ADS 503 - Team 7

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```
# R Libraries
library(caret)
library(AppliedPredictiveModeling)
library(Hmisc)
library(dplyr)
library(tidyverse)
library(ggplot2)
library(corrplot)
library(MASS)
library(ISLR)
library(rpart)
library(partykit)
library(randomForestSRC)
library(earth)
library(MARSS)
library(e1071)
library(summarytools)
library(grid)
library(MLeval)
library(pROC)
```

Load the Red Wine Quality data set from GitHub - data set copied from Kaggle and imported into GitHub.

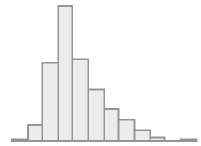
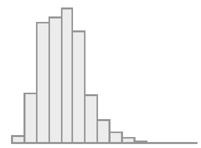
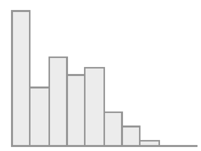
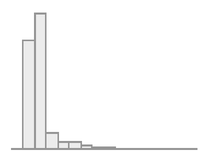
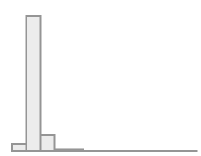
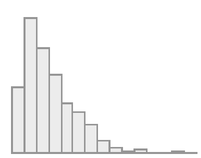
```
wine <- read.csv(
  url("https://raw.githubusercontent.com/OscarG-DataSci/ADS503/main/winequality-red.csv")
                      , header = TRUE)
```

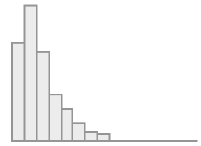
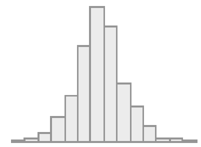
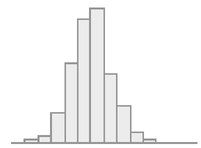
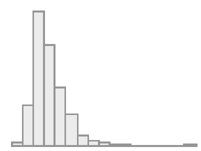
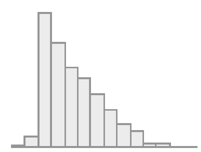
Data Summary

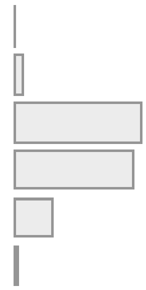
```
# use the view function to view in R Studio
#view(
dfSummary(wine,
          plain.ascii  = FALSE,
          style        = "grid",
          graph.magnif = 0.75,
          valid.col    = FALSE,
          tmp.img.dir  = "NA")
```

Data Frame Summary

wine **Dimensions:** 1599 x 12
Duplicates: 240

No	Variable	Stats / Values	Freqs (% of Valid)	Graph	Missing
1	fixed.acidity [numeric]	Mean (sd) : 8.3 (1.7) min < med < max: 4.6 < 7.9 < 15.9 IQR (CV) : 2.1 (0.2)	96 distinct values		0 (0.0%)
2	volatile.acidity [numeric]	Mean (sd) : 0.5 (0.2) min < med < max: 0.1 < 0.5 < 1.6 IQR (CV) : 0.2 (0.3)	143 distinct values		0 (0.0%)
3	citric.acid [numeric]	Mean (sd) : 0.3 (0.2) min < med < max: 0 < 0.3 < 1 IQR (CV) : 0.3 (0.7)	80 distinct values		0 (0.0%)
4	residual.sugar [numeric]	Mean (sd) : 2.5 (1.4) min < med < max: 0.9 < 2.2 < 15.5 IQR (CV) : 0.7 (0.6)	91 distinct values		0 (0.0%)
5	chlorides [numeric]	Mean (sd) : 0.1 (0) min < med < max: 0 < 0.1 < 0.6 IQR (CV) : 0 (0.5)	153 distinct values		0 (0.0%)
6	free.sulfur.dioxide [numeric]	Mean (sd) : 15.9 (10.5) min < med < max: 1 < 14 < 72 IQR (CV) : 14 (0.7)	60 distinct values		0 (0.0%)

No	Variable	Stats / Values	Freqs (% of Valid)	Graph	Missing
7	total.sulfur.dioxide [numeric]	Mean (sd) : 46.5 (32.9) min < med < max: 6 < 38 < 289 IQR (CV) : 40 (0.7)	144 distinct values		0 (0.0%)
8	density [numeric]	Mean (sd) : 1 (0) min < med < max: 1 < 1 < 1 IQR (CV) : 0 (0)	436 distinct values		0 (0.0%)
9	pH [numeric]	Mean (sd) : 3.3 (0.2) min < med < max: 2.7 < 3.3 < 4 IQR (CV) : 0.2 (0)	89 distinct values		0 (0.0%)
10	sulphates [numeric]	Mean (sd) : 0.7 (0.2) min < med < max: 0.3 < 0.6 < 2 IQR (CV) : 0.2 (0.3)	96 distinct values		0 (0.0%)
11	alcohol [numeric]	Mean (sd) : 10.4 (1.1) min < med < max: 8.4 < 10.2 < 14.9 IQR (CV) : 1.6 (0.1)	65 distinct values		0 (0.0%)

No	Variable	Stats / Values	Freqs (% of Valid)	Graph	Missing
12	quality [integer]	Mean (sd) : 5.6 (0.8) min < med < max: 3 < 6 < 8 IQR (CV) : 1 (0.1)	3 : 10 (0.6%) 4 : 53 (3.3%) 5 : 681 (42.6%) 6 : 638 (39.9%) 7 : 199 (12.4%) 8 : 18 (1.1%)		0 (0.0%)

```
#    )
```

Pre-processing

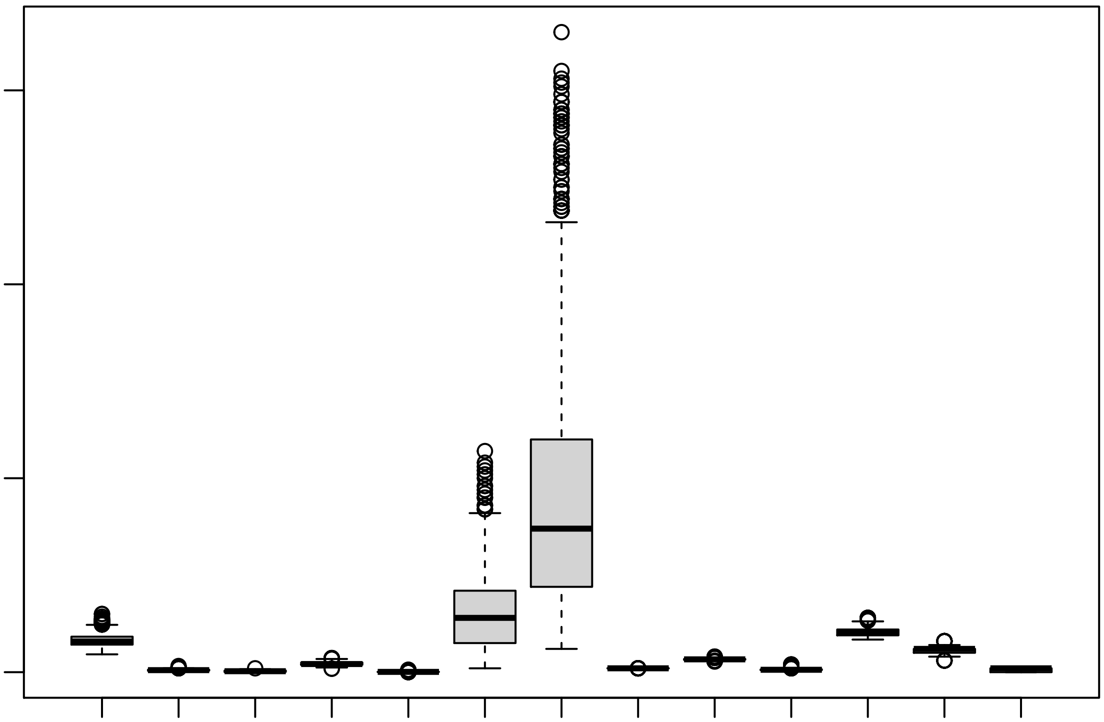
```
par(mar=c(1,1,1,1)) # to fix boxplot knit processing issues

# Create new variable, for quality values, split by half (0, 1)
wine$quality_target <- ifelse( wine$quality <= 5, 0, 1)

# Mean of new variable is at 0.5347 (close enough to 50% to maintain balance)
summary(wine$quality_target)
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  0.0000  0.0000  1.0000  0.5347  1.0000  1.0000
```

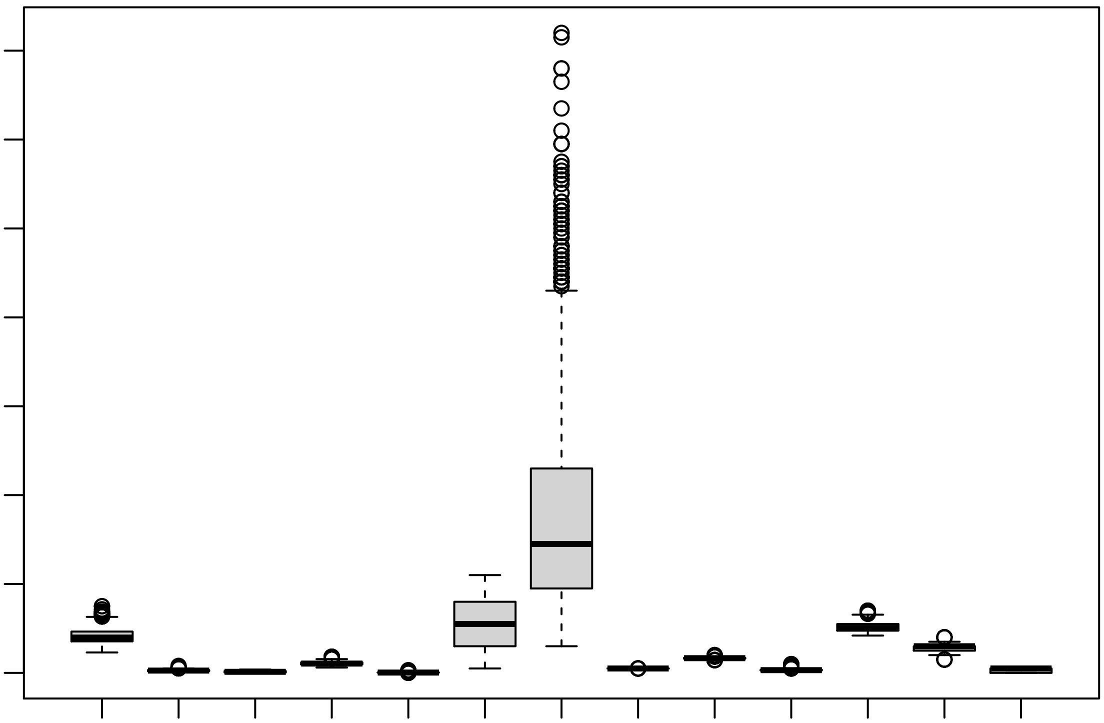
```
# Check for missing values in data set
wine %>% na.omit() %>% count() # there are no missing values
```

```
##      n
## 1 1599
```

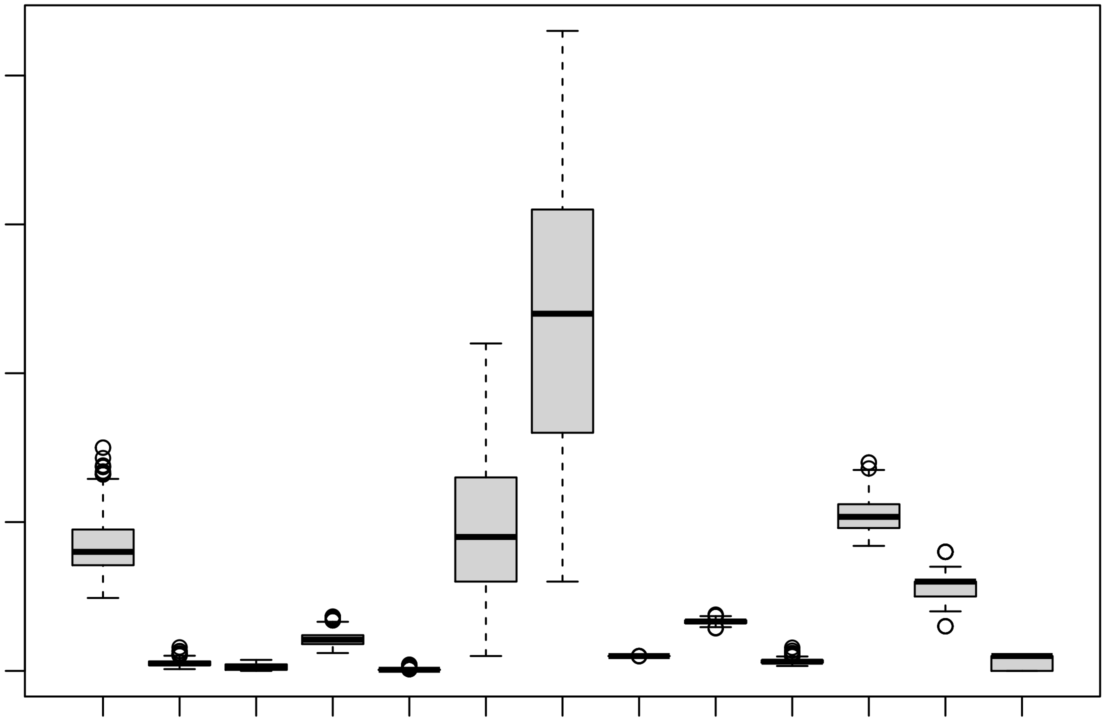
```
# Removing outliers for residual sugar:
Q <- quantile(wine$residual.sugar, probs=c(.25, .75), na.rm = FALSE)
iqr_rs <- IQR(wine$residual.sugar)
up_rs <-  Q[2]+1.5*iqr_rs # Upper Range
low_rs <- Q[1]-1.5*iqr_rs # Lower Range
eliminated_rs <- subset(wine, wine$residual.sugar > (Q[1] - 1.5*iqr_rs) & wine$residual.sugar < (Q[2]+1
boxplot(eliminated_rs)
```



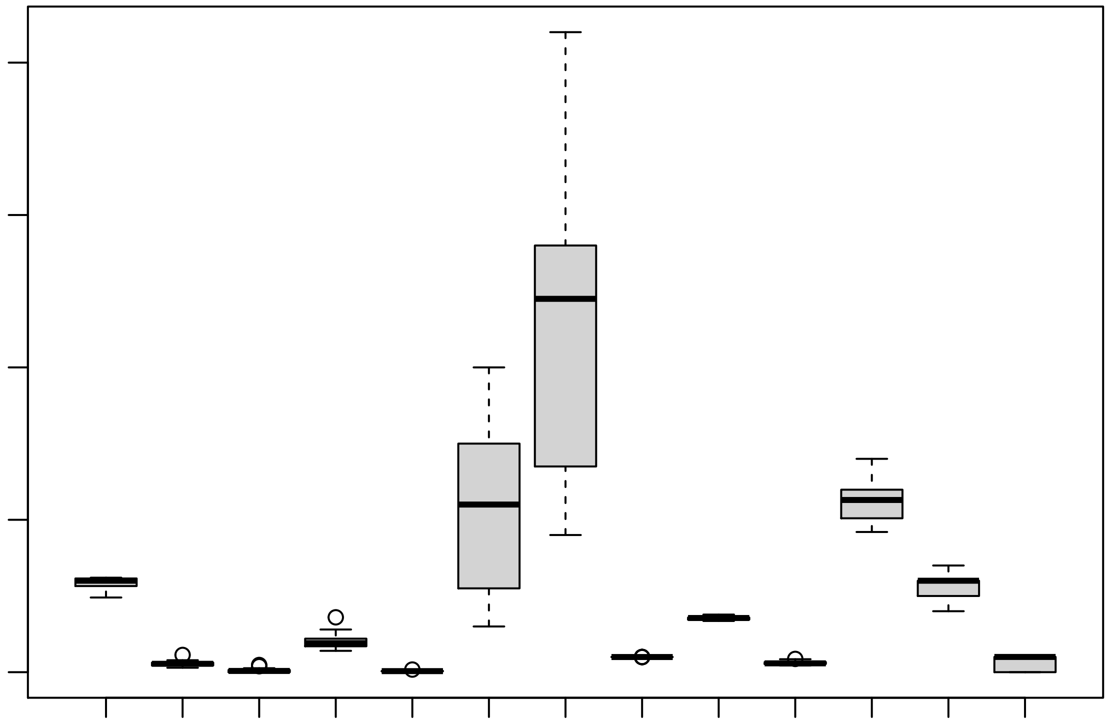
```
#Removing outliers for free.sulfur.dioxide:
Q2 <- quantile(wine$free.sulfur.dioxide, probs=c(.25, .75), na.rm = FALSE)
iqr_fs <- IQR(eliminated_rs$free.sulfur.dioxide)
up_fs <-  Q2[2]+1.5*iqr_fs # Upper Range
low_fs <- Q2[1]-1.5*iqr_fs # Lower Range
eliminated_fs <- subset(eliminated_rs, eliminated_rs$free.sulfur.dioxide > (Q[1] - 1.5*iqr_fs) & elimina
boxplot(eliminated_fs)
```



```
#Removing outliers for total.sulfur.dioxide:
Q3 <- quantile(wine$total.sulfur.dioxide, probs=c(.25, .75), na.rm = FALSE)
iqr_ts <- IQR(eliminated_fs$total.sulfur.dioxide)
up_ts <-  Q3[2]+1.5*iqr_ts # Upper Range
low_ts <- Q3[1]-1.5*iqr_ts # Lower Range
eliminated_ts <- subset(eliminated_fs, eliminated_fs$total.sulfur.dioxide > (Q[1] - 1.5*iqr_ts) & elimi
boxplot(eliminated_ts)
```



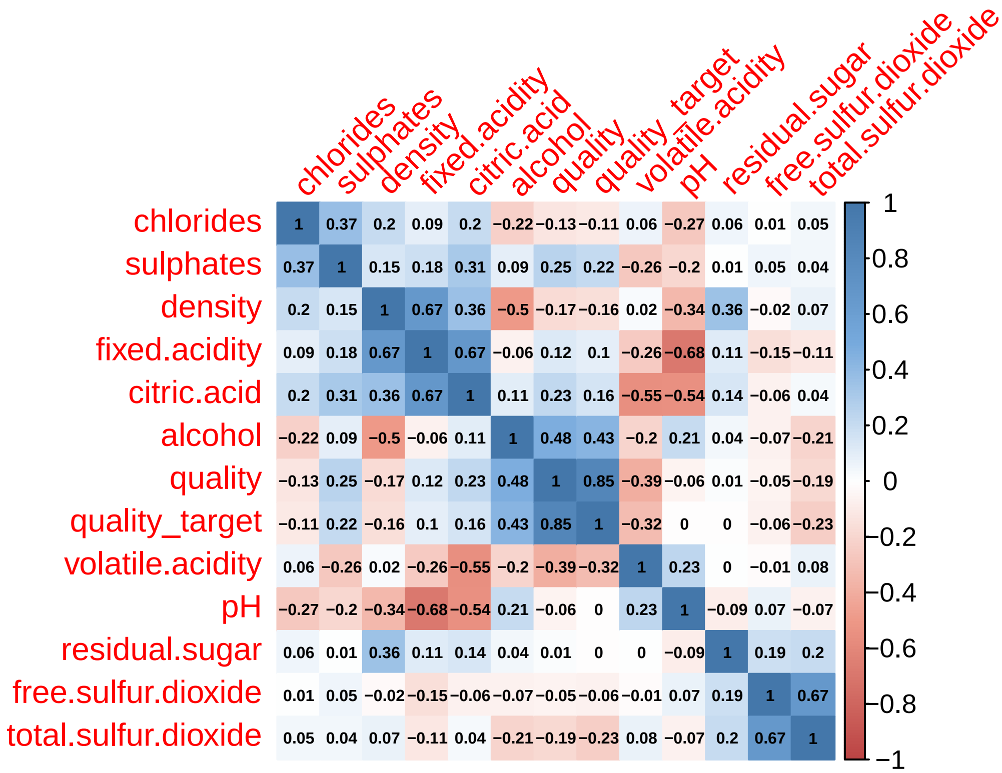
```
#Removing outliers for fixed.acidity:
Q4 <- quantile(wine$fixed.acidity, probs=c(.25, .75), na.rm = FALSE)
iqr_fa <- IQR(eliminated_ts$fixed.acidity)
up_fa <-  Q[2]+1.5*iqr_fa # Upper Range
low_fa <- Q[1]-1.5*iqr_fa # Lower Range
eliminated_fa <- subset(eliminated_ts, eliminated_ts$fixed.acidity > (Q[1] - 1.5*iqr_fa) & eliminated_t
boxplot(eliminated_fa)
```



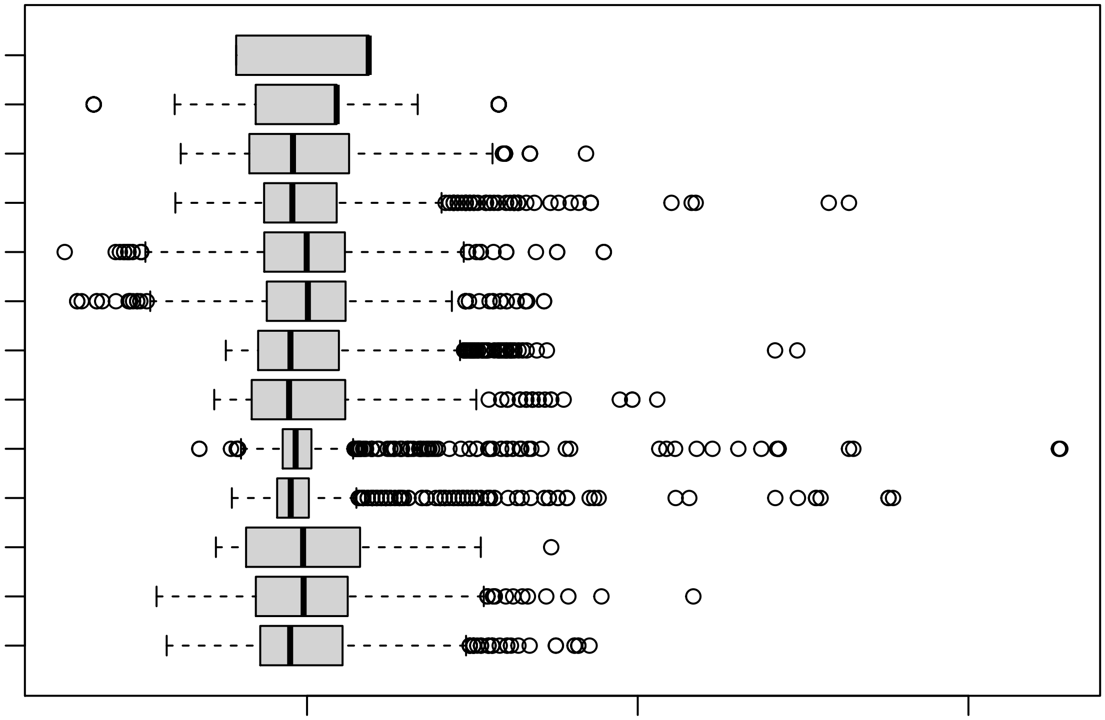
```r
new_wine_data <- eliminated_fa

# Removing outliers reduced dimension of data set from 1599 observations to 48
# team opted not to use new_wine_data and keep outlier data
dim(new_wine_data)
```

```
## [1] 48 13
```

```r
# Correlation Matrix
cor <- cor(wine)

# Colors for Correlation Matrix
colors <- colorRampPalette(c("#BB4444", "#EE9988", "#FFFFFF", "#77AADD", "#4477AA"))

corrplot(cor, order="hclust", method = "color", addCoef.col = "black"
         , tl.srt = 45, number.cex = 0.47, col=colors(200))
```




```r
# Cutoff Correlation features
cutoffCorr <- findCorrelation(cor, cutoff = .8)
cutoffCorrFeatures <- wine[, -cutoffCorr]

# Train and Test split
wine_split <- createDataPartition(wine$quality, p = .8, list = FALSE)
wine_train <- wine[ wine_split,]
wine_test  <- wine[-wine_split,]

# Transform Train Data
train_trans <- preProcess(wine_train, method = c("center", "scale"))
train_transformed <- predict(train_trans, wine_train)

# Transform Test Data
test_trans <- preProcess(wine_test, method = c("center", "scale"))
test_transformed <- predict(test_trans, wine_test)

# Boxplot of transformed train data
boxplot(train_transformed, horizontal = TRUE, las = 2, cex.axis = .65, cex.lab = 7)
```



Logistic Regression Model

```
# Cutoff Correlation string to copy + paste into feature area of model
subset(cutoffCorrFeatures, select = -c(quality_target)) %>%
      colnames() %>%
      paste0(collapse = " + ")
```

```
## [1] "fixed.acidity + volatile.acidity + citric.acid + residual.sugar + chlorides + free.sulfur.dioxi
```

```
set.seed(4)

# Model using "quality_target" as target variable
lmodel1 <- lm(quality_target~ volatile.acidity + sulphates + alcohol, data = wine_train)

summary(lmodel1)
```

```
##
## Call:
## lm(formula = quality_target ~ volatile.acidity + sulphates +
##     alcohol, data = wine_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.49852 -0.35196 -0.00665  0.38054  1.03178
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)      -1.28481    0.14349  -8.954  < 2e-16 ***
## volatile.acidity -0.57138    0.07048  -8.107 1.20e-15 ***
## sulphates         0.44466    0.07604   5.847 6.33e-09 ***
```

```
## alcohol           0.17554    0.01157  15.170  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4289 on 1277 degrees of freedom
## Multiple R-squared:  0.263,  Adjusted R-squared:  0.2613
## F-statistic: 151.9 on 3 and 1277 DF,  p-value: < 2.2e-16
```

```r
# Model using "quality" as target variable
lmodel2 <- lm(quality~ volatile.acidity + sulphates + alcohol, data = wine_train)

summary(lmodel2)
```

```
##
## Call:
## lm(formula = quality ~ volatile.acidity + sulphates + alcohol,
##     data = wine_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.73657 -0.38252 -0.05755  0.45741  2.17094
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)       2.52555    0.22310  11.320  < 2e-16 ***
## volatile.acidity -1.18982    0.10958 -10.858  < 2e-16 ***
## sulphates         0.78130    0.11824   6.608 5.71e-11 ***
## alcohol           0.30936    0.01799  17.194  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6668 on 1277 degrees of freedom
## Multiple R-squared:  0.3345, Adjusted R-squared:  0.333
## F-statistic:   214 on 3 and 1277 DF,  p-value: < 2.2e-16
```

```r
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(lmodel2, newdata = wine_test)) -> df

# Summary of predicted interval
predict(lmodel2, newdata = wine_test, interval = "prediction") %>%
  summary()
```

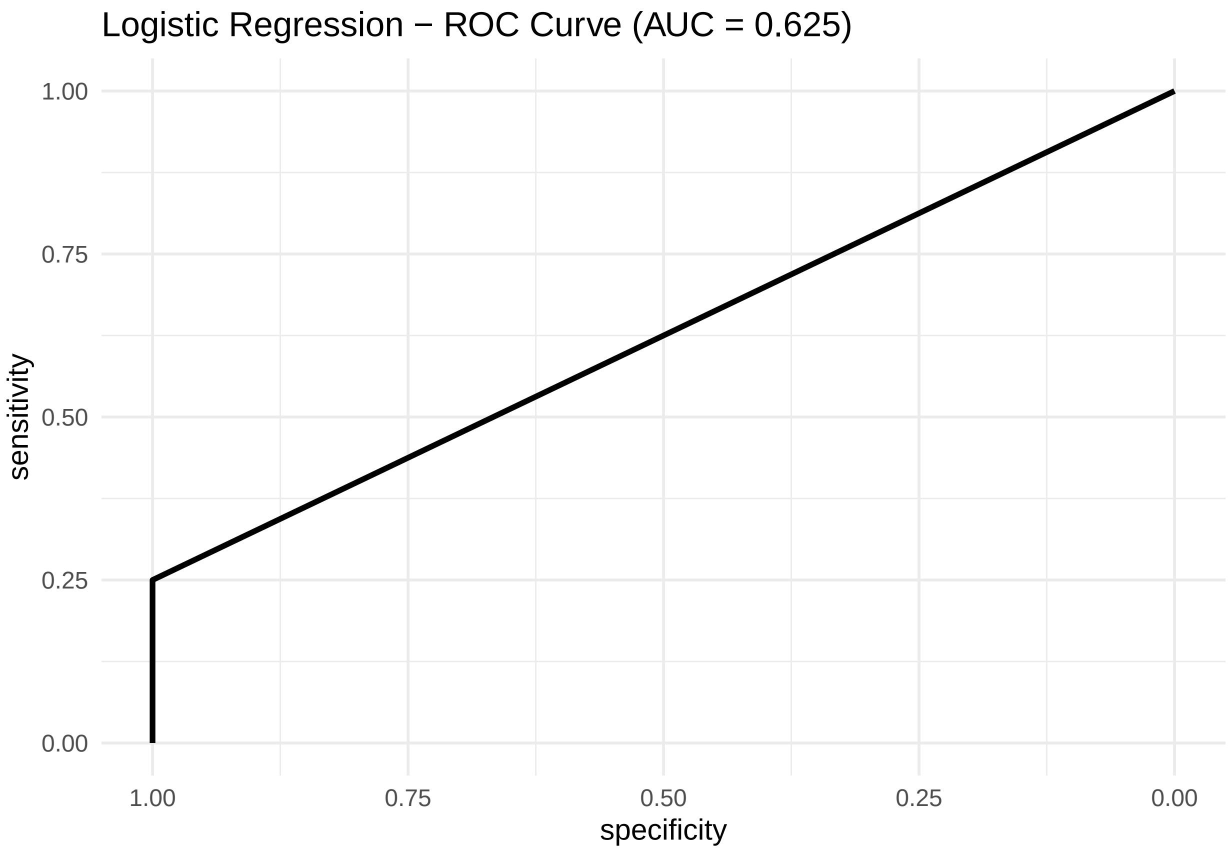
```
##       fit             lwr             upr
##  Min.   :4.642   Min.   :3.330   Min.   :5.955
##  1st Qu.:5.284   1st Qu.:3.975   1st Qu.:6.593
##  Median :5.522   Median :4.210   Median :6.832
##  Mean   :5.645   Mean   :4.335   Mean   :6.956
##  3rd Qu.:5.971   3rd Qu.:4.662   3rd Qu.:7.281
##  Max.   :6.990   Max.   :5.676   Max.   :8.305
```

```r
# Confusion Matrix
# Convert predicted values to whole numbers, so they match target values
df$predicted_int = as.integer(round(df$predicted, digits = 0))

union1 <- union(df$quality, df$predicted_int)
```

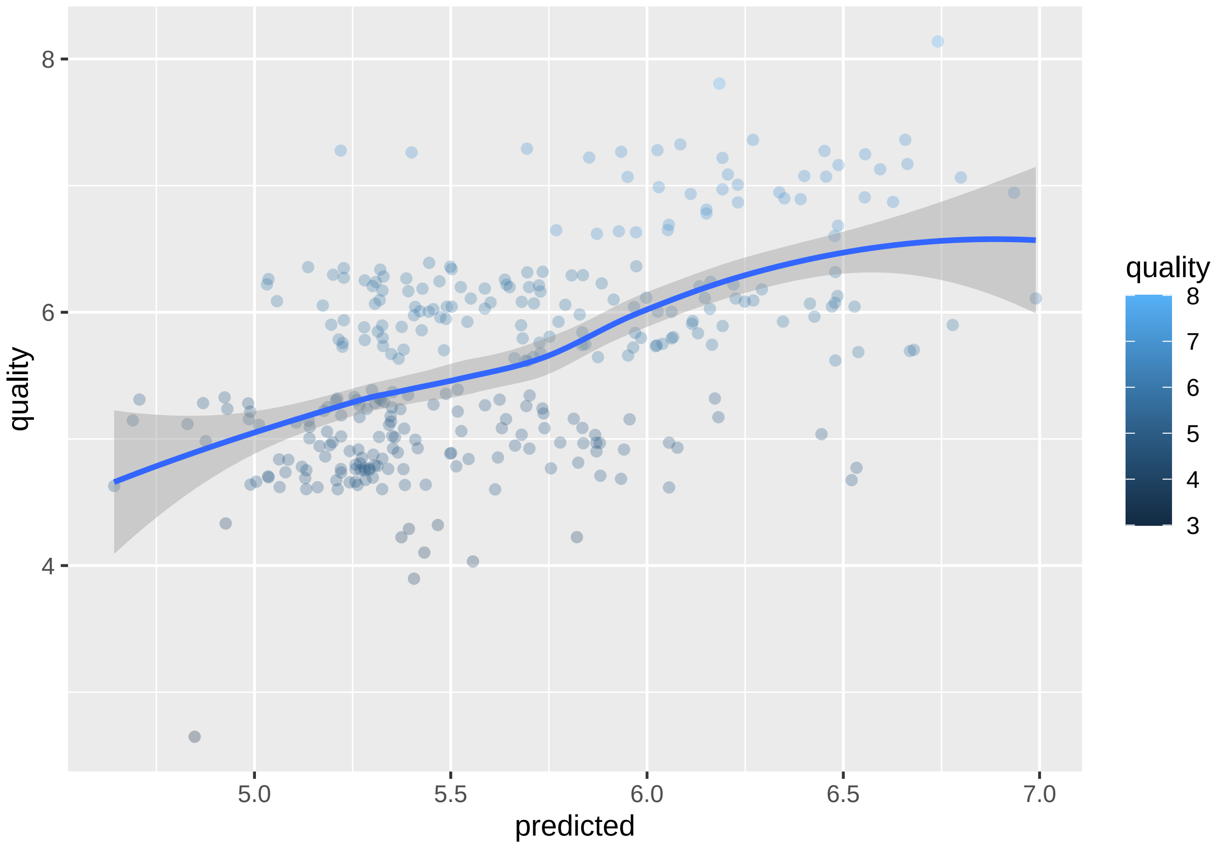
```r
table1 <- table(factor(df$quality, union1), factor(df$predicted_int, union1))

confusionMatrix(table1)
```

```
## Confusion Matrix and Statistics
##
##
##      5  7  6  4  8  3
##   5 97  2 40  0  0  0
##   7  2  8 31  0  0  0
##   6 47  6 74  0  0  0
##   4  6  0  2  0  0  0
##   8  0  1  1  0  0  0
##   3  1  0  0  0  0  0
##
## Overall Statistics
##
##                Accuracy : 0.5629
##                  95% CI : (0.5064, 0.6182)
##     No Information Rate : 0.4811
##     P-Value [Acc > NIR] : 0.002103
##
##                   Kappa : 0.2677
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 5 Class: 7 Class: 6 Class: 4 Class: 8 Class: 3
## Sensitivity            0.6340  0.47059   0.5000       NA       NA       NA
## Specificity            0.7455  0.89037   0.6882  0.97484 0.993711 0.996855
## Pos Pred Value         0.6978  0.19512   0.5827       NA       NA       NA
## Neg Pred Value         0.6872  0.96751   0.6126       NA       NA       NA
## Prevalence             0.4811  0.05346   0.4654  0.00000 0.000000 0.000000
## Detection Rate         0.3050  0.02516   0.2327  0.00000 0.000000 0.000000
## Detection Prevalence   0.4371  0.12893   0.3994  0.02516 0.006289 0.003145
## Balanced Accuracy      0.6897  0.68048   0.5941       NA       NA       NA
```

```r
# ROC plot
df$predicted_int = round(as.numeric(as.character(df$predicted)), digits = 0)

modelName1 <- 'Logistic Regression'
roc1 <- roc(df$quality, df$predicted_int)
auc1 <- round(auc(df$quality, df$predicted_int), 4)

ggroc(roc1, colours = 'red', size = 1) +
  ggtitle(paste0(modelName1, ' - ROC Curve ', '(AUC = ', auc1 , ')')) + theme_minimal()
```




```r
# Scatter plot of predicted
ggplot(df, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```

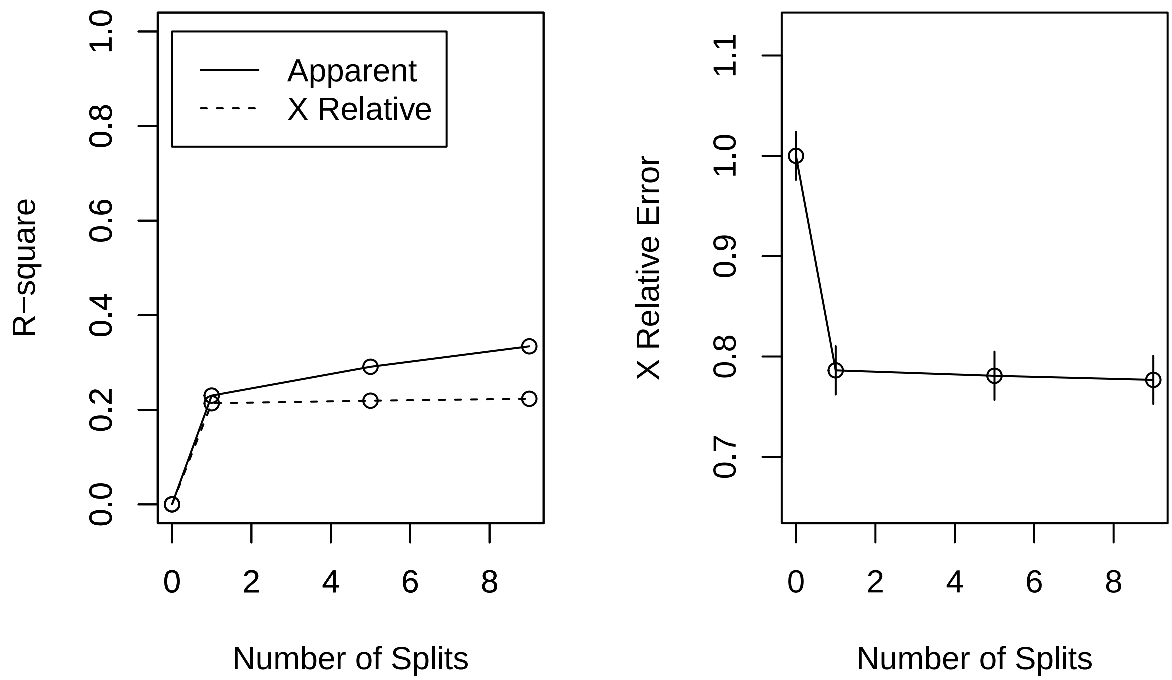



```
# The scatter plot supports the summary of the predicted interval, in the ranges of the fit,
# lower, and upper ranges. The R-squared value of 0.3283 of the model, indicates that this
# information can be predicted 33% of the time, with the data available, for the variance
# of the information.
```

CART

```
set.seed(4)
# Subset both train and test sets, to exclude "quality_target"
# Using non-transformed versions of train and test, to get actual values in the nodes
subset(wine_train, select = -c(quality_target)) -> rf_wine_train
subset(wine_test, select = -c(quality_target)) -> rf_wine_test

# Convert target variable to factor to ensure proper interpretation by model
rf_wine_train$quality <- as.factor(rf_wine_train$quality)

# Begin model...
rPartTree <- rpart(quality ~ ., data = rf_wine_train)

rpartTree2 <- as.party(rPartTree)

# R-Squared plot
par(mfrow=c(1,2))
rsq.rpart(rPartTree)
```

```
##
## Classification tree:
## rpart(formula = quality ~ ., data = rf_wine_train)
##
## Variables actually used in tree construction:
## [1] alcohol              fixed.acidity        sulphates
## [4] total.sulfur.dioxide volatile.acidity
##
## Root node error: 739/1281 = 0.57689
##
## n= 1281
##
##         CP nsplit rel error  xerror     xstd
## 1 0.230041      0   1.00000 1.00000 0.023928
## 2 0.014434      1   0.76996 0.78620 0.024111
## 3 0.010374      5   0.70907 0.78078 0.024097
## 4 0.010000      9   0.66576 0.77673 0.024085
```

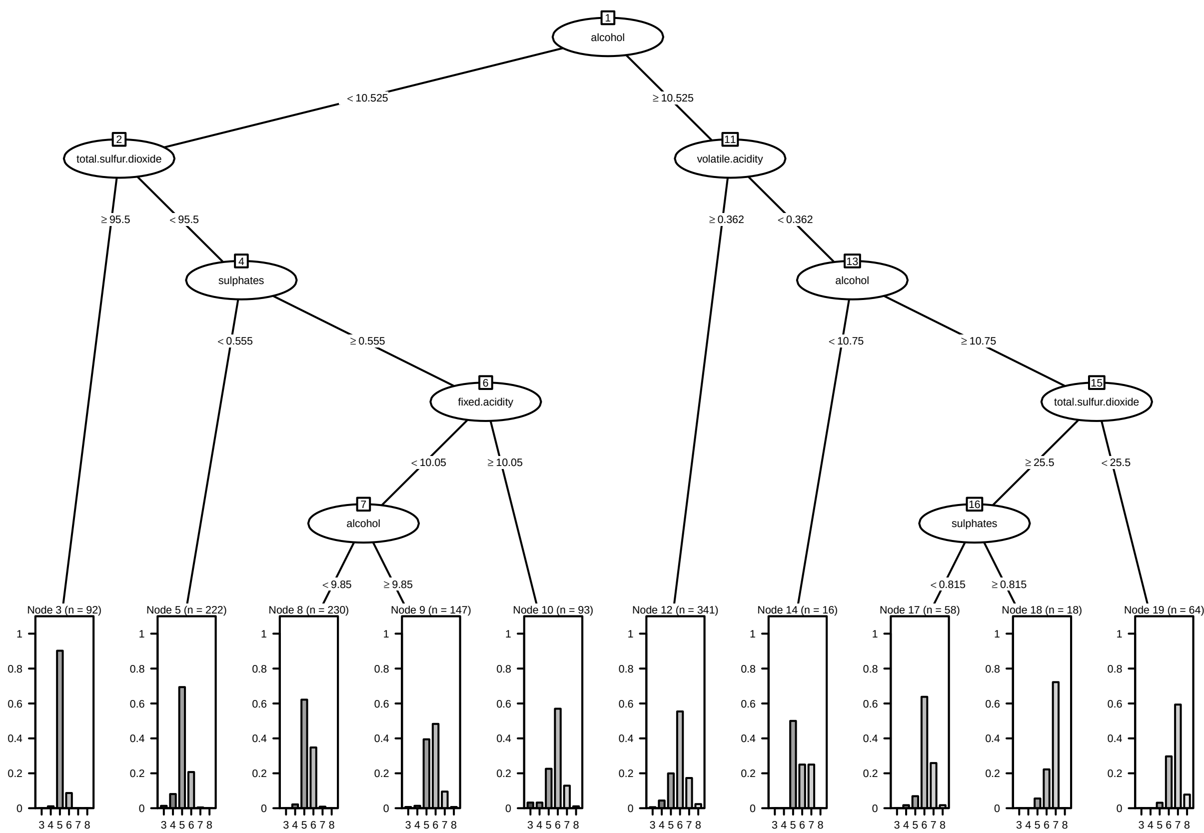



```
# Results
rpartTree2
```

```
##
## Model formula:
## quality ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar +
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
##     density + pH + sulphates + alcohol
##
## Fitted party:
## [1] root
## |   [2] alcohol < 10.525
## |   |   [3] total.sulfur.dioxide >= 95.5: 5 (n = 92, err = 9.8%)
## |   |   [4] total.sulfur.dioxide < 95.5
## |   |   |   [5] sulphates < 0.555: 5 (n = 222, err = 30.6%)
```

```
## |   |   |   [6] sulphates >= 0.555
## |   |   |   |   [7] fixed.acidity < 10.05
## |   |   |   |   |   [8] alcohol < 9.85: 5 (n = 230, err = 37.8%)
## |   |   |   |   |   [9] alcohol >= 9.85: 6 (n = 147, err = 51.7%)
## |   |   |   |   [10] fixed.acidity >= 10.05: 6 (n = 93, err = 43.0%)
## |   [11] alcohol >= 10.525
## |   |   [12] volatile.acidity >= 0.3625: 6 (n = 341, err = 44.6%)
## |   |   [13] volatile.acidity < 0.3625
## |   |   |   [14] alcohol < 10.75: 5 (n = 16, err = 50.0%)
## |   |   |   [15] alcohol >= 10.75
## |   |   |   |   [16] total.sulfur.dioxide >= 25.5
## |   |   |   |   |   [17] sulphates < 0.815: 6 (n = 58, err = 36.2%)
## |   |   |   |   |   [18] sulphates >= 0.815: 7 (n = 18, err = 27.8%)
## |   |   |   |   [19] total.sulfur.dioxide < 25.5: 7 (n = 64, err = 40.6%)
##
## Number of inner nodes:    9
## Number of terminal nodes: 10
```

```
plot(rpartTree2, gp = gpar(fontsize=4))
```




```
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(rpartTree2, newdata = wine_test)) -> df2

# Summary of predicted values
predict(rpartTree2, newdata = wine_test, interval = "prediction") %>%
  summary()
```

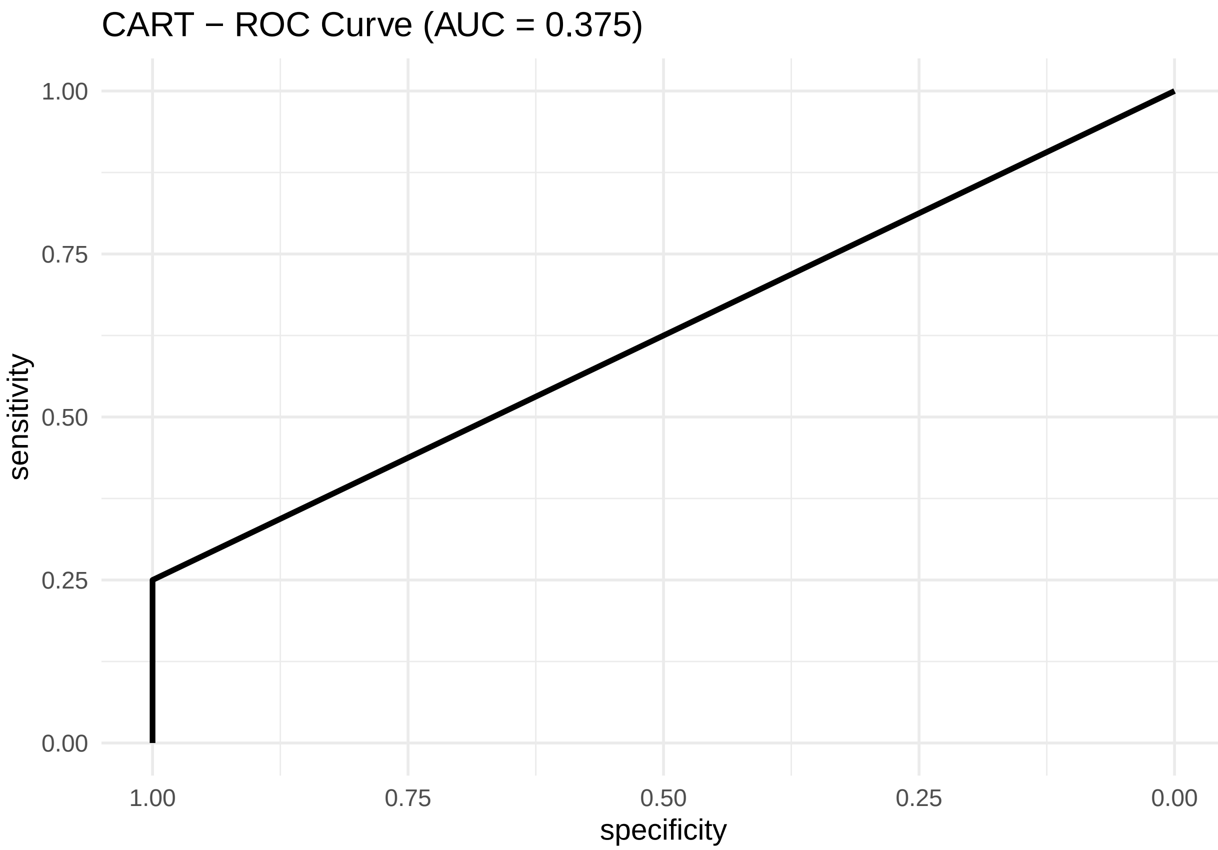
```
##    3    4    5    6    7    8
```

```
##   0   0 143 154  21   0
```

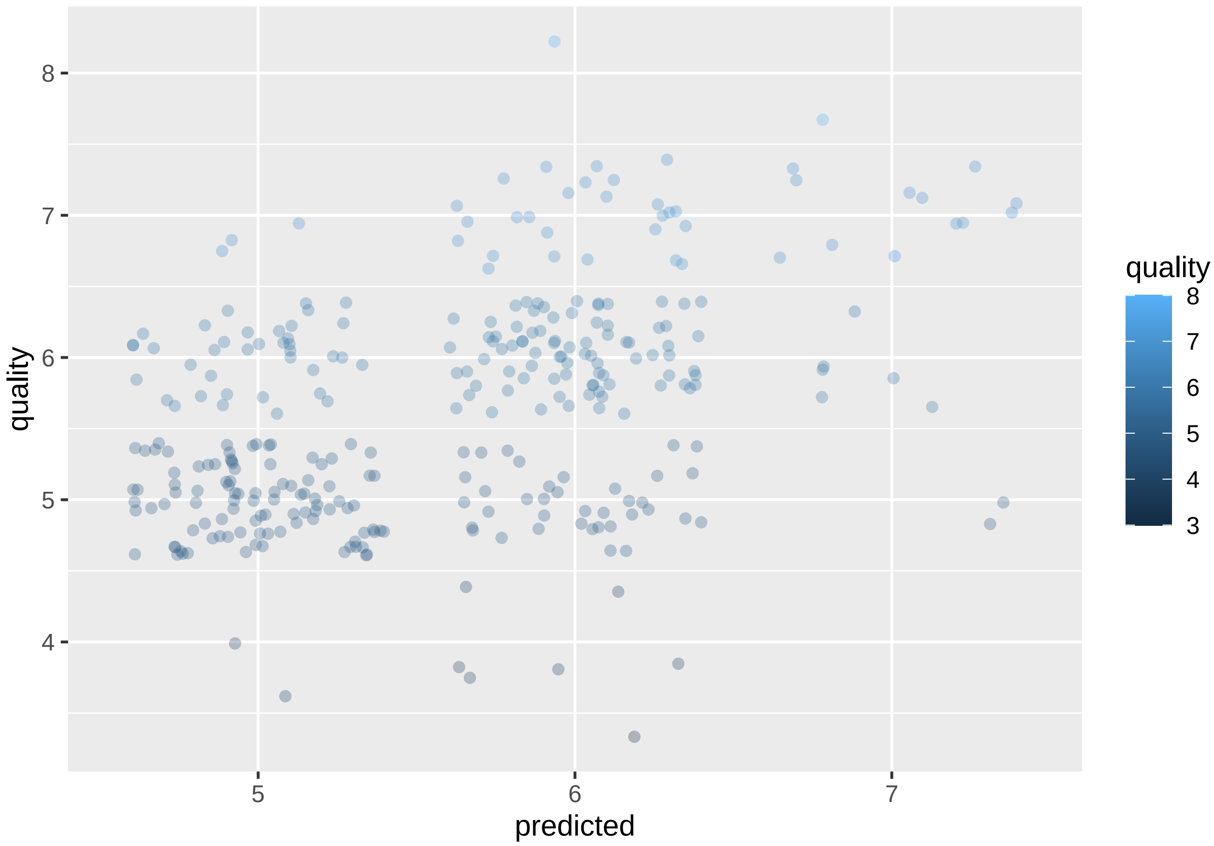
```r
# Confusion Matrix
confusionMatrix(table(df2$quality, df2$predicted))
```

```
## Confusion Matrix and Statistics
##
##
##       3   4   5   6   7   8
##   3   0   0   0   1   0   0
##   4   0   0   2   6   0   0
##   5   0   0 100  37   2   0
##   6   0   0  38  83   6   0
##   7   0   0   3  26  12   0
##   8   0   0   0   1   1   0
##
## Overall Statistics
##
##                Accuracy : 0.6132
##                  95% CI : (0.5573, 0.667)
##     No Information Rate : 0.4843
##     P-Value [Acc > NIR] : 2.6e-06
##
##                   Kappa : 0.357
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 3 Class: 4 Class: 5 Class: 6 Class: 7 Class: 8
## Sensitivity                NA       NA   0.6993   0.5390  0.57143       NA
## Specificity          0.996855  0.97484   0.7771   0.7317  0.90236 0.993711
## Pos Pred Value             NA       NA   0.7194   0.6535  0.29268       NA
## Neg Pred Value             NA       NA   0.7598   0.6283  0.96751       NA
## Prevalence           0.000000  0.00000   0.4497   0.4843  0.06604 0.000000
## Detection Rate       0.000000  0.00000   0.3145   0.2610  0.03774 0.000000
## Detection Prevalence 0.003145  0.02516   0.4371   0.3994  0.12893 0.006289
## Balanced Accuracy          NA       NA   0.7382   0.6353  0.73689       NA
```

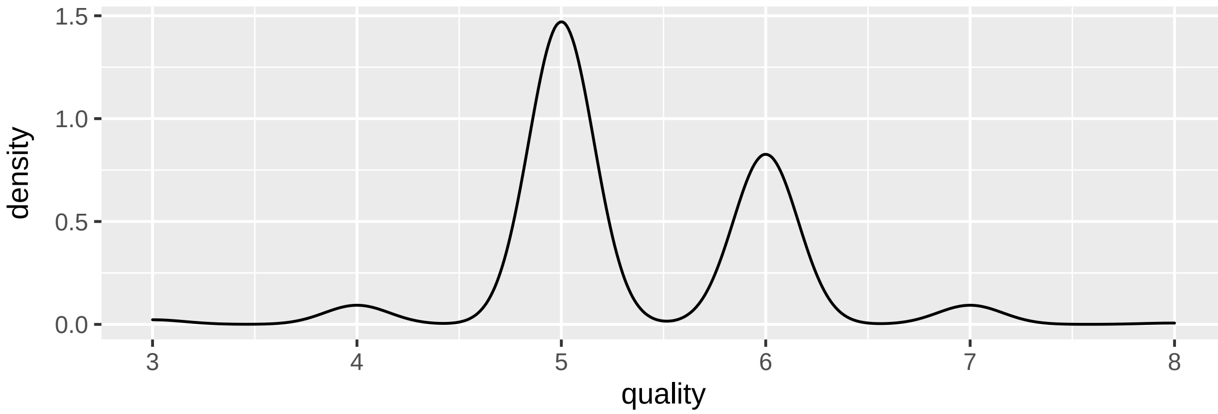
```r
# ROC plot
df2$predicted_int = round(as.numeric(as.character(df2$predicted)), digits = 0)

modelName2 <- 'CART'
roc2 <- roc(df2$quality, df2$predicted_int)
auc2 <- round(auc(df2$quality, df2$predicted_int), 4)

ggroc(roc1, colours = 'red', size = 1) +
  ggtitle(paste0(modelName2, ' - ROC Curve ', '(AUC = ', auc2 , ')')) + theme_minimal()
```

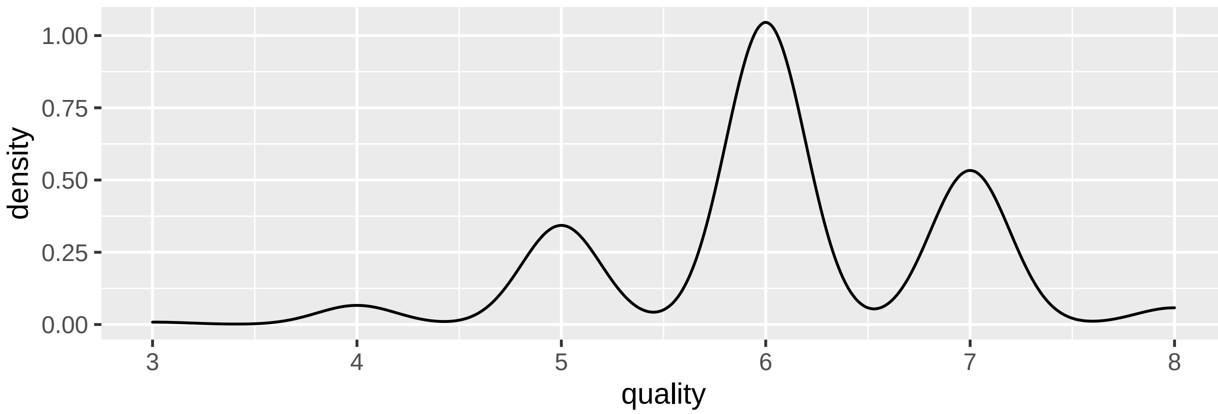



```r
# Scatter plot of predicted
ggplot(df2, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```




```
# Root Node Left vs Right, Quality Density Comparisons
grid.newpage()
filter(wine_train, alcohol < 10.525) %>%
  dplyr::select(quality, alcohol) %>%
  ggplot(aes(x = quality)) + geom_density() -> RootNodeLeft


filter(wine_train, alcohol >= 10.525) %>%
  dplyr::select(quality, alcohol) %>%
  ggplot(aes(x = quality)) + geom_density() -> RootNodeRight

grid.draw(rbind(ggplotGrob(RootNodeLeft), ggplotGrob(RootNodeRight), size = "last"))
```





Random Forest

```
set.seed(4)

rf <- rfsrc(quality ~ ., data = rf_wine_train)

print(rf)
```

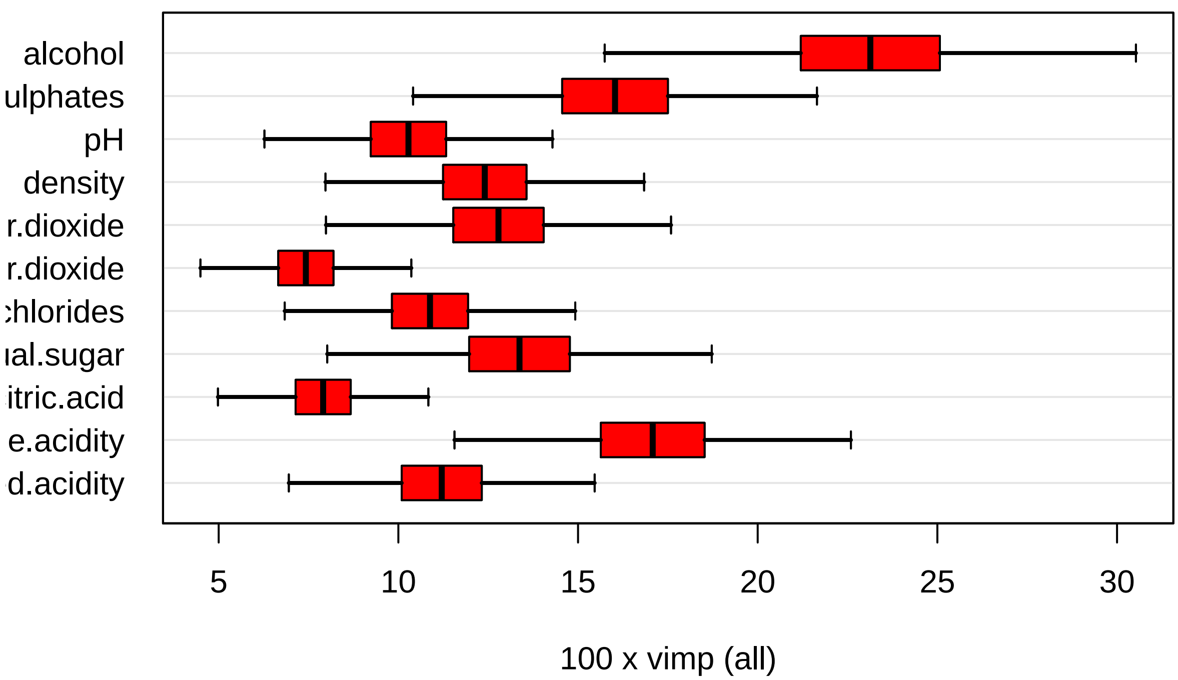
```
##                          Sample size: 1281
##            Frequency of class labels: 9, 45, 542, 511, 158, 16
##                      Number of trees: 500
##            Forest terminal node size: 1
##        Average no. of terminal nodes: 254.034
## No. of variables tried at each split: 4
##               Total no. of variables: 11
##        Resampling used to grow trees: swor
##     Resample size used to grow trees: 810
##                             Analysis: RF-C
##                               Family: class
##                       Splitting rule: gini
##                    (OOB) Brier score: 0.0694003
##         (OOB) Normalized Brier score: 0.49968218
##                            (OOB) AUC: 0.81564077
##    (OOB) Requested performance error: 0.30288837, 1, 0.97777778, 0.18819188, 0.2778865, 0.48734177, 0
##
```

```
## Confusion matrix:
##
##           predicted
##   observed 3 4   5   6  7 8 class.error
##          3 0 1   6   2  0 0      1.0000
##          4 0 1  27  16  1 0      0.9778
##          5 0 2 442  94  4 0      0.1845
##          6 0 2 105 370 34 0      0.2759
##          7 0 0   6  70 81 1      0.4873
##          8 0 0   0   9  5 2      0.8750
##
##       (OOB) Misclassification rate: 0.3005464
```

```r
# Variable Importance
vi <- subsample(rf, verbose = FALSE)

extract.subsample(vi)$var.jk.sel.Z
```

```
##                          lower      mean    upper       pvalue signif
## fixed.acidity         7.968889 11.207219 14.44555 5.883303e-12   TRUE
## volatile.acidity     12.880739 17.078132 21.27552 7.643822e-16   TRUE
## citric.acid           5.678804  7.907006 10.13521 1.761114e-12   TRUE
## residual.sugar        9.299919 13.371125 17.44233 6.087257e-11   TRUE
## chlorides             7.803877 10.880255 13.95663 2.077257e-12   TRUE
## free.sulfur.dioxide   5.193364  7.426327  9.65929 3.553201e-11   TRUE
## total.sulfur.dioxide  9.132848 12.786412 16.43998 3.459830e-12   TRUE
## density               9.031748 12.405096 15.77844 2.848544e-13   TRUE
## pH                    7.231599 10.281104 13.33061 1.950054e-11   TRUE
## sulphates            11.753794 16.029724 20.30565 1.009243e-13   TRUE
## alcohol              17.509637 23.134183 28.75873 3.768791e-16   TRUE
```

```r
# Variable Importance Plot
plot(vi)
```



```r
# Confusion Matrix
# https://www.rdocumentation.org/packages/randomForestSRC/versions/3.1.0/topics/predict.rfsrc
randomForestSRC::predict.rfsrc(rf, rf_wine_test)
```

```
##   Sample size of test (predict) data: 318
##                 Number of grow trees: 500
##   Average no. of grow terminal nodes: 254.034
##          Total no. of grow variables: 11
##        Resampling used to grow trees: swor
##     Resample size used to grow trees: 810
##                             Analysis: RF-C
##                               Family: class
##                          Brier score: 0.06901203
##               Normalized Brier score: 0.4968866
##                                  AUC: 0.84581745
##          Requested performance error: 0.31132075, 1, 1, 0.1942446, 0.2992126, 0.56097561, 1
##
## Confusion matrix:
##
##           predicted
##   observed 3 4   5  6  7 8 class.error
##          3 0 0   1  0  0 0      1.0000
##          4 0 0   6  2  0 0      1.0000
##          5 0 1 112 25  1 0      0.1942
##          6 0 0  36 89  2 0      0.2992
##          7 0 0   3 19 18 1      0.5610
##          8 0 0   0  1  1 0      1.0000
##
##           Misclassification error: 0.3113208
```

Partial Least Squares

```r
tctrl <- trainControl(method = "repeatedcv", repeats = 5, number =10)

set.seed(4)
pls_wine <- train(quality~ volatile.acidity + chlorides + total.sulfur.dioxide +
               sulphates + alcohol, data = wine_train,
                  method = "pls",
                  preProc = c("center", "scale", "BoxCox"),
                  tunelength =20,
                  trControl = tctrl)

pls_wine
```

```
## Partial Least Squares
##
## 1281 samples
##    5 predictor
##
## Pre-processing: centered (5), scaled (5), Box-Cox transformation (5)
## Resampling: Cross-Validated (10 fold, repeated 5 times)
## Summary of sample sizes: 1153, 1153, 1153, 1154, 1153, 1152, ...
```

```
## Resampling results across tuning parameters:
##
##   ncomp  RMSE       Rsquared   MAE
##   1      0.6576191  0.3546296  0.5091676
##   2      0.6570003  0.3558905  0.5088165
##   3      0.6569815  0.3559688  0.5079349
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was ncomp = 3.
```

```r
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(pls_wine, newdata = wine_test)) -> df3

# Summary of predicted interval
predict(pls_wine, newdata = wine_test, interval = "prediction") %>%
  summary()
```

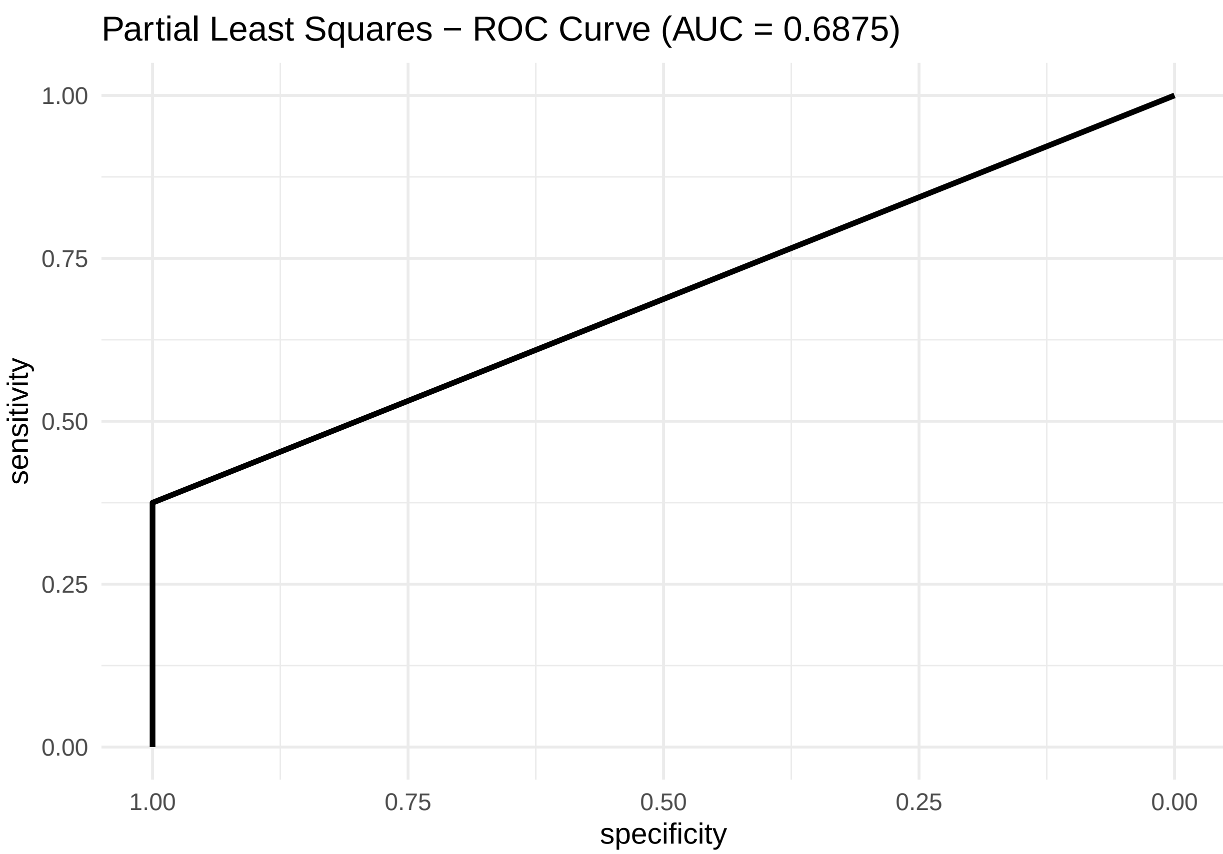
```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##   4.579   5.255   5.542   5.636   6.032   6.822
```

```r
# Confusion Matrix
# Convert predicted values to whole numbers, so they match target values
df3$predicted_int = as.integer(round(df3$predicted, digits = 0))

union3 <- union(df3$quality, df3$predicted_int)
table3 <- table(factor(df3$quality, union3), factor(df3$predicted_int, union3))

confusionMatrix(table3)
```

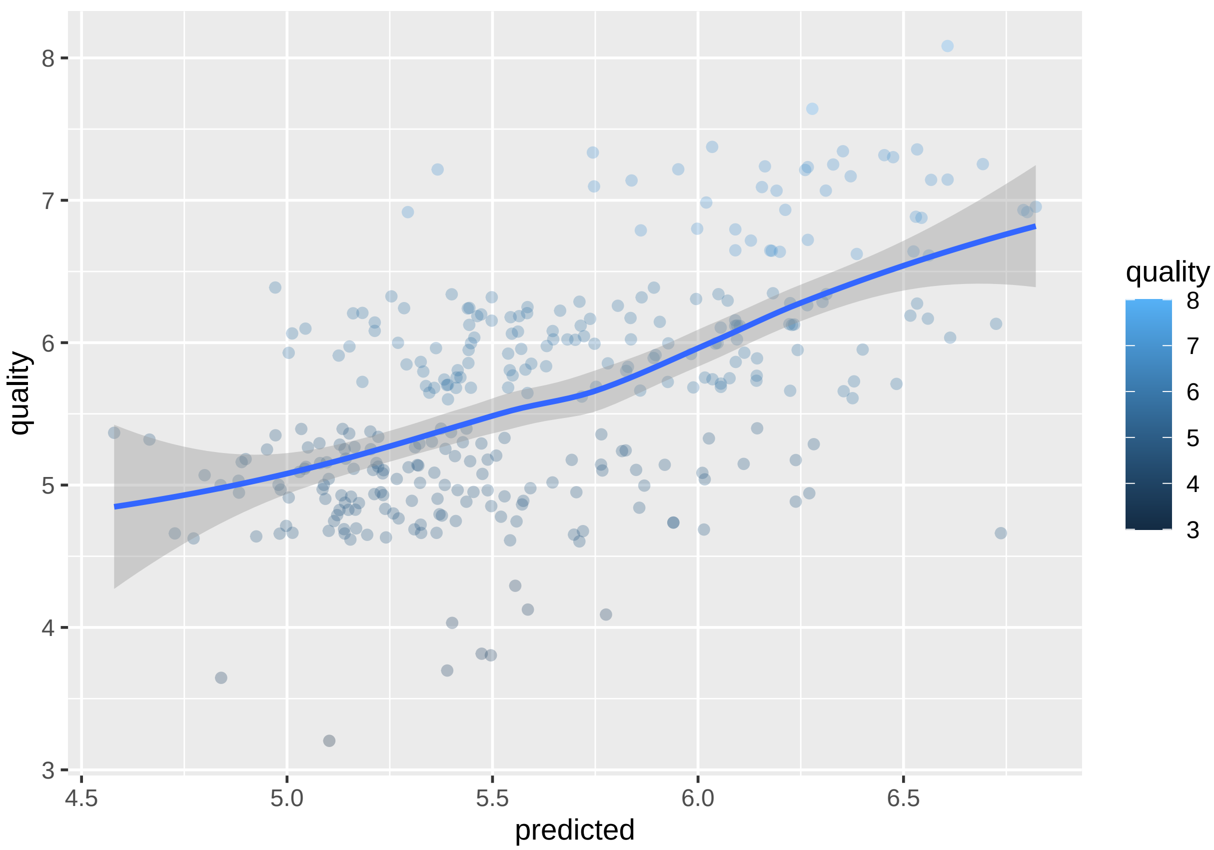
```
## Confusion Matrix and Statistics
##
##
##       5   7   6   4   8   3
##   5 102   1  36   0   0   0
##   7   2  11  28   0   0   0
##   6  42   5  80   0   0   0
##   4   5   0   3   0   0   0
##   8   0   1   1   0   0   0
##   3   1   0   0   0   0   0
##
## Overall Statistics
##
##                Accuracy : 0.6069
##                  95% CI : (0.5509, 0.661)
##     No Information Rate : 0.478
##     P-Value [Acc > NIR] : 2.631e-06
##
##                   Kappa : 0.3426
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 5 Class: 7 Class: 6 Class: 4 Class: 8 Class: 3
## Sensitivity            0.6711  0.61111   0.5405       NA       NA       NA
```

```
## Specificity            0.7771  0.90000   0.7235  0.97484 0.993711 0.996855
## Pos Pred Value         0.7338  0.26829   0.6299       NA       NA       NA
## Neg Pred Value         0.7207  0.97473   0.6440       NA       NA       NA
## Prevalence             0.4780  0.05660   0.4654  0.00000 0.000000 0.000000
## Detection Rate         0.3208  0.03459   0.2516  0.00000 0.000000 0.000000
## Detection Prevalence   0.4371  0.12893   0.3994  0.02516 0.006289 0.003145
## Balanced Accuracy      0.7241  0.75556   0.6320       NA       NA       NA
```

```
# ROC plot
df3$predicted_int = round(as.numeric(as.character(df3$predicted)), digits = 0)

modelName3 <- 'Partial Least Squares'
roc3 <- roc(df3$quality, df3$predicted_int)
auc3 <- round(auc(df3$quality, df3$predicted_int), 4)

ggroc(roc3, colours = 'red', size = 1) +
  ggtitle(paste0(modelName3, ' - ROC Curve ', '(AUC = ', auc3 , ')')) + theme_minimal()
```




```
# Scatter plot of predicted
ggplot(df3, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```



Mars Tuning

```
mars_wine <- earth(quality~ volatile.acidity + chlorides + total.sulfur.dioxide +
               sulphates + alcohol, data =wine_train)

mars_wine
```

```
## Selected 14 of 16 terms, and 5 of 5 predictors
## Termination condition: Reached nk 21
## Importance: alcohol, sulphates, volatile.acidity, total.sulfur.dioxide, ...
## Number of terms at each degree of interaction: 1 13 (additive model)
## GCV 0.4248782    RSS 521.5673    GRSq 0.3631477    RSq 0.388757
```

```
summary(mars_wine)
```

```
## Call: earth(formula=quality~volatile.acidity+chlorides+total.sulfur.di...),
##             data=wine_train)
##
##                               coefficients
## (Intercept)                      29.408320
## h(0.84-volatile.acidity)          0.830692
## h(volatile.acidity-0.84)         -1.983507
## h(chlorides-0.041)               38.221144
## h(0.152-chlorides)               39.984404
## h(chlorides-0.152)              -39.519916
## h(total.sulfur.dioxide-9)        -0.212396
```

```
## h(total.sulfur.dioxide-92)     -0.007246
## h(135-total.sulfur.dioxide)    -0.210830
## h(total.sulfur.dioxide-135)     0.228526
## h(0.82-sulphates)              -1.809642
## h(alcohol-9)                   -0.593061
## h(alcohol-9.6)                  0.453324
## h(12.5-alcohol)                -0.466959
##
## Selected 14 of 16 terms, and 5 of 5 predictors
## Termination condition: Reached nk 21
## Importance: alcohol, sulphates, volatile.acidity, total.sulfur.dioxide, ...
## Number of terms at each degree of interaction: 1 13 (additive model)
## GCV 0.4248782    RSS 521.5673    GRSq 0.3631477    RSq 0.388757
```

```
preProc_Arguments = c("center", "scale")
marsGrid_wine = expand.grid(.degree=1:2, .nprune=2:38)

set.seed(4)

marsModel_wine = train(quality~ volatile.acidity + chlorides + total.sulfur.dioxide +
                       sulphates + alcohol, data =wine_train,
                       method="earth",
                       preProc=preProc_Arguments,
                       tuneGrid=marsGrid_wine)

marsModel_wine
```

```
## Multivariate Adaptive Regression Spline
##
## 1281 samples
##    5 predictor
##
## Pre-processing: centered (5), scaled (5)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 1281, 1281, 1281, 1281, 1281, 1281, ...
## Resampling results across tuning parameters:
##
##   degree  nprune  RMSE       Rsquared   MAE
##   1        2      0.7233527  0.2262431  0.5666630
##   1        3      0.6868415  0.3022130  0.5295100
##   1        4      0.6657077  0.3447624  0.5160514
##   1        5      0.6661297  0.3445123  0.5154858
##   1        6      0.6657229  0.3452116  0.5156309
##   1        7      0.6664653  0.3442757  0.5154168
##   1        8      0.6650382  0.3471788  0.5139120
##   1        9      0.6678134  0.3427006  0.5146854
##   1       10      0.6678225  0.3431591  0.5147597
##   1       11      0.6690708  0.3411141  0.5152562
##   1       12      0.6724844  0.3351686  0.5172197
##   1       13      0.6725114  0.3353018  0.5171558
##   1       14      0.6738001  0.3332975  0.5179456
##   1       15      0.6739969  0.3329714  0.5180914
##   1       16      0.6741257  0.3327127  0.5181518
##   1       17      0.6741257  0.3327127  0.5181518
##   1       18      0.6741257  0.3327127  0.5181518
```

```
## 1 19 0.6741257 0.3327127 0.5181518
## 1 20 0.6741257 0.3327127 0.5181518
## 1 21 0.6741257 0.3327127 0.5181518
## 1 22 0.6741257 0.3327127 0.5181518
## 1 23 0.6741257 0.3327127 0.5181518
## 1 24 0.6741257 0.3327127 0.5181518
## 1 25 0.6741257 0.3327127 0.5181518
## 1 26 0.6741257 0.3327127 0.5181518
## 1 27 0.6741257 0.3327127 0.5181518
## 1 28 0.6741257 0.3327127 0.5181518
## 1 29 0.6741257 0.3327127 0.5181518
## 1 30 0.6741257 0.3327127 0.5181518
## 1 31 0.6741257 0.3327127 0.5181518
## 1 32 0.6741257 0.3327127 0.5181518
## 1 33 0.6741257 0.3327127 0.5181518
## 1 34 0.6741257 0.3327127 0.5181518
## 1 35 0.6741257 0.3327127 0.5181518
## 1 36 0.6741257 0.3327127 0.5181518
## 1 37 0.6741257 0.3327127 0.5181518
## 1 38 0.6741257 0.3327127 0.5181518
## 2  2 0.7231748 0.2268181 0.5654967
## 2  3 0.6868942 0.3017161 0.5284748
## 2  4 0.6631585 0.3501376 0.5110999
## 2  5 0.6624569 0.3546497 0.5108027
## 2  6 0.6620991 0.3563575 0.5088160
## 2  7 0.6618622 0.3567854 0.5087871
## 2  8 0.6615411 0.3577201 0.5081466
## 2  9 0.6666280 0.3504647 0.5100786
## 2 10 0.6716259 0.3427631 0.5125885
## 2 11 0.6701642 0.3454127 0.5114122
## 2 12 0.6715120 0.3432874 0.5122353
## 2 13 0.6729682 0.3412621 0.5127732
## 2 14 0.6751924 0.3396589 0.5130240
## 2 15 0.6752857 0.3394232 0.5132838
## 2 16 0.6760605 0.3382298 0.5136306
## 2 17 0.6759477 0.3383992 0.5135739
## 2 18 0.6759477 0.3383992 0.5135739
## 2 19 0.6759477 0.3383992 0.5135739
## 2 20 0.6759477 0.3383992 0.5135739
## 2 21 0.6759477 0.3383992 0.5135739
## 2 22 0.6759477 0.3383992 0.5135739
## 2 23 0.6759477 0.3383992 0.5135739
## 2 24 0.6759477 0.3383992 0.5135739
## 2 25 0.6759477 0.3383992 0.5135739
## 2 26 0.6759477 0.3383992 0.5135739
## 2 27 0.6759477 0.3383992 0.5135739
## 2 28 0.6759477 0.3383992 0.5135739
## 2 29 0.6759477 0.3383992 0.5135739
## 2 30 0.6759477 0.3383992 0.5135739
## 2 31 0.6759477 0.3383992 0.5135739
## 2 32 0.6759477 0.3383992 0.5135739
## 2 33 0.6759477 0.3383992 0.5135739
## 2 34 0.6759477 0.3383992 0.5135739
## 2 35 0.6759477 0.3383992 0.5135739
```

```
##   2       36      0.6759477  0.3383992  0.5135739
##   2       37      0.6759477  0.3383992  0.5135739
##   2       38      0.6759477  0.3383992  0.5135739
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were nprune = 8 and degree = 2.
```

```
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(marsModel_wine, newdata = wine_test)) -> df4

# Summary of predicted interval
predict(marsModel_wine, newdata = wine_test, interval = "prediction") %>%
  summary()
```

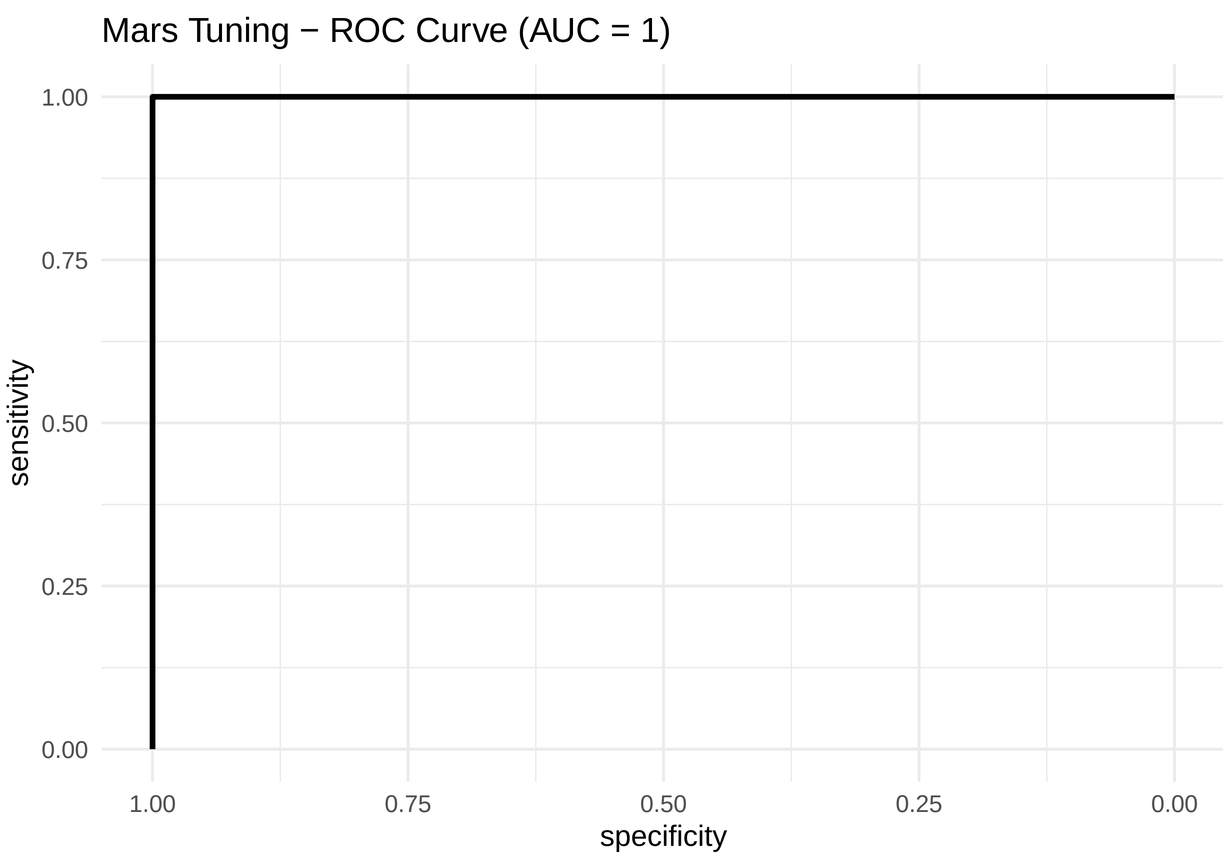
```
##        y
##  Min.   :4.045
##  1st Qu.:5.262
##  Median :5.493
##  Mean   :5.631
##  3rd Qu.:5.985
##  Max.   :7.158
```

```
# Confusion Matrix
# Convert predicted values to whole numbers, so they match target values
df4$predicted_int = as.integer(round(df4$predicted, digits = 0))

union4 <- union(df4$quality, df4$predicted_int)
table4 <- table(factor(df4$quality, union4), factor(df4$predicted_int, union4))

confusionMatrix(table4)
```

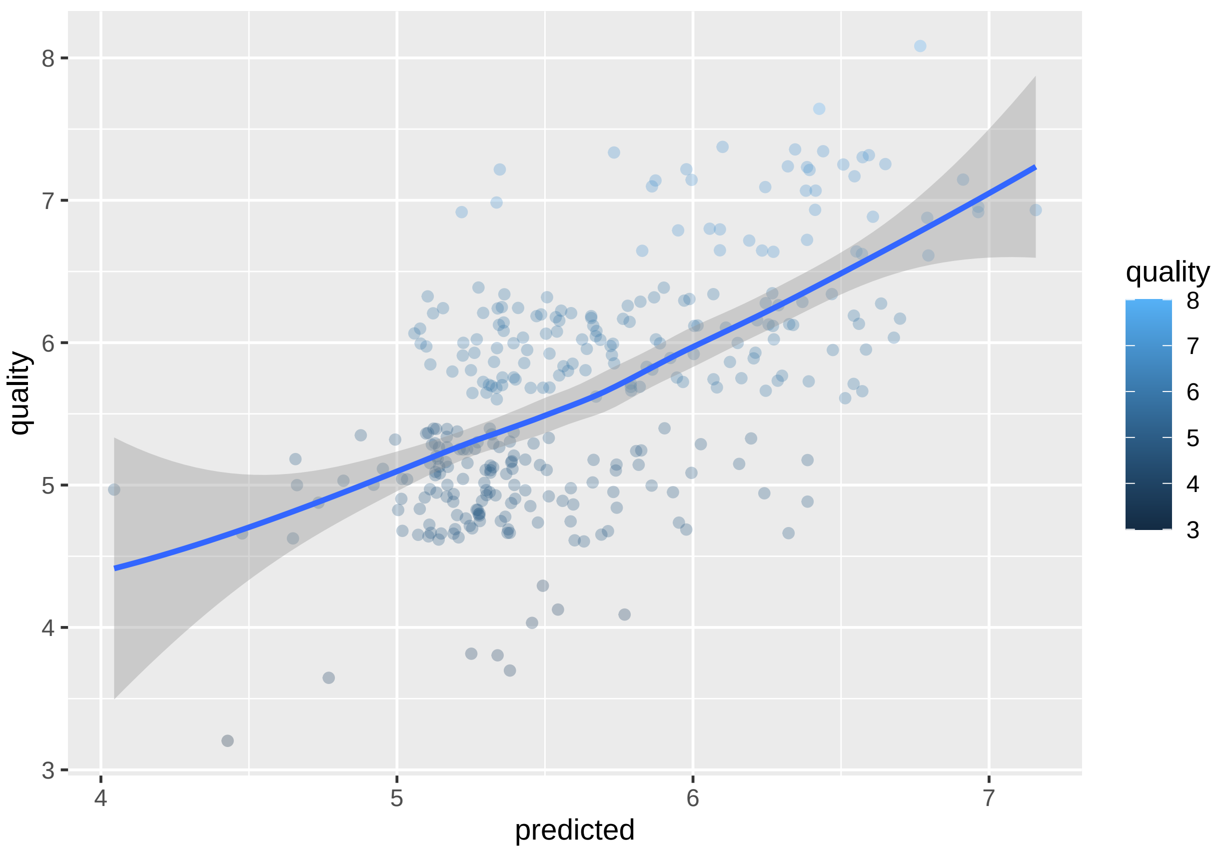
```
## Confusion Matrix and Statistics
##
##
##       5   7   6   4   8   3
##   5 104   0  33   2   0   0
##   7   3  14  24   0   0   0
##   6  44   9  74   0   0   0
##   4   6   0   2   0   0   0
##   8   0   1   1   0   0   0
##   3   0   0   0   1   0   0
##
## Overall Statistics
##
##                Accuracy : 0.6038
##                  95% CI : (0.5477, 0.6579)
##     No Information Rate : 0.4937
##     P-Value [Acc > NIR] : 5.208e-05
##
##                   Kappa : 0.3461
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
```

```
##                      Class: 5 Class: 7 Class: 6 Class: 4 Class: 8 Class: 3
## Sensitivity            0.6624  0.58333   0.5522 0.000000       NA       NA
## Specificity            0.7826  0.90816   0.7120 0.974603 0.993711 0.996855
## Pos Pred Value         0.7482  0.34146   0.5827 0.000000       NA       NA
## Neg Pred Value         0.7039  0.96390   0.6859 0.990323       NA       NA
## Prevalence             0.4937  0.07547   0.4214 0.009434 0.000000 0.000000
## Detection Rate         0.3270  0.04403   0.2327 0.000000 0.000000 0.000000
## Detection Prevalence   0.4371  0.12893   0.3994 0.025157 0.006289 0.003145
## Balanced Accuracy      0.7225  0.74575   0.6321 0.487302       NA       NA
```

```r
# ROC plot
df4$predicted_int = round(as.numeric(as.character(df4$predicted)), digits = 0)

modelName4 <- 'Mars Tuning'
roc4 <- roc(df4$quality, df4$predicted_int)
auc4 <- round(auc(df4$quality, df4$predicted_int), 4)

ggroc(roc4, colours = 'red', size = 1) +
  ggtitle(paste0(modelName4, ' - ROC Curve ', '(AUC = ', auc4 , ')')) + theme_minimal()
```




```r
# Scatter plot of predicted
ggplot(df4, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```



KNN Neighbors

```
set.seed(4)

knn_wine <- train(quality~ volatile.acidity + chlorides + total.sulfur.dioxide +
               sulphates + alcohol, data =wine_train,
               method = "knn",
               preProc = c("center", "scale"),
               tuneGrid = data.frame(.k = 1:50),
               trControl = trainControl(method = "cv"))

knn_wine
```

```
## k-Nearest Neighbors
##
## 1281 samples
##    5 predictor
##
## Pre-processing: centered (5), scaled (5)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1153, 1153, 1153, 1154, 1153, 1152, ...
## Resampling results across tuning parameters:
##
##   k   RMSE       Rsquared   MAE
##    1  0.7611645  0.3095018  0.4418281
```

```
##    2  0.7059464  0.3221223  0.4923622
##    3  0.6978592  0.3201862  0.4995266
##    4  0.6918078  0.3179160  0.5105364
##    5  0.6774652  0.3336540  0.5054629
##    6  0.6667031  0.3468976  0.5008060
##    7  0.6586993  0.3588673  0.4951389
##    8  0.6537894  0.3649030  0.4946392
##    9  0.6532109  0.3637033  0.4973384
##   10  0.6544274  0.3609880  0.4999216
##   11  0.6521244  0.3649248  0.4998247
##   12  0.6522693  0.3644235  0.4995611
##   13  0.6522334  0.3645066  0.4987153
##   14  0.6512748  0.3666665  0.4973378
##   15  0.6501829  0.3685282  0.4972328
##   16  0.6516641  0.3656231  0.4991521
##   17  0.6496509  0.3694799  0.4970775
##   18  0.6488745  0.3707600  0.4977312
##   19  0.6482618  0.3717198  0.4976589
##   20  0.6489652  0.3706964  0.4986046
##   21  0.6504049  0.3680175  0.4996562
##   22  0.6505565  0.3679427  0.5007805
##   23  0.6502980  0.3687124  0.5005675
##   24  0.6486853  0.3721803  0.4990811
##   25  0.6497087  0.3704544  0.4998703
##   26  0.6481956  0.3733048  0.4989776
##   27  0.6476405  0.3746132  0.4985409
##   28  0.6483439  0.3730679  0.5003046
##   29  0.6487146  0.3726818  0.5006378
##   30  0.6486947  0.3729127  0.5005301
##   31  0.6490613  0.3723327  0.5007166
##   32  0.6489346  0.3727020  0.5010819
##   33  0.6484185  0.3741388  0.5012523
##   34  0.6482329  0.3744969  0.5015616
##   35  0.6484952  0.3741138  0.5016705
##   36  0.6494802  0.3724373  0.5022773
##   37  0.6501885  0.3711916  0.5023928
##   38  0.6498152  0.3721481  0.5021523
##   39  0.6498068  0.3722171  0.5024646
##   40  0.6491849  0.3732611  0.5022056
##   41  0.6495999  0.3726338  0.5021190
##   42  0.6485574  0.3745594  0.5013595
##   43  0.6486343  0.3742573  0.5016012
##   44  0.6483522  0.3749460  0.5016836
##   45  0.6480208  0.3756090  0.5012867
##   46  0.6477996  0.3759857  0.5015260
##   47  0.6474121  0.3767748  0.5013182
##   48  0.6471637  0.3774581  0.5016746
##   49  0.6471179  0.3776970  0.5017991
##   50  0.6472295  0.3776650  0.5016013
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 49.
```

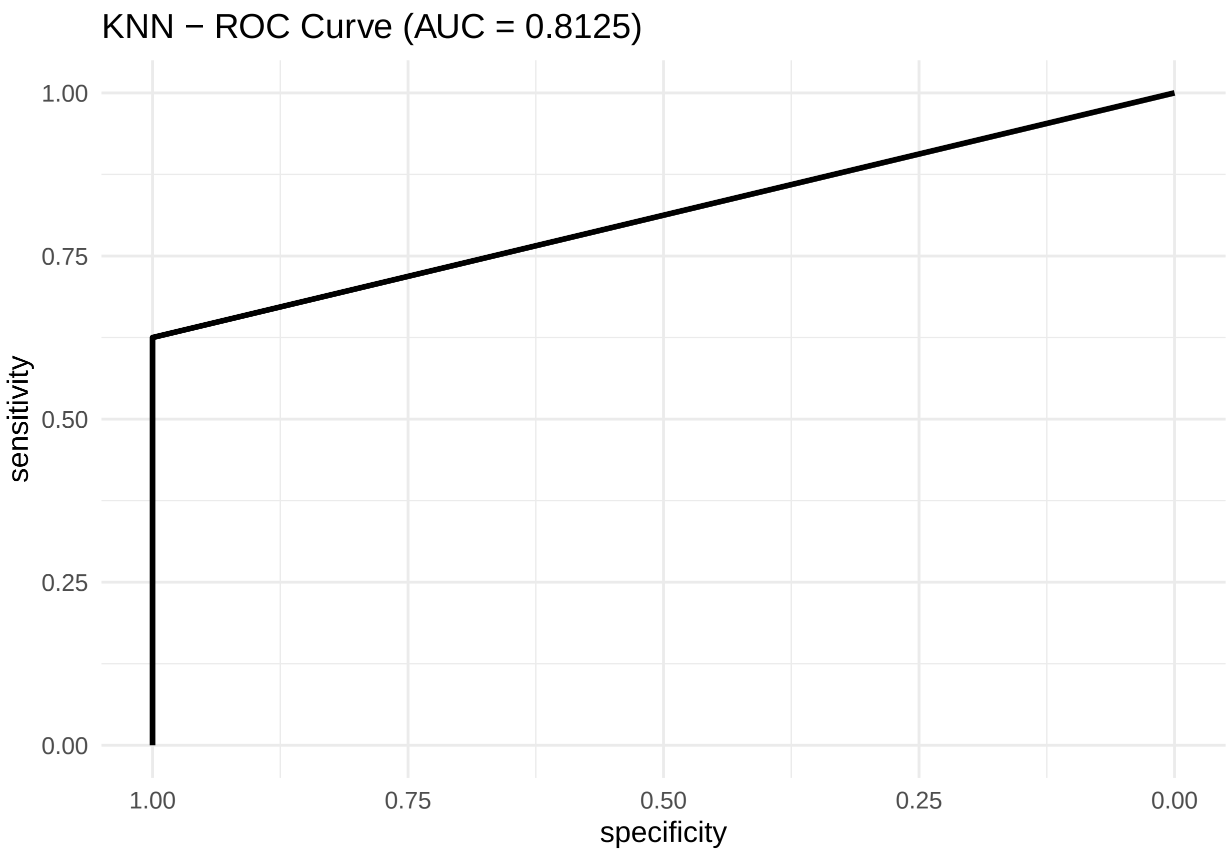
```r
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(knn_wine, newdata = wine_test)) -> df5

# Summary of predicted interval
predict(knn_wine, newdata = wine_test, interval = "prediction") %>%
  summary()
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##   4.878   5.265   5.551   5.651   6.000   6.796
```

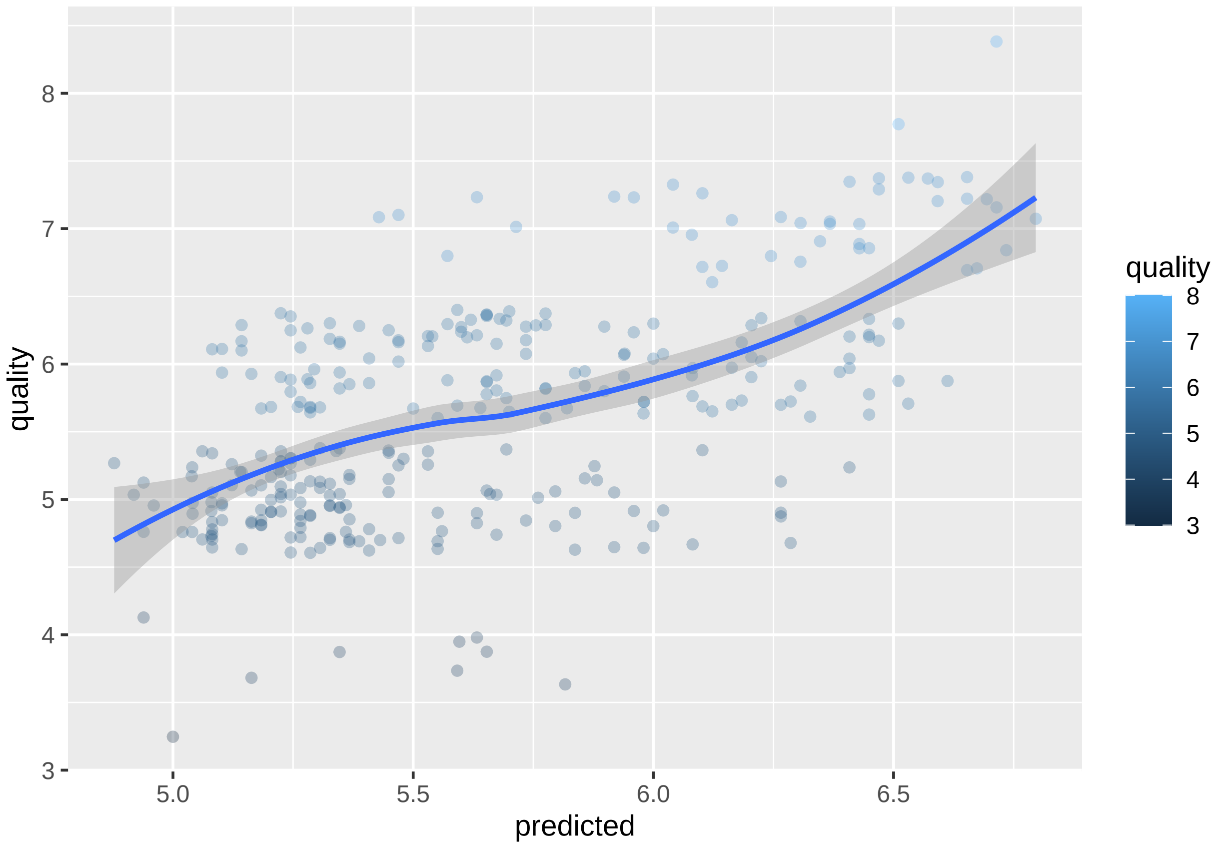
```r
# Confusion Matrix
# Convert predicted values to whole numbers, so they match target values
df5$predicted_int = as.integer(round(df5$predicted, digits = 0))

union5 <- union(df5$quality, df5$predicted_int)
table5 <- table(factor(df5$quality, union5), factor(df5$predicted_int, union5))

confusionMatrix(table5)
```

```
## Confusion Matrix and Statistics
##
##
##       5   7   6   4   8   3
##   5 104   0  35   0   0   0
##   7   2  12  27   0   0   0
##   6  40   4  83   0   0   0
##   4   3   0   5   0   0   0
##   8   0   2   0   0   0   0
##   3   1   0   0   0   0   0
##
## Overall Statistics
##
##                Accuracy : 0.6258
##                  95% CI : (0.5701, 0.6792)
##     No Information Rate : 0.4717
##     P-Value [Acc > NIR] : 2.392e-08
##
##                   Kappa : 0.3744
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 5 Class: 7 Class: 6 Class: 4 Class: 8 Class: 3
## Sensitivity            0.6933  0.66667   0.5533       NA       NA       NA
## Specificity            0.7917  0.90333   0.7381  0.97484 0.993711 0.996855
## Pos Pred Value         0.7482  0.29268   0.6535       NA       NA       NA
## Neg Pred Value         0.7430  0.97834   0.6492       NA       NA       NA
## Prevalence             0.4717  0.05660   0.4717  0.00000 0.000000 0.000000
## Detection Rate         0.3270  0.03774   0.2610  0.00000 0.000000 0.000000
## Detection Prevalence   0.4371  0.12893   0.3994  0.02516 0.006289 0.003145
## Balanced Accuracy      0.7425  0.78500   0.6457       NA       NA       NA
```

```r
# ROC plot
df5$predicted_int = round(as.numeric(as.character(df5$predicted)), digits = 0)

modelName5 <- 'KNN'
roc5 <- roc(df5$quality, df5$predicted_int)
auc5 <- round(auc(df5$quality, df5$predicted_int), 4)

ggroc(roc5, colours = 'red', size = 1) +
  ggtitle(paste0(modelName5, ' - ROC Curve ', '(AUC = ', auc5 , ')')) + theme_minimal()
```




```r
# Scatter plot of predicted
ggplot(df5, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```



SVM

```
set.seed(4)


svmTune <- train(quality ~ volatile.acidity + sulphates + alcohol, data = rf_wine_train, # using the su
                 method = "svmRadial",
                 preProc = c("center", "scale"),
                 tuneLength= 5,
                 trControl = trainControl(method = "cv"))
svmTune
```

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 1281 samples
##    3 predictor
##    6 classes: '3', '4', '5', '6', '7', '8'
##
## Pre-processing: centered (3), scaled (3)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1153, 1154, 1152, 1151, 1154, 1153, ...
## Resampling results across tuning parameters:
##
##   C     Accuracy   Kappa
##   0.25  0.5877289  0.3089678
```

```
##   0.50  0.5892976  0.3141981
##   1.00  0.5861540  0.3116337
##   2.00  0.5877290  0.3191442
##   4.00  0.5923682  0.3275874
##
## Tuning parameter 'sigma' was held constant at a value of 0.5592836
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were sigma = 0.5592836 and C = 4.
```

```r
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(svmTune, newdata = wine_test)) -> df6

# Summary of predicted interval
predict(svmTune, newdata = wine_test, interval = "prediction") %>%
  summary()
```

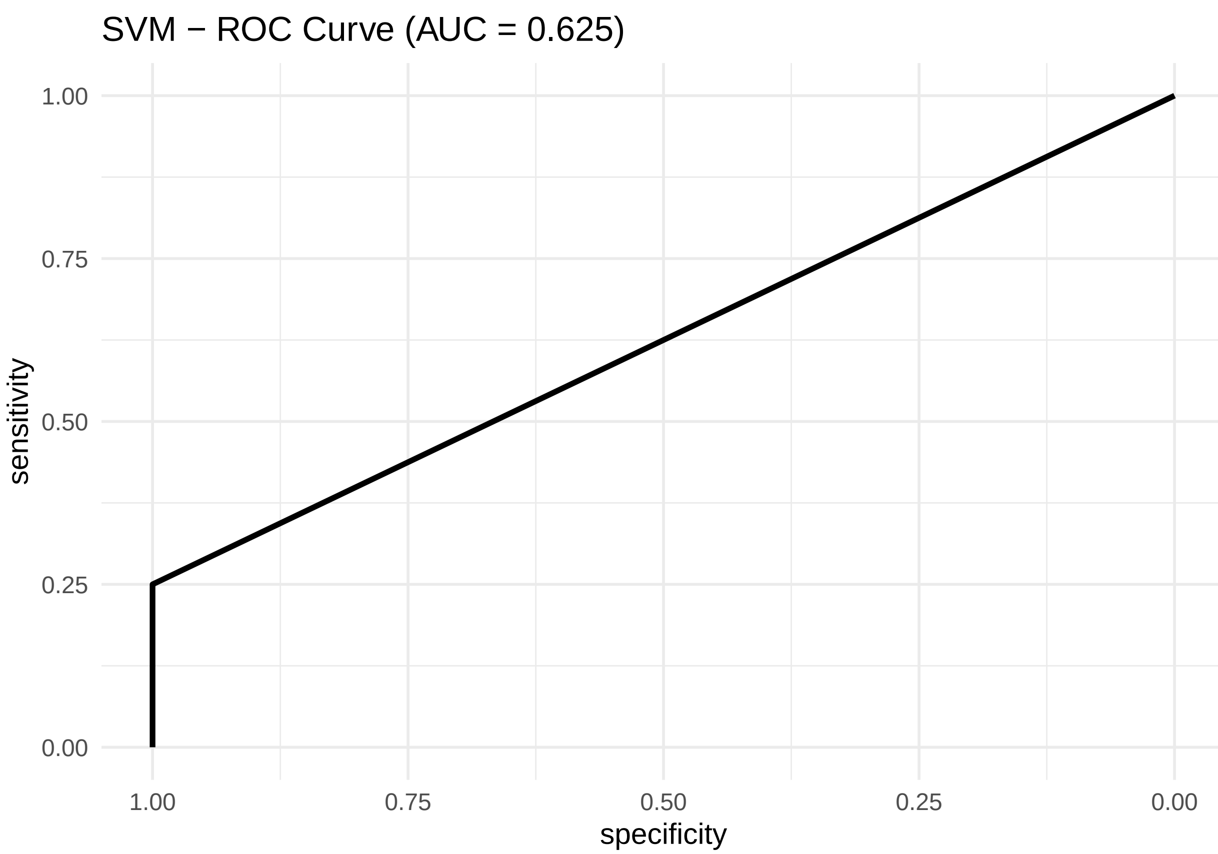
```
##   3   4   5   6   7   8
##   0   1 162 133  22   0
```

```r
# Confusion Matrix
confusionMatrix(table(df6$quality, df6$predicted))
```

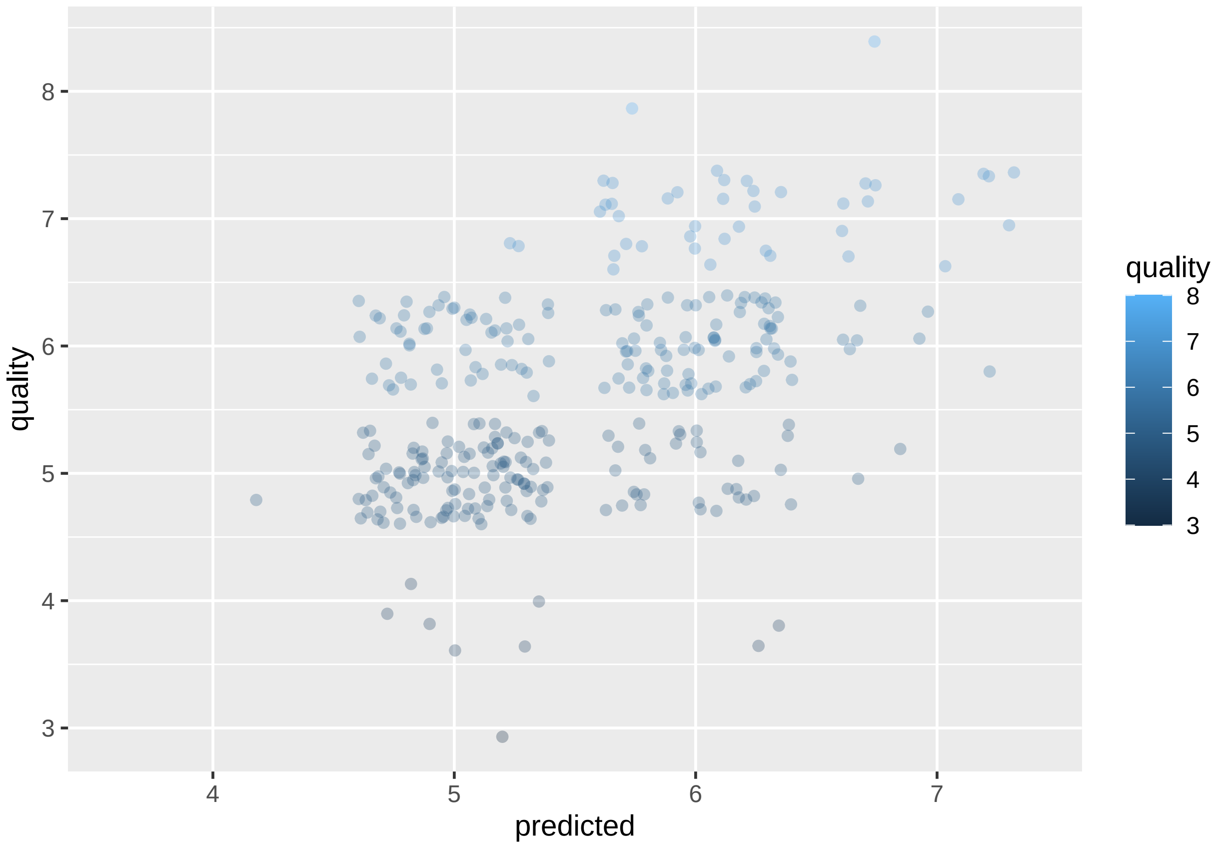
```
## Confusion Matrix and Statistics
##
##
##       3   4   5   6   7   8
##   3   0   0   1   0   0   0
##   4   0   0   6   2   0   0
##   5   0   1 105  31   2   0
##   6   0   0  48  72   7   0
##   7   0   0   2  27  12   0
##   8   0   0   0   1   1   0
##
## Overall Statistics
##
##                Accuracy : 0.5943
##                  95% CI : (0.5381, 0.6488)
##     No Information Rate : 0.5094
##     P-Value [Acc > NIR] : 0.001434
##
##                   Kappa : 0.3254
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 3 Class: 4 Class: 5 Class: 6 Class: 7 Class: 8
## Sensitivity                NA 0.000000   0.6481   0.5414  0.54545       NA
## Specificity          0.996855 0.974763   0.7821   0.7027  0.90203 0.993711
## Pos Pred Value             NA 0.000000   0.7554   0.5669  0.29268       NA
## Neg Pred Value             NA 0.996774   0.6816   0.6806  0.96390       NA
## Prevalence           0.000000 0.003145   0.5094   0.4182  0.06918 0.000000
## Detection Rate       0.000000 0.000000   0.3302   0.2264  0.03774 0.000000
## Detection Prevalence 0.003145 0.025157   0.4371   0.3994  0.12893 0.006289
```

```
## Balanced Accuracy          NA 0.487382   0.7151   0.6220  0.72374       NA
```

```r
# ROC plot
df6$predicted_int = round(as.numeric(as.character(df6$predicted)), digits = 0)

modelName6 <- 'SVM'
roc6 <- roc(df6$quality, df6$predicted_int)
auc6 <- round(auc(df6$quality, df6$predicted_int), 4)

ggroc(roc6, colours = 'red', size = 1) +
  ggtitle(paste0(modelName6, ' - ROC Curve ', '(AUC = ', auc6 , ')')) + theme_minimal()
```




```r
# Scatter plot of predicted
ggplot(df6, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```



Penalized Logistic Regression Tuning

```r
#tuning parameters, alpha is associated with the ridge(0) versus lasso regression(1)
glmnGrid <- expand.grid(alpha = c(0,  .1,  .2, .4, .6, .8, 1),
                        lambda = seq(.01, .2, length = 5))
glmnTune <- train(quality ~ ., data = rf_wine_train, # using the subset data as used in random forest,
                 method = "glmnet",
                 tuneGrid = glmnGrid,
                 preProc = c("center", "scale"),
                 trControl = trainControl(method = "cv"))
glmnTune
```

```
## glmnet
##
## 1281 samples
##   11 predictor
##    6 classes: '3', '4', '5', '6', '7', '8'
##
## Pre-processing: centered (11), scaled (11)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1152, 1153, 1153, 1153, 1152, 1153, ...
## Resampling results across tuning parameters:
##
##   alpha  lambda  Accuracy   Kappa
##   0.0    0.0100  0.5885118  0.3162331
```

```
##   0.0    0.0575  0.5822860  0.2987068
##   0.0    0.1050  0.5768173  0.2840738
##   0.0    0.1525  0.5791549  0.2860009
##   0.0    0.2000  0.5815109  0.2891512
##   0.1    0.0100  0.5893053  0.3205317
##   0.1    0.0575  0.5799362  0.2926301
##   0.1    0.1050  0.5799484  0.2875440
##   0.1    0.1525  0.5814985  0.2890215
##   0.1    0.2000  0.5728985  0.2741068
##   0.2    0.0100  0.5877184  0.3160999
##   0.2    0.0575  0.5783858  0.2886395
##   0.2    0.1050  0.5775800  0.2825011
##   0.2    0.1525  0.5705670  0.2701028
##   0.2    0.2000  0.5690290  0.2667256
##   0.4    0.0100  0.5869371  0.3144909
##   0.4    0.0575  0.5783613  0.2855434
##   0.4    0.1050  0.5689984  0.2672190
##   0.4    0.1525  0.5697922  0.2676438
##   0.4    0.2000  0.5580733  0.2471184
##   0.6    0.0100  0.5877306  0.3139489
##   0.6    0.0575  0.5666546  0.2647442
##   0.6    0.1050  0.5705612  0.2690615
##   0.6    0.1525  0.5479108  0.2294916
##   0.6    0.2000  0.5510361  0.2335781
##   0.8    0.0100  0.5861681  0.3104682
##   0.8    0.0575  0.5705427  0.2702880
##   0.8    0.1050  0.5549422  0.2420563
##   0.8    0.1525  0.5549425  0.2407836
##   0.8    0.2000  0.5370280  0.2087613
##   1.0    0.0100  0.5830552  0.3047040
##   1.0    0.0575  0.5728866  0.2735412
##   1.0    0.1050  0.5541673  0.2397724
##   1.0    0.1525  0.5471541  0.2268064
##   1.0    0.2000  0.4387409  0.0288173
##
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were alpha = 0.1 and lambda = 0.01.
```

```r
# Add predicted values to new data frame
wine_test %>%
  mutate(predicted = predict(glmnTune, newdata = wine_test)) -> df7

# Summary of predicted interval
predict(svmTune, newdata = wine_test, interval = "prediction") %>%
  summary()
```

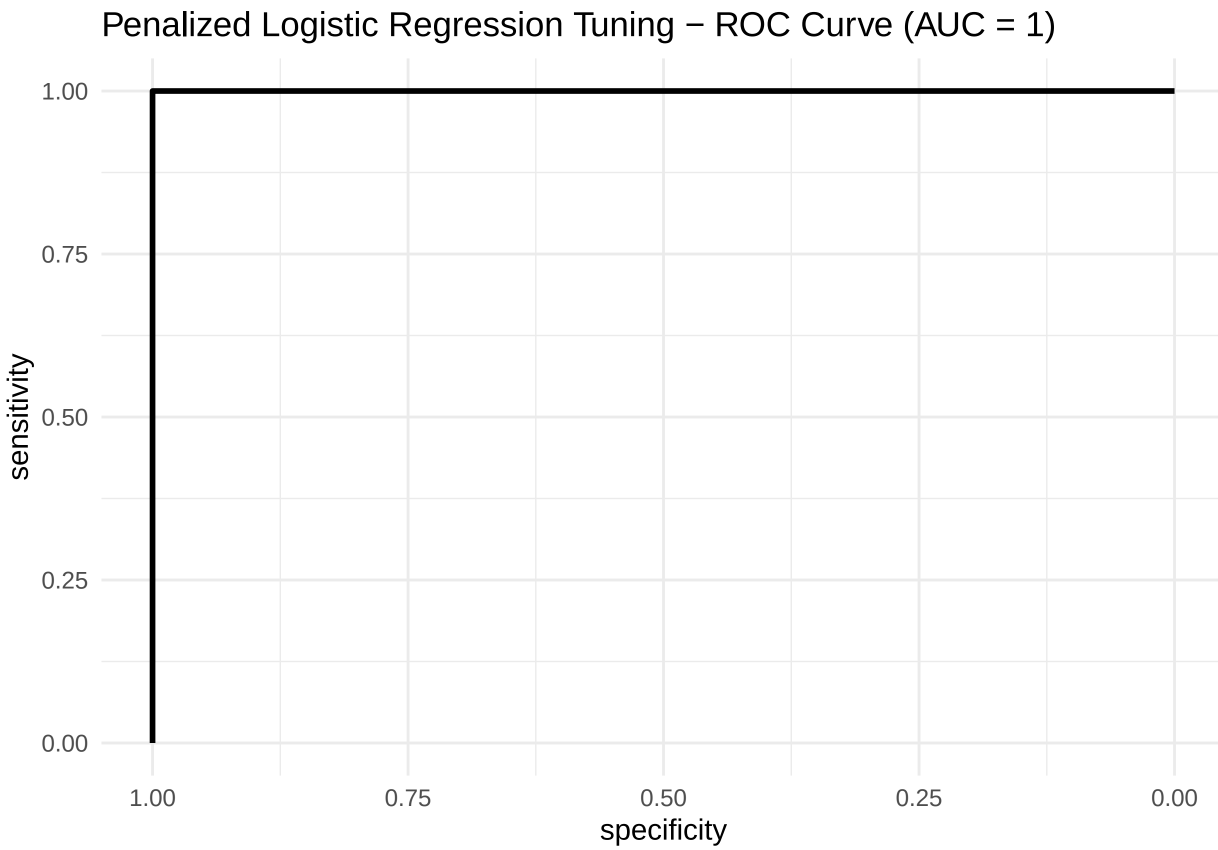
```
##   3   4   5   6   7   8
##   0   1 162 133  22   0
```

```r
# Confusion Matrix
confusionMatrix(table(df7$quality, df7$predicted))
```

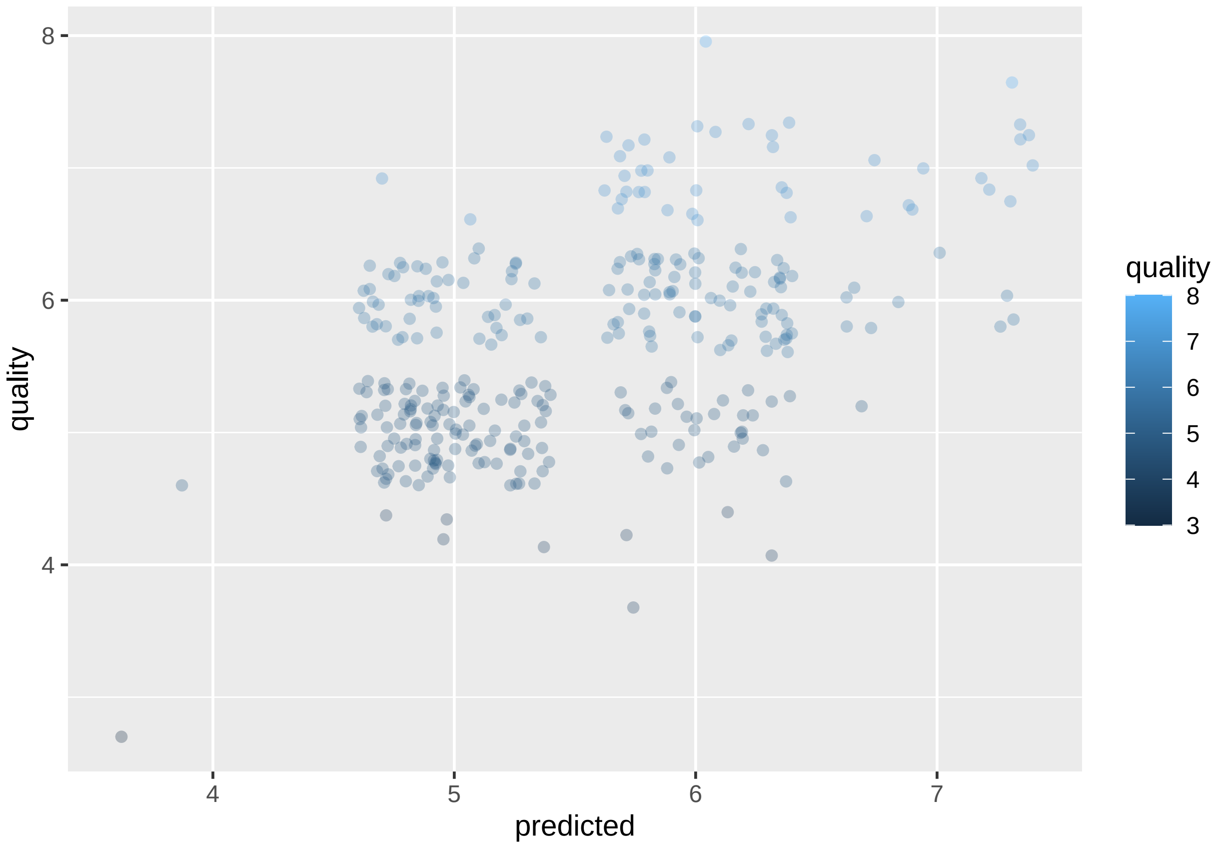
```
## Confusion Matrix and Statistics
##
##
```

```
##       3   4   5   6   7   8
##   3   0   1   0   0   0   0
##   4   0   0   4   4   0   0
##   5   0   1 107  30   1   0
##   6   0   0  48  70   9   0
##   7   0   0   2  27  12   0
##   8   0   0   0   1   1   0
##
## Overall Statistics
##
##                Accuracy : 0.5943
##                  95% CI : (0.5381, 0.6488)
##     No Information Rate : 0.5063
##     P-Value [Acc > NIR] : 0.0009891
##
##                   Kappa : 0.3278
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 3 Class: 4 Class: 5 Class: 6 Class: 7 Class: 8
## Sensitivity                NA 0.000000   0.6646   0.5303  0.52174       NA
## Specificity          0.996855 0.974684   0.7962   0.6935  0.90169 0.993711
## Pos Pred Value             NA 0.000000   0.7698   0.5512  0.29268       NA
## Neg Pred Value             NA 0.993548   0.6983   0.6754  0.96029       NA
## Prevalence           0.000000 0.006289   0.5063   0.4151  0.07233 0.000000
## Detection Rate       0.000000 0.000000   0.3365   0.2201  0.03774 0.000000
## Detection Prevalence 0.003145 0.025157   0.4371   0.3994  0.12893 0.006289
## Balanced Accuracy          NA 0.487342   0.7304   0.6119  0.71172       NA
```

```r
# ROC plot
df7$predicted_int = round(as.numeric(as.character(df7$predicted)), digits = 0)

modelName7 <- 'Penalized Logistic Regression Tuning'
roc7 <- roc(df7$quality, df7$predicted_int)
auc7 <- round(auc(df7$quality, df7$predicted_int), 4)

ggroc(roc7, colours = 'red', size = 1) +
  ggtitle(paste0(modelName7, ' - ROC Curve ', '(AUC = ', auc7 , ')')) + theme_minimal()
```




```
# Scatter plot of predicted
ggplot(df7, aes(x = predicted, y = quality, colour = quality ))+
geom_point(alpha = 0.3, position = position_jitter()) + stat_smooth()
```



quality
8
6
4
4
5
6
7
predicted
quality
8
7
6
5
4
3