Predicting Wine Quality

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Problem: Predict wine quality using Multiclass Classification analysis.The data contains quality ratings for a few thousands of wines (1599 red wine samples), along with their physical and chemical properties (11 predictors). We want to use these properties to predict a rating for a wine. The goal is to model wine quality based on physicochemical tests.

(**data from** https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv (https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv))
Azure ML experiment at https://gallery.cortanaintelligence.com/Experiment/Predict-Wine-Quality-Classification-10 (https://gallery.cortanaintelligence.com/Experiment/Predict-Wine-Quality-Classification-10)

In [107]:
```
#download data from
#https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.dat
a
data_wine = read.table("https://archive.ics.uci.edu/ml/machine-learning-
databases/wine-quality/winequality-red.csv",
                       header=T,sep=";",na.strings="NA") #1599 12
class(data_wine)  #"data.frame"

#Relabel quality ratings as follows
#3,4,5 as Low
#6 as Med
#7,8 as High

data_wine$qualityV2 = ifelse(data_wine$quality <=5, 'Low','None')
TorF = data_wine$quality == 6
data_wine$qualityV2[TorF] = 'Med'
TorF = data_wine$quality > 6
data_wine$qualityV2[TorF] = 'High'

data_wine$quality = NULL
names(data_wine)[names(data_wine)=='qualityV2'] = 'quality'

#convert data frame to xdf object using rxDataStep()
pathc     = getwd()
dataclassi_xdf = file.path(pathc,'dataclassi_xdf.xdf')
data_classi = rxDataStep(inData = data_wine, outFile = dataclassi_xdf ,
                       rowsPerRead=500, overwrite=TRUE, reportProgress=
0)
class(data_classi)  # "RxXdfData"
```

Out[107]: "data.frame"

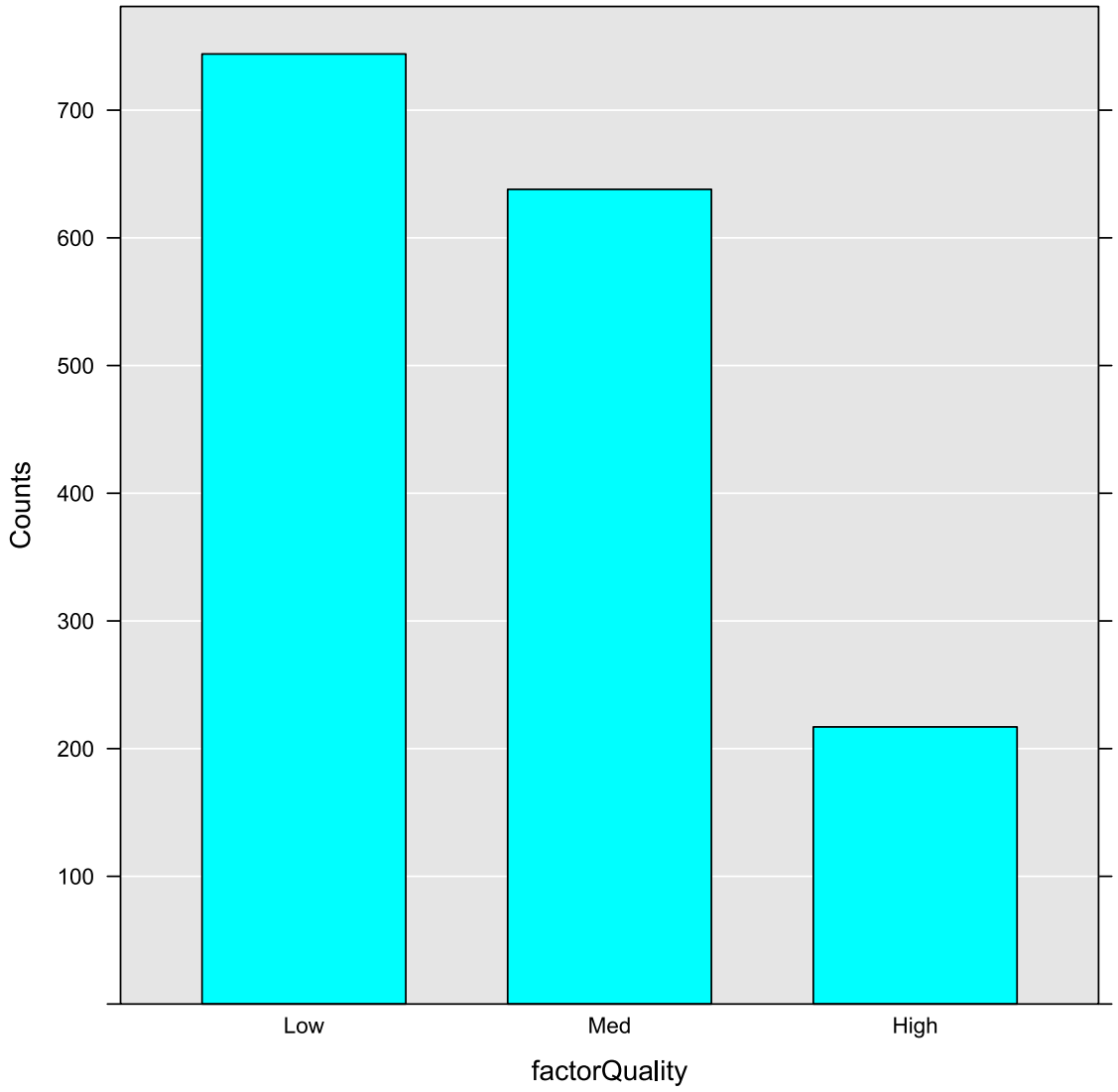
Out[107]: "RxXdfData"

In [111]:
```
#make a new column factorQuality from quality col -- make it categorical
rxFactors(inData = data_classi, outFile = data_classi, overwrite = TRUE,
          factorInfo = list(factorQuality = list(varName = "quality")),
reportProgress=0)

#can remove the col quality now
ColsToKeep = setdiff(names(data_classi),c('quality'))

data_classi = rxDataStep(inData = data_classi, outFile = 'data_classi_te
mp.xdf',varsToKeep = ColsToKeep, overwrite = TRUE, reportProgress=0)
```

Data Exploration

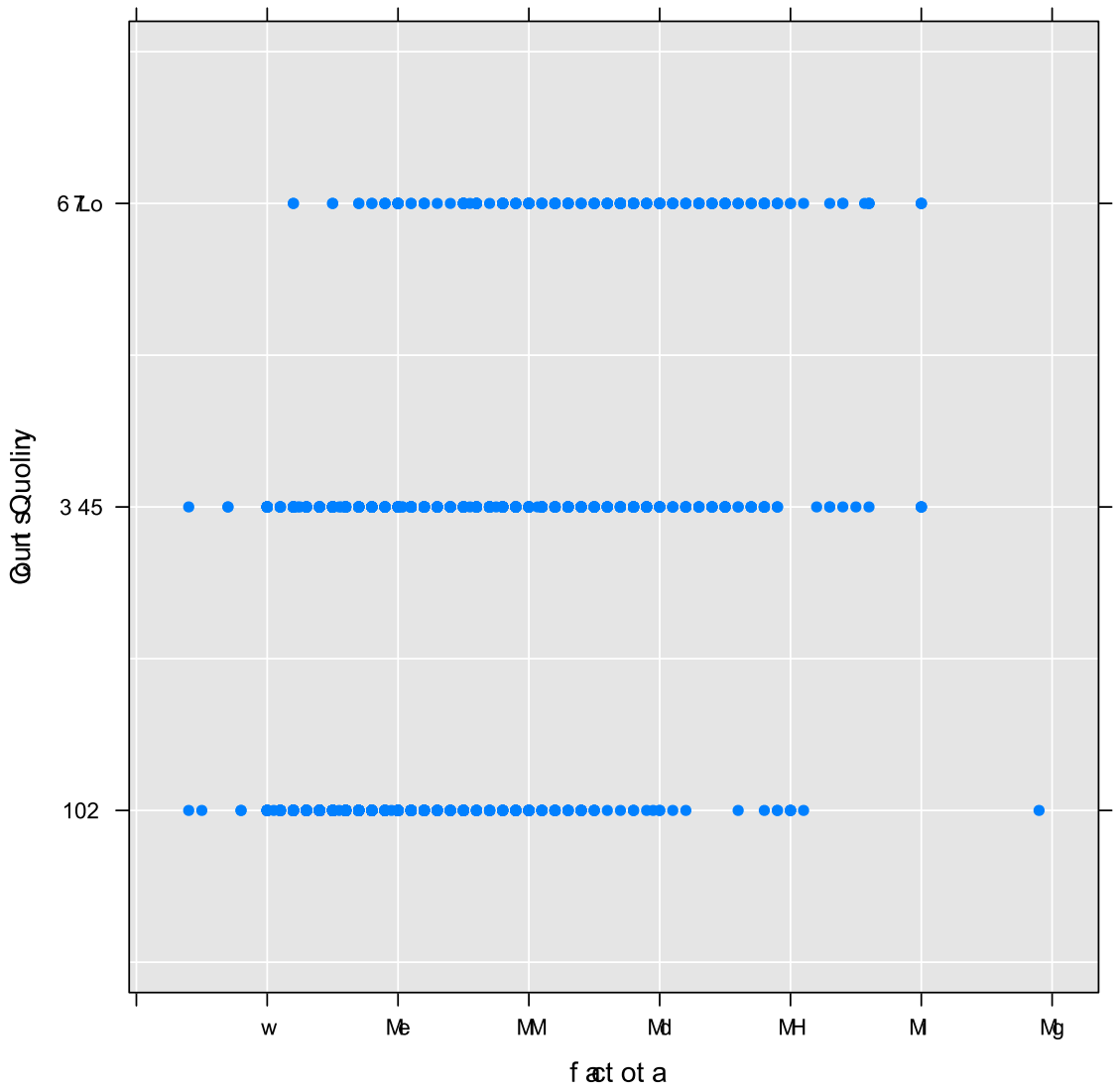
In [113]:
```
cat("Data distribution \n")
rxHistogram(formula = ~ factorQuality, data = data_classi)
```

```
Data distribution
Rows Read: 500, Total Rows Processed: 500, Total Chunk Time: 0.001 seco
nds
Rows Read: 500, Total Rows Processed: 1000, Total Chunk Time: Less than
.001 seconds
Rows Read: 500, Total Rows Processed: 1500, Total Chunk Time: Less than
.001 seconds
Rows Read: 99, Total Rows Processed: 1599, Total Chunk Time: Less than
.001 seconds
Computation time: 0.005 seconds.
```



In [115]:
```
cat("A line plot \n")
rxLinePlot(factorQuality ~ alcohol, type = "p", data = data_classi)
```

```
A line plot
Rows Read: 500, Total Rows Processed: 500, Total Chunk Time: 0.002 se
conds
Rows Read: 500, Total Rows Processed: 1000, Total Chunk Time: Less th
an .001 seconds
Rows Read: 500, Total Rows Processed: 1500, Total Chunk Time: 0.001 s
econds
Rows Read: 99, Total Rows Processed: 1599, Total Chunk Time: Less tha
n .001 seconds
```



In [87]:
```
#rename the label col 'factorQuality' as 'LabelsCol'
names(data_classi)[names(data_classi)=='factorQuality'] = 'LabelsCol'
names(data_classi)
```

Out[87]:
```
"fixed.acidity"    "volatile.acidity"    "citric.acid"    "residual.sugar"    "chlorides"
"free.sulfur.dioxide"    "total.sulfur.dioxide"    "density"    "pH"    "sulphates"
"alcohol"    "LabelsCol"
```

In [88]:
```
#use rxDataStep() to create a col called 'splitcol' to use for splitting
rxDataStep(inData=data_classi,outFile=data_classi,transforms=list(splitc
ol=factor(rbinom(.rxNumRows,1,0.8),labels=c('test','train'))),
           overwrite=T, reportProgress=0)
names(data_classi)

#split using the col "splitcol"
#rxSplit() -- Splits an input '.xdf' file or data frame into multiple '.
xdf' files or a list of data frames.
listofxdfs = rxSplit(data_classi,outFileBase='data_classi_split',outFile
Suffixes=c("Train", "Test"),splitByFactor = "splitcol",
                     overwrite=T, reportProgress=0 )

trainingdata = listofxdfs[[2]]
testdata = listofxdfs[[1]]
dim(trainingdata)
dim(testdata)
dim(data_classi)
```

Out[88]:
```
"fixed.acidity"    "volatile.acidity"    "citric.acid"    "residual.sugar"    "chlorides"
"free.sulfur.dioxide"    "total.sulfur.dioxide"    "density"    "pH"    "sulphates"
"alcohol"    "LabelsCol"    "splitcol"
```

Out[88]:
```
1250  13
```

Out[88]:
```
349  13
```

Out[88]:
```
1599  13
```

In [89]:
```
#collect names of columns (features) to be used for modelling
allfeatures = setdiff(names(data_classi),c('LabelsCol','splitcol'))

#create formula for modelling
formula = as.formula(paste('LabelsCol',paste(allfeatures,collapse=' +
'),sep=' ~ '))
formula
```

Out[89]:
```
LabelsCol ~ fixed.acidity + volatile.acidity + citric.acid +
    residual.sugar + chlorides + free.sulfur.dioxide + total.sulfur.dio
xide +
    density + pH + sulphates + alcohol
```

In [90]:
```
Algorithms <- c("Decision Forest Classification",
                "Boosted Decision Tree Classification",
                "Decision Tree Classification")
```

In [91]:
```
##########################################################################
########
## Decision forest modeling
##########################################################################
########
#Decision Forest
#using rxDForest() to build ML model
DForest_model <- rxDForest(formula = formula,
                           data = trainingdata,
                           seed = 10,
                           cp = 0.01,
                           nTree = 50,
                           mTry = 2,
                           overwrite = TRUE,
                           reportProgress = 0)
DForest_model
class(DForest_model) #"rxDForest"
```

Out[91]:
```
Call:
rxDForest(formula = formula, data = trainingdata, overwrite = TRUE,
    cp = 0.01, nTree = 50, mTry = 2, seed = 10, reportProgress = 0)


             Type of decision forest: class
                    Number of trees: 50
No. of variables tried at each split: 2

         OOB estimate of error rate: 38.16%
Confusion matrix:
         Predicted
LabelsCol Low Med High class.error
     Low  439 144    1   0.2482877
     Med  183 304    7   0.3846154
     High  11 131   30   0.8255814
```

Out[91]: "rxDForest"

In [92]:
```
################################################################################
########
## Boosted tree modeling
################################################################################
########
BoostedTree_model = rxBTrees(formula = formula,
                             data = trainingdata,
                             learningRate = 0.2,
                             minSplit = 10,
                             minBucket = 10,
                             nTree = 100,
                             lossFunction = "multinomial",
                             reportProgress = 0)
BoostedTree_model
class(BoostedTree_model)
```

Out[92]:
```
Call:
rxBTrees(formula = formula, data = trainingdata, minSplit = 10,
    minBucket = 10, nTree = 100, lossFunction = "multinomial",
    learningRate = 0.2, reportProgress = 0)


      Loss function of boosted trees: multinomial
       Number of boosting iterations: 100
No. of variables tried at each split: 3

            OOB estimate of deviance: 0.6543003
```

Out[92]: "rxBTrees" "rxDForest"

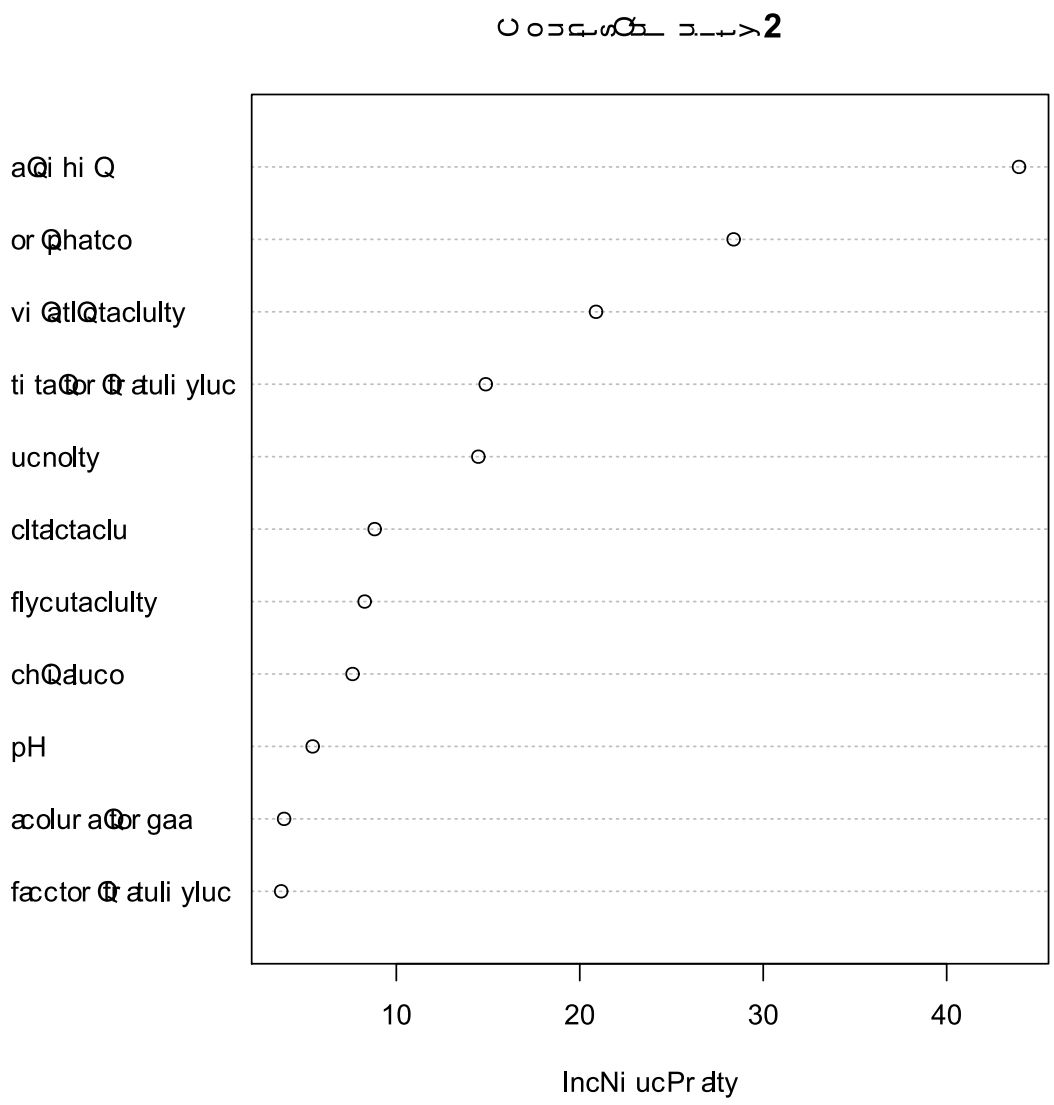
In [93]:
```
################################################################################
########
## Decision Tree Modelling
################################################################################
########

#rxDTree
DTree_model = rxDTree(formula = formula,
                          data = trainingdata,
                          minSplit = 10,
                          minBucket = 10,
                          nTree = 100,
                          reportProgress = 0)
DTree_model
class(DTree_model)
```

Out[93]:
```
Call:
rxDTree(formula = formula, data = trainingdata, minSplit = 10,
    minBucket = 10, reportProgress = 0, nTree = 100)


             Type of decision forest: class
                    Number of trees: 100
No. of variables tried at each split: 0
```

Out[93]: "rxDForest"

In [106]:
```
#For feature importance plot we must have importance = TRUE
DForest_model2 <- rxDForest(formula = formula,
                            data = trainingdata,
                            seed = 10,
                            cp = 0.01,
                            nTree = 50,
                            mTry = 2,
                            importance = TRUE,
                            overwrite = TRUE,
                            reportProgress = 0)
class(DForest_model2) #"rxDForest"

#Feature Importance plot
rxVarImpPlot(DForest_model2)
```

```
Out[106]: "rxDForest"
```



In [96]:
```
#Function to compute accuracy of the trained model on the given data
computeaccuracy <- function(ML_model,scoredata){
  if(file.exists("modelout_xdf.xdf") ) {  file.remove("modelout_xdf.xd
f") }
  modelout_xdf = RxXdfData("modelout_xdf.xdf") #initialise xdf object
  rxPredict(ML_model, data = scoredata, outData = modelout_xdf, overwrit
e = TRUE,
            writeModelVars = TRUE, reportProgress = 0)
  #head(modelout_xdf)  #contains the actual and predicted cols

  #get the columns "LabelsCol_Pred" and "LabelsCol" from modelout_xdf


  mytemp_xdf = RxXdfData("mytemp_xdf.xdf") #initialise an xdf object
  results_model = rxDataStep(inData = modelout_xdf, outFile = mytemp_xd
f,varsToKeep = c('LabelsCol_Pred','LabelsCol'),
                             overwrite = TRUE, reportProgress = 0 )

  cm = rxCrossTabs(~LabelsCol_Pred:LabelsCol,results_model,returnXtabs =
T, reportProgress=0) #create a confusion matrix
  cm
  accuracy = sum(diag(cm)) / sum(cm)
  accuracy

  #cat('The model produced an accuracy = ',accuracy,'\n')
  return(accuracy)
}
# to invoke function:
# computeaccuracy(ML_model,testdata)
# computeaccuracy(ML_model,trainingdata)
# where
# ML_model = DForest_model
# ML_model = BoostedTree_model
# ML_model = DTree_model
```

In [97]:
```
#=====================================================

ML_model = DForest_model

cat('For Decision Forest: accuracy = ',computeaccuracy(ML_model,training
data),'\n')
cat('For Decision Forest: accuracy on test data = ',computeaccuracy(ML_m
odel,testdata),'\n')
#=====================================================
ML_model = BoostedTree_model

cat('For Boosted tree: accuracy = ',computeaccuracy(ML_model,trainingdat
a),'\n')
cat('For Boosted tree: accuracy on test data = ',computeaccuracy(ML_mode
l,testdata),'\n')
#=====================================================
ML_model = DTree_model

cat('For Decision Tree: accuracy = ',computeaccuracy(ML_model,trainingda
ta),'\n')
cat('For Decision Tree: accuracy on test data = ',computeaccuracy(ML_mod
el,testdata),'\n')
```

```
For Decision Forest: accuracy =  0.6712
For Decision Forest: accuracy on test data =  0.6418338
For Boosted tree: accuracy =  0.7216
For Boosted tree: accuracy on test data =  0.6561605
For Decision Tree: accuracy =  0.7624
For Decision Tree: accuracy on test data =  0.5644699
```