DSC 680 Project 3 White Wine R

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```
#Set the working directory
setwd("C:/Users/Christine/Documents/Bellevue/DSC 680/Project 3")
```

Import data from file

```
# Read data to www dataframe
# row.names = 1 to avoid an index column creation upon dataset reading into a dataframe
www <- read.csv('C:/Users/Christine/Documents/Bellevue/DSC 680/Project 3/winequality-white.csv', sep = '</pre>
```

Display first five records of file

```
head(ww)
```

```
##
     fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1
               7.0
                                0.27
                                            0.36
                                                            20.7
## 2
               6.3
                                0.30
                                            0.34
                                                             1.6
                                                                      0.049
## 3
               8.1
                                0.28
                                            0.40
                                                             6.9
                                                                      0.050
## 4
               7.2
                                0.23
                                            0.32
                                                             8.5
                                                                      0.058
## 5
               7.2
                                0.23
                                            0.32
                                                             8.5
                                                                      0.058
## 6
               8.1
                                0.28
                                            0.40
                                                             6.9
                                                                      0.050
                                                          pH sulphates alcohol
     free.sulfur.dioxide total.sulfur.dioxide density
## 1
                      45
                                            170 1.0010 3.00
                                                                  0.45
## 2
                       14
                                           132 0.9940 3.30
                                                                   0.49
                                                                            9.5
## 3
                      30
                                            97 0.9951 3.26
                                                                  0.44
                                                                           10.1
## 4
                      47
                                           186 0.9956 3.19
                                                                  0.40
                                                                            9.9
## 5
                      47
                                           186 0.9956 3.19
                                                                  0.40
                                                                           9.9
                                            97 0.9951 3.26
                                                                  0.44
## 6
                      30
                                                                           10.1
##
     quality
## 1
## 2
           6
## 3
           6
## 4
           6
## 5
           6
## 6
           6
```

Find dimensions of ww dataframe

```
dim(ww)
```

```
## [1] 4898 12
```

List www dataframe's column names, types and a subset of values

str(ww)

```
'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
                                 0.27\ 0.3\ 0.28\ 0.23\ 0.23\ 0.28\ 0.32\ 0.27\ 0.3\ 0.22\ \dots
                          : num
## $ citric.acid
                                 0.36 0.34 0.4 0.32 0.32 0.4 0.16 0.36 0.34 0.43 ...
                          : num
                                 20.7 1.6 6.9 8.5 8.5 6.9 7 20.7 1.6 1.5 ...
## $ residual.sugar
                          : 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
##
   Hq $
                                 3 3.3 3.26 3.19 3.19 3.26 3.18 3 3.3 3.22 ...
                          : num
## $ sulphates
                                 0.45 0.49 0.44 0.4 0.4 0.44 0.47 0.45 0.49 0.45 ...
                          : num
## $ alcohol
                                 8.8 9.5 10.1 9.9 9.9 10.1 9.6 8.8 9.5 11 ...
                          : num
##
   $ quality
                          : int
                                 6 6 6 6 6 6 6 6 6 6 . . .
```

Display summary statistics for each variable

summary(ww)

```
fixed.acidity
                     volatile.acidity citric.acid
                                                       residual.sugar
          : 3.800
                            :0.0800 Min.
                                                              : 0.600
##
  Min.
                    Min.
                                             :0.0000
                                                       Min.
   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
                            :0.2782
                                      Mean
                                             :0.3342
                                                              : 6.391
                     Mean
                                                       Mean
##
   3rd Qu.: 7.300
                     3rd Qu.:0.3200
                                      3rd Qu.:0.3900
                                                       3rd Qu.: 9.900
  \mathtt{Max}.
           :14.200
                     Max.
                            :1.1000
                                      Max.
                                             :1.6600
                                                       Max.
                                                              :65.800
                      free.sulfur.dioxide total.sulfur.dioxide
##
      chlorides
                                                                  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
                                                :138.4
                                                               Mean
                                                                       :0.9940
                                          Mean
   3rd Qu.:0.05000
                      3rd Qu.: 46.00
                                          3rd Qu.:167.0
                                                               3rd Qu.:0.9961
##
   Max.
                      Max.
                            :289.00
                                                                      :1.0390
          :0.34600
                                          Max.
                                                 :440.0
                                                               Max.
##
                                        alcohol
         рН
                      sulphates
                                                        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
```

Check how many missing values (NA) are in each column/variable, sum them up per column

colSums(is.na(ww))

```
##
          fixed.acidity
                                                        citric.acid
                             volatile.acidity
##
                       0
                                             0
##
         residual.sugar
                                     chlorides
                                               free.sulfur.dioxide
##
                       0
                                             0
## total.sulfur.dioxide
                                       density
                                                                  рΗ
```

```
sulphates
                                                           quality
##
                                            0
                                                                 0
# Draw a histogram for a given dataframe and variable
# Use deparse() and substitute() functions to decode column name from
# a variable passed as an argument to the function, to be displayed
# on x axis (xlab())
draw_hist <- function(dataframe, variable)</pre>
  # Save histogram definition to the plot variable
 plot <- ggplot(data = dataframe, aes(x = variable)) +</pre>
           geom_histogram(color = 'black', fill = '#099DD9') +
           xlab(deparse(substitute(variable)))
  return(plot)
}
# Build a matrix of small histograms with 3 columns
# using customly defined draw_hist() function
grid.arrange(draw_hist(ww, ww$fixed.acidity),
             draw_hist(ww, ww$volatile.acidity),
             draw_hist(ww, ww$citric.acid),
             draw_hist(ww, ww$residual.sugar),
             draw_hist(ww, ww$chlorides),
             draw hist(ww, ww$free.sulfur.dioxide),
             draw_hist(ww, ww$total.sulfur.dioxide),
             draw_hist(ww, ww$density),
             draw hist(ww, ww$pH),
             draw hist(ww, ww$sulphates),
             draw_hist(ww, ww$alcohol),
```

0

alcohol

0

##

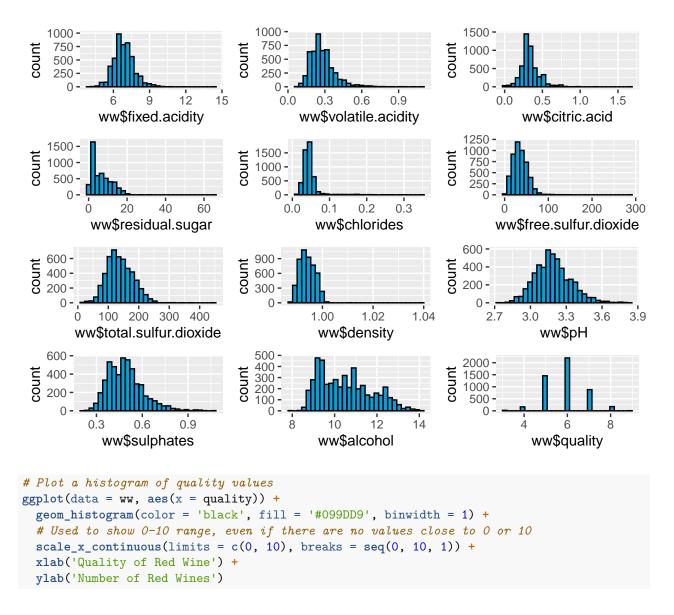
##

0

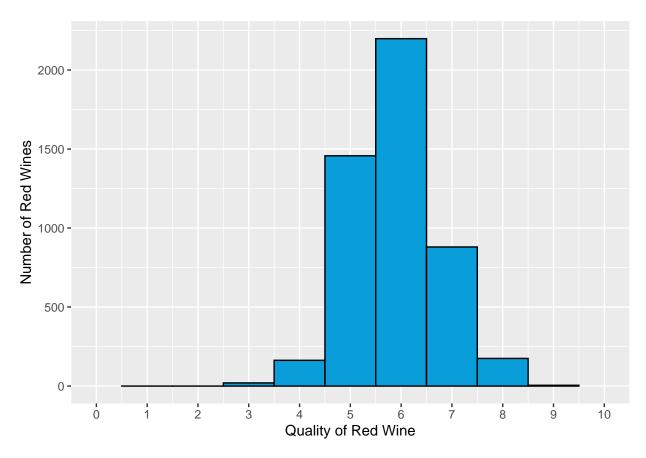
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
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## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

draw_hist(ww, ww\$quality),

ncol = 3)



Warning: Removed 2 rows containing missing values (geom_bar).



```
# Set boundaries for intervals
breaks <-c(0, 5, 7, 10)
# Bucket data points into intervals
ww$quality.category <- cut(ww$quality, breaks, include.lowest = TRUE, right = FALSE)</pre>
# Check intervals
summary(ww$quality.category)
##
    [0,5)
           [5,7) [7,10]
##
      183
            3655
# Add labels to intervals
labels <- c("Low", "Medium", "High")</pre>
ww$quality.category <- cut(ww$quality, breaks, include.lowest = TRUE, right = FALSE, labels=labels)</pre>
# Check if labels are applied properly
table(ww$quality.category)
##
                   High
##
      Low Medium
```

##

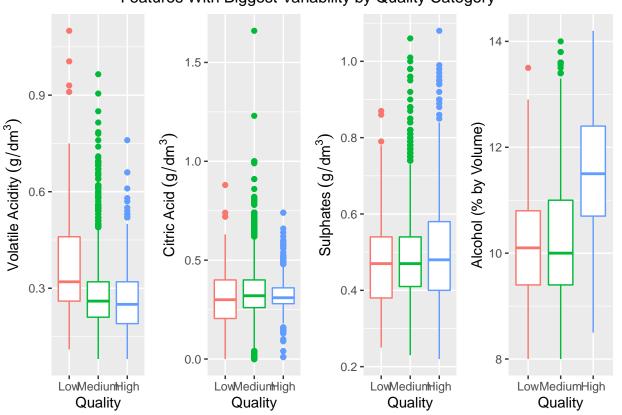
183

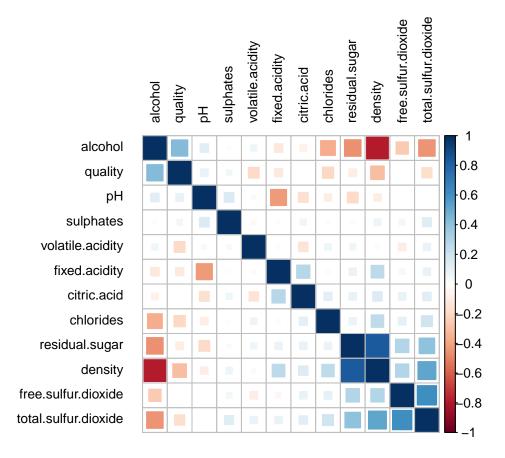
3655

1060

```
draw_boxplot <- function(dataframe, variable, ylab)</pre>
  plot <- ggplot(data = dataframe, aes(x = quality.category, y = variable, color = quality.category)) +</pre>
    geom_boxplot() +
    xlab('Quality') +
    #ylab(deparse(substitute(variable))) +
    ylab(ylab) +
    theme(legend.position = "none")
  return(plot)
}
\# Build 4 boxplots summarizing distributions of 4 selected features
draw_univ_summary <- function()</pre>
  grid.arrange(draw_boxplot(ww, ww$volatile.acidity, expression(Volatile~Acidity~(g/dm^{3}))),
             draw_boxplot(ww, ww$citric.acid, expression(Citric~Acid~(g/dm^{3}))),
             draw_boxplot(ww, ww$sulphates, expression(Sulphates~(g/dm^{3}))),
             draw_boxplot(ww, ww$alcohol, 'Alcohol (% by Volume)'),
             ncol = 4,
             top = 'Features With Biggest Variability by Quality Category')
}
draw_univ_summary()
```

Features With Biggest Variability by Quality Category





Regession models using binomial

```
# create categorical variables

ww$category[ww$quality <= 5] <- 0
ww$category[ww$quality > 5] <- 1
ww$quality2 <- as.factor(ww$quality)

ww$category <- as.factor(ww$category)</pre>
```

```
fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
##
## 1
               7.0
                                0.27
                                            0.36
                                                            20.7
                                                                     0.045
## 2
               6.3
                                            0.34
                                                                     0.049
                                0.30
                                                             1.6
## 3
               8.1
                                0.28
                                            0.40
                                                             6.9
                                                                     0.050
## 4
               7.2
                                0.23
                                            0.32
                                                             8.5
                                                                     0.058
```

```
## 5
               7.2
                                0.23
                                            0.32
                                                            8.5
                                                                     0.058
## 6
               8.1
                                0.28
                                            0.40
                                                             6.9
                                                                     0.050
                                                         pH sulphates alcohol
     free.sulfur.dioxide total.sulfur.dioxide density
## 1
                                           170 1.0010 3.00
                                                                  0.45
                      45
## 2
                      14
                                           132 0.9940 3.30
                                                                  0.49
                                                                           9.5
## 3
                      30
                                            97 0.9951 3.26
                                                                  0.44
                                                                          10.1
## 4
                      47
                                           186 0.9956 3.19
                                                                  0.40
                                                                           9.9
## 5
                                           186 0.9956 3.19
                      47
                                                                  0.40
                                                                           9.9
## 6
                      30
                                            97 0.9951 3.26
                                                                  0.44
                                                                          10.1
     quality quality.category category quality2
## 1
           6
                       Medium
                                      1
## 2
           6
                       Medium
                                               6
                                      1
## 3
           6
                       Medium
                                      1
                                               6
## 4
           6
                       Medium
                                      1
                                               6
## 5
           6
                       Medium
                                      1
                                               6
## 6
           6
                       Medium
                                      1
                                               6
```

Split data into Train Test sets

```
set.seed(3000)
spl = sample.split(ww$category, SplitRatio = 0.7)
wwtrain = subset(ww, spl==TRUE)
wwtest = subset(ww, spl==FALSE)
head(wwtrain)
```

```
fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 2
                6.3
                                 0.30
                                             0.34
                                                              1.6
                                                                      0.049
## 5
                7.2
                                 0.23
                                              0.32
                                                              8.5
                                                                      0.058
## 6
                8.1
                                 0.28
                                             0.40
                                                              6.9
                                                                      0.050
## 8
                7.0
                                 0.27
                                             0.36
                                                             20.7
                                                                      0.045
## 9
                6.3
                                 0.30
                                              0.34
                                                              1.6
                                                                      0.049
## 10
                8.1
                                 0.22
                                             0.43
                                                              1.5
                                                                      0.044
##
      free.sulfur.dioxide total.sulfur.dioxide density pH sulphates alcohol
## 2
                        14
                                             132 0.9940 3.30
                                                                   0.49
                                                                             9.5
## 5
                        47
                                             186 0.9956 3.19
                                                                   0.40
                                                                             9.9
## 6
                        30
                                             97 0.9951 3.26
                                                                   0.44
                                                                            10.1
## 8
                        45
                                                                            8.8
                                             170 1.0010 3.00
                                                                   0.45
## 9
                        14
                                             132 0.9940 3.30
                                                                   0.49
                                                                             9.5
## 10
                        28
                                             129 0.9938 3.22
                                                                   0.45
                                                                            11.0
##
      quality quality.category category quality2
## 2
                        Medium
                                                 6
            6
                                       1
                         Medium
## 5
            6
                                                 6
                                       1
## 6
            6
                        Medium
                                       1
                                                 6
            6
                        Medium
                                                6
## 8
                                       1
## 9
            6
                        Medium
                                       1
                                                 6
## 10
            6
                        Medium
                                       1
                                                 6
```

Create model

```
model_glm <- glm(category ~ . - quality - quality2, data = wwtrain, family=binomial(link = "logit"))</pre>
```

Stepwise model

```
model_gl <- step(model_glm)</pre>
## Start: AIC=2985.57
## category ~ (fixed.acidity + volatile.acidity + citric.acid +
##
      residual.sugar + chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
      density + pH + sulphates + alcohol + quality + quality.category +
##
##
      quality2) - quality - quality2
##
##
                         Df Deviance
                                        ATC
## - chlorides
                              2957.6 2983.6
## - citric.acid
                              2957.8 2983.8
                          1
## - fixed.acidity
                             2957.8 2983.8
                          1
## - total.sulfur.dioxide 1 2958.0 2984.0
## - pH
                          1 2958.1 2984.1
                              2957.6 2985.6
## <none>
## - density
                          1 2960.9 2986.9
## - free.sulfur.dioxide 1 2963.8 2989.8
## - sulphates
                          1 2965.3 2991.3
                          1 2970.4 2996.4
## - residual.sugar
## - alcohol
                          1 3003.0 3029.0
## - volatile.acidity
                          1 3046.7 3072.7
## - quality.category
                          2 3475.8 3499.8
##
## Step: AIC=2983.57
## category ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar +
##
      free.sulfur.dioxide + total.sulfur.dioxide + density + pH +
##
      sulphates + alcohol + quality.category
##
##
                         Df Deviance
                          1 2957.8 2981.8
## - citric.acid
## - fixed.acidity
                          1
                              2957.9 2981.9
## - total.sulfur.dioxide 1
                            2958.0 2982.0
## - pH
                          1 2958.1 2982.1
## <none>
                              2957.6 2983.6
## - density
                            2961.0 2985.0
                          1
## - free.sulfur.dioxide 1 2963.9 2987.9
## - sulphates
                          1 2965.3 2989.3
                          1 2970.9 2994.9
## - residual.sugar
## - alcohol
                            3003.1 3027.1
                          1
## - volatile.acidity
                          1 3047.2 3071.2
## - quality.category
                          2 3475.8 3497.8
##
## Step: AIC=2981.81
## category ~ fixed.acidity + volatile.acidity + residual.sugar +
      free.sulfur.dioxide + total.sulfur.dioxide + density + pH +
##
##
      sulphates + alcohol + quality.category
##
##
                         Df Deviance
```

1 2958.1 2980.1

- fixed.acidity

```
## - total.sulfur.dioxide 1
                           2958.3 2980.3
## - pH
                             2958.3 2980.3
                         1
## <none>
                             2957.8 2981.8
## - density
                             2961.1 2983.1
## - free.sulfur.dioxide
                         1
                           2964.3 2986.3
## - sulphates
                         1 2965.6 2987.6
## - residual.sugar
                         1 2971.0 2993.0
                         1 3004.2 3026.2
## - alcohol
## - volatile.acidity
                         1 3050.1 3072.1
## - quality.category
                         2 3476.1 3496.1
## Step: AIC=2980.05
## category ~ volatile.acidity + residual.sugar + free.sulfur.dioxide +
      total.sulfur.dioxide + density + pH + sulphates + alcohol +
##
##
      quality.category
##
##
                        Df Deviance
                                      AIC
## - total.sulfur.dioxide 1
                            2958.5 2978.5
## - pH
                           2959.7 2979.7
## <none>
                            2958.1 2980.1
## - free.sulfur.dioxide 1
                           2964.5 2984.5
## - density
                         1 2966.1 2986.1
## - sulphates
                         1 2966.2 2986.2
                         1 2983.4 3003.4
## - residual.sugar
## - alcohol
                         1 3038.1 3058.1
## - volatile.acidity
                         1 3050.9 3070.9
## - quality.category
                         2 3476.1 3494.1
##
## Step: AIC=2978.5
## category ~ volatile.acidity + residual.sugar + free.sulfur.dioxide +
##
      density + pH + sulphates + alcohol + quality.category
##
##
                       Df Deviance
                                     AIC
## - pH
                            2960.1 2978.1
## <none>
                            2958.5 2978.5
## - free.sulfur.dioxide 1
                           2965.7 2983.7
## - sulphates
                       1 2966.2 2984.2
## - density
                        1 2968.0 2986.0
                        1 2985.8 3003.8
## - residual.sugar
## - alcohol
                        1 3038.1 3056.1
## - volatile.acidity
                       1 3059.1 3077.1
                        2 3476.2 3492.2
## - quality.category
## Step: AIC=2978.1
## category ~ volatile.acidity + residual.sugar + free.sulfur.dioxide +
##
      density + sulphates + alcohol + quality.category
##
##
                       Df Deviance
                                     AIC
## <none>
                            2960.1 2978.1
## - free.sulfur.dioxide 1
                            2967.5 2983.5
                           2968.2 2984.2
## - density
                       1
## - sulphates
                       1 2968.4 2984.4
## - residual.sugar
                       1 2985.9 3001.9
                        1 3053.4 3069.4
## - alcohol
```

```
1 3062.5 3078.5
## - volatile.acidity
                            3482.1 3496.1
## - quality.category
head(fitted(model_gl))
##
                                                         10
## 0.3055928 0.6111362 0.5462353 0.4965432 0.3055928 0.6881878
head(predict(model_gl))
                       5
                                   6
                                              8
                                                                    10
head(predict(model_gl, type = "response"))
##
                    5
                             6
                                       8
                                                         10
## 0.3055928 0.6111362 0.5462353 0.4965432 0.3055928 0.6881878
Categorize wine
trn_pred <- ifelse(predict(model_gl, type = "response") > 0.5, "Good Wine", "Bad Wine")
head(trn_pred)
##
                                   6
## "Bad Wine" "Good Wine" "Bad Wine"
                                                "Bad Wine" "Good Wine"
Confusion matrix
trn_tab <- table(predicted = trn_pred, actual = wwtrain$category)</pre>
trn_tab
##
             actual
## predicted
                     1
##
    Bad Wine
               664 295
    Good Wine 484 1986
##
Checking accuracy of the training set.
sum(diag(trn_tab))/length(wwtrain$category)
## [1] 0.7728201
Confusion matrix for the test data.
# Making predictions on the test set.
tst_pred <- ifelse(predict(model_gl, newdata = wwtest, type = "response") > 0.5, "Good Wine", "Bad Wine
tst_tab <- table(predicted = tst_pred, actual = wwtest$category)</pre>
tst_tab
```

```
## actual
## predicted 0 1
## Bad Wine 294 120
## Good Wine 198 857
```

Checking accuracy for the test data.

```
sum(diag(tst_tab))/length(wwtest$category)
```

[1] 0.7835262