## Decision trees and random forest

*Objective:* to predict wine quality rankings from its chemical properties.

Data set: Red wine dataset from <a href="https://archive.ics.uci.edu/ml/machine-learning-">https://archive.ics.uci.edu/ml/machine-learning-</a>

databases/wine-quality/winequality-red.csv.

First, I prepared the environment, set the working directory and loaded the libraries using the following:

```
> ### Assignment: Decision trees and random forest
> rm(list=ls()) #Clear the environment
> setwd("YOUR_PATH") #Set working directory for the assignment
> getwd() #Check working directory
[1] "YOUR_PATH"
>
> ### Assignment: Decision tree working directory for the assignment
> getwd() #Check working directory
[1] "YOUR_PATH"
>
> #Use decision trees and random forest to predict wine quality from its chemical properties
> #Dataset red wine from https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv
> #Load packages
> #Load packages
> library(rpart)
> library (caret)
> library(randomForest)
```

Next, I loaded the red wine dataset from the previously downloaded csv file (

https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv)

using the following code:

```
#Load data from the CSV file
> redwine <- read.csv2("winequality-red.csv", header = TRUE, sep= ";", quote= "", stringsAsFactor
s= FALSE)</pre>
```

To make sure that the data was loaded correctly, I previewed the data and looked at the internal structure of the data frame:

```
> #Check
> View(redwine) #Preview data
> str(redwine) #Check internal structure of the data frame
'data.frame': 1599 obs. of 12 variables:
$ X.fixed.acidity. : chr "7.4" "7.8" "7.8" "11.2" ...
$ X.volatile.acidity. : chr "0.7" "0.88" "0.76" "0.28" ...
$ X.citric.acid. : chr "0" "0" "0.04" "0.56" ...
$ X.residual.sugar. : chr "1.9" "2.6" "2.3" "1.9" ...
$ X.chlorides. : chr "0.076" "0.098" "0.092" "0.075" ...
$ X.free.sulfur.dioxide. : chr "11" "25" "15" "17" ...
$ X.total.sulfur.dioxide. : chr "34" "67" "54" "60" ...
$ X.density. : chr "0.9978" "0.9968" "0.997" "0.998" ...
$ X.pH. : chr "3.51" "3.2" "3.26" "3.16" ...
$ X.sulphates. : chr "0.56" "0.68" "0.65" "0.58" ...
$ X.alcohol. : chr "9.4" "9.8" "9.8" "9.8" ...
$ X.quality. : int 5 5 5 6 5 5 5 7 7 5 ...
```

The data was loaded correctly. The data set contains 1599 observations of 12 variables. X.quality variable has int type, the rest of the variables loaded as char. First, for convenience purposes, I decided to change column names – delete X. in the beginning and delete the period in the end of each column name. I used the gsub() function to replace X. and .\$ patterns:

```
> ###Change column names to easier to read
> #Delete X. in the beginning of column names
> names(redwine) <- qsub(pattern = "X.", replacement = "", names(redwine))</pre>
> #Delete the period in the end of column names
> names(redwine) <- qsub(pattern = ".$", replacement = "", names(redwine))</pre>
> #Check results
> str(redwine)
'data.frame': 1599 obs. of 12 variables:
$ fixed.acidity : chr "7.4" "7.8" "7.8" "11.2" ...
$ volatile.acidity : chr "0.7" "0.88" "0.76" "0.28" ...
$ citric.acid : chr "0" "0.04" "0.56" ... $ residual.sugar : chr "1.9" "2.6" "2.3" "1.9" ... $ chlorides : chr "0.076" "0.098" "0.092" "0.075" ...
$ free.sulfur.dioxide : chr "11" "25" "15" "17" ...
 $ total.sulfur.dioxide: chr "34" "67" "54" "60" ...
$ density : chr "0.9978" "0.9968" "0.997" "0.998" ...
                      : chr "3.51" "3.2" "3.26" "3.16" ...
$ pH
$ sulphates : chr "0.56" "0.68" "0.65" "0.58" ...
 $ alcohol
                      : chr "9.4" "9.8" "9.8" "9.8" ...
                : int 5 5 5 6 5 5 5 7 7 5 ...
 $ quality
```

As the above output shows, the column names were changed successfully. So, I proceeded to the data type conversions. I converted the output variable quality to a factor, and the rest of the variables to numeric using lapply(0 function:

```
> ###Data type conversions
> #Convert the response variable to factor
> redwine$quality <- as.factor(redwine$quality)</pre>
> #Convert all other columns to numeric
> redwine[1:11] <- lapply(redwine[1:11], as.numeric)</pre>
> #Check results
> str(redwine)
'data.frame':
                  1599 obs. of 12 variables:
$ fixed.acidity
                     : num 7.4 7.8 7.8 11.2 7.4 7.4 7.9 7.3 7.8 7.5 ...
$ volatile.acidity
                      : num 0.7 0.88 0.76 0.28 0.7 0.66 0.6 0.65 0.58 0.5 ...
 $ citric.acid
                      : num 0 0 0.04 0.56 0 0 0.06 0 0.02 0.36 ...
 $ residual.sugar
                      : num 1.9 2.6 2.3 1.9 1.9 1.8 1.6 1.2 2 6.1 ...
 $ chlorides
                      : num 0.076 0.098 0.092 0.075 0.076 0.075 0.069 0.065 0.073 0.071 ...
 $ free.sulfur.dioxide : num 11 25 15 17 11 13 15 15 9 17 ...
 $ total.sulfur.dioxide: num 34 67 54 60 34 40 59 21 18 102 ...
 $ density
                      : num 0.998 0.997 0.997 0.998 0.998 ...
                      : num 3.51 3.2 3.26 3.16 3.51 3.51 3.3 3.39 3.36 3.35 ...
 $ pH
 $ sulphates
                      : num 0.56 0.68 0.65 0.58 0.56 0.56 0.46 0.47 0.57 0.8 ...
 $ alcohol
                      : num 9.4 9.8 9.8 9.8 9.4 9.4 9.4 10 9.5 10.5 ...
                      : Factor w/ 6 levels "3", "4", "5", "6", ...: 3 3 3 4 3 3 3 5 5 3 ...
 $ quality
```

The above conversion was successful, no warnings about any conversion errors (N/As etc.). To make sure that there was no irregularities in the data that would affect the model, I displayed the summary statistics for all 12 variables in the data set:

```
> ###Summary statistics for all variables in the dataset
> summary(redwine)
fixed acidity volatile acidity citric acid residu.
                                                                                                                                         free.sulfur.dioxide total.sulfur.dioxide
                                                                                residual.sugar
                                                                                                               chlorides
                                                                                                                                                                                                                density
Min. : 4.60
1st Qu.: 7.10
Median : 7.90
Mean : 8.32
3rd Qu.: 9.20
                                                                               Min. : 0.900
1st Qu.: 1.900
Median : 2.200
Mean : 2.539
3rd Qu.: 2.600
                          Min. :0.1200
1st Qu.:0.3900
                                                     Min. :0.000
1st Qu.:0.090
                                                                                                           Min. :0.01200
1st Qu.:0.07000
                                                                                                                                         Min. : 1.00
1st Qu.: 7.00
                                                                                                                                                                         Min. : 6.00
1st Qu.: 22.00
                                                                                                                                                                                                          Min. :0.9901
1st Qu.:0.9956
                                                                                                                                                                                                                                       Min. :2.740
1st Qu.:3.210
                          Median :0.5200
Mean :0.5278
                                                                                                                                         Median :14.00
Mean :15.87
                                                                                                                                                                          Median : 38.00
                                                      Median :0.260
Mean :0.271
                                                                                                            Median :0.07900
Mean :0.08747
                                                                                                                                                                                                            Median :0.9968
                                                                                                                                                                                                                                       Median :3.310
Mean :3.311
                                                                                                                                                                                     : 46.47
: 62.00
                                                                                                                                                                                                            Mean :0.9967
3rd Qu.:0.9978
                                                                                                                                                                         Mean
                                                                                                                                                                                                            Mean
                           3rd Qu.:0.6400
                                                       3rd Qu.:0.420
                                                                                                            3rd Qu.:0.09000
                                                                                                                                         3rd Qu.:21.00
                                                                                                                                                                          3rd Qu.:
                                                                                                                                                                                                                                       3rd Qu.:3.400
                         Max. :1...
alcohol
            :15.90
                                                      Max.
quality
3: 10
4: 53
                                                                                           :15,500
                                                                                                                       :0.61100
                                                                                                                                                                                     :289.00
                                                                                                                                                                                                                       :1.0037
                                      :1.5800
                                                                 :1.000
                                                                               Max.
                                                                                                           Max.
                                                                                                                                                                                                           Max.
                                                                                                                                                                                                                                                   :4.010
    sulphates
Min. :0.3300
1st Qu.:0.5500
                           Min. : 8.40
1st Qu.: 9.50
Median :0.6200
Mean :0.6581
                           Median :10.20
Mean :10.42
                                                      5:681
 3rd Qu.: 0.7300
                            3rd Qu.:11.10
            :2.0000
```

The above output shows that the target variable quality which contains wine expert ratings on a scale from 1 to 10 actually has only observations with levels 3 through 8. In addition the sample contains very few observations for both extremes and the bulk of observations is in the 5-6 range. For example, there is just 10 wine samples with the rating 3 in the whole dataset, and after splitting it in the training and testing sets the resulting number will not be sufficient to train the algorithm. So I decided to groups observation into three levels of quality –

low (for quality 3 and 4), medium (for quality 5 and 6), and high (for quality 7 and 8). I used nested ifelse() statements as follows:

```
> redwine$quality <- as.factor(with(redwine, ifelse(quality%in%c("3","4"), "low", (ifelse(quality</pre>
%in%c("5", "6"), "medium", "high"))))
 > summary(redwind fixed.acidity  
Min. : 4.60  
1st Qu.: 7.10  
Median : 7.90  
Mean : 8.32  
3rd Qu.: 9.20  
Max. :15.90
                                   volatile.acidity citric.acid
                                                                                                     residual.sugar
                                                                                                                                            chlorides
                                                                                                                                                                             free.sulfur.dioxide total.sulfur.dioxide
                                                                                                                                                                                                                                                                      density
                                                                                                                                                                                                                    Min. : 6.00
1st Qu.: 22.00
Median : 38.00
Mean : 46.47
3rd Qu.: 62.00
                                                                                                     Min. : 0.900
1st Qu.: 1.900
Median : 2.200
Mean : 2.539
                                                                                                                                       Min. :0.01200
1st Qu.:0.07000
Median :0.07900
Mean :0.08747
                                                                                                                                                                             Min. : 1.00
1st Qu.: 7.00
Median :14.00
                                                                                                                                                                                                                                                                Min. :0.9901
1st Qu.:0.9956
Median :0.9968
                                 Min. :0.1200
1st Qu.:0.3900
                                                                   Min. :0.000
1st Qu.:0.090
                                                                    Median :0.260
                                  Median :0.5200
                                  Mean
                                                :0.5278
                                                                    Mean
                                                                                   :0.271
                                                                                                                                                                             Mean
                                                                                                                                                                                           :15.87
                                                                                                                                                                                                                                                                Mean
                                                                                                                                                                                                                                                                              :0.9967
                                   3rd Qu.:0.6400
                                                                     3rd Qu.:0.420
                                                                                                      3rd Qu.:
                                                                                                                                         3rd Qu.:0.09000
                                                                                                                                                                             3rd Qu.:21.00
                                                                                                                                                                                                                                                                 3rd Qu.:0.9978
                                                                                                    Max. ... quality high : 217
 Max. :1
pH
Min. :2
                                                                                                                                                      :0.61100
                                                                                                                                                                                                                                   :289.00
                                 мах.
                                                 :1.5800
                                                                   Max. :1.0
alcohol
                                                                                    :1.000
                                                                                                                    :15.500
                                                                                                                                        Max.
                                                                                                                                                                            Max.
                                                                                                                                                                                          :72.00
                                                                                                                                                                                                                     Max.
                                                                                                                                                                                                                                                               Max.
                                                                                                                                                                                                                                                                              :1.0037
                                       sulphates
  Min. :2.740
1st Qu.:3.210
                                 Min. :0.3300
1st Qu.:0.5500
                                                                    Min. : 8.40
1st Qu.: 9.50
  Median :3.310
Mean :3.311
                                 Median :0.6200
Mean :0.6581
3rd Qu.:0.7300
                                                                    Median :10.20
Mean :10.42
                                                                                                     medium:1319
  Mean :3.311
3rd Qu.:3.400
                                                                     3rd Qu.:11.10
                :4.010
                                               :2.0000
                               1599 obs. of 12 variables:
 'data.frame': 1599 obs. of 12 variables:
$ fixed.acidity : num 7.4 7.8 7.8 11.2 7.4 7.4 7.9 7.3 7.8 7.5 ...
$ volatific.acidity : num 0.7 0.88 0.76 0.28 0.7 0.66 0.6 0.65 0.58 0.5 ...
$ citric.acid : num 0.7 0.88 0.76 0.28 0.7 0.66 0.6 0.65 0.58 0.5 ...
$ residual.sugar : num 1.9 2.6 2.3 1.9 1.9 1.8 1.6 1.2 2 6.1 ...
$ chlorides : num 5 chlorides : num 5 total.sulfur.dioxide : num 5 total.sulfur.dioxide : num 5 total.sulfur.dioxide : num 6 density : num 7 density : num 7 density : num 8 density : num 8 density : num 9.4 6.8 0.56 0.68 0.65 0.58 0.56 0.64 0.47 0.57 0.8 ...
$ sulphates : num 9.4 9.8 9.8 9.8 9.4 9.4 10 9.5 10.5 ...
$ quality : Factor w/ 3 levels "high", "low", "medium": 3 3 3 3 3 3 1 1 3 ...
  data.frame':
```

As a result, the dataset contains 217 high quality wine samples, 63 low quality samples, and 1319 medium quality samples.

Next, I used the following code to split the data into training (80%) and testing (20%)

sets:

```
> #Prepare training and testing datasets (80% training, 20% testing)
>
> set.seed(15)
> ind <- sample.int(n=nrow(redwine), size=floor(0.8*nrow(redwine)), replace = FALSE)
> redwine_train <- redwine[ind, ] #training set
> redwine_test <- redwine[ -ind, ] #testing set
> #Prepare training and testing datasets (80% training, 20% testing)
> set.seed(15)
> ind <- sample.int(n=nrow(redwine), size=floor(0.8*nrow(redwine)), replace = FALSE)
> redwine_train <- redwine[ind, ] #training set
> redwine_test <- redwine[ -ind, ] #testing set</pre>
```

The resulting training set contains 1279 observations of 12 variables and testing set contains 320 observations of 12 variables.

> #Check resulting datasets

```
> dim(redwine_train)
[1] 1279   12
> dim(redwine_test)
[1] 320   12
```

I compared proportion between the three levels of wine quality in the training and testing sets, and they were approximately equal:

```
> #Compare proportions between low, medium and high quality wines in testing and training data
> prop.table(table(redwine_train$quality))
    high    low    medium
0.1422987 0.0398749 0.8178264
> prop.table(table(redwine_test$quality))
    high    low    medium
0.109375 0.037500 0.853125
```

Next step is to build the classification model. I used rpart() function from the rpart package, and included all variables:

```
> #Build classification tree model
> winequality_rp <- rpart(quality ~ ., data = redwine_train)</pre>
> #Retrieve node details
> winequality_rp
n = 1279
node), split, n, loss, yval, (yprob)
     * denotes terminal node
1) root 1279 233 medium (0.142298671 0.039874902 0.817826427)
  2) alcohol>=11.55 201 95 medium (0.462686567 0.009950249 0.527363184)
    4) sulphates>=0.685 89 26 high (0.707865169 0.000000000 0.292134831)
      8) free.sulfur.dioxide< 18.5 62 12 high (0.806451613 0.000000000 0.193548387) *
      9) free.sulfur.dioxide>=18.5 27 13 medium (0.481481481 0.000000000 0.518518519)
       18) free.sulfur.dioxide>=27.5 11 2 high (0.818181818 0.000000000 0.18181818182) *
       5) sulphates< 0.685 112 32 medium (0.267857143 0.017857143 0.714285714)
     10) total.sulfur.dioxide< 15.5 29 13 high (0.551724138 0.034482759 0.413793103)
       21) sulphates< 0.585 15 5 medium (0.266666667 0.066666667 0.666666667) *
     11) total.sulfur.dioxide>=15.5 83 15 medium (0.168674699 0.012048193 0.819277108)
       22) free.sulfur.dioxide>=31.5 9 2 high (0.777777778 0.000000000 0.222222222) *
       23) free.sulfur.dioxide< 31.5 74 8 medium (0.094594595 0.013513514 0.891891892) *
  3) alcohol< 11.55 1078 138 medium (0.082560297 0.045454545 0.871985158)
    6) volatile.acidity< 0.405 254 64 medium (0.236220472 0.015748031 0.748031496)
     12) alcohol>=10.45 118 51 medium (0.415254237 0.016949153 0.567796610)
       24) sulphates>=0.735 59 25 high (0.576271186 0.000000000 0.423728814)
         48) density>=0.99757 17  2 high (0.882352941 0.000000000 0.117647059) *
```

```
49) density< 0.99757 42 19 medium (0.452380952 0.000000000 0.547619048)
98) density< 0.9958 15 3 high (0.800000000 0.000000000 0.200000000) *
99) density>=0.9958 27 7 medium (0.259259259 0.0000000000 0.740740741) *
25) sulphates< 0.735 59 17 medium (0.254237288 0.033898305 0.711864407) *
13) alcohol< 10.45 136 13 medium (0.080882353 0.014705882 0.904411765) *
7) volatile.acidity>=0.405 824 74 medium (0.035194175 0.054611650 0.910194175)
14) volatile.acidity>=0.8375 65 19 medium (0.000000000 0.292307692 0.707692308)
28) citric.acid< 0.085 29 13 low (0.000000000 0.551724138 0.448275862)
56) citric.acid>=0.015 16 4 low (0.000000000 0.750000000 0.250000000) *
57) citric.acid< 0.015 13 4 medium (0.000000000 0.307692308 0.692307692) *
29) citric.acid>=0.085 36 3 medium (0.000000000 0.083333333 0.916666667) *
15) volatile.acidity< 0.8375 759 55 medium (0.038208169 0.034255599 0.927536232) *
```

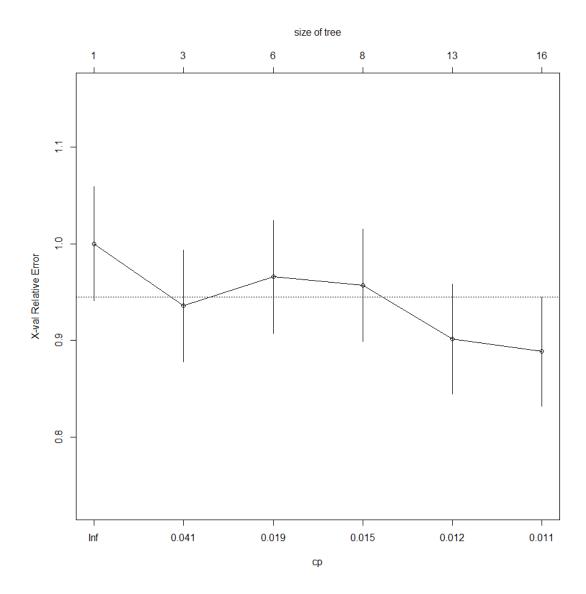
Then, I used printcp() to examine the complexity parameter:

```
> #Examine complexity
> printcp(winequality_rp)
Classification tree:
rpart(formula = quality ~ ., data = redwine_train)
Variables actually used in tree construction:
                                       density
                                                         free.sulfur.dioxide sulphates
[1] alcohol
                   citric.acid
total.sulfur.dioxide volatile.acidity
Root node error: 233/1279 = 0.18217
n = 1279
      CP nsplit rel error xerror
1 0.079399 0 1.00000 1.00000 0.059245
2 0.021459
            2 0.84120 0.93562 0.057716
3 0.017167 5 0.77682 0.96567 0.058441
4 0.012876
            7 0.74249 0.95708 0.058236
6 0.010000 15 0.61373 0.88841 0.056532
```

The output above shows that the following seven variables were actually used in the tree construction: alcohol, citric.acid, density, free.sulfur.dioxide, sulphates, total.sulfur.dioxide and volatile.acidity. It also list the number od splits (nsplit), the relative error (xerror) and the standard error (xstand).

It is convenient to visually analyze the cost complexity parameters using plotcp(0 function:

```
> #Plot cost complexity parameters
> plotcp(winequality_rp)
```



The graph above shows that the minimum relative error estimated by a 10-fold classification (Xerror) is observed with the tree size of 16.

A detailed summary of the model can be displayed using the summary() command: I list the importance of the variables and characteristics of each node (how observations were split in each node):

```
> #Examine the model
> summary(winequality_rp)
Call:
rpart(formula = quality ~ ., data = redwine_train)
    n= 1279
```

```
CP nsplit rel error
                                xerror
1 0.07939914
                 0 1.0000000 1.0000000 0.05924512
2 0.02145923
                 2 0.8412017 0.9356223 0.05771580
3 0.01716738
                 5 0.7768240 0.9656652 0.05844137
                 7 0.7424893 0.9570815 0.05823622
4 0.01287554
5 0.01144492
                12 0.6480687 0.9012876 0.05686006
6 0.01000000
                15 0.6137339 0.8884120 0.05653161
Variable importance
            alcohol
                               sulphates
                                                      density
                                                                  volatile.acidity free.sulfur.
dioxide total.sulfur.dioxide
                                     citric.acid
                 23
                                                                                11
                                      13
                                                           13
                                         7
                    8
                                                                    residual.sugar
       fixed.acidity
                               chlorides
                                                           рН
                  6
                                                            4
Node number 1: 1279 observations,
                                    complexity param=0.07939914
  predicted class=medium expected loss=0.1821736 P(node) =1
   class counts: 182
                          51 1046
  probabilities: 0.142 0.040 0.818
  left son=2 (201 obs) right son=3 (1078 obs)
  Primary splits:
     alcohol
                      < 11.55
                                 to the right, improve=44.81302, (0 missing)
                                 to the right, improve=26.88087, (0 missing)
     sulphates
                      < 0.685
     volatile.acidity < 0.3625
                                 to the left, improve=25.95614, (0 missing)
                                 to the right, improve=20.18783, (0 missing)
                     < 0.315
     citric.acid
     density
                      < 0.99535 to the left, improve=19.75534, (0 missing)
  Surrogate splits:
                          < 0.993785 to the left, agree=0.887, adj=0.279, (0 split)
     density
                          < 0.0525 to the left, agree=0.860, adj=0.109, (0 split)
     chlorides
                          < 5.55
                                     to the left, agree=0.856, adj=0.085, (0 split)
     fixed.acidity
                          < 3.695
                                     to the right, agree=0.850, adj=0.045, (0 split)
     total.sulfur.dioxide < 162.5
                                     to the right, agree=0.845, adj=0.015, (0 split)
Node number 2: 201 observations,
                                   complexity param=0.07939914
  predicted class=medium expected loss=0.4726368 P(node) =0.157154
   class counts: 93
                          2 106
   probabilities: 0.463 0.010 0.527
  left son=4 (89 obs) right son=5 (112 obs)
  Primary splits:
     sulphates
                      < 0.685
                                to the right, improve=18.455050, (0 missing)
     рН
                      < 3.365
                                 to the left, improve= 9.083775, (0 missing)
                                 to the right, improve= 7.901565, (0 missing)
     citric.acid
                      < 0.315
                      < 7.85
                                 to the right, improve= 7.333158, (0 missing)
     fixed.acidity
                                 to the left, improve= 4.739165, (0 missing)
     volatile.acidity < 0.335
  Surrogate splits:
                                     to the right, agree=0.647, adj=0.202, (0 split)
     fixed.acidity
                          < 8.05
                          < 0.325
                                     to the right, agree=0.632, adj=0.169, (0 split)
     citric.acid
                          < 0.345
                                     to the left, agree=0.627, adj=0.157, (0 split)
     volatile.acidity
                          < 12.85
                                     to the right, agree=0.612, adj=0.124, (0 split)
      total.sulfur.dioxide < 51
                                     to the right, agree=0.607, adj=0.112, (0 split)
Node number 3: 1078 observations,
                                    complexity param=0.01287554
  predicted class=medium expected loss=0.1280148 P(node) =0.842846
   class counts:
                    89
                          49
                              940
  probabilities: 0.083 0.045 0.872
```

```
left son=6 (254 obs) right son=7 (824 obs)
  Primary splits:
     volatile.acidity
                         < 0.405
                                    to the left, improve=13.244800, (0 missing)
                          < 10.45
                                    to the right, improve=13.187220, (0 missing)
     alcohol
     sulphates
                          < 0.675
                                   to the right, improve= 9.555997, (0 missing)
     total.sulfur.dioxide < 49.5 to the left. improve= 6.863008. (0 missing)
     citric.acid
                         < 0.295 to the right, improve= 6.501941, (0 missing)
 Surrogate splits:
     citric.acid
                         < 0.395
                                    to the right, agree=0.793, adj=0.122, (0 split)
     fixed.acidity
                         < 10.45
                                    to the right, agree=0.773, adj=0.035, (0 split)
     free.sulfur.dioxide < 3.5
                                    to the left, agree=0.768, adj=0.016, (0 split)
     total.sulfur.dioxide < 10.5
                                    to the left, agree=0.768, adj=0.016, (0 split)
Node number 4: 89 observations.
                                complexity param=0.01716738
 predicted class=high
                        expected loss=0.2921348 P(node) =0.06958561
   class counts: 63
                        0
                             26
  probabilities: 0.708 0.000 0.292
 left son=8 (62 obs) right son=9 (27 obs)
 Primary splits:
     free.sulfur.dioxide < 18.5
                                    to the left, improve=3.972669, (0 missing)
     total.sulfur.dioxide < 56.5
                                    to the left, improve=3.750644, (0 missing)
     density
                         < 0.99533 to the left, improve=3.280533, (0 missing)
                                   to the left, improve=1.804469, (0 missing)
                         < 3.365
     рН
                                    to the left, improve=1.185295, (0 missing)
     alcohol
                         < 13.8
 Surrogate splits:
     total.sulfur.dioxide < 44
                                    to the left, agree=0.865, adj=0.556, (0 split)
     alcohol
                        < 11.65
                                    to the right, agree=0.742, adj=0.148, (0 split)
     density
                         < 0.99176 to the right, agree=0.730, adj=0.111, (0 split)
                                    to the left, agree=0.730, adj=0.111, (0 split)
     пΗ
                         < 3.59
                                    to the left, agree=0.719, adj=0.074, (0 split)
     citric.acid
                         < 0.72
Node number 5: 112 observations,
                                  complexity param=0.02145923
 predicted class=medium expected loss=0.2857143 P(node) =0.08756841
   class counts:
                    30
                          2
                             80
   probabilities: 0.268 0.018 0.714
 left son=10 (29 obs) right son=11 (83 obs)
  Primary splits:
     total.sulfur.dioxide < 15.5 to the left, improve=6.697638, (0 missing)
                                   to the left, improve=5.081589, (0 missing)
     free.sulfur.dioxide < 7.5
                         < 3.275 to the left, improve=4.984568, (0 missing)
     citric.acid
                         < 0.265 to the right, improve=4.472894, (0 missing)
                         < 3.9
                                   to the right, improve=3.386447, (0 missing)
     residual.sugar
 Surrogate splits:
     free.sulfur.dioxide < 7.5</pre>
                                   to the left, agree=0.920, adj=0.690, (0 split)
                        < 0.1225 to the right, agree=0.768, adj=0.103, (0 split)
     chlorides
                                   to the right, agree=0.750, adj=0.034, (0 split)
     residual.sugar
                        < 5.85
Node number 6: 254 observations.
                                  complexity param=0.01287554
 predicted class=medium expected loss=0.2519685 P(node) =0.1985927
   class counts:
                          4 190
                  60
  probabilities: 0.236 0.016 0.748
 left son=12 (118 obs) right son=13 (136 obs)
  Primary splits:
     alcohol
                                    to the right, improve=14.223290, (0 missing)
                          < 10.45
     chlorides
                         < 0.0755 to the left, improve= 8.651214, (0 missing)
                         < 0.715
     sulphates
                                    to the right, improve= 7.886671, (0 missing)
     total.sulfur.dioxide < 49.5
                                    to the left, improve= 6.499420, (0 missing)
```

```
< 0.99554 to the left, improve= 6.368964, (0 missing)
     density
 Surrogate splits:
     density
                         < 0.996785 to the left, agree=0.669, adj=0.288, (0 split)
                          < 0.0705 to the left, agree=0.650, adj=0.246, (0 split)
     chlorides
     sulphates
                         < 0.705
                                    to the right, agree=0.618, adj=0.178, (0 split)
                                    to the right, agree=0.602, adj=0.144, (0 split)
     citric.acid
                          < 0.315
     total.sulfur.dioxide < 47.5
                                    to the left, agree=0.594, adj=0.127, (0 split)
Node number 7: 824 observations,
                                  complexity param=0.01144492
 predicted class=medium expected loss=0.08980583 P(node) =0.6442533
   class counts:
                   29
                         45 750
   probabilities: 0.035 0.055 0.910
  left son=14 (65 obs) right son=15 (759 obs)
  Primary splits:
     volatile.acidity
                         < 0.8375 to the right, improve=6.968096, (0 missing)
                                    to the left, improve=4.245303, (0 missing)
     total.sulfur.dioxide < 14.5
     citric.acid
                   < 0.105
                                    to the left, improve=2.525045, (0 missing)
     free.sulfur.dioxide < 6.5
                                    to the left, improve=2.250605, (0 missing)
     residual.sugar < 1.55
                                    to the left, improve=2.026013, (0 missing)
 Surrogate splits:
     chlorides
                         < 0.048
                                    to the left, agree=0.925, adj=0.046, (0 split)
     fixed.acidity
                         < 5.15
                                    to the left, agree=0.924, adj=0.031, (0 split)
     total.sulfur.dioxide < 144.5
                                    to the right, agree=0.924, adj=0.031, (0 split)
                          < 3.73
                                    to the right, agree=0.924, adj=0.031, (0 split)
Node number 8: 62 observations
 predicted class=high
                         expected loss=0.1935484 P(node) =0.04847537
   class counts:
                    50
                           0
                              12
  probabilities: 0.806 0.000 0.194
Node number 9: 27 observations,
                                 complexity param=0.01716738
 predicted class=medium expected loss=0.4814815 P(node) =0.02111024
   class counts:
                  13
                          0
  probabilities: 0.481 0.000 0.519
 left son=18 (11 obs) right son=19 (16 obs)
  Primary splits:
     free.sulfur.dioxide < 27.5</pre>
                                    to the right, improve=4.208754, (0 missing)
                                    to the left, improve=3.333754, (0 missing)
                          < 3.37
                                    to the left, improve=3.114815, (0 missing)
     total.sulfur.dioxide < 56.5
                                    to the right, improve=1.814815, (0 missing)
     sulphates
                         < 0.755
     density
                         < 0.995365 to the left, improve=1.514449, (0 missing)
 Surrogate splits:
     рН
                      < 3.345
                                 to the left, agree=0.741, adj=0.364, (0 split)
                                to the right, agree=0.741, adj=0.364, (0 split)
     sulphates
                     < 0.81
     volatile.acidity < 0.415
                                to the right, agree=0.704, adj=0.273, (0 split)
                                to the right, agree=0.704, adj=0.273, (0 split)
     citric.acid
                  < 0.445
     fixed.acidity
                      < 9.15
                                to the right, agree=0.667, adj=0.182, (0 split)
Node number 10: 29 observations,
                                   complexity param=0.02145923
                         expected loss=0.4482759 P(node) =0.02267396
 predicted class=high
   class counts:
                   16
                           1
                               12
  probabilities: 0.552 0.034 0.414
 left son=20 (14 obs) right son=21 (15 obs)
  Primary splits:
     sulphates
                         < 0.585
                                    to the right, improve=4.543842, (0 missing)
     chlorides
                         < 0.0665 to the right, improve=2.484102, (0 missing)
                         < 0.99413 to the left, improve=1.656624, (0 missing)
     density
```

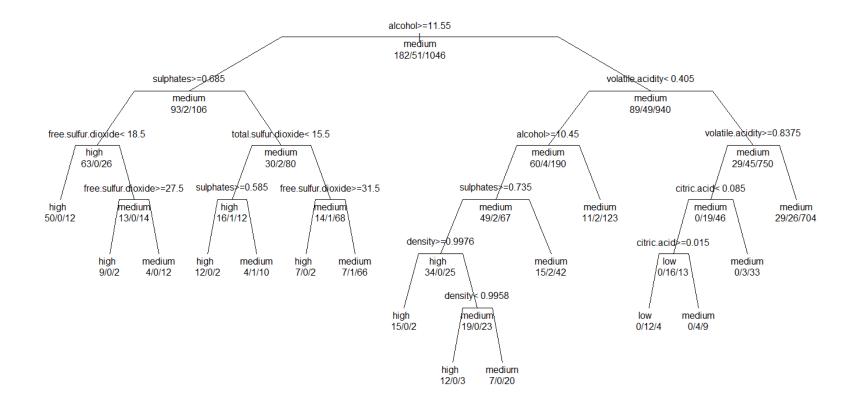
```
total.sulfur.dioxide < 9
                                   to the right, improve=1.497089, (0 missing)
     residual.sugar < 3.9
                                   to the right, improve=1.029557, (0 missing)
 Surrogate splits:
     chlorides
                     < 0.072 to the right, agree=0.759, adj=0.500, (0 split)
     residual.sugar < 2.05 to the right, agree=0.724, adj=0.429, (0 split)
     volatile.acidity < 0.445 to the right, agree=0.655, adj=0.286, (0 split)
     density
                    < 0.995855 to the right, agree=0.655, adj=0.286, (0 split)
                     < 8.25 to the right, agree=0.621, adj=0.214, (0 split)
     fixed.acidity
Node number 11: 83 observations, complexity param=0.02145923
 predicted class=medium expected loss=0.1807229 P(node) =0.06489445
   class counts: 14
                        1 68
  probabilities: 0.169 0.012 0.819
 left son=22 (9 obs) right son=23 (74 obs)
  Primary splits:
     free.sulfur.dioxide < 31.5</pre>
                                   to the right, improve=7.345092, (0 missing)
                         < 3.27
                                   to the left, improve=3.073070, (0 missing)
     total.sulfur.dioxide < 99.5 to the right, improve=2.408144, (0 missing)
     volatile.acidity < 0.355 to the left, improve=2.397998, (0 missing)
     residual.sugar
                       < 4.15 to the right, improve=1.999179, (0 missing)
 Surrogate splits:
     total.sulfur.dioxide < 99.5 to the right, agree=0.952, adj=0.556, (0 split)
                       < 0.991555 to the left, agree=0.928, adj=0.333, (0 split)
                         < 3.035 to the left, agree=0.928, adj=0.333, (0 split)
                        < 0.023
                                 to the left, agree=0.916, adj=0.222, (0 split)
     chlorides
                         < 0.395 to the left, agree=0.916, adj=0.222, (0 split)
     sulphates
Node number 12: 118 observations, complexity param=0.01287554
 predicted class=medium expected loss=0.4322034 P(node) =0.09225958
   class counts:
                   49
                         2 67
  probabilities: 0.415 0.017 0.568
  left son=24 (59 obs) right son=25 (59 obs)
  Primary splits:
     sulphates
                         < 0.735
                                   to the right, improve=5.542373, (0 missing)
                                   to the left, improve=3.812779, (0 missing)
     total.sulfur.dioxide < 50
                       < 0.0565 to the left, improve=3.398901, (0 missing)
                         < 3.265 to the left, improve=2.145792, (0 missing)
     рН
                         < 0.99757 to the right, improve=2.046632, (0 missing)
     density
 Surrogate splits:
     total.sulfur.dioxide < 20.5
                                   to the right, agree=0.644, adj=0.288, (0 split)
     volatile.acidity < 0.335 to the left, agree=0.619, adj=0.237, (0 split)
     free.sulfur.dioxide < 7.5 to the right, agree=0.619, adj=0.237, (0 split)
                         < 11.05 to the left, agree=0.619, adj=0.237, (0 split)
     alcohol
                         < 0.99491 to the right, agree=0.610, adj=0.220, (0 split)
     density
Node number 13: 136 observations
 predicted class=medium expected loss=0.09558824 P(node) =0.1063331
   class counts: 11
                        2 123
  probabilities: 0.081 0.015 0.904
Node number 14: 65 observations,
                                  complexity param=0.01144492
 predicted class=medium expected loss=0.2923077 P(node) =0.05082095
   class counts: 0
                        19
                             46
  probabilities: 0.000 0.292 0.708
  left son=28 (29 obs) right son=29 (36 obs)
 Primary splits:
     citric.acid
                        < 0.085 to the left, improve=7.047480, (0 missing)
```

```
рН
                      < 3.28 to the right, improve=4.936752, (0 missing)
                      < 7.65 to the left, improve=3.798438, (0 missing)
     fixed.acidity
 Surrogate splits:
     total.sulfur.dioxide < 34
                               to the left, agree=0.769, adj=0.483, (0 split)
     fixed.acidity < 7.65 to the left, agree=0.723, adj=0.379, (0 split)
     free.sulfur.dioxide < 6.5
                                to the left, agree=0.692, adj=0.310, (0 split)
                       < 3.38
     рΗ
                                 to the right, agree=0.692, adj=0.310, (0 split)
     density
                       < 0.99671 to the left, agree=0.662, adj=0.241, (0 split)
Node number 15: 759 observations
 predicted class=medium expected loss=0.07246377 P(node) =0.5934324
   class counts: 29 26 704
  probabilities: 0.038 0.034 0.928
Node number 18: 11 observations
 predicted class=high
                       expected loss=0.1818182 P(node) =0.008600469
                      0 2
   class counts: 9
  probabilities: 0.818 0.000 0.182
Node number 19: 16 observations
 predicted class=medium expected loss=0.25 P(node) =0.01250977
   class counts: 4
                       0 12
  probabilities: 0.250 0.000 0.750
Node number 20: 14 observations
 predicted class=high expected loss=0.1428571 P(node) =0.01094605
   class counts: 12
                      0
                             2
  probabilities: 0.857 0.000 0.143
Node number 21: 15 observations
 predicted class=medium expected loss=0.3333333 P(node) =0.01172791
   class counts: 4 1 10
  probabilities: 0.267 0.067 0.667
Node number 22: 9 observations
 predicted class=high expected loss=0.2222222 P(node) =0.007036747
                  7
                      0
   class counts:
  probabilities: 0.778 0.000 0.222
Node number 23: 74 observations
 predicted class=medium expected loss=0.1081081 P(node) =0.0578577
   class counts: 7 1
                           66
  probabilities: 0.095 0.014 0.892
Node number 24: 59 observations, complexity param=0.01287554
                       expected loss=0.4237288 P(node) =0.04612979
 predicted class=high
                        0 25
   class counts: 34
  probabilities: 0.576 0.000 0.424
 left son=48 (17 obs) right son=49 (42 obs)
 Primary splits:
     density
                       < 0.99757 to the right, improve=4.474624, (0 missing)
                                 to the left, improve=2.523763, (0 missing)
     chlorides
                       < 0.061
     total.sulfur.dioxide < 56.5
                                 to the left, improve=2.405533, (0 missing)
     sulphates
                   < 0.765 to the left, improve=1.651795, (0 missing)
     free.sulfur.dioxide < 21.5 to the left, improve=1.422582, (0 missing)
```

```
Surrogate splits:
                                   to the right, agree=0.847, adj=0.471, (0 split)
     residual.sugar
                        < 2.55
     fixed.acidity
                        < 9.95
                                   to the right, agree=0.814, adj=0.353, (0 split)
     citric.acid
                        < 0.575 to the right, agree=0.763, adj=0.176, (0 split)
     free.sulfur.dioxide < 7.5 to the left, agree=0.763, adj=0.176, (0 split)
                        < 0.745 to the left, agree=0.763, adj=0.176, (0 split)
     sulphates
Node number 25: 59 observations
 predicted class=medium expected loss=0.2881356 P(node) =0.04612979
   class counts: 15 2 42
  probabilities: 0.254 0.034 0.712
Node number 28: 29 observations,
                                  complexity param=0.01144492
 predicted class=low
                        expected loss=0.4482759 P(node) =0.02267396
   class counts:
                   0
                        16 13
  probabilities: 0.000 0.552 0.448
  left son=56 (16 obs) right son=57 (13 obs)
  Primary splits:
                                   to the right, improve=2.806366, (0 missing)
     citric.acid
                        < 0.015
     free.sulfur.dioxide < 5.5
                                   to the left, improve=1.881670, (0 missing)
                                  to the right, improve=1.609533, (0 missing)
     volatile.acidity < 0.97
                        < 10.95
                                   to the right, improve=1.333716, (0 missing)
     alcohol
                                   to the right, improve=1.244828, (0 missing)
     fixed.acidity
                        < 6.65
 Surrogate splits:
                                to the left, agree=0.690, adj=0.308, (0 split)
     chlorides
                     < 0.08
                     < 0.99558 to the right, agree=0.690, adj=0.308, (0 split)
     density
                     < 3.545 to the left, agree=0.690, adj=0.308, (0 split)
     fixed.acidity < 6.45
                               to the right, agree=0.655, adj=0.231, (0 split)
     volatile.acidity < 1.1375 to the left, agree=0.655, adj=0.231, (0 split)
Node number 29: 36 observations
 predicted class=medium expected loss=0.08333333 P(node) =0.02814699
   class counts:
                  0
                         3
  probabilities: 0.000 0.083 0.917
Node number 48: 17 observations
 predicted class=high
                        expected loss=0.1176471 P(node) =0.01329163
   class counts: 15
                        0
                               2
  probabilities: 0.882 0.000 0.118
Node number 49: 42 observations,
                                complexity param=0.01287554
 predicted class=medium expected loss=0.452381 P(node) =0.03283815
   class counts:
                   19
                          0
                             23
  probabilities: 0.452 0.000 0.548
  left son=98 (15 obs) right son=99 (27 obs)
  Primary splits:
                           to the left, improve=5.639153, (0 missing)
     density
                 < 0.9958
                           to the left, improve=3.530112, (0 missing)
     chlorides
                 < 0.061
     рН
                 < 3.39
                           to the right, improve=3.172024, (0 missing)
                          to the left, improve=2.742857, (0 missing)
     citric.acid < 0.47
               < 10.95 to the right, improve=2.484581, (0 missing)
 Surrogate splits:
                    < 7.25
     fixed.acidity
                                to the left, agree=0.738, adj=0.267, (0 split)
                                to the right, agree=0.738, adj=0.267, (0 split)
     volatile.acidity < 0.355
                  < 0.061 to the left, agree=0.738, adj=0.267, (0 split)
     chlorides
     На
                     < 3.2
                               to the left, agree=0.690, adj=0.133, (0 split)
                     < 10.95 to the right, agree=0.667, adj=0.067, (0 split)
     alcohol
```

```
Node number 56: 16 observations
 predicted class=low expected loss=0.25 P(node) =0.01250977
   class counts: 0 12 4
  probabilities: 0.000 0.750 0.250
Node number 57: 13 observations
 predicted class=medium expected loss=0.3076923 P(node) =0.01016419
   class counts: 0 4
  probabilities: 0.000 0.308 0.692
Node number 98: 15 observations
 predicted class=high expected loss=0.2 P(node) =0.01172791
   class counts: 12 0 3
  probabilities: 0.800 0.000 0.200
Node number 99: 27 observations
  predicted class=medium expected loss=0.2592593 P(node) =0.02111024
    class counts: 7 0 20
   probabilities: 0.259 0.000 0.741
```

It is more convenient to present this information by visualizing the tree. I used the uniform tree presentation and displayed all textual information on the tree:



Next step is to use the model to generate predictions on the testing dataset.

The classification table above shows that out of 320 test observation the model correctly predicted 17 high quality samples, and 255 medium quality samples. At the same time 18 high quality samples were classified as medium quality, 12 low quality samples were included in the medium category and 13 medium samples were classified as high quality, when 5 medium samples were included in the low-quality category.

A more detailed analysis of predictive performance of the classification model can be done using confusion matrix from the caret package:

```
> #generate confusion matrix using caret package
> confusionMatrix(table(predictions, redwine_test$quality))
Confusion Matrix and Statistics
predictions high low medium
    high
            17 0
                      13
    low
            0 0
                      5
    medium 18 12
                      255
Overall Statistics
             Accuracy: 0.85
               95% CI: (0.8061, 0.8873)
   No Information Rate: 0.8531
   P-Value [Acc > NIR] : 0.6004
                Kappa : 0.346
Mcnemar's Test P-Value : NA
Statistics by Class:
                   Class: high Class: low Class: medium
                     0.48571 0.00000 0.9341
Sensitivity
```

Specificity	0.95439	0.98377	0.3617
Pos Pred Value	0.56667	0.00000	0.8947
Neg Pred Value	0.93793	0.96190	0.4857
Prevalence	0.10938	0.03750	0.8531
Detection Rate	0.05312	0.00000	0.7969
Detection Prevalence	0.09375	0.01562	0.8906
Balanced Accuracy	0.72005	0.49188	0.6479

The above output shows that the overall accuracy of the model is 85%. At the same time the low wine quality category has the lowest balanced accuracy of 49% ((sensitivity + specificity)/2) compared to 72% for high quality wines and about 65% for medium quality wines.

One way to improve the classification model would be to prune the tree. However, previously plotcp(winequality\_rp) command demonstrated that the minimum error was obtained on the maximum size tree, so pruning based on minimum cross validation error will not work in this case.

In order to check, I proceeded to find the minimum cross-validation error:

```
> ###Pruning the tree
> #Find minimum cross-validation error
> min(winequality_rp$cptable[ ,"xerror"])
[1] 0.888412
```

And the record that had the minimum error:

```
> #Find the record with the minimum cross-validation error
> which.min(winequality_rp$cptable[ ,"xerror"])
6
```

I used the 6th record to estimate the cost complexity parameter and prune the tree based on it:

```
> #Get the cost complexity parameter of the record with min cross-validation error
> winequality_rp.cp <- winequality_rp$cptable[6, "CP"]
> #Prune the tree
> winequality_prune <- prune(winequality_rp, cp=winequality_rp.cp)</pre>
```

As the summary() command's sample output below shows, it resulted in the exactly the same

#### model:

```
> #Examine the pruned model
> summary(winequality_prune)
call:
rpart(formula = quality ~ ., data = redwine_train)
 n = 1279
         CP nsplit rel error
                                xerror
                                             xstd
1 0.07939914
                 0 1.0000000 1.0000000 0.05924512
2 0.02145923
                 2 0.8412017 0.9356223 0.05771580
3 0.01716738
                 5 0.7768240 0.9656652 0.05844137
4 0.01287554
                 7 0.7424893 0.9570815 0.05823622
                12 0.6480687 0.9012876 0.05686006
5 0.01144492
6 0.01000000
                15 0.6137339 0.8884120 0.05653161
Variable importance
            alcohol
                                                                  volatile.acidity free.sulfur.
                               sulphates
                                                       density
dioxide total.sulfur.dioxide
                                     citric.acid
                 23
                                      13
                                                            13
                                                                                11
                                         7
       fixed.acidity
                                chlorides
                                                            рН
                                                                     residual.sugar
Node number 1: 1279 observations,
                                    complexity param=0.07939914
  predicted class=medium expected loss=0.1821736 P(node) =1
                           51 1046
   class counts:
                   182
  probabilities: 0.142 0.040 0.818
  left son=2 (201 obs) right son=3 (1078 obs)
  Primary splits:
     alcohol
                      < 11.55
                                 to the right, improve=44.81302, (0 missing)
     sulphates
                      < 0.685
                                 to the right, improve=26.88087, (0 missing)
     volatile.acidity < 0.3625 to the left, improve=25.95614, (0 missing)
     citric.acid
                      < 0.315
                                 to the right, improve=20.18783, (0 missing)
                      < 0.99535 to the left, improve=19.75534, (0 missing)
     density
  Surrogate splits:
                          < 0.993785 to the left, agree=0.887, adj=0.279, (0 split)
     density
                          < 0.0525 to the left, agree=0.860, adj=0.109, (0 split)
     chlorides
                                     to the left, agree=0.856, adj=0.085, (0 split)
      fixed.acidity
                          < 5.55
                                     to the right, agree=0.850, adj=0.045, (0 split)
                          < 3.695
     total.sulfur.dioxide < 162.5
                                     to the right, agree=0.845, adj=0.015, (0 split)
Node number 2: 201 observations,
                                   complexity param=0.07939914
  predicted class=medium expected loss=0.4726368 P(node) =0.157154
   class counts:
                  93
                           2 106
   probabilities: 0.463 0.010 0.527
  left son=4 (89 obs) right son=5 (112 obs)
  Primary splits:
      sulphates
                      < 0.685
                                 to the right, improve=18.455050, (0 missing)
     рН
                      < 3.365
                                 to the left, improve= 9.083775, (0 missing)
     citric.acid
                      < 0.315
                                 to the right, improve= 7.901565, (0 missing)
                      < 7.85
     fixed.acidity
                                 to the right, improve= 7.333158, (0 missing)
     volatile.acidity < 0.335
                                 to the left, improve= 4.739165, (0 missing)
  Surrogate splits:
```

```
fixed.acidity < 8.05 to the right, agree=0.647, adj=0.202, (0 split) citric.acid < 0.325 to the right, agree=0.632, adj=0.169, (0 split) volatile.acidity < 0.345 to the left, agree=0.627, adj=0.157, (0 split) alcohol < 12.85 to the right, agree=0.612, adj=0.124, (0 split) total.sulfur.dioxide < 51 to the right, agree=0.607, adj=0.112, (0 split)
```

(the rest of the output is omitted for brevity)

Naturally, the tree visualization and confusion matrix resulted in the same output.

```
> #Visualize the prunned model
> #using the uniform tree presentation
> plot(winequality_prune, uniform = TRUE, branch = 0.6, margin = 0.1)
> text(winequality_prune, all=TRUE, use.n=TRUE)
> #Generate classification table
  predictions <- predict(winequality_prune, redwine_test, type = "class")
table(redwine_test$quality, predictions)</pre>
            predictions
             high low medium
17 0 18
                                18
12
   high
   low
                 0
                       0
   medium
                13
   #Grenrate confusion matrix
   confusionMatrix(table(predictions, redwine_test$quality))
Confusion Matrix and Statistics
predictions high low medium
       high
                                  13
                      0
       low
       medium
Overall Statistics
      Accuracy : 0.85
95% CI : (0.8061, 0.8873)
No Information Rate : 0.8531
P-Value [Acc > NIR] : 0.6004
 Kappa : 0.346
Mcnemar's Test P-Value : NA
Statistics by Class:
                              Class: high Class: low Class: medium 0.48571 0.00000 0.9341 0.95439 0.98377 0.3617
Sensitivity
Specificity
                                                    0.00000
Pos Pred Value
Neg Pred Value
                                    0.56667
                                                                          0.8947
                                    0.93793
                                                                          0.4857
                                                    0.96190
                                    0.10938
Prevalence
                                                    0.03750
                                                                          0.8531
Detection Rate
                                    0.05312
                                                    0.00000
                                                                          0.7969
Detection Prevalence
                                                    0.01562
                                    0.09375
                                                                          0.8906
Balanced Accuracy
                                    0.72005
                                                    0.49188
                                                                          0.6479
```

In an effort to improve the predictive power, I tried to use the random forest approach. I fit the random forest classifier with the training set using the randomForest() command and displayed its results:

```
> ######Random Forest###########
```

```
> winequality_rf <- randomForest(quality ~ ., data = redwine_train, importance = T)</pre>
> #display model details
> winequality_rf
Call:
randomForest(formula = quality ~ ., data = redwine_train, importance = T)
              Type of random forest: classification
                    Number of trees: 500
No. of variables tried at each split: 3
       OOB estimate of error rate: 13.29%
Confusion matrix:
      high low medium class.error
high
        99 0 83 0.45604396
        1 2
                  48 0.96078431
low
medium
        34 4
                 1008 0.03632887
```

The estimated error rate for the random forest model shows some improvement over the previously constructed recursive partitioning model. However, the real test is to use the model on the previously unseen data. So, I used this model to generate predictions on the testing data set

The classification table above shows that 24 high quality samples and 259 medium samples were classified correctly, when overall 37 samples (11+12+14) were misclassified (or 11.56% of the testing dataset).

The below output of the confusion matrix shows that the random forest model has an improved overall accuracy of 88.44% (compared to 85% for the recursive partitioning tree). The balanced accuracy also improved for all three classes, however it remains low for the low quality wines.

```
> #Confusion matrix
```

next:

# > confusionMatrix(table(predictions\_rf, redwine\_test\$quality))

Confusion Matrix and Statistics

Overall Statistics

Accuracy : 0.8844

95% CI: (0.8442, 0.9173)

No Information Rate : 0.8531 P-Value [Acc > NIR] : 0.06341

Kappa : 0.5084 Mcnemar's Test P-Value : NA

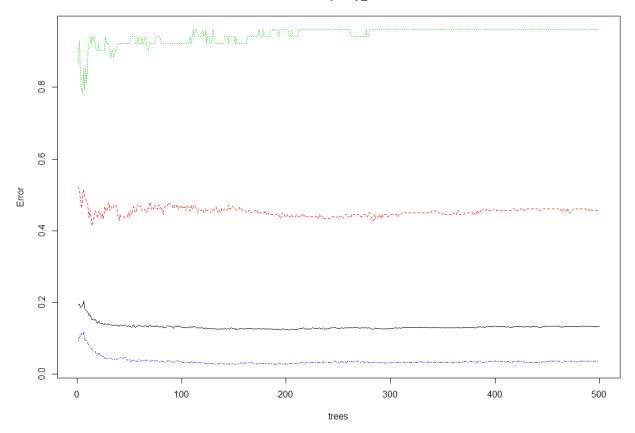
#### Statistics by Class:

	Class: high	class: low	Class: medium
Sensitivity	0.6857	0.0000	0.9487
Specificity	0.9509	1.0000	0.5106
Pos Pred Value	0.6316	Nan	0.9184
Neg Pred Value	0.9610	0.9625	0.6316
Prevalence	0.1094	0.0375	0.8531
Detection Rate	0.0750	0.0000	0.8094
Detection Prevalence	0.1187	0.0000	0.8812
Balanced Accuracy	0.8183	0.5000	0.7297

The mean square error of the forest object is plotted below:

- > #Plot the mean square error of the forest object
- > plot(winequality\_rf)





The randomForrest package allow us to analyze the most influential factors in the model using the importance() function:

# > #Examine importance of each attribute

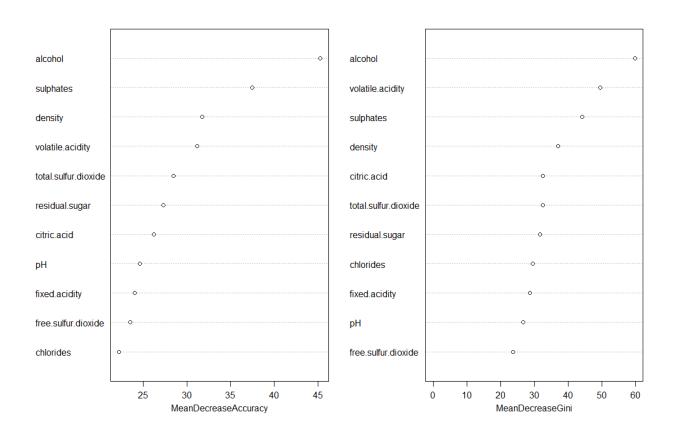
> importance(winequality\_rf)

	high	low	medium	MeanDecreaseAccuracy	MeanDecreaseGini
fixed.acidity	17.54848	-3.038072	18.67693	24.03245	28.55228
volatile.acidity	30.83032	19.299514	12.00160	31.16631	49.40767
citric.acid	22.00919	7.790991	15.85684	26.20611	32.51236
residual.sugar	19.42921	3.930668	21.47767	27.31235	31.62724
chlorides	13.77201	-3.212559	19.14726	22.21225	29.50768
free.sulfur.dioxide	13.79151	3.297954	19.71502	23.52889	23.60979
total.sulfur.dioxide	24.62445	5.058901	21.10894	28.49398	32.43242
density	23.29300	-2.489272	26.05187	31.76683	36.92529
рН	17.51735	4.519130	18.66730	24.59749	26.68204
sulphates	42.25236	8.857301	17.37636	37.48310	44.07924
alcohol	45.45322	3.330081	27.25061	45.30108	59.74893

The top three most important for classification attributes are alcohol, volatile.acidity and sulphates as they have the highest mean decrease in Gini index. The variables' importance can be presented visually using varImpPlot() function:

- > #Plot varaible importance
- > varImpPlot(winequality\_rf)

### winequality\_rf

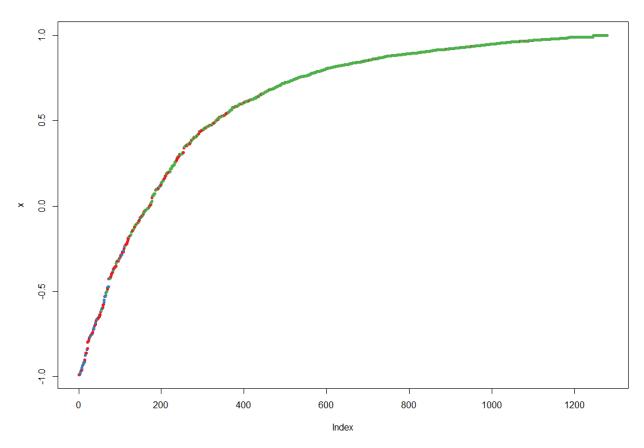


In order to assess certainty of the classification, we should look at the margins, which are calculated as the difference between the support of the correct class and the maximum support for the incorrect class. Correctly classified examples have positive margins and incorrectly classified examples have negative margins. The closer the margin is to one, the higher the degree of confidence for the classification. Low margins imply uncertain classification.

```
> #calculate margins and plot the margin cumulative distribution
```

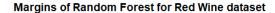
<sup>&</sup>gt; margins\_rf <- margin(winequality\_rf, redwine\_train)</pre>

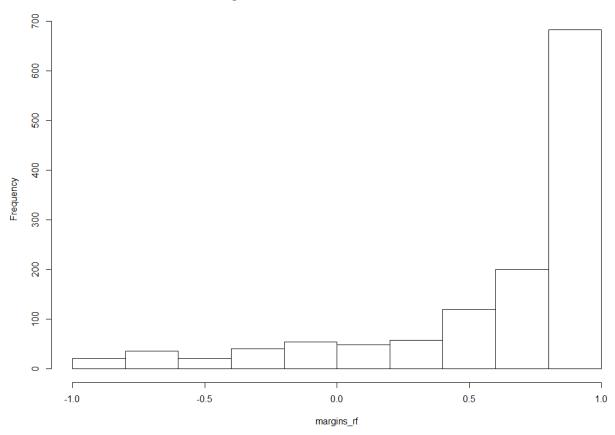
<sup>&</sup>gt; plot(margins\_rf)



The above plot shows, for about of 400 training observations out of 1279 the margin was below 0.5 suggesting uncertain classifications. The histogram of margin distributions confirms that only about 700 training observations were classified reliably.

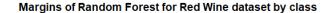
- > #Visualize margin distribution
- > hist(margins\_rf, main="Margins of Random Forest for Red Wine dataset")

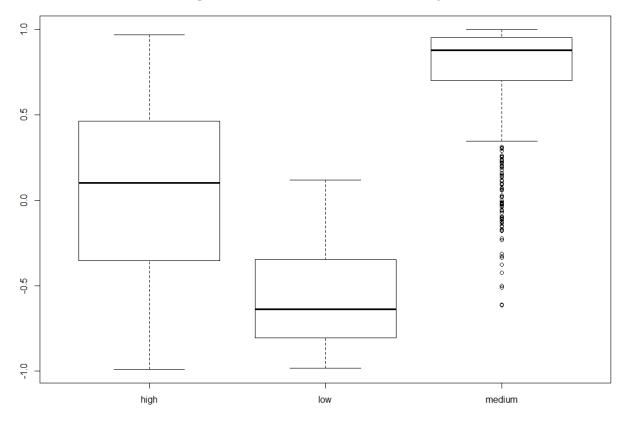




Visualizing margin by class of wine quality (see below) shows that the medium wine quality group had the margins closest to 1, but at the same time it had the highest number of outliers (in this case samples that could not be classified reliably). The low wine quality group had the lowest margins, followed by the high wine quality group.

```
> #Visualize margins by class
> boxplot(margins_rf ~ redwine_train$quality, main = "Margins of Random Forest for Red Wine datas
et by class")
```





Overall, the random forest classifier yielded more accurate predictions compared to the recursive partitioning tree. However, the predictive accuracy remained lower for the two extreme classes – low and high quality wines. It can partially be explained by how the quality ratings were collected for the data set as a median of at least three subjective evaluations made by wine experts. As a result, the ratings show evidence of an extremity avoidance bias, when a medium quality classification becomes a de-facto default classification.

In order to further improve the predictive power of the model, since no additional samples (observations) for the two extreme classes are available, it might be necessary to focus on the most important attributes for those classes separately. It might happen that the attributes that were not significant for the model as a whole might have more relative significance for the extreme classes. In this case, they need to intentionally be included in the model. In addition, fine tuning the parameters for the random forest algorithm (ex., number of trees, depth of trees and the number of features used for a split) can also be helpful.