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Assignment 2

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```r
library(class)

# Read CSV from working directory into R

MyData <- read.csv(file="redwine.csv", header=TRUE, sep=",")

### Question 2

## a.

# Numerical summary of data

str(MyData)
```

```
## '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 ...
##  $ pH                  : num  3.51 3.2 3.26 3.16 3.51 3.51 3.3 3.39 3.36 3.35 ...
##  $ 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 ...
##  $ quality             : int  5 5 5 6 5 5 5 7 7 5 ...
```

```r
library(psych)
describe(MyData)
```

```
##                       vars    n  mean    sd median trimmed   mad  min
## fixed.acidity            1 1599  8.32  1.74   7.90    8.15  1.48 4.60
## volatile.acidity         2 1599  0.53  0.18   0.52    0.52  0.18 0.12
## citric.acid              3 1599  0.27  0.19   0.26    0.26  0.25 0.00
## residual.sugar           4 1599  2.54  1.41   2.20    2.26  0.44 0.90
## chlorides                5 1599  0.09  0.05   0.08    0.08  0.01 0.01
## free.sulfur.dioxide      6 1599 15.87 10.46  14.00   14.58 10.38 1.00
## total.sulfur.dioxide     7 1599 46.47 32.90  38.00   41.84 26.69 6.00
## density                  8 1599  1.00  0.00   1.00    1.00  0.00 0.99
## pH                       9 1599  3.31  0.15   3.31    3.31  0.15 2.74
## sulphates               10 1599  0.66  0.17   0.62    0.64  0.12 0.33
## alcohol                 11 1599 10.42  1.07  10.20   10.31  1.04 8.40
## quality                 12 1599  5.64  0.81   6.00    5.59  1.48 3.00
##                          max  range skew kurtosis   se
## fixed.acidity          15.90  11.30 0.98     1.12 0.04
## volatile.acidity        1.58   1.46 0.67     1.21 0.00
## citric.acid             1.00   1.00 0.32    -0.79 0.00
## residual.sugar         15.50  14.60 4.53    28.49 0.04
## chlorides               0.61   0.60 5.67    41.53 0.00
## free.sulfur.dioxide    72.00  71.00 1.25     2.01 0.26
## total.sulfur.dioxide 289.00 283.00 1.51     3.79 0.82
## density                1.00   0.01 0.07     0.92 0.00
```

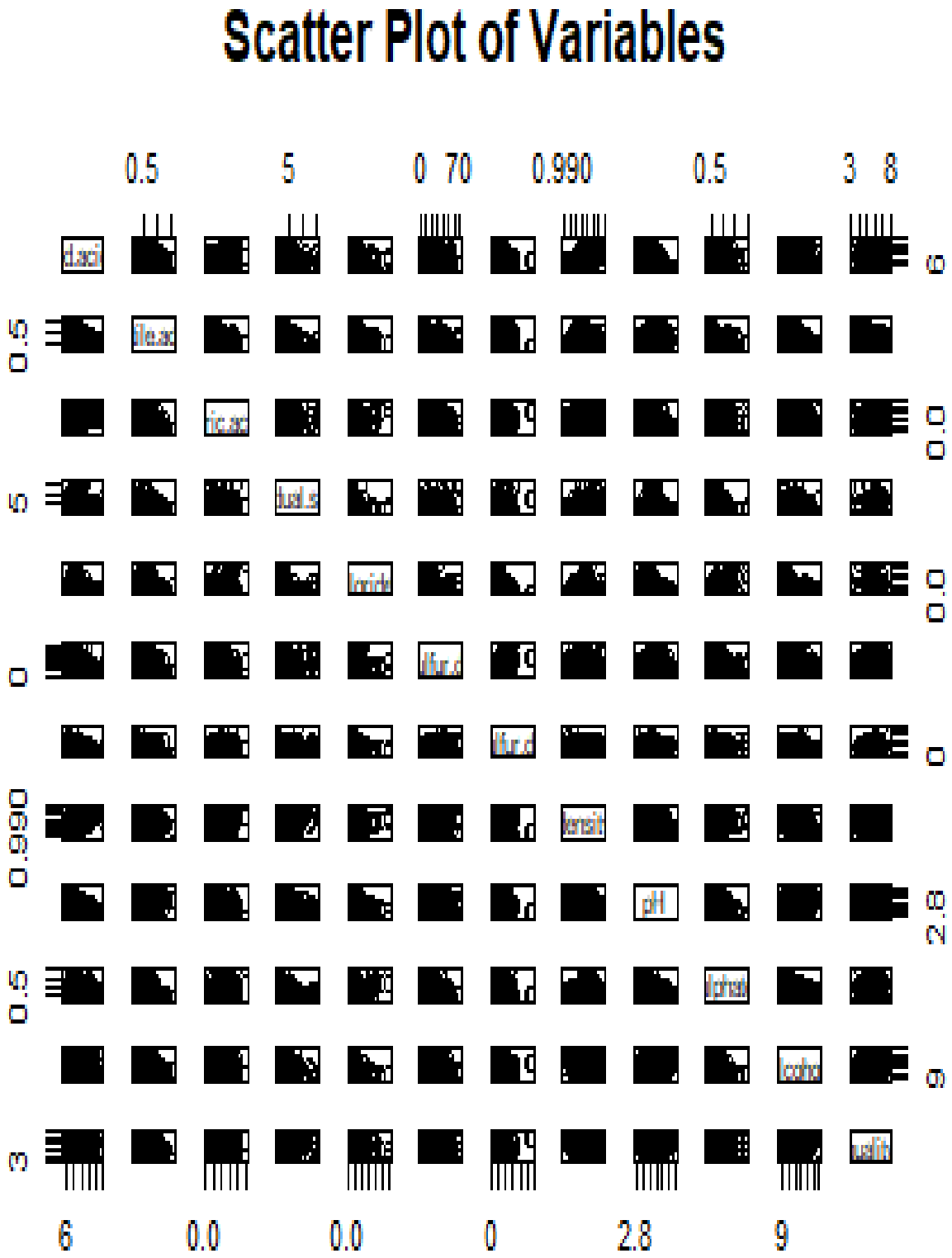
```
## pH                    4.01   1.27 0.19     0.80 0.00
## sulphates             2.00   1.67 2.42    11.66 0.00
## alcohol              14.90   6.50 0.86     0.19 0.03
## quality               8.00   5.00 0.22     0.29 0.02
```

```
summary(MyData)
```

```
##  fixed.acidity   volatile.acidity  citric.acid    residual.sugar
##  Min.   : 4.60   Min.   :0.1200   Min.   :0.000   Min.   : 0.900
##  1st Qu.: 7.10   1st Qu.:0.3900   1st Qu.:0.090   1st Qu.: 1.900
##  Median : 7.90   Median :0.5200   Median :0.260   Median : 2.200
##  Mean   : 8.32   Mean   :0.5278   Mean   :0.271   Mean   : 2.539
##  3rd Qu.: 9.20   3rd Qu.:0.6400   3rd Qu.:0.420   3rd Qu.: 2.600
##  Max.   :15.90   Max.   :1.5800   Max.   :1.000   Max.   :15.500
##    chlorides       free.sulfur.dioxide total.sulfur.dioxide
##  Min.   :0.01200   Min.   : 1.00       Min.   :  6.00
##  1st Qu.:0.07000   1st Qu.: 7.00       1st Qu.: 22.00
##  Median :0.07900   Median :14.00       Median : 38.00
##  Mean   :0.08747   Mean   :15.87       Mean   : 46.47
##  3rd Qu.:0.09000   3rd Qu.:21.00       3rd Qu.: 62.00
##  Max.   :0.61100   Max.   :72.00       Max.   :289.00
##     density             pH          sulphates         alcohol
##  Min.   :0.9901   Min.   :2.740   Min.   :0.3300   Min.   : 8.40
##  1st Qu.:0.9956   1st Qu.:3.210   1st Qu.:0.5500   1st Qu.: 9.50
##  Median :0.9968   Median :3.310   Median :0.6200   Median :10.20
##  Mean   :0.9967   Mean   :3.311   Mean   :0.6581   Mean   :10.42
##  3rd Qu.:0.9978   3rd Qu.:3.400   3rd Qu.:0.7300   3rd Qu.:11.10
##  Max.   :1.0037   Max.   :4.010   Max.   :2.0000   Max.   :14.90
##     quality
##  Min.   :3.000
##  1st Qu.:5.000
##  Median :6.000
##  Mean   :5.636
##  3rd Qu.:6.000
##  Max.   :8.000
```

```r
# Graphical summary of data

pairs(MyData, main="Scatter Plot of Variables")
```



```r
# Correlation of attributes

z <- cor(MyData)
z[lower.tri(z,diag=TRUE)]=NA
z=as.data.frame(as.table(z))
z=na.omit(z)
z=z[order(-abs(z$Freq)),]
head(z, n=10)
```

```
##                    Var1                 Var2       Freq
## 97        fixed.acidity                   pH -0.6829782
## 25        fixed.acidity          citric.acid  0.6717034
## 85        fixed.acidity              density  0.6680473
## 78  free.sulfur.dioxide total.sulfur.dioxide  0.6676665
## 26     volatile.acidity          citric.acid -0.5524957
## 99           citric.acid                   pH -0.5419041
## 128             density              alcohol -0.4961798
## 143             alcohol              quality  0.4761663
## 134    volatile.acidity              quality -0.3905578
## 113           chlorides            sulphates  0.3712605
```

```r
  # After exploring the dataset, I generated a correlation matrix to understand
  # how the attributes are related to each other. I created a list of these
  # relationships, sorted them, and printed out the ones with the largest absolute
  # values. Obviously, a correlation of 1 would be the highest signify a perfect,
  # positive correlation whereas a -1 would signify a perfect, negative
  # correlation.

  # The highest correlation patterns in the data seem to be between fixed.acidity
  # & pH, fixed.acidity % citric.acid, fixed.acidity & density, and
  # freesulfur.dioxide & total.sulfur.dioxide. All of them have roughly a 0.68
  # correlation - only fixed.acidity and pH have an inverse relationship. Although
  # these correlations are not extremely high, they indicate that there is some
  # dependency of variables on each other which is potentially harmful to us when
  # building a model.

## b.

# Create binary variable final_quality using mean

MyData$final_quality <- with(ifelse(quality>mean(quality), 1, 0), data=MyData)


# Creating dataset without original quality attribute

myvars <- names(MyData) %in% c("quality")
fulldataset <- MyData[!myvars]
head(fulldataset, n=1)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.4              0.7           0            1.9     0.076
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  11                  34  0.9978 3.51      0.56     9.4
##   final_quality
## 1             0
```

```r
# Splitting data into train and test

set.seed(1)
rows <- sample(x=nrow(fulldataset), size=.80*nrow(fulldataset))
trainset <- fulldataset[rows, ]
testset <- fulldataset[-rows, ]

# Logistic Regression

glm.fit <- glm(final_quality ~ fixed.acidity+volatile.acidity+citric.acid+residual.sugar+
chlorides+free.sulfur.dioxide+total.sulfur.dioxide+density+pH+sulphates+alcohol, data=tra
inset, family=binomial)
summary(glm.fit)

##
## Call:
## glm(formula = final_quality ~ fixed.acidity + volatile.acidity +
##     citric.acid + residual.sugar + chlorides + free.sulfur.dioxide +
##     total.sulfur.dioxide + density + pH + sulphates + alcohol,
##     family = binomial, data = trainset)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -3.3285  -0.8640   0.3094   0.8477   2.2338
##
## Coefficients:
##                        Estimate Std. Error z value Pr(>|z|)
## (Intercept)           19.150545  85.590617   0.224  0.82296
## fixed.acidity          0.111649   0.105894   1.054  0.29173
## volatile.acidity      -2.844256   0.534364  -5.323 1.02e-07 ***
## citric.acid           -0.988874   0.630212  -1.569  0.11662
## residual.sugar         0.006617   0.061182   0.108  0.91388
## chlorides             -4.933251   1.738512  -2.838  0.00454 **
## free.sulfur.dioxide    0.016142   0.009139   1.766  0.07734 .
## total.sulfur.dioxide  -0.014461   0.003119  -4.636 3.55e-06 ***
## density              -25.095517  87.419908  -0.287  0.77406
## pH                    -0.921976   0.793994  -1.161  0.24557
## sulphates              2.567119   0.499801   5.136 2.80e-07 ***
## alcohol                0.872373   0.113699   7.673 1.68e-14 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 1770.7  on 1278  degrees of freedom
## Residual deviance: 1352.0  on 1267  degrees of freedom
## AIC: 1376
##
## Number of Fisher Scoring iterations: 4

  # Atleast 4 of the predictors appear to be statistically significant. alcohol,
  # sulphates, total.sulfur.dioxide, and volative.acidity all have very small p
  # values meaning they have the largest impact on the response variable of final
  # quality.
```

```
## c.

# Confusion Matrix

glm.probs <- predict(glm.fit, testset, type="response")
glm.preds <- ifelse(glm.probs>0.5, 1, 0)
confusion_matrix_glm <- table(testset$final_quality,glm.preds)
print(confusion_matrix_glm)

##    glm.preds
##       0   1
##   0 105  27
##   1  45 143

# Fraction of Correct Predictions

Correct_Predictions_fraction = (confusion_matrix_glm[1,1]+confusion_matrix_glm[2,2])/sum(
confusion_matrix_glm)
sprintf("Overall Fraction of Correct Predictions are: %f",Correct_Predictions_fraction)

## [1] "Overall Fraction of Correct Predictions are: 0.775000"

  # The confusion tells us about the performance of the model. There were True
  # Negatives (105) and True Positives (143) and, as can be seen above, constitute
  # about 77.5% of results. The rest were misclassified - so about 22.5%. 27
  # points were False Positives and 45 were False Negatives. This tells us our
  # logistic regression model is wrong about one fourth of the time and tends to
  # be too conservative. It is wrongly classifying good wine (in class 1 that have
  # quality above the mean) as bad wine (in class 0 with quality below mean) more
  # than it is classifying bad wine as good wine (although that is happening a
  # fair bit as well).

## d.

variables <- which(names(fulldataset)%in%c("fixed.acidity","volatile.acidity","citric.aci
d","residual.sugar","chlorides","free.sulfur.dioxide","total.sulfur.dioxide","density","p
H","sulphates","alcohol"))

test_error <- data.frame("k"=1:11)

set.seed(1)
for(k in 1:11)
  {
    knn.pred <- knn(train=trainset[, variables], test=testset[, variables], cl=trainset$f
inal_quality, k=k)
    test_error$error[k]= round(sum(knn.pred!=testset$final_quality)/nrow(testset)*100,2)
  }

print(test_error)

##     k error
## 1   1 25.62
## 2   2 35.00
## 3   3 34.06
## 4   4 37.19
```

```
## 5   5 36.25
## 6   6 37.50
## 7   7 32.81
## 8   8 32.50
## 9   9 34.06
## 10 10 34.69
## 11 11 31.87

# As seen above, the model with the lowest test error is when k=1 with an error
# of approximately 25 and therefore can be concluded to be performing the best
# on this dataset.


### Question 3

## a.

# Split data into training and test - 80/20

set.seed(1)

rows <- sample(x=nrow(fulldataset), size=0.8*nrow(fulldataset))
trainset <- fulldataset[rows, ]
testset <- fulldataset[-rows, ]

## b.

# LDA

library (MASS)

## Warning: package 'MASS' was built under R version 3.4.3

lda.fit <- lda(final_quality ~ fixed.acidity+volatile.acidity+citric.acid+residual.sugar+
chlorides+free.sulfur.dioxide+total.sulfur.dioxide+density+pH+sulphates+alcohol, data=tra
inset)
lda.pred <- predict(lda.fit, testset)
confusion_matrix_lda <- table(testset$final_quality, lda.pred$class)
print(confusion_matrix_lda)

##
##       0   1
##   0 105  27
##   1  47 141

test_error_lda <- sum(lda.pred$class!=testset$final_quality)/nrow(testset)
sprintf("The test error for LDA is: %f", test_error_lda)

## [1] "The test error for LDA is: 0.231250"
```

```
## c.

# QDA

qda.fit <- qda(final_quality ~ fixed.acidity+volatile.acidity+citric.acid+residual.sugar+
chlorides+free.sulfur.dioxide+total.sulfur.dioxide+density+pH+sulphates+alcohol, data=tra
inset)
qda.pred <- predict(qda.fit, testset)
confusion_matrix_qda <- table(testset$final_quality, qda.pred$class)
print(confusion_matrix_qda)

##
##       0   1
##   0  90  42
##   1  36 152

test_error_qda <- sum(qda.pred$class!=testset$final_quality)/nrow(testset)
sprintf("The test error for QDA is: %f", test_error_qda)

## [1] "The test error for QDA is: 0.243750"
```

SUMMARY OF SECTION 4.5 – COMPARISON OF CLASSIFICATION METHODS

Logistic regression, LDA, QDA, and kNN are all different classification methods that each have their streng ths and weaknesses – understanding the scenarios in which they are most useful can help us build more a ccurate models. Logistic regression and LDA both create linear decision boundaries (only difference betw een the two is their fitting procedures) and therefore when the true decision boundary is linear in form, t hese methods perform well. kNN, on the other hand, is completely non-parametric (does not assume shap e), and hence performs better when the true boundary is highly-nonlinear. The disadvantage with kNN is that we cannot infer anything about the individual predictors and their impact. QDA falls somewhere in b etween the two: able to fit a wider range of shapes than linear methods but not as flexible as kNN. By mak ing assumptions about the data, it is able to perform better at lower number of training examples than kN N. There are several in between states as well – such as transformations of the predictors – that can be pe rformed to move between these four main types of classification methods. It is important to realize the be nefits and shortcomings of each method so that we can apply the correct one when the problem needs it.