 9	0.5649924
1e-02	0.4095029	0.4115330	6.193869	6.206721	0.0697435 1	0.7529775
1e-01	0.3123559	0.3149953	7.420396	7.429738	0.0943222 0	0.9853778




Log Determinant vs Lambda
Log(Determinant)
-20
-30
-40
0.00
0.02
0.04
0.06
0.08
0.10
Lambda

c) Regression tree of maximum depth 1, 2, ... up to 7, for a total of 7 regression trees. On the same plot, plot the average training and test R2 vs the tree depth as two separate curves. On another plot, plot the average training and test MSE vs the tree depth, and show the null model MSE from a) as a horizontal line. (2 points)



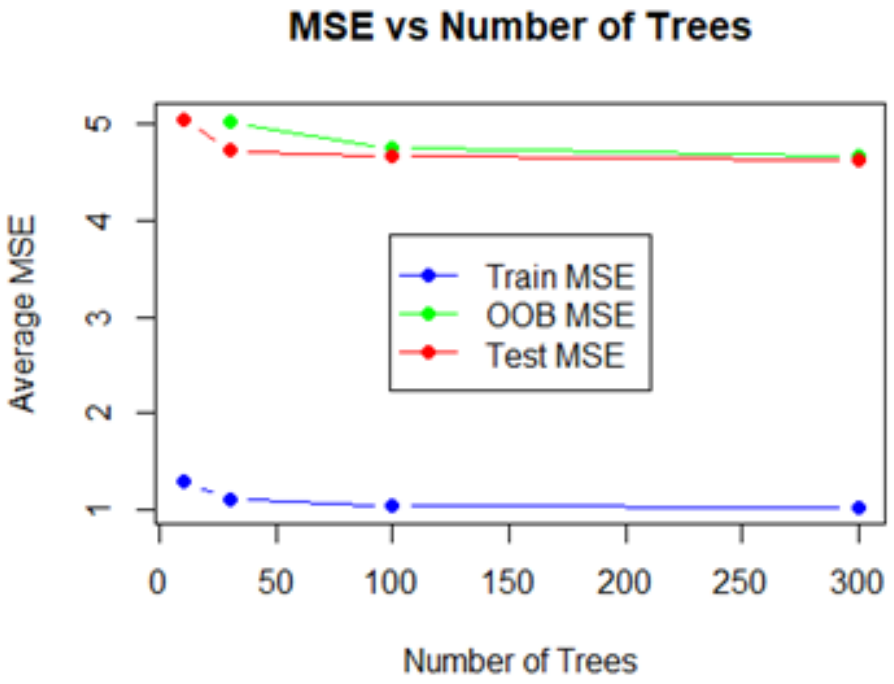


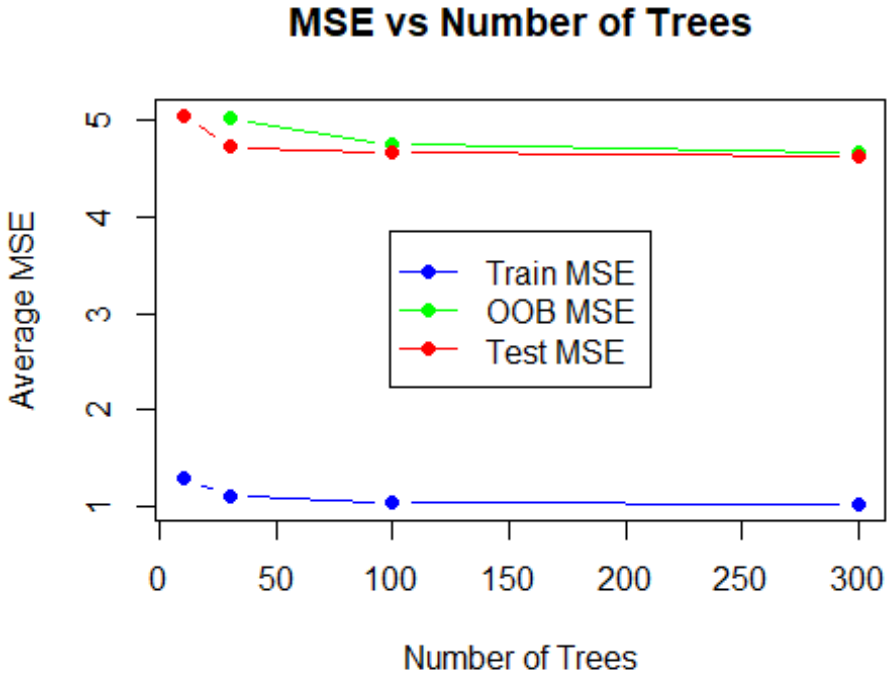
d) Random forest regression with 10, 30, 100 and 300 trees. Report the average training, OOB, and test R2 and MSE and their standard deviations in each case. On the same plot, plot the average training, OOB and test R2 vs the number of trees as three separate curves. How does the average OOB R2 compare to the test R2? (2 points)

- **Answer:** The OOB R2 average is always smaller than the Test R2 average, but the gap between them narrows substantially around 300 trees. The OOB R2 average being constantly smaller might suggest that the model is overfitting the training data, since the OOB is incorporated into the training and the test set is withheld in its entirety.
- **Note that the graphs are on the following page (page 6).**

Trees	Train R2 avg	OOB R2 avg	Test R2 avg	Train MSE avg	OOB MSE avg	Test MSE avg
10	0.8865525	0.4072991	0.5156062	1.286288	NA	5.052605
30	0.9094320	0.5160888	0.5452158	1.101971	5.028956	4.731017
100	0.9182881	0.5424960	0.5519620	1.033360	4.754497	4.663469
300	0.9203430	0.5502045	0.5552729	1.017506	4.674341	4.626219

Trees	Train R2 std	OOB R2 std	Test R2 std	Train MSE std	OOB MSE std	Test MSE std
10	0.0028843811	0.011475763	0.02301231	0.0369152 8	NA	0.3970279
30	0.0012358099	0.004527119	0.0239414 6	0.0134324 1	0.0651533 3	0.3484426
100	0.0011129689	0.004065406	0.0174770 0	0.0125675 6	0.0577512 3	0.3859143
300	0.0005341447	0.002480689	0.0202952 9	0.0109854 6	0.0410344 9	0.3608691


MSE vs Number of Trees
Average MSE
1
2
3
4
5
0
50
100
150
200
250
300
Number of Trees
Train MSE
OOB MSE
Test MSE


MSE vs Number of Trees
Average MSE
1
2
3
4
5
0
50
100
150
200
250
300
Number of Trees
Train MSE
OOB MSE
Test MSE

- **This is where all of the preparations take place (loading in data and generating folds).**

```
df <- read.csv("C:/Users/Bryce/Downloads/STA 5635/HW2/abalone.csv", header = FALSE, sep = ",")

set.seed(0)

n <- nrow(df)
k <- 10

RandPerm <- sample(n)

# Split data
foldSize <- rep(floor(n/k), k)

foldSize[1:(n %% k)] <- foldSize[1:(n %% k)] + 1

folds <- split(RandPerm, rep(1:k, foldSize))

foldedData <- lapply(folds, function(indices) df[indices, ])

# Check folds
sapply(foldedData, nrow)
```

```
##   1   2   3   4   5   6   7   8   9  10
## 418 418 418 418 418 418 418 417 417 417
```

- **Part a) begins here**

```r
library(Metrics)

# Model Training for the Null Model
trainMSE <- numeric(10)
testMSE <- numeric(10)

for (i in 1:10) {

  testIndices <- folds[[i]]
  trainIndices <- setdiff(1:nrow(df), testIndices)

  trainData <- df[trainIndices, ]
  testData <- df[testIndices, ]

  yTrain <- trainData$V8
  yTest <- testData$V8
  yTrainMean <- mean(yTrain)

  trainMSE[i] <- mse(yTrain, rep(yTrainMean, length(yTrain)))
  testMSE[i] <- mse(yTest, rep(yTrainMean, length(yTest)))
}

averageTrainMSE <- mean(trainMSE)
averageTestMSE <- mean(testMSE)

cat("Average Training MSE (Null Model):", averageTrainMSE, "\n")

## Average Training MSE (Null Model): 10.39242

cat("Average Test MSE (Null Model):", averageTestMSE, "\n")

## Average Test MSE (Null Model): 10.40003
```

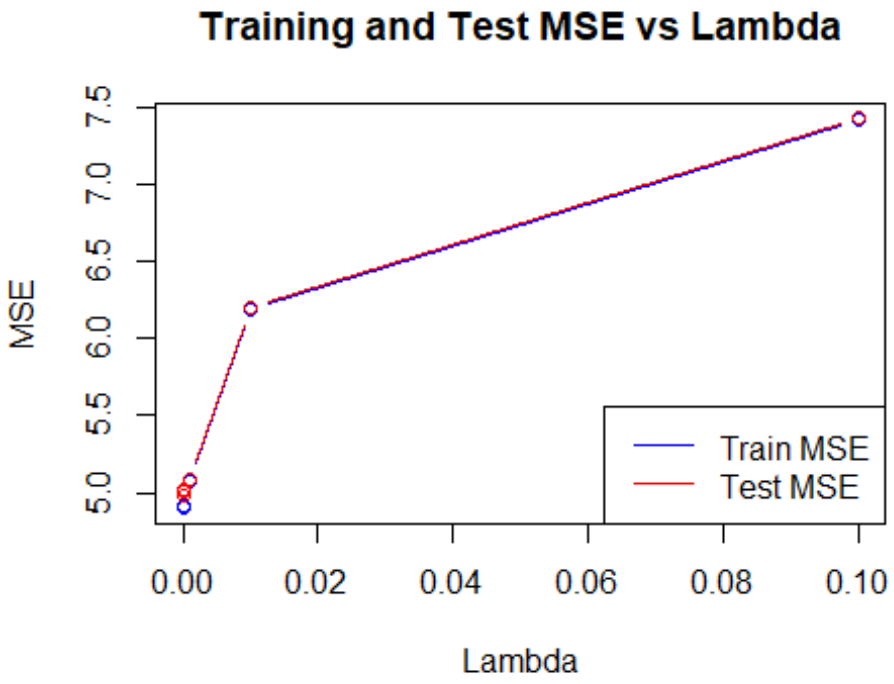
- **Part b) begins here**

```
library(caret)

library(Matrix)

lambdas <- c(0, 10^(-5), 10^(-4), 10^(-3), 10^(-2), 10^(-1))

trainMSE <- testMSE <- trainR2 <- testR2 <- logDet <- matrix(NA, nrow = lengt
h(lambdas), ncol = k)

# cv and fitting
for (lambdaIDX in 1:length(lambdas)) {
  lambda <- lambdas[lambdaIDX]

  for (foldIDX in 1:k) {

    testData <- foldedData[[foldIDX]]
    trainData <- do.call(rbind, foldedData[-foldIDX])

    xTrain <- cbind(1, as.matrix(trainData[, -ncol(df)]))
    yTrain <- trainData[, ncol(df)]
    xTest <- cbind(1, as.matrix(testData[, -ncol(df)]))
    yTest <- testData[, ncol(df)]

    # Normal equation
    XTX <- t(xTrain) %*% xTrain / nrow(xTrain)
    XTXlambda <- XTX + lambda * diag(ncol(xTrain))
    XTY <- t(xTrain) %*% yTrain / nrow(xTrain)

    beta <- solve(XTXlambda, XTY)

    # Train pred and perf
    yTrainPred <- xTrain %*% beta
    trainMSE[lambdaIDX, foldIDX] <- mse(yTrain, yTrainPred)
    trainR2[lambdaIDX, foldIDX] <- R2(yTrain, yTrainPred)

    # Test pred and perf
    yTestPred <- xTest %*% beta
    testMSE[lambdaIDX, foldIDX] <- mse(yTest, yTestPred)
    testR2[lambdaIDX, foldIDX] <- R2(yTest, yTestPred)

    # Log det
    logDet[lambdaIDX, foldIDX] <- determinant(XTXlambda, logarithm = TRUE)$mo
dulus
  }
}
```

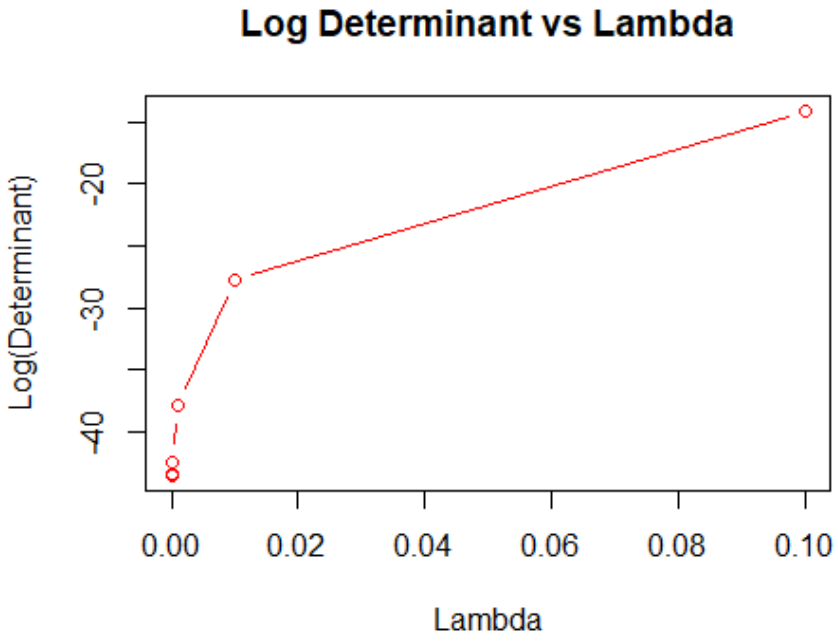
```r
# avg and std dev
trainMSEavg <- apply(trainMSE, 1, mean)
testMSEavg <- apply(testMSE, 1, mean)
trainMSEsd <- apply(trainMSE, 1, sd)
testMSEsd <- apply(testMSE, 1, sd)

trainR2avg <- apply(trainR2, 1, mean)
testR2avg <- apply(testR2, 1, mean)

logDetavg <- apply(logDet, 1, mean)

results <- data.frame(
  Lambda = lambdas,
  TrainR2avg = trainR2avg,
  TestR2avg = testR2avg,
  TrainMSEavg = trainMSEavg,
  TestMSEavg = testMSEavg,
  TrainMSEsd = trainMSEsd,
  TestMSEsd = testMSEsd,
  LogDetavg = logDetavg
)

# Print results
print(results)
```

```
##   Lambda TrainR2avg TestR2avg TrainMSEavg TestMSEavg TrainMSEsd TestMSEsd
## 1  0e+00  0.5280324 0.5216713    4.904990   5.016222 0.07380305 0.8108113
## 2  1e-05  0.5280203 0.5221116    4.905133   5.009041 0.07376744 0.7887751
## 3  1e-04  0.5273338 0.5241585    4.913411   4.977585 0.07182748 0.6703977
## 4  1e-03  0.5154296 0.5162472    5.071642   5.091793 0.06024019 0.5649924
## 5  1e-02  0.4095029 0.4115330    6.193869   6.206721 0.06974351 0.7529775
## 6  1e-01  0.3123559 0.3149953    7.420396   7.429738 0.09432220 0.9853778
##   LogDetavg
## 1 -43.53125
## 2 -43.40539
## 3 -42.45541
## 4 -37.90852
## 5 -27.73346
## 6 -14.12231
```

```r
plot(lambdas, trainMSEavg, type = "b", col = "blue", xlab = "Lambda", ylab =
"MSE", main = "Training and Test MSE vs Lambda")
lines(lambdas, testMSEavg, type = "b", col = "red")
legend("bottomright", legend = c("Train MSE", "Test MSE"), col = c("blue", "r
ed"), lty = 1)
```




```r
plot(lambdas, logDetavg, type = "b", col = "red", xlab = "Lambda", ylab = "Log(Determinant)", main = "Log Determinant vs Lambda")
```



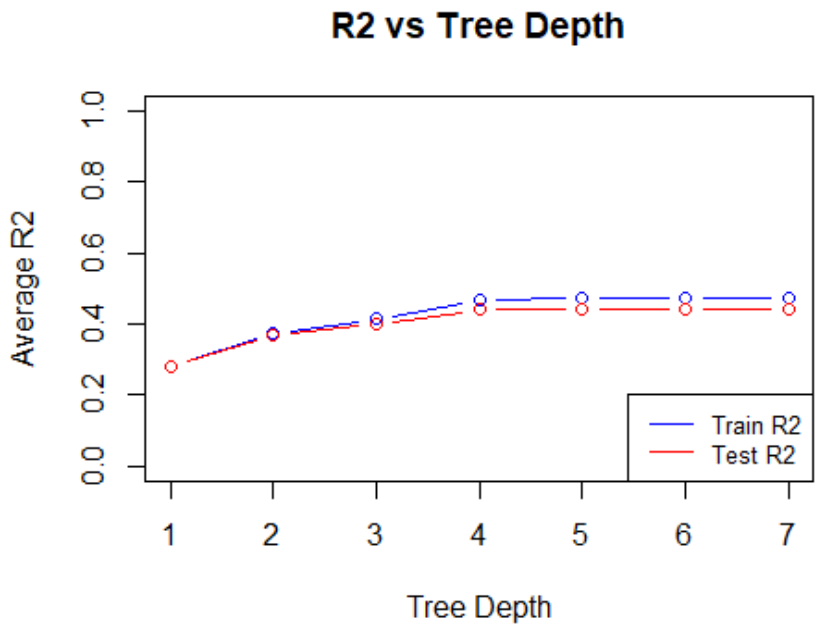
- **Part c) begins here**

```r
library(rpart)
library(dplyr)

k <- length(foldedData)

trainMSE <- matrix(NA, nrow = length(1:7), ncol = k)
testMSE <- matrix(NA, nrow = length(1:7), ncol = k)
trainR2 <- matrix(NA, nrow = length(1:7), ncol = k)
testR2 <- matrix(NA, nrow = length(1:7), ncol = k)


for (depth in 1:7) {

  for (foldIDX in 1:k) {

    testData <- foldedData[[foldIDX]]
    trainData <- do.call(rbind, foldedData[-foldIDX])

    # Tree
    tree_model <- rpart(
      V8 ~ .,
      data = trainData,
      method = "anova",
      control = rpart.control(maxdepth = depth)
    )

    # Train preds
    yTrainPred <- predict(tree_model, trainData)
    yTrain <- trainData$V8
    trainMSE[depth, foldIDX] <- mse(yTrain, yTrainPred)
    trainR2[depth, foldIDX] <- R2(yTrain, yTrainPred)

    # Test preds
    yTestPred <- predict(tree_model, testData)
    yTest <- testData$V8
    testMSE[depth, foldIDX] <- mse(yTest, yTestPred)
    testR2[depth, foldIDX] <- R2(yTest, yTestPred)
  }
}

trainMSEavg <- apply(trainMSE, 1, mean)
testMSEavg <- apply(testMSE, 1, mean)
trainR2avg <- apply(trainR2, 1, mean)
testR2avg <- apply(testR2, 1, mean)

results <- data.frame(
  Depth = 1:7,
```

```
  TrainMSEavg = trainMSEavg,
  TestMSEavg = testMSEavg,
  TrainR2avg = trainR2avg,
  TestR2avg = testR2avg)

print(results)
```

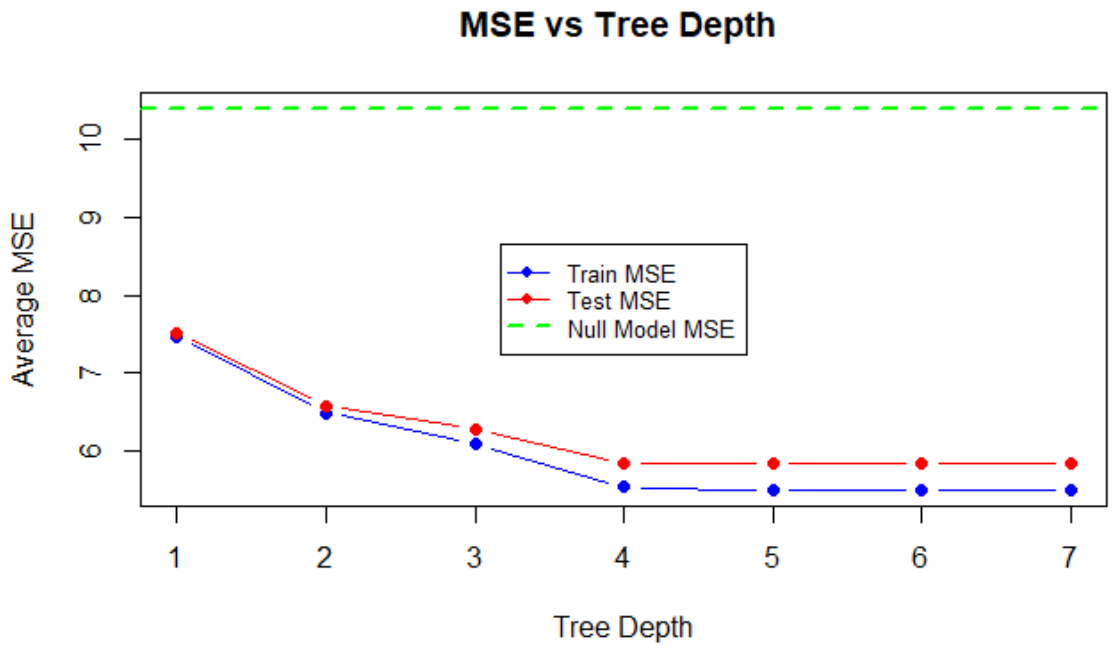
```
##   Depth TrainMSEavg TestMSEavg TrainR2avg TestR2avg
## 1     1    7.458863   7.514351  0.2822763 0.2788266
## 2     2    6.487685   6.579579  0.3757303 0.3696510
## 3     3    6.088498   6.273050  0.4141116 0.3984290
## 4     4    5.529737   5.837267  0.4678603 0.4399638
## 5     5    5.491621   5.832157  0.4715848 0.4400065
## 6     6    5.491621   5.832157  0.4715848 0.4400065
## 7     7    5.491621   5.832157  0.4715848 0.4400065
```

```
plot(1:7, trainR2avg, type = "b", col = "blue", ylim = c(0, 1),
     xlab = "Tree Depth", ylab = "Average R2", main = "R2 vs Tree Depth")

lines(1:7, testR2avg, type = "b", col = "red")

legend("bottomright", legend = c("Train R2", "Test R2"), col = c("blue", "red
"), lty = 1, cex = 0.8)
```




```
plot(1:7, trainMSEavg, type = "b", col = "blue", pch = 16, ylim = range(c(tra
inMSEavg, testMSEavg, averageTestMSE)),
     xlab = "Tree Depth", ylab = "Average MSE", main = "MSE vs Tree Depth")

lines(1:7, testMSEavg, type = "b", col = "red", pch = 16)
```

```r
abline(h = averageTestMSE, col = "green", lty = 2, lwd = 2)

legend("center", legend = c("Train MSE", "Test MSE", "Null Model MSE"),
       col = c("blue", "red", "green"), lty = c(1, 1, 2), pch = c(16, 16, NA)
, lwd = c(1, 1, 2), cex = 0.8)
```



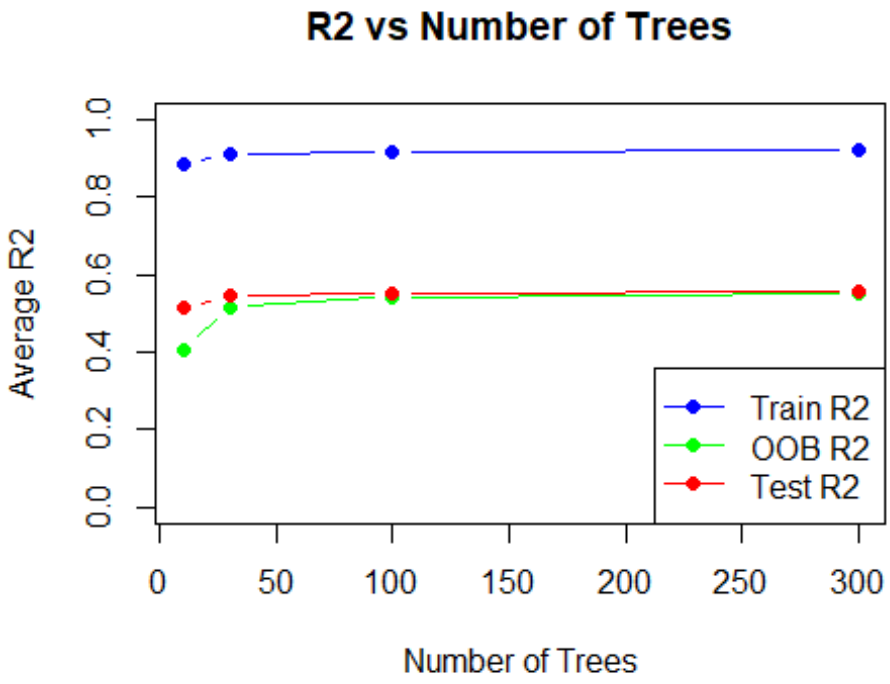
- **Part d) begins here**

```
library(randomForest)

treeCount <- c(10, 30, 100, 300)
trainR2 <- testR2 <- oobR2 <- trainMSE <- testMSE <- oobMSE <- matrix(NA, nro
w = length(treeCount), ncol = k)

for (nTrees in treeCount) {
  for (i in 1:k) {

    testIndices <- folds[[i]]
    trainIndices <- setdiff(1:nrow(df), testIndices)

    trainData <- df[trainIndices, ]
    testData <- df[testIndices, ]

    rfModel <- randomForest(V8 ~ ., data = trainData, ntree = nTrees)

    # Train preds
    yTrainPred <- predict(rfModel, newdata = trainData)
    trainR2[nTrees == treeCount, i] <- R2(trainData$V8, yTrainPred)
    trainMSE[nTrees == treeCount, i] <- mse(trainData$V8, yTrainPred)

    # OOB
    oobR2[nTrees == treeCount, i] <- rfModel$rsq[length(rfModel$rsq)]
    oobMSE[nTrees == treeCount, i] <- mean((rfModel$y - rfModel$predicted)^2)

    # test preds
    yTestPred <- predict(rfModel, newdata = testData)
    testR2[nTrees == treeCount, i] <- R2(testData$V8, yTestPred)
    testMSE[nTrees == treeCount, i] <- mse(testData$V8, yTestPred)
  }
}

# avg and std dev
trainR2avg <- apply(trainR2, 1, mean)
testR2avg <- apply(testR2, 1, mean)
oobR2avg <- apply(oobR2, 1, mean)
```

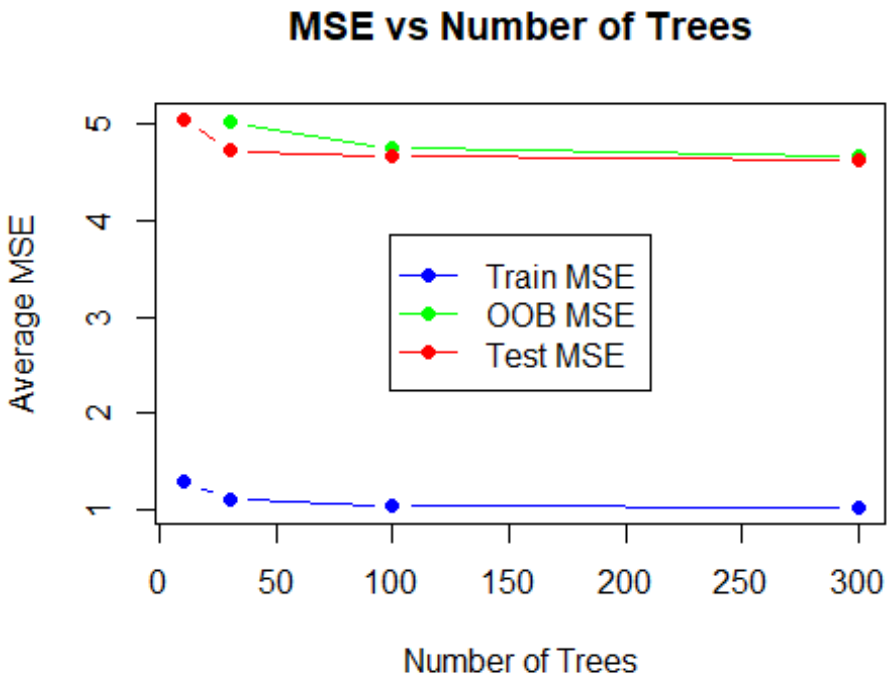
```r
trainMSEavg <- apply(trainMSE, 1, mean)
testMSEavg <- apply(testMSE, 1, mean)
oobMSEavg <- apply(oobMSE, 1, mean)

trainR2sd <- apply(trainR2, 1, sd)
testR2sd <- apply(testR2, 1, sd)
oobR2sd <- apply(oobR2, 1, sd)

trainMSEsd <- apply(trainMSE, 1, sd)
testMSEsd <- apply(testMSE, 1, sd)
oobMSEsd <- apply(oobMSE, 1, sd)

results <- data.frame(
  Trees = treeCount,
  TrainR2avg = trainR2avg,
  OOBR2avg = oobR2avg,
  TestR2avg = testR2avg,
  TrainMSEavg = trainMSEavg,
  OOBMSEavg = oobMSEavg,
  TestMSEavg = testMSEavg,
  TrainR2sd = trainR2sd,
  OOBR2sd = oobR2sd,
  TestR2sd = testR2sd,
  TrainMSEsd = trainMSEsd,
  OOBMSEsd = oobMSEsd,
  TestMSEsd = testMSEsd
)

print(results)
```

```
##   Trees TrainR2avg  OOBR2avg TestR2avg TrainMSEavg OOBMSEavg TestMSEavg
## 1    10  0.8865525 0.4072991 0.5156062    1.286288        NA   5.052605
## 2    30  0.9094320 0.5160888 0.5452158    1.101971  5.028956   4.731017
## 3   100  0.9182881 0.5424960 0.5519620    1.033360  4.754497   4.663469
## 4   300  0.9203430 0.5502045 0.5552729    1.017506  4.674341   4.626219
##      TrainR2sd     OOBR2sd   TestR2sd TrainMSEsd   OOBMSEsd TestMSEsd
## 1 0.0028843811 0.011475763 0.02301231 0.03691528         NA 0.3970279
## 2 0.0012358099 0.004527119 0.02394146 0.01343241 0.06515333 0.3484426
## 3 0.0011129689 0.004065406 0.01747700 0.01256756 0.05775123 0.3859143
## 4 0.0005341447 0.002480689 0.02029529 0.01098546 0.04103449 0.3608691
```

```r
plot(treeCount, trainR2avg, type = "b", col = "blue", ylim = c(0, 1), pch = 16,
     xlab = "Number of Trees", ylab = "Average R2", main = "R2 vs Number of Trees")
lines(treeCount, oobR2avg, type = "b", col = "green", pch = 16)
lines(treeCount, testR2avg, type = "b", col = "red", pch = 16)
legend("bottomright", legend = c("Train R2", "OOB R2", "Test R2"), col = c("blue", "green", "red"), lty = 1, pch = 16)
```




```r
ymin <- min(c(trainMSEavg, oobMSEavg, testMSEavg), na.rm = TRUE)
ymax <- max(c(trainMSEavg, oobMSEavg, testMSEavg), na.rm = TRUE)

plot(treeCount, trainMSEavg, type = "b", col = "blue", pch = 16,
     xlab = "Number of Trees", ylab = "Average MSE", main = "MSE vs Number of
Trees",
     ylim = c(ymin, ymax))
lines(treeCount, oobMSEavg, type = "b", col = "green", pch = 16)
lines(treeCount, testMSEavg, type = "b", col = "red", pch = 16)
legend("center", legend = c("Train MSE", "OOB MSE", "Test MSE"), col = c("blu
e", "green", "red"), lty = 1, pch = 16)
```


MSE vs Number of Trees
Average MSE
1
2
3
4
5
0
50
100
150
200
250
300
Number of Trees
Train MSE
OOB MSE
Test MSE