# Tree-based methods

# Load the packages that we will use in the workshop

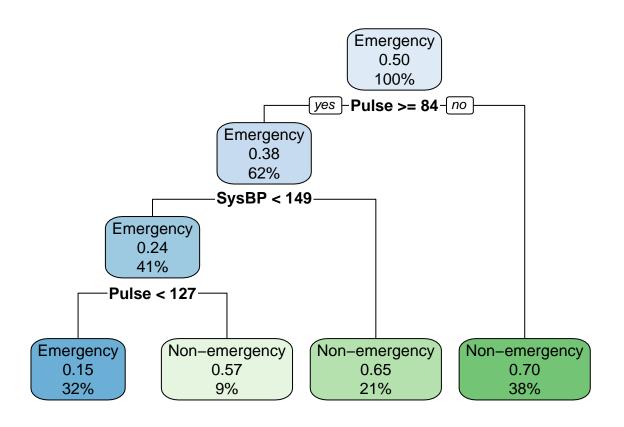
```
library(caret)
library(tidyverse)
library(rpart)
library(rpart.plot)
library(ipred)
library(bst)
library(ranger)
```

#### Classification trees

# Exercise 1 - Classification trees using rpart package

Using the rpart() function, create a classification tree using the adapted ICU data (made from the ICU dataset available in the Stat2Data package).

```
# Read in the data
ICU = read.delim("ICU.adapted.txt")
# Check the structure of the data
str(ICU)
## 'data.frame':
                   80 obs. of 10 variables:
             : int 38 104 107 40 79 70 110 157 188 116 ...
              : int 170 438 442 180 331 292 462 727 877 505 ...
## $ Survive : int 1 1 0 1 0 1 1 1 1 1 ...
            : int 51 80 69 64 63 61 69 75 88 40 ...
## $ AgeGroup : int 2 3 2 2 2 2 2 3 3 1 ...
## $ Sex
             : int 0 1 1 1 1 0 1 0 1 0 ...
## $ Infection: int 0 0 0 1 1 1 0 0 0 0 ...
             : int 110 162 170 158 36 68 150 144 190 130 ...
## $ SysBP
              : int 99 44 60 90 86 124 85 120 88 65 ...
## $ Pulse
## $ Emergency: Factor w/ 2 levels "Emergency", "Non-emergency": 1 1 1 1 1 1 1 1 1 1 ...
ICU.tree = rpart(Emergency ~ SysBP + Pulse, data = ICU)
# Plot the tree using the rpart.plot() function
# Shows predicted class, predicted probability of class, percentage of observations in node
rpart.plot(ICU.tree)
```



```
# What are the splitting rules for this tree?
rpart.rules(ICU.tree)
##
    Emergency
         0.15 when Pulse is 84 to 127 & SysBP < 149 \,
##
##
         0.57 when Pulse >= 127 & SysBP < 149
         0.65 when Pulse >=
                                 84 & SysBP >= 149
##
##
         0.70 when Pulse < 84
# Is the tree the same as before? What is your explanation for this?
# Use the predict() function to classify the data and calculate the classification
# error rate of our tree.
predicted.emergency = predict(ICU.tree)
predicted.emergency = predict(ICU.tree, type = "class")
ICU.table = table(predicted.emergency, ICU$Emergency)
ICU.table
## predicted.emergency Emergency Non-emergency
##
         Emergency
                              22
                                             4
##
         Non-emergency
                              18
                                            36
```

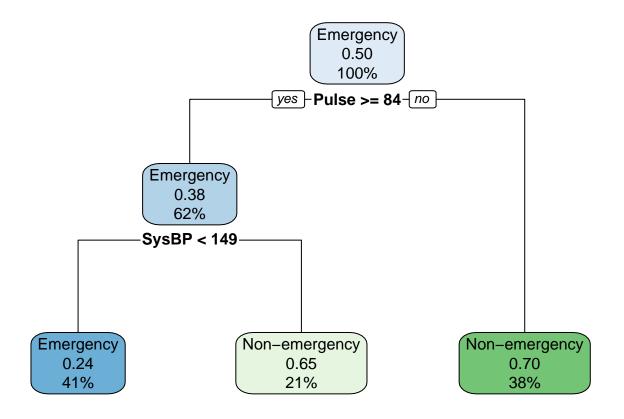
```
ICU.error = (ICU.table[2,1] + ICU.table[1,2]) / sum(ICU.table)
```

# Exercise 2 - How large should my tree be?

```
# Set the Cp parameter to 0.1 and construct another tree with the ICU data. What do you notice?

ICU.tree.cp.01 = rpart(Emergency ~ SysBP + Pulse, data = ICU, control = rpart.control(cp = 0.1))
## Higher cp - smaller tree and vice versa

rpart.plot(ICU.tree.cp.01)
```



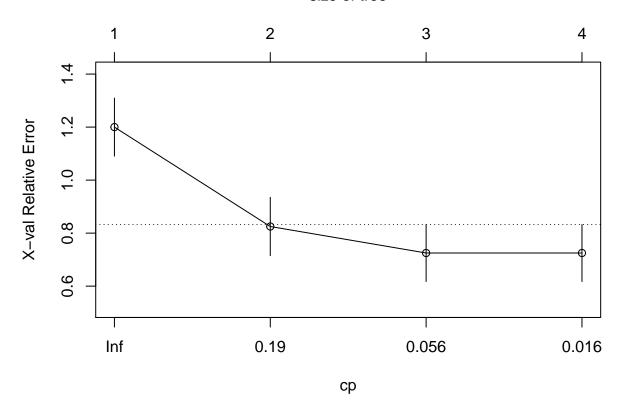
```
# Check the cp parameter of the original tree that you created (ICU.tree object) -
# use the summary() and plotcp() functions
summary(ICU.tree)$cptable
```

```
## Call:
## rpart(formula = Emergency ~ SysBP + Pulse, data = ICU)
## n= 80
##
## CP nsplit rel error xerror xstd
## 1 0.300 0 1.000 1.200 0.1095445
## 2 0.125 1 0.700 0.825 0.1100781
## 3 0.025 2 0.575 0.725 0.1074927
## 4 0.010 3 0.550 0.725 0.1074927
```

```
##
## Variable importance
## Pulse SysBP
##
      62
##
## Node number 1: 80 observations,
                                       complexity param=0.3
     predicted class=Emergency
                                    expected loss=0.5 P(node) =1
##
##
       class counts:
                        40
##
      probabilities: 0.500 0.500
##
     left son=2 (50 obs) right son=3 (30 obs)
##
     Primary splits:
##
         Pulse < 83.5 to the right, improve=3.840000, (0 missing)
##
         SysBP < 149
                       to the left, improve=2.849003, (0 missing)
##
## Node number 2: 50 observations,
                                       complexity param=0.125
##
     predicted class=Emergency
                                    expected loss=0.38 P(node) =0.625
##
       class counts:
                        31
##
      probabilities: 0.620 0.380
##
     left son=4 (33 obs) right son=5 (17 obs)
##
     Primary splits:
##
         SysBP < 149
                       to the left,
                                     improve=3.674082, (0 missing)
##
         Pulse < 119.5 to the left, improve=1.007619, (0 missing)
##
     Surrogate splits:
         Pulse < 87.5 to the right, agree=0.68, adj=0.059, (0 split)
##
##
## Node number 3: 30 observations
     predicted class=Non-emergency
                                    expected loss=0.3 P(node) =0.375
##
##
       class counts:
##
      probabilities: 0.300 0.700
##
## Node number 4: 33 observations,
                                       complexity param=0.025
##
     predicted class=Emergency
                                    expected loss=0.2424242 P(node) =0.4125
##
       class counts:
                        25
##
      probabilities: 0.758 0.242
##
     left son=8 (26 obs) right son=9 (7 obs)
##
     Primary splits:
##
         Pulse < 126.5 to the left,
                                     improve=1.9234100, (0 missing)
##
         SysBP < 105 to the left, improve=0.4267677, (0 missing)
##
## Node number 5: 17 observations
     predicted class=Non-emergency
                                    expected loss=0.3529412 P(node) =0.2125
##
##
                         6
       class counts:
##
      probabilities: 0.353 0.647
##
## Node number 8: 26 observations
     predicted class=Emergency
                                     expected loss=0.1538462 P(node) =0.325
##
##
       class counts:
                        22
##
      probabilities: 0.846 0.154
##
## Node number 9: 7 observations
##
     predicted class=Non-emergency
                                    expected loss=0.4285714 P(node) =0.0875
##
       class counts:
                         3
##
      probabilities: 0.429 0.571
```

```
CP nsplit rel error xerror
## 1 0.300
                      1.000 1.200 0.1095445
                0
                             0.825 0.1100781
## 2 0.125
                      0.700
## 3 0.025
                2
                             0.725 0.1074927
                      0.575
## 4 0.010
                3
                      0.550
                             0.725 0.1074927
plotcp(ICU.tree)
```

#### size of tree



```
# What is the prediction accuracy of the original tree (ICU.tree object) but on
# new data?

ICU.test = read.delim("ICU.adapted.test.txt")
predicted.test.emergency = predict(ICU.tree, newdata = ICU.test, type = "class")

ICU.test.table = table(predicted.test.emergency, ICU.test$Emergency)

ICU.test.error = (ICU.test.table[1,2] + ICU.test.table[2,1]) / sum(ICU.test.table)
ICU.test.error
```

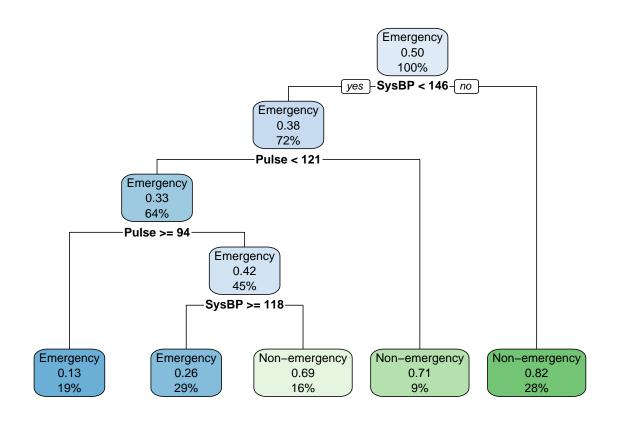
This exercise shows the influence of the cp parameter on the tree size and the prediction accuracy

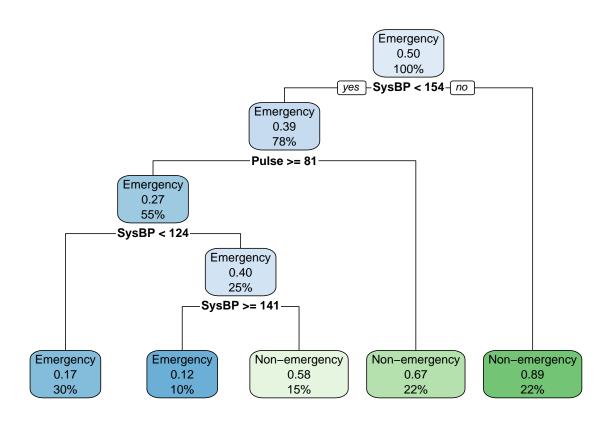
## Exercise 3 - Stability of trees

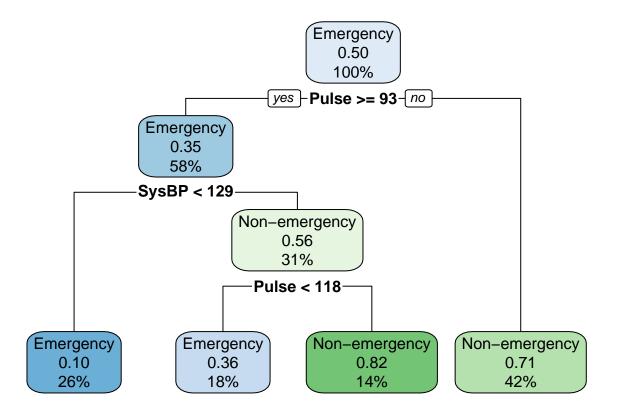
## [1] 0.7

Read in the original ICU dataset from the Stat2Data package. You want to construct a training set with 50 Emergency and 50 Non-emergency patients and train a classification tree. Repeat this process 3 times and

compare the resulting classification trees. Set the seed to 1, 2 and 3 respectively. What do you notice?







You are supposed to notice the instability of trees when change input data (take different samples of patients from the same dataset)

# Regression trees

#### Exercise 4 - Training a regression tree using the Caret package

Using the rpart method implemented in caret package, train a regression tree to predict gene expression from histone modifications. Report the accuracy of your model (hcp.model)

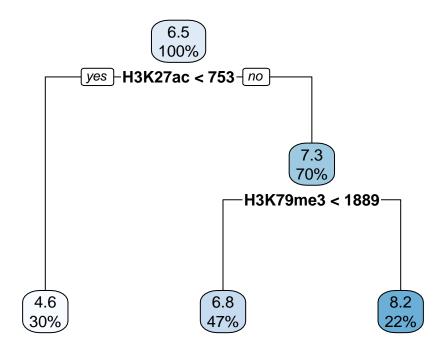
```
## [1] 400 32
dim(testing.hcp)
## [1] 100 32
# Define the control parameters for the model using the trainControl() function.
# Use 5-fold cross-validation and return all resampled measures.
# Also print the training log.
# Save the control parameters in an object hcp.ctrl since we will use them in
# subsequent models.
hcp.ctrl <- trainControl(method = "cv",
                     number = 5,
                     returnResamp = "all",
                     verboseIter = TRUE)
# Train the regression tree using the train() function
hcp.model <- train( expression ~ .,
                training.hcp,
               method = "rpart",
               trControl = hcp.ctrl)
## + Fold1: cp=0.03009
## - Fold1: cp=0.03009
## + Fold2: cp=0.03009
## - Fold2: cp=0.03009
## + Fold3: cp=0.03009
## - Fold3: cp=0.03009
## + Fold4: cp=0.03009
## - Fold4: cp=0.03009
## + Fold5: cp=0.03009
## - Fold5: cp=0.03009
## Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info =
## trainInfo, : There were missing values in resampled performance measures.
## Aggregating results
## Selecting tuning parameters
## Fitting cp = 0.0301 on full training set
# Test the model on the test data
# Predict expression values for test data
predicted.hcp = predict(hcp.model, newdata = testing.hcp)
# Calculate the accuracy of the model using the postResample() function
test.hcp.accuracy = postResample(pred = predicted.hcp, obs = testing.hcp$expression)
test.hcp.accuracy
        RMSE Rsquared
                             MAE
## 1.6603689 0.2530859 1.1663846
```

#### Exercise 5 - Visualize the regression tree and the predictions

Plot the binary tree representing the model and visualize the observed and predicted expression data. What do you notice?

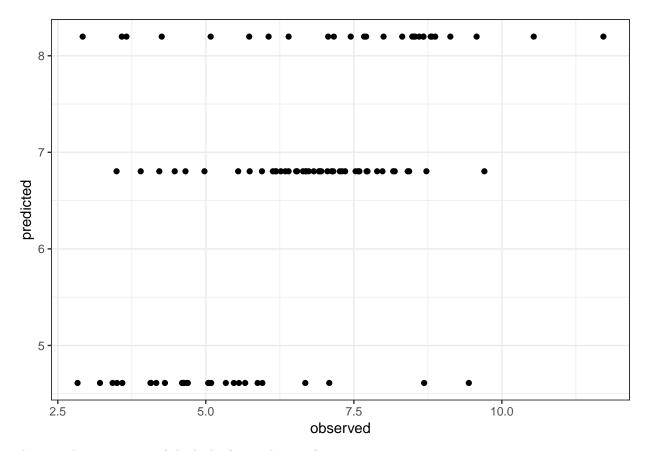
```
# What does our model actually look like? Print the final model and
# visualize the regression tree using rpart.plot()
hcp.model$finalModel
```

```
## n= 400
##
## node), split, n, deviance, yval
##    * denotes terminal node
##
## 1) root 400 1488.4150 6.454349
## 2) H3K27ac< 753 121 228.6196 4.611699 *
## 3) H3K27ac>=753 279 670.7795 7.253491
## 6) H3K79me3< 1889 189 389.1397 6.803634 *
## 7) H3K79me3>=1889 90 163.0704 8.198191 *
rpart.plot(hcp.model$finalModel)
```



```
# Create a scatterplot of predicted and observed values of gene expression
# on the test set. What do you notice?
hcp.results = data.frame(observed = testing.hcp$expression, predicted = predicted.hcp)

ggplot(hcp.results, aes(x = observed, y = predicted)) +
    geom_point() +
    theme_bw()
```



This is a demonstration of the lack of smoothness of regression trees

## Ensemble methods

#### Exercise 6 - Random Forest

Using the ranger method implemented in caret package, train a regression tree to predict gene expression from histone modifications. Report the accuracy of your model (hcp.model.rf)

```
## + Fold1: mtry= 2, min.node.size=5, splitrule=variance
## - Fold1: mtry= 2, min.node.size=5, splitrule=variance
## + Fold1: mtry= 5, min.node.size=5, splitrule=variance
## - Fold1: mtry= 5, min.node.size=5, splitrule=variance
```

```
## + Fold1: mtry= 8, min.node.size=5, splitrule=variance
## - Fold1: mtry= 8, min.node.size=5, splitrule=variance
## + Fold1: mtry=11, min.node.size=5, splitrule=variance
## - Fold1: mtry=11, min.node.size=5, splitrule=variance
## + Fold1: mtry=14, min.node.size=5, splitrule=variance
## - Fold1: mtry=14, min.node.size=5, splitrule=variance
## + Fold1: mtry=18, min.node.size=5, splitrule=variance
## - Fold1: mtry=18, min.node.size=5, splitrule=variance
## + Fold1: mtry=21, min.node.size=5, splitrule=variance
## - Fold1: mtry=21, min.node.size=5, splitrule=variance
## + Fold1: mtry=24, min.node.size=5, splitrule=variance
## - Fold1: mtry=24, min.node.size=5, splitrule=variance
## + Fold1: mtry=27, min.node.size=5, splitrule=variance
## - Fold1: mtry=27, min.node.size=5, splitrule=variance
## + Fold1: mtry=31, min.node.size=5, splitrule=variance
## - Fold1: mtry=31, min.node.size=5, splitrule=variance
## + Fold1: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold1: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold1: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold1: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold1: mtry= 8, min.node.size=5, splitrule=extratrees
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## - Fold1: mtry=18, min.node.size=5, splitrule=extratrees
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## + Fold1: mtry=24, min.node.size=5, splitrule=extratrees
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## + Fold1: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold2: mtry= 2, min.node.size=5, splitrule=variance
## - Fold2: mtry= 2, min.node.size=5, splitrule=variance
## + Fold2: mtry= 5, min.node.size=5, splitrule=variance
## - Fold2: mtry= 5, min.node.size=5, splitrule=variance
## + Fold2: mtry= 8, min.node.size=5, splitrule=variance
## - Fold2: mtry= 8, min.node.size=5, splitrule=variance
## + Fold2: mtry=11, min.node.size=5, splitrule=variance
## - Fold2: mtry=11, min.node.size=5, splitrule=variance
## + Fold2: mtry=14, min.node.size=5, splitrule=variance
## - Fold2: mtry=14, min.node.size=5, splitrule=variance
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## - Fold2: mtry=24, min.node.size=5, splitrule=variance
## + Fold2: mtry=27, min.node.size=5, splitrule=variance
## - Fold2: mtry=27, min.node.size=5, splitrule=variance
```

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## + Fold2: mtry=31, min.node.size=5, splitrule=variance
## - Fold2: mtry=31, min.node.size=5, splitrule=variance
## + Fold2: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold2: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold2: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold2: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold2: mtry= 8, min.node.size=5, splitrule=extratrees
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## - Fold2: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold3: mtry= 2, min.node.size=5, splitrule=variance
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## - Fold3: mtry= 8, min.node.size=5, splitrule=variance
## + Fold3: mtry=11, min.node.size=5, splitrule=variance
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## - Fold3: mtry=27, min.node.size=5, splitrule=variance
## + Fold3: mtry=31, min.node.size=5, splitrule=variance
## - Fold3: mtry=31, min.node.size=5, splitrule=variance
## + Fold3: mtry= 2, min.node.size=5, splitrule=extratrees
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## + Fold3: mtry= 5, min.node.size=5, splitrule=extratrees
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## + Fold3: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=14, min.node.size=5, splitrule=extratrees
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## + Fold3: mtry=21, min.node.size=5, splitrule=extratrees
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## + Fold3: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold4: mtry= 2, min.node.size=5, splitrule=variance
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## - Fold4: mtry=24, min.node.size=5, splitrule=variance
## + Fold4: mtry=27, min.node.size=5, splitrule=variance
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## + Fold4: mtry=31, min.node.size=5, splitrule=variance
## - Fold4: mtry=31, min.node.size=5, splitrule=variance
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## + Fold4: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold4: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold4: mtry= 8, min.node.size=5, splitrule=extratrees
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## + Fold4: mtry=14, min.node.size=5, splitrule=extratrees
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## + Fold4: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold5: mtry= 2, min.node.size=5, splitrule=variance
## - Fold5: mtry= 2, min.node.size=5, splitrule=variance
## + Fold5: mtry= 5, min.node.size=5, splitrule=variance
## - Fold5: mtry= 5, min.node.size=5, splitrule=variance
## + Fold5: mtry= 8, min.node.size=5, splitrule=variance
## - Fold5: mtry= 8, min.node.size=5, splitrule=variance
```

```
## + Fold5: mtry=11, min.node.size=5, splitrule=variance
## - Fold5: mtry=11, min.node.size=5, splitrule=variance
## + Fold5: mtry=14, min.node.size=5, splitrule=variance
## - Fold5: mtry=14, min.node.size=5, splitrule=variance
## + Fold5: mtry=18, min.node.size=5, splitrule=variance
## - Fold5: mtry=18, min.node.size=5, splitrule=variance
## + Fold5: mtry=21, min.node.size=5, splitrule=variance
## - Fold5: mtry=21, min.node.size=5, splitrule=variance
## + Fold5: mtry=24, min.node.size=5, splitrule=variance
## - Fold5: mtry=24, min.node.size=5, splitrule=variance
## + Fold5: mtry=27, min.node.size=5, splitrule=variance
## - Fold5: mtry=27, min.node.size=5, splitrule=variance
## + Fold5: mtry=31, min.node.size=5, splitrule=variance
## - Fold5: mtry=31, min.node.size=5, splitrule=variance
## + Fold5: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold5: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold5: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold5: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold5: mtry= 8, min.node.size=5, splitrule=extratrees
## - Fold5: mtry= 8, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=14, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=14, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=18, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=31, min.node.size=5, splitrule=extratrees
## Aggregating results
## Selecting tuning parameters
## Fitting mtry = 5, splitrule = variance, min.node.size = 5 on full training set
# Inspect the final randomForest model
hcp.model.rf$finalModel
## Ranger result
##
## Call:
   ranger::ranger(dependent.variable.name = ".outcome", data = x,
                                                                        mtry = min(param$mtry, ncol(x))
## Type:
                                     Regression
## Number of trees:
                                     500
                                     400
## Sample size:
## Number of independent variables:
## Mtry:
## Target node size:
## Variable importance mode:
                                     permutation
## Splitrule:
                                     variance
## 00B prediction error (MSE):
                                     1.761024
```

```
0.5279217
## R squared (00B):
# Using the predict() function, predict the expression values of the test dataset
predicted.hcp.rf <- predict(hcp.model.rf , newdata = testing.hcp)</pre>
# Calculate the accuracy of the model using the postResample() function
test.hcp.accuracy.rf = postResample(pred = predicted.hcp.rf, obs = testing.hcp$expression)
test.hcp.accuracy.rf
##
        RMSE Rsquared
                             MAE
## 1.5527371 0.3295244 1.0956180
```

Notice that random forest gives a higher prediction accuracy than individual regression tree from exercise 4

#### Exercise 7 - Variable importance of Random Forest models

## H3K27me1 19.65

18.20

13.68

13.56

11.53

13.24

plot(rfImp.hcp,top = 20)

## H4K12ac

## H4K16ac

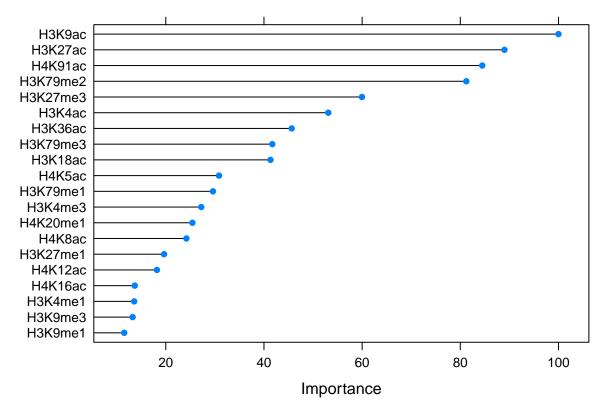
## H3K4me1

## H3K9me3

## H3K9me1

Compare variable importance of random forest models used for predicting expression of genes with HCP or LCP promoters.

```
# Inspect and visualize the variable importance of randomForest model used to
# predict gene expression from histone modifications. Use the varImp() function
rfImp.hcp <- varImp(hcp.model.rf)
rfImp.hcp
## ranger variable importance
##
##
     only 20 most important variables shown (out of 31)
##
            Overall
##
## H3K9ac
             100.00
## H3K27ac
              89.00
              84.47
## H4K91ac
## H3K79me2
              81.23
## H3K27me3
              59.96
## H3K4ac
              53.11
## H3K36ac
              45.65
## H3K79me3
              41.70
## H3K18ac
              41.33
## H4K5ac
              30.84
## H3K79me1
              29.61
## H3K4me3
              27.23
## H4K20me1
              25.43
## H4K8ac
              24.19
```



```
# Using the ranger method implemented in caret package, train a regression tree
# to predict gene expression from histone modifications but for LCP promoters.
# Report the accuracy of your model (lcp.model.rf)
# Read in expression and histone modification data for genes with LCP promoters
hm.data.lcp = read.delim("hm.data.lcp.txt")
# Create training and test sets using the createDataPartition() function (80:20)
index.train <- createDataPartition(y = hm.data.lcp$expression, p= 0.8, list = FALSE)
training.lcp <- hm.data.lcp[index.train,]</pre>
testing.lcp <- hm.data.lcp[-index.train,]</pre>
# Train the model using 'ranger' method. Set the number of trees to 500 and
# importance to "permutation"
lcp.model.rf <- train(expression ~ .,</pre>
                 data = training.lcp,
                 method = 'ranger',
                # should be set high at least p/3
                 tuneLength = 10,
                 trControl = hcp.ctrl,
                ## parameters passed onto the ranger function
                # the bigger the better.
                 num.trees = 500,
                 importance = "permutation")
```

## + Fold1: mtry= 2, min.node.size=5, splitrule=variance

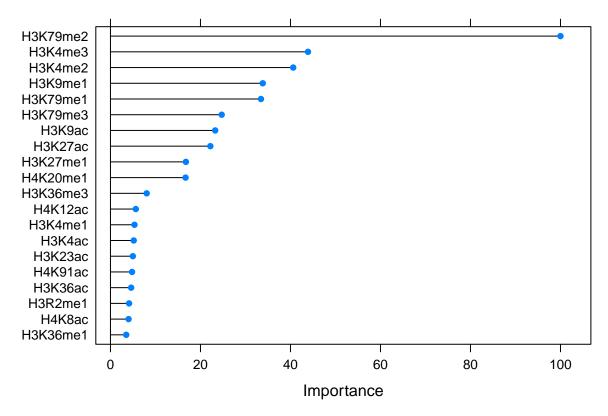
```
## - Fold1: mtry= 2, min.node.size=5, splitrule=variance
## + Fold1: mtry= 5, min.node.size=5, splitrule=variance
## - Fold1: mtry= 5, min.node.size=5, splitrule=variance
## + Fold1: mtry= 8, min.node.size=5, splitrule=variance
## - Fold1: mtry= 8, min.node.size=5, splitrule=variance
## + Fold1: mtry=11, min.node.size=5, splitrule=variance
## - Fold1: mtry=11, min.node.size=5, splitrule=variance
## + Fold1: mtry=14, min.node.size=5, splitrule=variance
## - Fold1: mtry=14, min.node.size=5, splitrule=variance
## + Fold1: mtry=18, min.node.size=5, splitrule=variance
## - Fold1: mtry=18, min.node.size=5, splitrule=variance
## + Fold1: mtry=21, min.node.size=5, splitrule=variance
## - Fold1: mtry=21, min.node.size=5, splitrule=variance
## + Fold1: mtry=24, min.node.size=5, splitrule=variance
## - Fold1: mtry=24, min.node.size=5, splitrule=variance
## + Fold1: mtry=27, min.node.size=5, splitrule=variance
## - Fold1: mtry=27, min.node.size=5, splitrule=variance
## + Fold1: mtry=31, min.node.size=5, splitrule=variance
## - Fold1: mtry=31, min.node.size=5, splitrule=variance
## + Fold1: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold1: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold1: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold1: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold1: mtry= 8, min.node.size=5, splitrule=extratrees
## - Fold1: mtry= 8, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=14, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=14, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=18, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold1: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold1: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold2: mtry= 2, min.node.size=5, splitrule=variance
## - Fold2: mtry= 2, min.node.size=5, splitrule=variance
## + Fold2: mtry= 5, min.node.size=5, splitrule=variance
## - Fold2: mtry= 5, min.node.size=5, splitrule=variance
## + Fold2: mtry= 8, min.node.size=5, splitrule=variance
## - Fold2: mtry= 8, min.node.size=5, splitrule=variance
## + Fold2: mtry=11, min.node.size=5, splitrule=variance
## - Fold2: mtry=11, min.node.size=5, splitrule=variance
## + Fold2: mtry=14, min.node.size=5, splitrule=variance
## - Fold2: mtry=14, min.node.size=5, splitrule=variance
## + Fold2: mtry=18, min.node.size=5, splitrule=variance
## - Fold2: mtry=18, min.node.size=5, splitrule=variance
## + Fold2: mtry=21, min.node.size=5, splitrule=variance
## - Fold2: mtry=21, min.node.size=5, splitrule=variance
## + Fold2: mtry=24, min.node.size=5, splitrule=variance
```

```
## - Fold2: mtry=24, min.node.size=5, splitrule=variance
## + Fold2: mtry=27, min.node.size=5, splitrule=variance
## - Fold2: mtry=27, min.node.size=5, splitrule=variance
## + Fold2: mtry=31, min.node.size=5, splitrule=variance
## - Fold2: mtry=31, min.node.size=5, splitrule=variance
## + Fold2: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold2: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold2: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold2: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold2: mtry= 8, min.node.size=5, splitrule=extratrees
## - Fold2: mtry= 8, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=14, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=14, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=18, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold2: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold2: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold3: mtry= 2, min.node.size=5, splitrule=variance
## - Fold3: mtry= 2, min.node.size=5, splitrule=variance
## + Fold3: mtry= 5, min.node.size=5, splitrule=variance
## - Fold3: mtry= 5, min.node.size=5, splitrule=variance
## + Fold3: mtry= 8, min.node.size=5, splitrule=variance
## - Fold3: mtry= 8, min.node.size=5, splitrule=variance
## + Fold3: mtry=11, min.node.size=5, splitrule=variance
## - Fold3: mtry=11, min.node.size=5, splitrule=variance
## + Fold3: mtry=14, min.node.size=5, splitrule=variance
## - Fold3: mtry=14, min.node.size=5, splitrule=variance
## + Fold3: mtry=18, min.node.size=5, splitrule=variance
## - Fold3: mtry=18, min.node.size=5, splitrule=variance
## + Fold3: mtry=21, min.node.size=5, splitrule=variance
## - Fold3: mtry=21, min.node.size=5, splitrule=variance
## + Fold3: mtry=24, min.node.size=5, splitrule=variance
## - Fold3: mtry=24, min.node.size=5, splitrule=variance
## + Fold3: mtry=27, min.node.size=5, splitrule=variance
## - Fold3: mtry=27, min.node.size=5, splitrule=variance
## + Fold3: mtry=31, min.node.size=5, splitrule=variance
## - Fold3: mtry=31, min.node.size=5, splitrule=variance
## + Fold3: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold3: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold3: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold3: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold3: mtry= 8, min.node.size=5, splitrule=extratrees
## - Fold3: mtry= 8, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=14, min.node.size=5, splitrule=extratrees
```

```
## - Fold3: mtry=14, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=18, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold3: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold3: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold4: mtry= 2, min.node.size=5, splitrule=variance
## - Fold4: mtry= 2, min.node.size=5, splitrule=variance
## + Fold4: mtry= 5, min.node.size=5, splitrule=variance
## - Fold4: mtry= 5, min.node.size=5, splitrule=variance
## + Fold4: mtry= 8, min.node.size=5, splitrule=variance
## - Fold4: mtry= 8, min.node.size=5, splitrule=variance
## + Fold4: mtry=11, min.node.size=5, splitrule=variance
## - Fold4: mtry=11, min.node.size=5, splitrule=variance
## + Fold4: mtry=14, min.node.size=5, splitrule=variance
## - Fold4: mtry=14, min.node.size=5, splitrule=variance
## + Fold4: mtry=18, min.node.size=5, splitrule=variance
## - Fold4: mtry=18, min.node.size=5, splitrule=variance
## + Fold4: mtry=21, min.node.size=5, splitrule=variance
## - Fold4: mtry=21, min.node.size=5, splitrule=variance
## + Fold4: mtry=24, min.node.size=5, splitrule=variance
## - Fold4: mtry=24, min.node.size=5, splitrule=variance
## + Fold4: mtry=27, min.node.size=5, splitrule=variance
## - Fold4: mtry=27, min.node.size=5, splitrule=variance
## + Fold4: mtry=31, min.node.size=5, splitrule=variance
## - Fold4: mtry=31, min.node.size=5, splitrule=variance
## + Fold4: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold4: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold4: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold4: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold4: mtry= 8, min.node.size=5, splitrule=extratrees
## - Fold4: mtry= 8, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=14, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=14, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=18, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold4: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold4: mtry=31, min.node.size=5, splitrule=extratrees
## + Fold5: mtry= 2, min.node.size=5, splitrule=variance
## - Fold5: mtry= 2, min.node.size=5, splitrule=variance
## + Fold5: mtry= 5, min.node.size=5, splitrule=variance
```

```
## - Fold5: mtry= 5, min.node.size=5, splitrule=variance
## + Fold5: mtry= 8, min.node.size=5, splitrule=variance
## - Fold5: mtry= 8, min.node.size=5, splitrule=variance
## + Fold5: mtry=11, min.node.size=5, splitrule=variance
## - Fold5: mtry=11, min.node.size=5, splitrule=variance
## + Fold5: mtry=14, min.node.size=5, splitrule=variance
## - Fold5: mtry=14, min.node.size=5, splitrule=variance
## + Fold5: mtry=18, min.node.size=5, splitrule=variance
## - Fold5: mtry=18, min.node.size=5, splitrule=variance
## + Fold5: mtry=21, min.node.size=5, splitrule=variance
## - Fold5: mtry=21, min.node.size=5, splitrule=variance
## + Fold5: mtry=24, min.node.size=5, splitrule=variance
## - Fold5: mtry=24, min.node.size=5, splitrule=variance
## + Fold5: mtry=27, min.node.size=5, splitrule=variance
## - Fold5: mtry=27, min.node.size=5, splitrule=variance
## + Fold5: mtry=31, min.node.size=5, splitrule=variance
## - Fold5: mtry=31, min.node.size=5, splitrule=variance
## + Fold5: mtry= 2, min.node.size=5, splitrule=extratrees
## - Fold5: mtry= 2, min.node.size=5, splitrule=extratrees
## + Fold5: mtry= 5, min.node.size=5, splitrule=extratrees
## - Fold5: mtry= 5, min.node.size=5, splitrule=extratrees
## + Fold5: mtry= 8, min.node.size=5, splitrule=extratrees
## - Fold5: mtry= 8, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=11, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=11, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=14, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=14, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=18, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=18, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=21, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=21, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=24, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=24, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=27, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=27, min.node.size=5, splitrule=extratrees
## + Fold5: mtry=31, min.node.size=5, splitrule=extratrees
## - Fold5: mtry=31, min.node.size=5, splitrule=extratrees
## Aggregating results
## Selecting tuning parameters
## Fitting mtry = 11, splitrule = variance, min.node.size = 5 on full training set
#Inspect the final model
lcp.model.rf$finalModel
## Ranger result
##
## Call:
   ranger::ranger(dependent.variable.name = ".outcome", data = x,
                                                                        mtry = min(param$mtry, ncol(x))
                                     Regression
## Type:
## Number of trees:
                                     500
## Sample size:
                                     400
## Number of independent variables:
                                     31
## Mtry:
                                     11
## Target node size:
                                     5
```

```
permutation
## Variable importance mode:
## Splitrule:
                                    variance
## OOB prediction error (MSE):
                                     1.313338
## R squared (00B):
                                     0.5535528
# Using the predict() function, predict the expression values of the test dataset
# of genes with LCP promoters
predicted.lcp.rf <- predict(lcp.model.rf , testing.lcp)</pre>
# Calculate the accuracy of the model using the postResample() function
test.accuracy.lcp.rf = postResample(pred = predicted.lcp.rf, obs = testing.lcp$expression)
test.accuracy.lcp.rf
       RMSE Rsquared
                          MAE
## 1.208272 0.494549 0.992078
# Inspect and visualize the variable importance of randomForest model used to
# predict gene expression from histone modifications for genes with LCP promoters.
# Use the varImp() function
rfImp.lcp <- varImp(lcp.model.rf)</pre>
rfImp.lcp
## ranger variable importance
##
##
     only 20 most important variables shown (out of 31)
##
##
            Overall
## H3K79me2 100.000
## H3K4me3 43.888
## H3K4me2 40.611
## H3K9me1 33.841
## H3K79me1 33.444
## H3K79me3 24.720
## H3K9ac
            23.273
## H3K27ac 22.202
## H3K27me1 16.763
## H4K20me1 16.688
## H3K36me3 8.051
## H4K12ac
             5.632
## H3K4me1
             5.336
## H3K4ac
             5.172
## H3K23ac 4.970
## H4K91ac 4.793
## H3K36ac
             4.594
## H3R2me1
             4.138
## H4K8ac
              4.024
## H3K36me1 3.500
plot(rfImp.lcp,top = 20)
```



The purpose of this exercise was to demonstrate how we can use variable importance to infer biological mechanisms - genes with high-CpG (HCP) and low-CpG (LCP) promoters seem to be regulated by different histone modifications. For more information you can check out https://www.pnas.org/content/107/7/2926 where we used linear regression with feature selection to choose important variables but the final results are similar.

#### Exercise 8 - Bagging

Using the "treebag" method implemented in caret package, train a regression tree to predict gene expression from histone modifications for genes with HCP promoters. Report the accuracy of your model (hcp.model.bag)

```
## + Fold1: parameter=none
## - Fold1: parameter=none
## + Fold2: parameter=none
## - Fold2: parameter=none
## - Fold3: parameter=none
## - Fold4: parameter=none
## - Fold4: parameter=none
## + Fold5: parameter=none
```

```
## - Fold5: parameter=none
## Aggregating results
## Fitting final model on full training set
# Using the predict() function, predict the expression values of the test dataset
predicted.hcp.bag <- predict(hcp.model.bag, newdata = testing.hcp)
# Calculate the accuracy of the model using the postResample() function
test.hcp.accuracy.bag = postResample(pred = predicted.hcp.bag, obs = testing.hcp$expression)
test.hcp.accuracy.bag
## RMSE Rsquared MAE
## 1.5901745 0.3140327 1.1200287</pre>
```

#### Exercise 9 - Boosting

Using the "bstTree" method implemented in caret package, train a regression tree to predict gene expression from histone modifications for genes with HCP promoters. Report the accuracy of your model (hcp.model.boost)

```
## + Fold1: maxdepth=1, nu=0.1, mstop=150
## - Fold1: maxdepth=1, nu=0.1, mstop=150
## + Fold1: maxdepth=2, nu=0.1, mstop=150
## - Fold1: maxdepth=2, nu=0.1, mstop=150
## + Fold1: maxdepth=3, nu=0.1, mstop=150
## - Fold1: maxdepth=3, nu=0.1, mstop=150
## + Fold2: maxdepth=1, nu=0.1, mstop=150
## - Fold2: maxdepth=1, nu=0.1, mstop=150
## + Fold2: maxdepth=2, nu=0.1, mstop=150
## - Fold2: maxdepth=2, nu=0.1, mstop=150
## + Fold2: maxdepth=3, nu=0.1, mstop=150
## - Fold2: maxdepth=3, nu=0.1, mstop=150
## + Fold3: maxdepth=1, nu=0.1, mstop=150
## - Fold3: maxdepth=1, nu=0.1, mstop=150
## + Fold3: maxdepth=2, nu=0.1, mstop=150
## - Fold3: maxdepth=2, nu=0.1, mstop=150
## + Fold3: maxdepth=3, nu=0.1, mstop=150
## - Fold3: maxdepth=3, nu=0.1, mstop=150
## + Fold4: maxdepth=1, nu=0.1, mstop=150
## - Fold4: maxdepth=1, nu=0.1, mstop=150
## + Fold4: maxdepth=2, nu=0.1, mstop=150
## - Fold4: maxdepth=2, nu=0.1, mstop=150
## + Fold4: maxdepth=3, nu=0.1, mstop=150
## - Fold4: maxdepth=3, nu=0.1, mstop=150
## + Fold5: maxdepth=1, nu=0.1, mstop=150
## - Fold5: maxdepth=1, nu=0.1, mstop=150
## + Fold5: maxdepth=2, nu=0.1, mstop=150
## - Fold5: maxdepth=2, nu=0.1, mstop=150
```

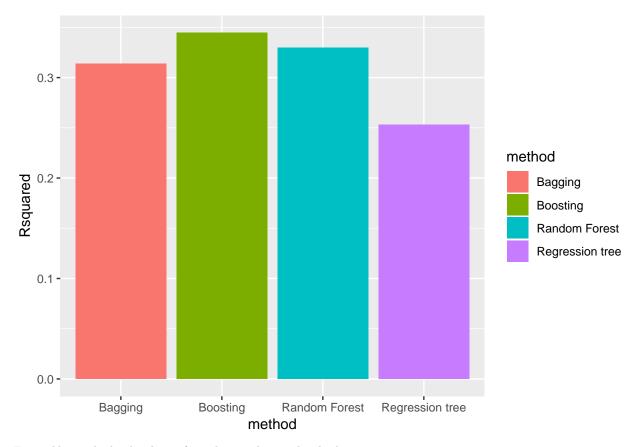
```
## + Fold5: maxdepth=3, nu=0.1, mstop=150
## - Fold5: maxdepth=3, nu=0.1, mstop=150
## Aggregating results
## Selecting tuning parameters
## Fitting mstop = 150, maxdepth = 1, nu = 0.1 on full training set
## Using the predict() function, predict the expression values of the test dataset
predicted.hcp.boost <- predict(hcp.model.boost, newdata = testing.hcp)

## Calculate the accuracy of the model using the postResample() function
test.hcp.accuracy.boost = postResample(pred = predicted.hcp.boost, obs = testing.hcp$expression)
test.hcp.accuracy.boost

## RMSE Rsquared MAE
## 1.5358010 0.3447751 1.0675493</pre>
```

# Exercise 10 - Compare the performance of different models

Use the previously obtained Rsquared values (from postResample() funciton) to compare the accuracy of regression tree, random forest, bagging and boosting models.



 $Ensemble\ methods\ clearly\ perform\ better\ than\ individual\ trees.$