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 ...
                               0.36 0.34 0.4 0.32 0.32 0.4 0.16 0.36 0.34 0.43 ...
## $ citric.acid
                         : num
## $ residual.sugar
                               20.7 1.6 6.9 8.5 8.5 6.9 7 20.7 1.6 1.5 ...
                        : num
## $ 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
                               1.001 0.994 0.995 0.996 0.996 ...
                       : num
                               3 3.3 3.26 3.19 3.19 3.26 3.18 3 3.3 3.22 ...
## $ pH
## $ sulphates
                        : num
                               0.45 0.49 0.44 0.4 0.4 0.44 0.47 0.45 0.49 0.45 ...
                         : num 8.8 9.5 10.1 9.9 9.9 10.1 9.6 8.8 9.5 11 ...
## $ alcohol
                         : int 6666666666...
## $ quality
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
          : 6.855
##
    Mean
                     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
                            :1.1000
##
                     Max.
                                       {\tt Max.}
                                              :1.6600
                                                        Max.
                                                                :65.800
##
      chlorides
                      free.sulfur.dioxide total.sulfur.dioxide
                                                                    density
##
                      Min. : 2.00
                                                  : 9.0
   Min.
           :0.00900
                                           Min.
                                                                        :0.9871
                                                                \mathtt{Min}.
    1st Qu.:0.03600
                      1st Qu.: 23.00
                                           1st Qu.:108.0
                                                                 1st Qu.:0.9917
                      Median : 34.00
##
   Median :0.04300
                                           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
           :0.34600
                      Max.
                             :289.00
                                           Max.
                                                  :440.0
                                                                 Max.
                                                                        :1.0390
##
          рΗ
                      sulphates
                                         alcohol
                                                          quality
                                      Min.
##
  Min.
           :2.720
                            :0.2200
                                             : 8.00
                                                      Min.
                                                              :3.000
                    Min.
   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
                           :1.0800
                                            :14.20
                                                              :9.000
                    Max.
                                      Max.
                                                      Max.
```

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

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

[1] 0

```
# no missing data
```

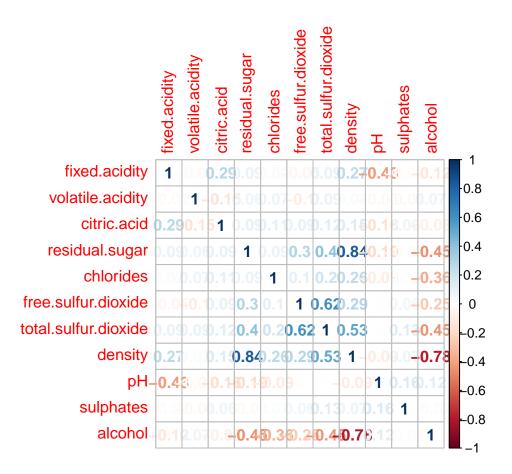
```
# INSERT YOUR CODE HERE.
wineNoEquality <- wine[, -grep("quality", names(wine))]
winecor <- cor(wineNoEquality)
winecor</pre>
```

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

```
##
                        fixed.acidity volatile.acidity citric.acid residual.sugar
                           1.00000000
                                           -0.02269729 0.28918070
                                                                        0.08902070
## fixed.acidity
## volatile.acidity
                          -0.02269729
                                            1.00000000 -0.14947181
                                                                        0.06428606
## citric.acid
                           0.28918070
                                           -0.14947181 1.00000000
                                                                        0.09421162
## residual.sugar
                                            0.06428606 0.09421162
                           0.08902070
                                                                        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
                                           -0.0493958591
## fixed.acidity
                         0.02308564
                                                                  0.091069756
                                           -0.0970119393
                                                                  0.089260504
## volatile.acidity
                         0.07051157
## citric.acid
                                            0.0940772210
                                                                  0.121130798
                         0.11436445
## 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
                        0.25721132
## density
                                           0.2942104109
                                                                  0.529881324
## pH
                                          -0.0006177961
                        -0.09043946
                                                                  0.002320972
## sulphates
                        0.01676288
                                          0.0592172458
                                                                  0.134562367
## alcohol
                                           -0.2501039415
                        -0.36018871
                                                                 -0.448892102
                                                pH sulphates
                                                                   alcohol
                            density
## fixed.acidity
                       0.26533101 -0.4258582910 -0.01714299 -0.12088112
## fixed.acidity 0.26533101 -0.4258582910 -0.01714299 -0.12088112 ## volatile.acidity 0.02711385 -0.0319153683 -0.03572815 0.06771794
                        0.14950257 -0.1637482114 0.06233094 -0.07572873
## citric.acid
                    0.83896645 -0.1941334540 -0.02666437 -0.45063122
0.25721132 -0.0904394560 0.01676288 -0.36018871
## residual.sugar
## chlorides
## 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
#install.packages("corrplot")
library(corrplot)
## Warning: package 'corrplot' was built under R version 4.0.2
## corrplot 0.84 loaded
```

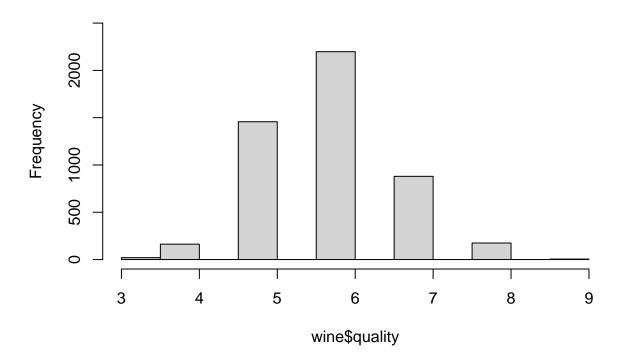
corrplot(winecor, method="number")



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

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

Histogram of wine\$quality



```
# 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)</pre>
```

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.</pre>
```

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

wine[1:11] <- sapply(wine[1:11], normalize)</pre>

summary(wine)

```
fixed.acidity
                   volatile.acidity citric.acid
                                                   residual.sugar
          :0.0000
                                                          :0.00000
##
   Min.
                   Min.
                          :0.0000 Min.
                                         :0.0000
                                                   Min.
  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
##
                                      alcohol
         рΗ
                    sulphates
                                                     quality
## Min.
         :0.0000
                   Min.
                         :0.0000 Min.
                                         :0.0000
                                                   high :1060
## 1st Qu.:0.3364
                   1st Qu.:0.2209 1st Qu.:0.2419
                                                         : 183
                                                   low
## 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,]</pre>
```

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))]</pre> test.set_new <- test.set[, -grep("quality", names(wine))]</pre> wine_train_labels <- train.set\$quality</pre> wine_test_labels <- test.set\$quality</pre> wine_knn_prediction <- knn(train = train.set_new, test = test.set_new, cl= wine_train_labels, k = 3)</pre> head(wine_knn_prediction) ## [1] 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)</pre> ConfusionMatrix 10. Display the confusion matrix to evaluate the model performance. (12 points) ## predicted ## actual high low medium 175 1 ## high 147 6 3 ## low 34 medium 109 18 977 CrossTable(x=wine_test_labels, y=wine_knn_prediction, prop.chisq=FALSE) ## ## ## Cell Contents ## | 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
##	١	0.542	0.003	0.455	0.220
##	I	0.603	0.045	0.127	l I
##	I	0.119	0.001	0.100	l l
## -					
##	low	6	3	l 34	43
##	I	0.140	0.070	0.791	0.029
##	I	0.021	0.136	0.029	1
##	I	0.004	0.002	0.023	
##					
##	medium	109	18	977	1104
##	I	0.099	0.016	0.885	0.751
##	I	0.376	0.818	0.844	1
##	I	0.074	0.012	0.665	l I
## -					
##	Column Total	290	22	1158	1470
##	I	0.197	0.015	0.788	1
##					
##					
##					

```
# INSERT YOUR CODE HERE.
sum(diag(ConfusionMatrix))/nrow(test.set)
```

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

[1] 0.7857143

This is the end of Assignment 3

Ceni Babaoglu, PhD