CMTH 642 Data Analytics: Advanced Methods

Assignment 3 (10%)

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```
# INSERT YOUR CODE HERE.
wine <- read.csv("http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-whi
```

1. Import to R the following fiel: http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white.csv (The dataset is related to white Portuguese "Vinho Verde" wine. For more info: https://archive.ics.uci.edu/ml/datasets/Wine+Quality) (3 points)

```
# INSERT YOUR CODE HERE.
str(wine)
```

2. Check the datatypes of the attributes. (3 points)

```
## 'data.frame':    4898 obs. of  12 variables:
##  $ fixed.acidity       : num  7 6.3 8.1 7.2 7.2 8.1 6.2 7 6.3 8.1 ...
##  $ volatile.acidity    : num  0.27 0.3 0.28 0.23 0.23 0.28 0.32 0.27 0.3 0.22 ...
##  $ citric.acid         : num  0.36 0.34 0.4 0.32 0.32 0.4 0.16 0.36 0.34 0.43 ...
##  $ residual.sugar      : num  20.7 1.6 6.9 8.5 8.5 6.9 7 20.7 1.6 1.5 ...
##  $ chlorides           : num  0.045 0.049 0.05 0.058 0.058 0.05 0.045 0.045 0.049 0.044 ...
##  $ free.sulfur.dioxide : num  45 14 30 47 47 30 30 45 14 28 ...
##  $ total.sulfur.dioxide: num  170 132 97 186 186 97 136 170 132 129 ...
##  $ density             : num  1.001 0.994 0.995 0.996 0.996 ...
##  $ pH                  : num  3 3.3 3.26 3.19 3.19 3.26 3.18 3 3.3 3.22 ...
##  $ sulphates           : num  0.45 0.49 0.44 0.4 0.4 0.44 0.47 0.45 0.49 0.45 ...
##  $ alcohol             : num  8.8 9.5 10.1 9.9 9.9 10.1 9.6 8.8 9.5 11 ...
##  $ quality             : int  6 6 6 6 6 6 6 6 6 6 ...
```

```
summary(wine)
```

```
##  fixed.acidity    volatile.acidity  citric.acid     residual.sugar
##  Min.   : 3.800   Min.   :0.0800   Min.   :0.0000   Min.   : 0.600
##  1st Qu.: 6.300   1st Qu.:0.2100   1st Qu.:0.2700   1st Qu.: 1.700
##  Median : 6.800   Median :0.2600   Median :0.3200   Median : 5.200  
##  Mean   : 6.855   Mean   :0.2782   Mean   :0.3342   Mean   : 6.391  
##  3rd Qu.: 7.300   3rd Qu.:0.3200   3rd Qu.:0.3900   3rd Qu.: 9.900  
##  Max.   :14.200   Max.   :1.1000   Max.   :1.6600   Max.   :65.800  
##    chlorides       free.sulfur.dioxide total.sulfur.dioxide    density      
##  Min.   :0.00900   Min.   :  2.00      Min.   :  9.0        Min.   :0.9871  
##  1st Qu.:0.03600   1st Qu.: 23.00      1st Qu.:108.0        1st Qu.:0.9917  
##  Median :0.04300   Median : 34.00      Median :134.0        Median :0.9937  
##  Mean   :0.04577   Mean   : 35.31      Mean   :138.4        Mean   :0.9940  
##  3rd Qu.:0.05000   3rd Qu.: 46.00      3rd Qu.:167.0        3rd Qu.:0.9961  
##  Max.   :0.34600   Max.   :289.00      Max.   :440.0        Max.   :1.0390  
##        pH          sulphates         alcohol         quality     
##  Min.   :2.720   Min.   :0.2200   Min.   : 8.00   Min.   :3.000  
##  1st Qu.:3.090   1st Qu.:0.4100   1st Qu.: 9.50   1st Qu.:5.000  
##  Median :3.180   Median :0.4700   Median :10.40   Median :6.000  
##  Mean   :3.188   Mean   :0.4898   Mean   :10.51   Mean   :5.878  
##  3rd Qu.:3.280   3rd Qu.:0.5500   3rd Qu.:11.40   3rd Qu.:6.000  
##  Max.   :3.820   Max.   :1.0800   Max.   :14.20   Max.   :9.000
```

```r
# INSERT YOUR CODE HERE.
sum(is.na(wine))
```

3. Are there any missing values in the dataset? (4 points)

```
## [1] 0
```

```r
# no missing data
```

```r
# INSERT YOUR CODE HERE.
wineNoEquality <- wine[, -grep("quality", names(wine))]
winecor <- cor(wineNoEquality)
winecor
```

4. What is the correlation between the attributes other than Quality? (10 points)

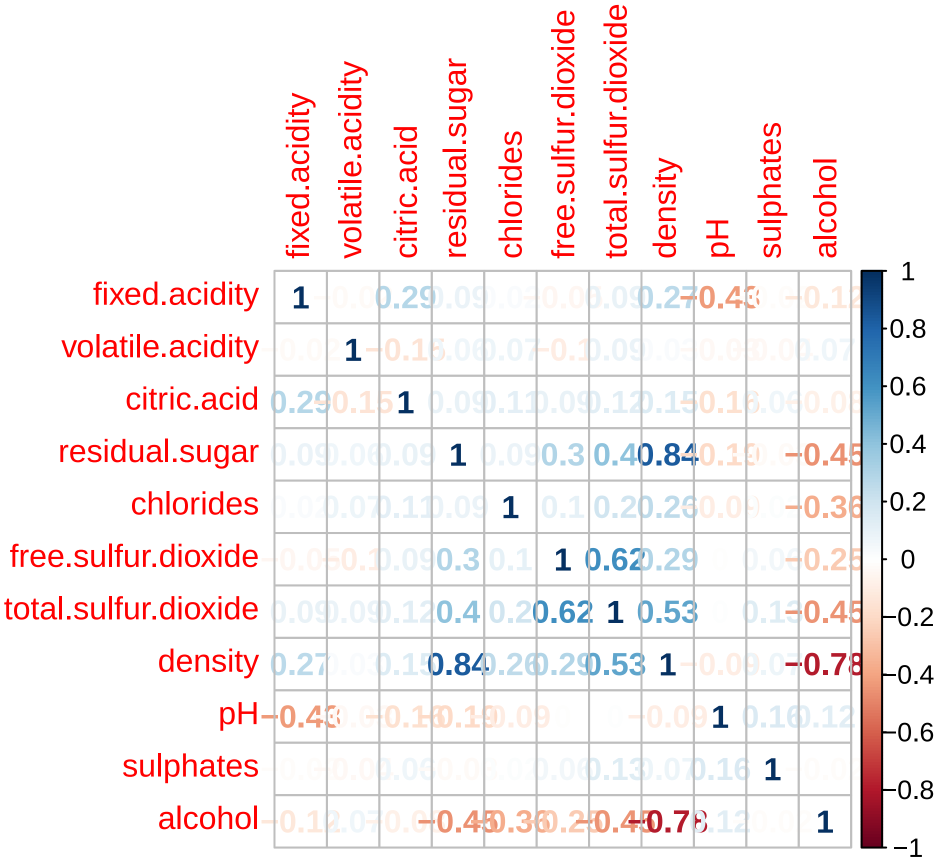
```
##                      fixed.acidity volatile.acidity citric.acid residual.sugar
## fixed.acidity           1.00000000      -0.02269729  0.28918070     0.08902070
## volatile.acidity       -0.02269729       1.00000000 -0.14947181     0.06428606
## citric.acid             0.28918070      -0.14947181  1.00000000     0.09421162
## residual.sugar          0.08902070       0.06428606  0.09421162     1.00000000
## chlorides               0.02308564       0.07051157  0.11436445     0.08868454
## free.sulfur.dioxide    -0.04939586      -0.09701194  0.09407722     0.29909835
## total.sulfur.dioxide    0.09106976       0.08926050  0.12113080     0.40143931
## density                 0.26533101       0.02711385  0.14950257     0.83896645
## pH                     -0.42585829      -0.03191537 -0.16374821    -0.19413345
## sulphates              -0.01714299      -0.03572815  0.06233094    -0.02666437
## alcohol                -0.12088112       0.06771794 -0.07572873    -0.45063122
##                          chlorides free.sulfur.dioxide total.sulfur.dioxide
## fixed.acidity          0.02308564       -0.0493958591          0.091069756
## volatile.acidity       0.07051157       -0.0970119393          0.089260504
## citric.acid            0.11436445        0.0940772210          0.121130798
## residual.sugar         0.08868454        0.2990983537          0.401439311
## chlorides              1.00000000        0.1013923521          0.198910300
## free.sulfur.dioxide    0.10139235        1.0000000000          0.615500965
## total.sulfur.dioxide   0.19891030        0.6155009650          1.000000000
## density                0.25721132        0.2942104109          0.529881324
## pH                    -0.09043946       -0.0006177961          0.002320972
## sulphates              0.01676288        0.0592172458          0.134562367
## alcohol               -0.36018871       -0.2501039415         -0.448892102
##                            density            pH   sulphates     alcohol
## fixed.acidity          0.26533101 -0.4258582910 -0.01714299 -0.12088112
## volatile.acidity       0.02711385 -0.0319153683 -0.03572815  0.06771794
## citric.acid            0.14950257 -0.1637482114  0.06233094 -0.07572873
## residual.sugar         0.83896645 -0.1941334540 -0.02666437 -0.45063122
## chlorides              0.25721132 -0.0904394560  0.01676288 -0.36018871
## free.sulfur.dioxide    0.29421041 -0.0006177961  0.05921725 -0.25010394
## total.sulfur.dioxide   0.52988132  0.0023209718  0.13456237 -0.44889210
## density                1.00000000 -0.0935914935  0.07449315 -0.78013762
## pH                    -0.09359149  1.0000000000  0.15595150  0.12143210
## sulphates              0.07449315  0.1559514973  1.00000000 -0.01743277
## alcohol               -0.78013762  0.1214320987 -0.01743277  1.00000000
```

```r
#install.packages("corrplot")
library(corrplot)
```

```
## Warning: package 'corrplot' was built under R version 4.0.2
```

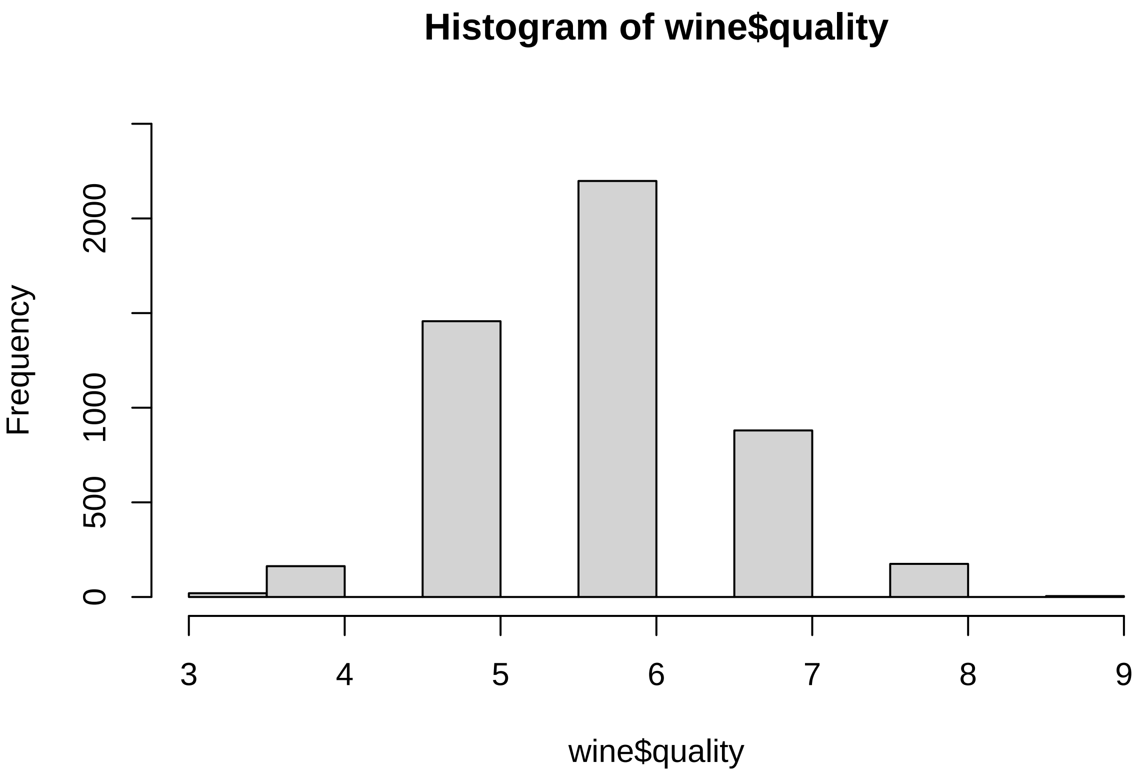
```
## corrplot 0.84 loaded
```

```r
corrplot(winecor, method="number")
```



```
# INSERT YOUR CODE
hist(wine$quality, ylim=c(0, 2500))
```

5. Graph the frequency distribution of wine quality by using Quality. (10 points)



```
# INSERT YOUR CODE HERE.
wine$quality <- sapply(wine$quality, function(x) {
  if (x < 5) {
    return("low")
  } else if (x < 7) {
    return("medium")
  } else {
    return("high")
  }
})
wine$quality <- as.factor(wine$quality)
round(prop.table(table(wine$quality)) * 100, digits = 1)
```

6. Reduce the levels of rating for quality to three levels as high, medium and low. Assign the levels of 3 and 4 to level 0; 5 and 6 to level 1; and 7,8 and 9 to level 2. (10 points)

```
##
##   high    low medium
##   21.6    3.7   74.6
```

```
normalize <- function(x){
  return ((x - min(x)) / (max(x) - min(x)))
}
```

```
# INSERT YOUR CODE HERE.
wine[1:11] <- sapply(wine[1:11], normalize)
summary(wine)
```

7. Normalize the data set by using the following function: (12 points)

```
##  fixed.acidity    volatile.acidity  citric.acid     residual.sugar
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000   Min.   :0.00000
##  1st Qu.:0.2404   1st Qu.:0.1275   1st Qu.:0.1627   1st Qu.:0.01687
##  Median :0.2885   Median :0.1765   Median :0.1928   Median :0.07055
##  Mean   :0.2937   Mean   :0.1944   Mean   :0.2013   Mean   :0.08883
##  3rd Qu.:0.3365   3rd Qu.:0.2353   3rd Qu.:0.2349   3rd Qu.:0.14264
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000   Max.   :1.00000
##    chlorides        free.sulfur.dioxide total.sulfur.dioxide    density
##  Min.   :0.00000   Min.   :0.00000     Min.   :0.0000       Min.   :0.00000
##  1st Qu.:0.08012   1st Qu.:0.07317     1st Qu.:0.2297       1st Qu.:0.08892
##  Median :0.10089   Median :0.11150     Median :0.2900       Median :0.12782
##  Mean   :0.10912   Mean   :0.11606     Mean   :0.3001       Mean   :0.13336
##  3rd Qu.:0.12166   3rd Qu.:0.15331     3rd Qu.:0.3666       3rd Qu.:0.17332
##  Max.   :1.00000   Max.   :1.00000     Max.   :1.0000       Max.   :1.00000
##        pH           sulphates         alcohol          quality
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000   high  :1060
##  1st Qu.:0.3364   1st Qu.:0.2209   1st Qu.:0.2419   low   : 183
##  Median :0.4182   Median :0.2907   Median :0.3871   medium:3655
##  Mean   :0.4257   Mean   :0.3138   Mean   :0.4055
##  3rd Qu.:0.5091   3rd Qu.:0.3837   3rd Qu.:0.5484
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000
```

```
# INSERT YOUR CODE HERE.
set.seed(1)
train_index <- sample(1:nrow(wine), 0.7 * nrow(wine))
train.set <- wine[train_index,]
test.set <- wine[-train_index,]
```

8. Divide the dataset to training and test sets. (12 points)

```
# INSERT YOUR CODE HERE.
library("class")
library("gmodels")
```

9. Use the KNN algorithm to predict the quality of wine using its attributes. (12 points)

```
## Warning: package 'gmodels' was built under R version 4.0.2
```

```
train.set_new <- train.set[,-grep("quality", names(wine))]
test.set_new <- test.set[, -grep("quality", names(wine))]
wine_train_labels <- train.set$quality
wine_test_labels <- test.set$quality
wine_knn_prediction <- knn(train = train.set_new, test = test.set_new, cl= wine_train_labels, k = 3)
head(wine_knn_prediction)
```

```
## [1] medium medium medium medium medium medium
## Levels: high low medium
```

```
summary(wine_knn_prediction)
```

```
##   high    low medium
##    290     22   1158
```

```


# INSERT YOUR CODE HERE.
ConfusionMatrix <- table(actual =wine_test_labels, predicted = wine_knn_prediction)
ConfusionMatrix
```

10. Display the confusion matrix to evaluate the model performance. (12 points)

```
##         predicted
## actual   high low medium
##   high    175   1    147
##   low       6   3     34
##   medium  109  18    977
```

```
CrossTable(x=wine_test_labels, y=wine_knn_prediction, prop.chisq=FALSE)
```

```
##
##
##    Cell Contents
## |-------------------------|
## |                       N |
## |           N / Row Total |
## |           N / Col Total |
## |         N / Table Total |
## |-------------------------|
##
##
## Total Observations in Table:  1470
##
##
##                  | wine_knn_prediction
## wine_test_labels |      high |       low |    medium | Row Total |
## ------------------|-----------|-----------|-----------|-----------|
##             high |       175 |         1 |       147 |       323 |
##                  |     0.542 |     0.003 |     0.455 |     0.220 |
##                  |     0.603 |     0.045 |     0.127 |           |
##                  |     0.119 |     0.001 |     0.100 |           |
## ------------------|-----------|-----------|-----------|-----------|
##              low |         6 |         3 |        34 |        43 |
##                  |     0.140 |     0.070 |     0.791 |     0.029 |
##                  |     0.021 |     0.136 |     0.029 |           |
##                  |     0.004 |     0.002 |     0.023 |           |
## ------------------|-----------|-----------|-----------|-----------|
##           medium |       109 |        18 |       977 |      1104 |
##                  |     0.099 |     0.016 |     0.885 |     0.751 |
##                  |     0.376 |     0.818 |     0.844 |           |
##                  |     0.074 |     0.012 |     0.665 |           |
## ------------------|-----------|-----------|-----------|-----------|
##     Column Total |       290 |        22 |      1158 |      1470 |
##                  |     0.197 |     0.015 |     0.788 |           |
## ------------------|-----------|-----------|-----------|-----------|
##
##
```

```
# INSERT YOUR CODE HERE.
ConfusionMatrix
```

11. Evaluate the model performance by computing Accuracy, Sensitivity and Specificity. (12 points)

```
##         predicted
## actual   high low medium
##   high    175   1    147
##   low       6   3     34
##   medium  109  18    977
```

```
sum(diag(ConfusionMatrix))/nrow(test.set)
```

```
## [1] 0.7857143
```

```
#Sensitivity = TP/(TP+FN)
(ConfusionMatrix[2,2]+ConfusionMatrix[2,3]+ConfusionMatrix[3,2]+ConfusionMatrix[3,3])/(ConfusionMatrix[
```

```
## [1] 0.8997384
```

```
#Specificity = TN / (FP + TN)
ConfusionMatrix[1,1]/(ConfusionMatrix[1,1]+ConfusionMatrix[1,2]+ConfusionMatrix[1,3])
```

```
## [1] 0.5417957
```

This is the end of Assignment 3

Ceni Babaoglu, PhD