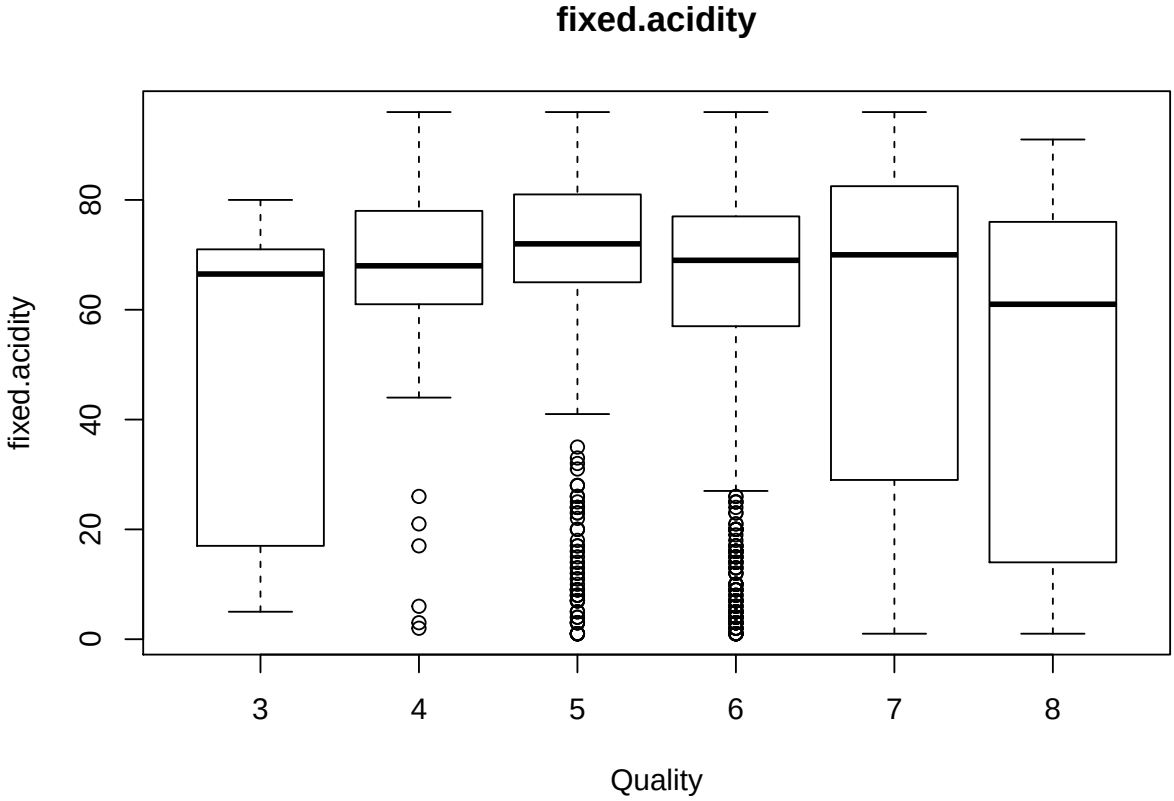
Bruce Campbell Final Project

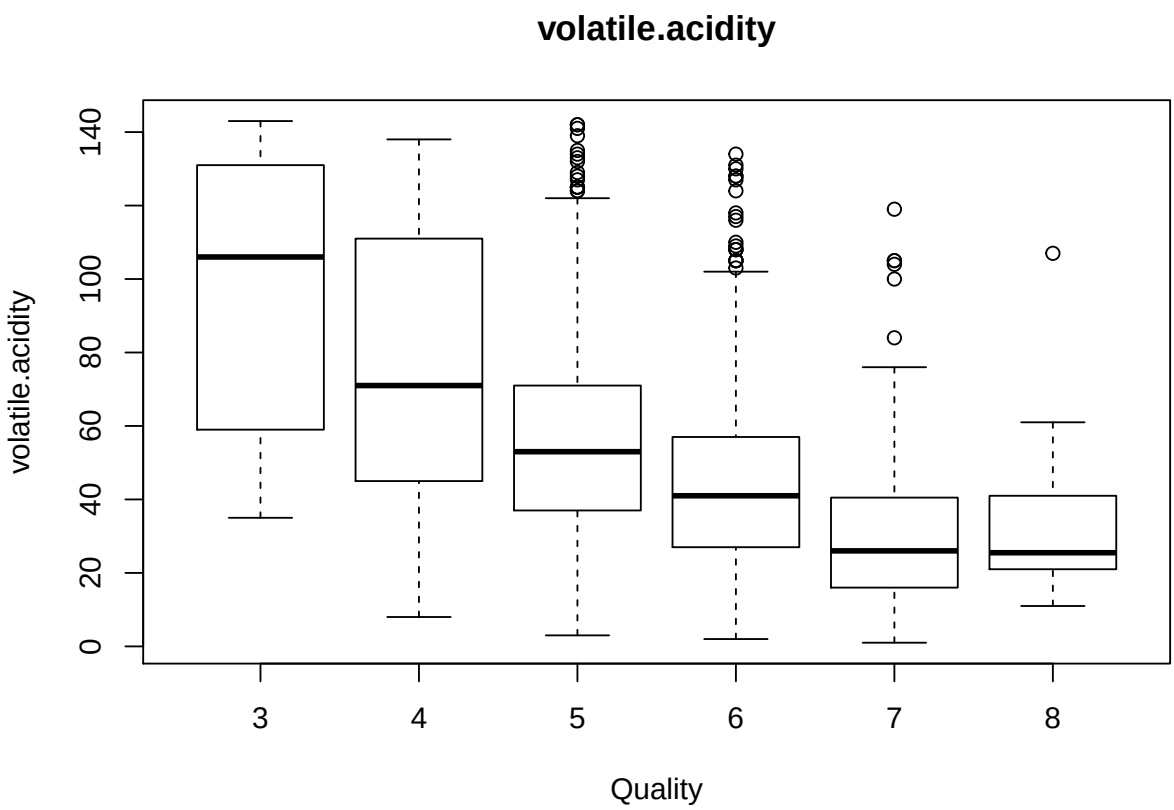
Thu Jul 28 15:02:46 2016

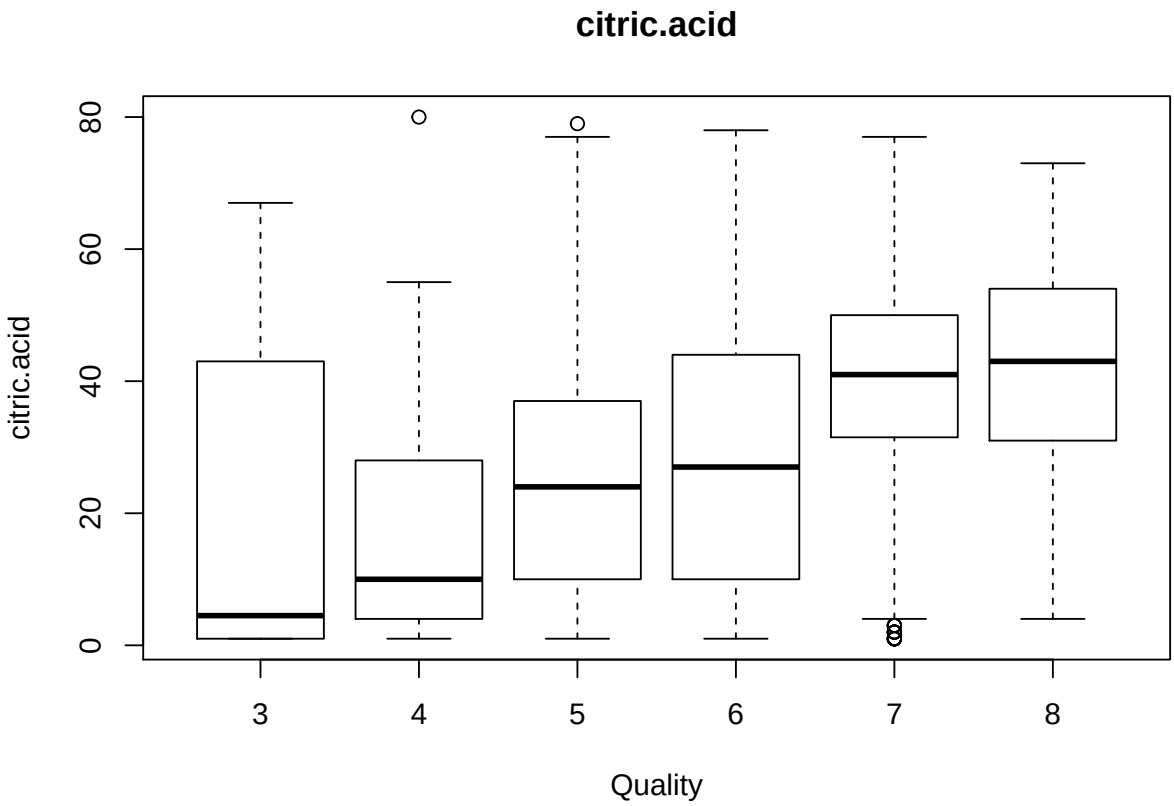
```
rm(list = ls())
set.seed(7)

setwd("C:/st-617/")

## use read.csv2 since data fields are delimited by semicolons (;)

cls = c(rep("numeric", 11), "integer")

wine.data <- read.csv2("FinalProject/winequality-red.csv")

# Specifying the data type via colClasses did not work - so we sapply
# as.numeric to convert the factor data to numeric.  We may want to convert
# some of the variables to factors later - but for visualization of the raw
# features we should use numeric type.
wine.data[, c(1:12)] <- sapply(wine.data[, c(1:12)], as.numeric)

DF <- wine.data
```

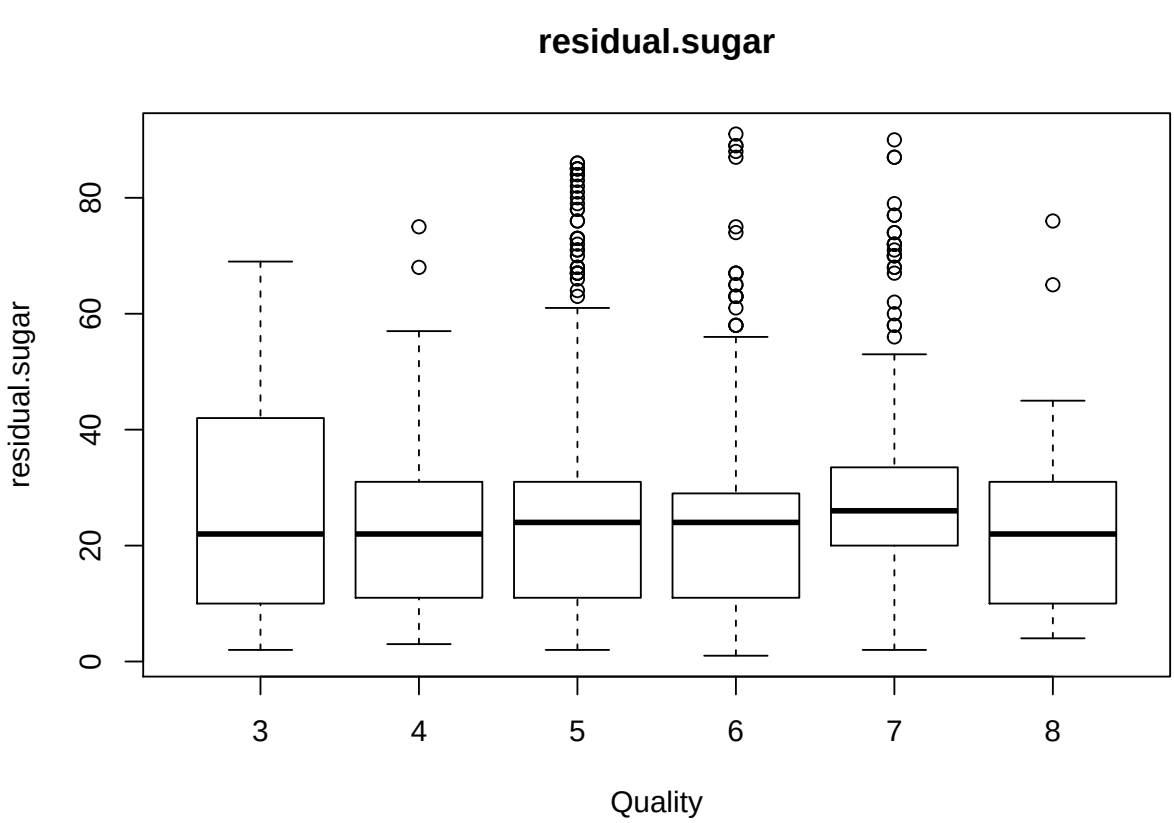
Box plots of features by quality

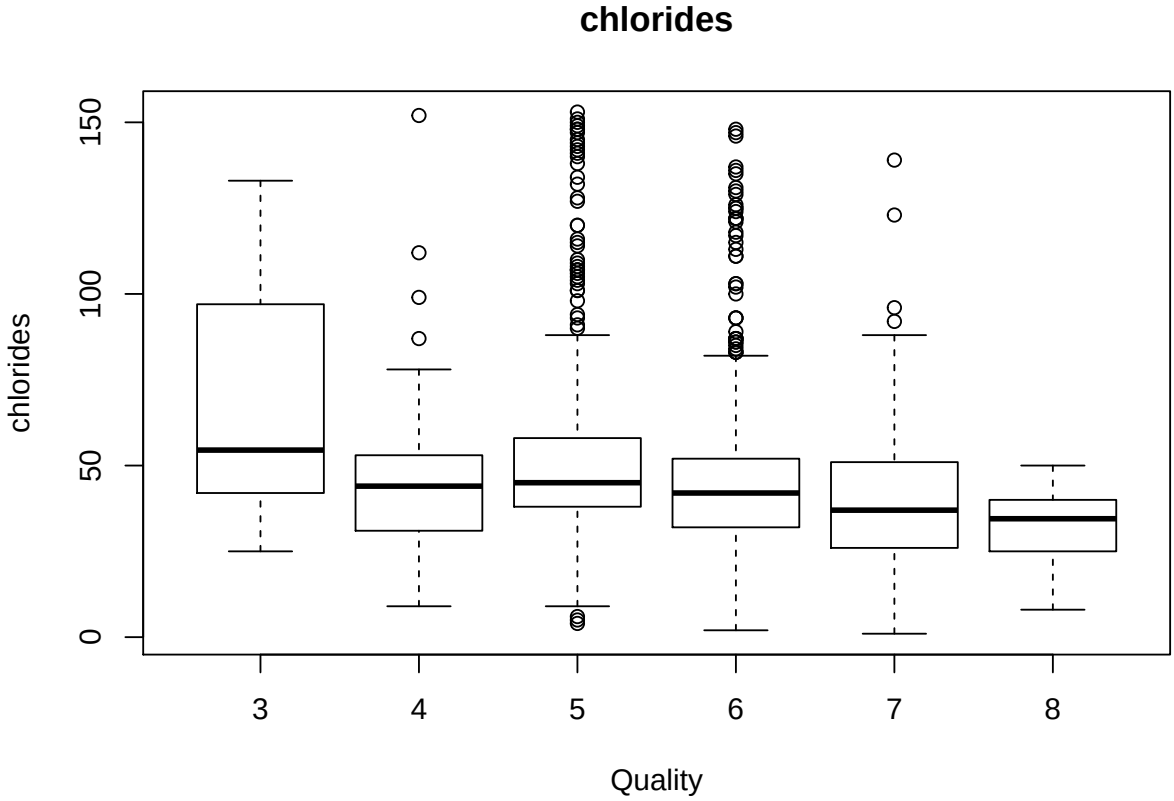
```
for (i in 1:(ncol(wine.data) - 1)) {
    feature = wine.data[, i]
    featureName = names(wine.data)[i]
    boxplot(feature ~ DF$quality, xlab = "Quality", ylab = featureName, main = featureName)
}
```

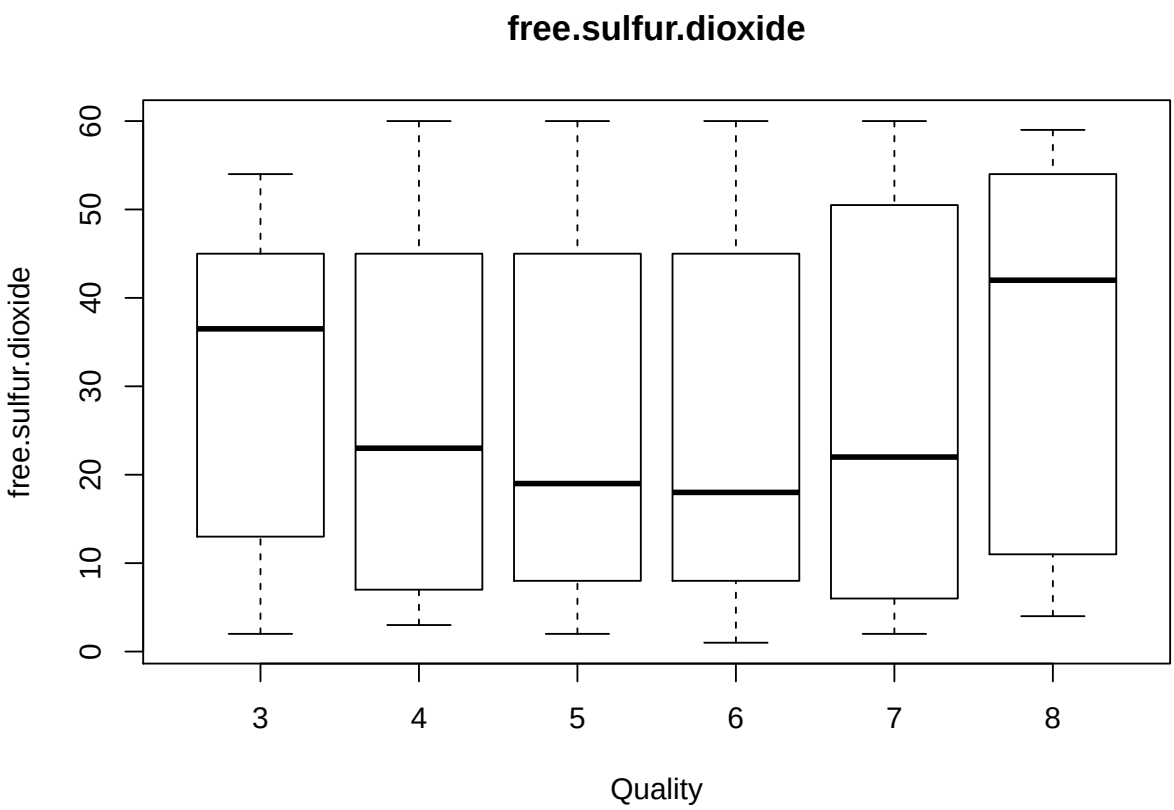

fixed.acidity
fixed.acidity
0
20
40
60
80
3
4
5
6
7
8
Quality

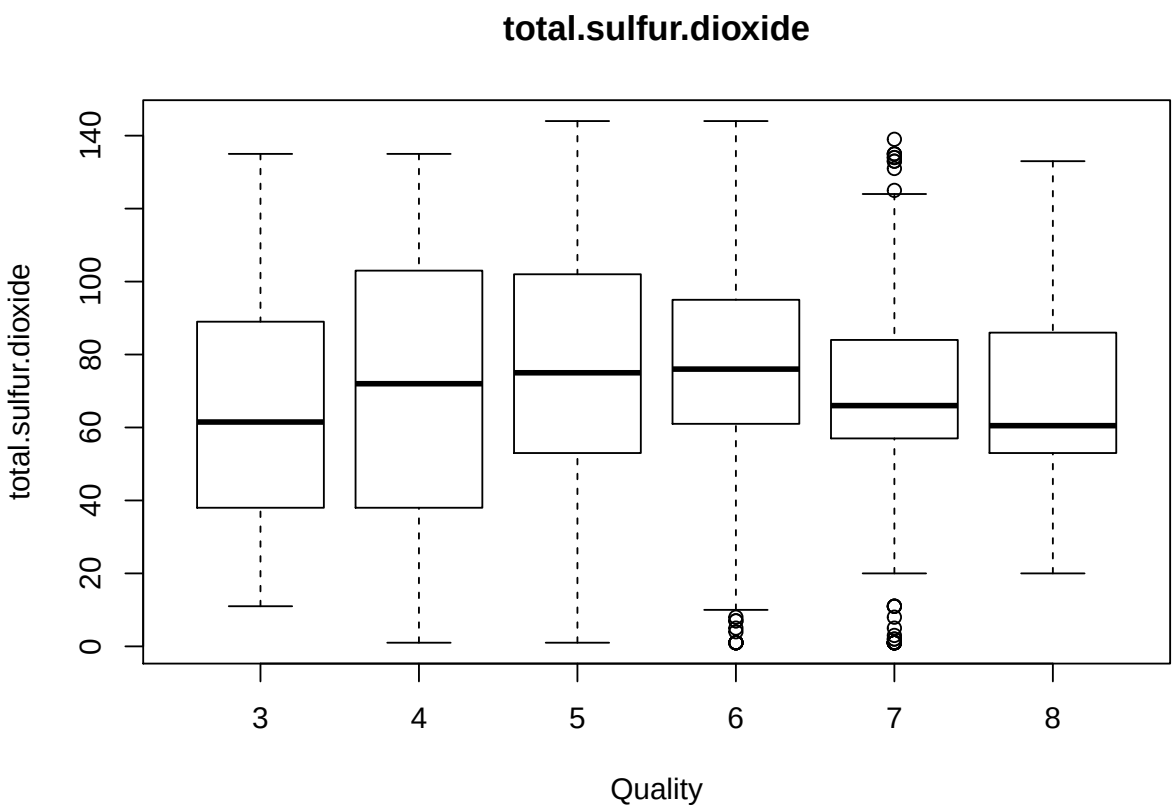

volatile.acidity
volatile.acidity
0
20
40
60
80
100
140
3
4
5
6
7
8
Quality

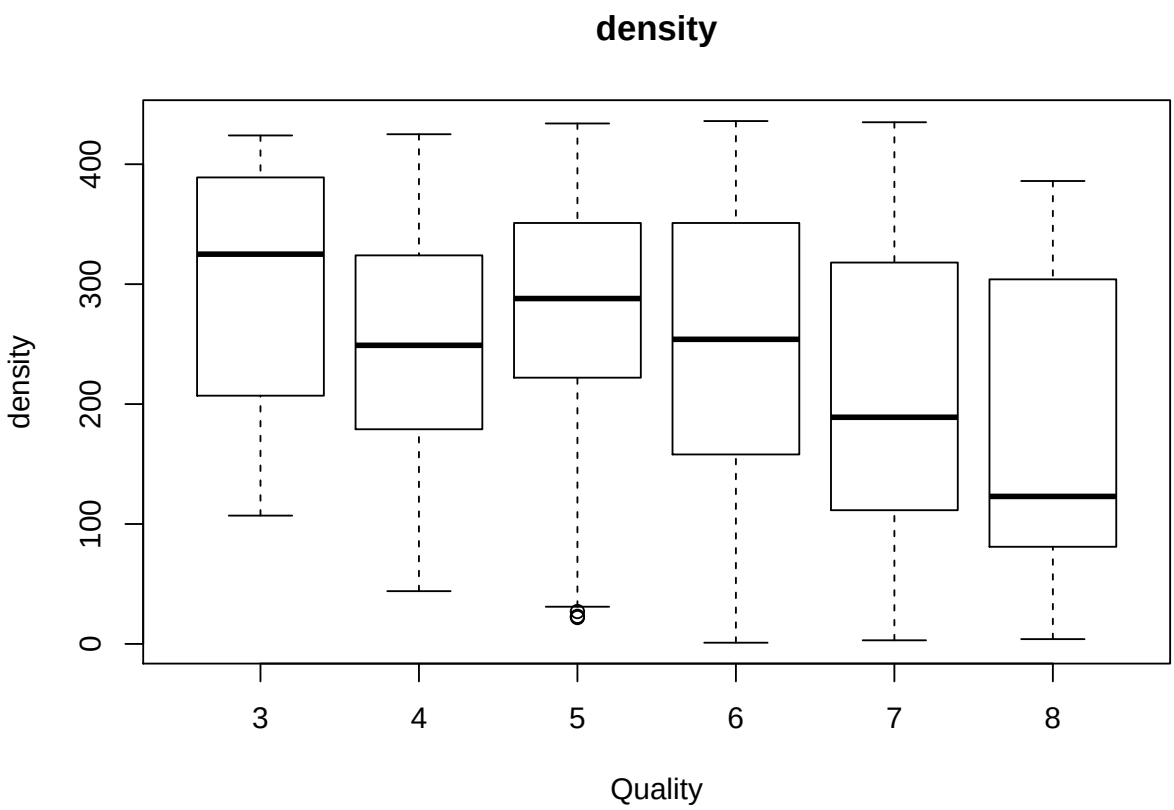

citric.acid
citric.acid
0
20
40
60
80
3
4
5
6
7
8
Quality

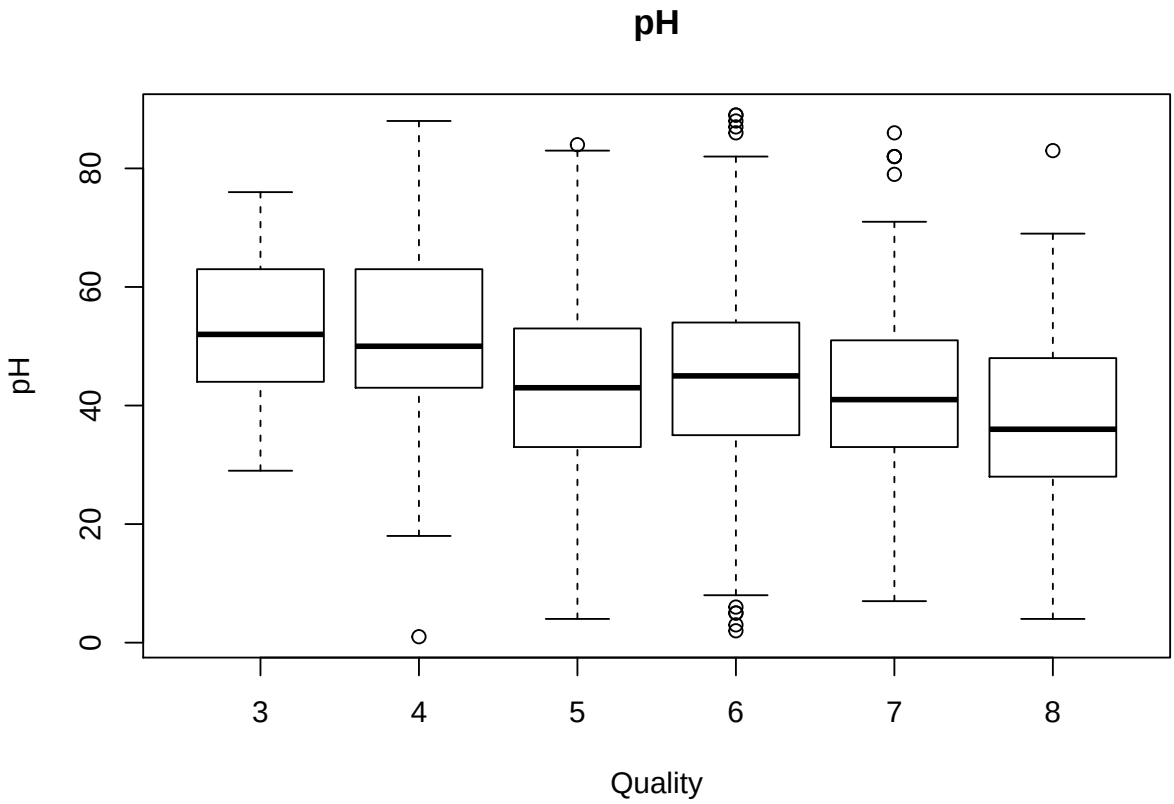

residual.sugar
residual.sugar
0
20
40
60
80
3
4
5
6
7
8
Quality

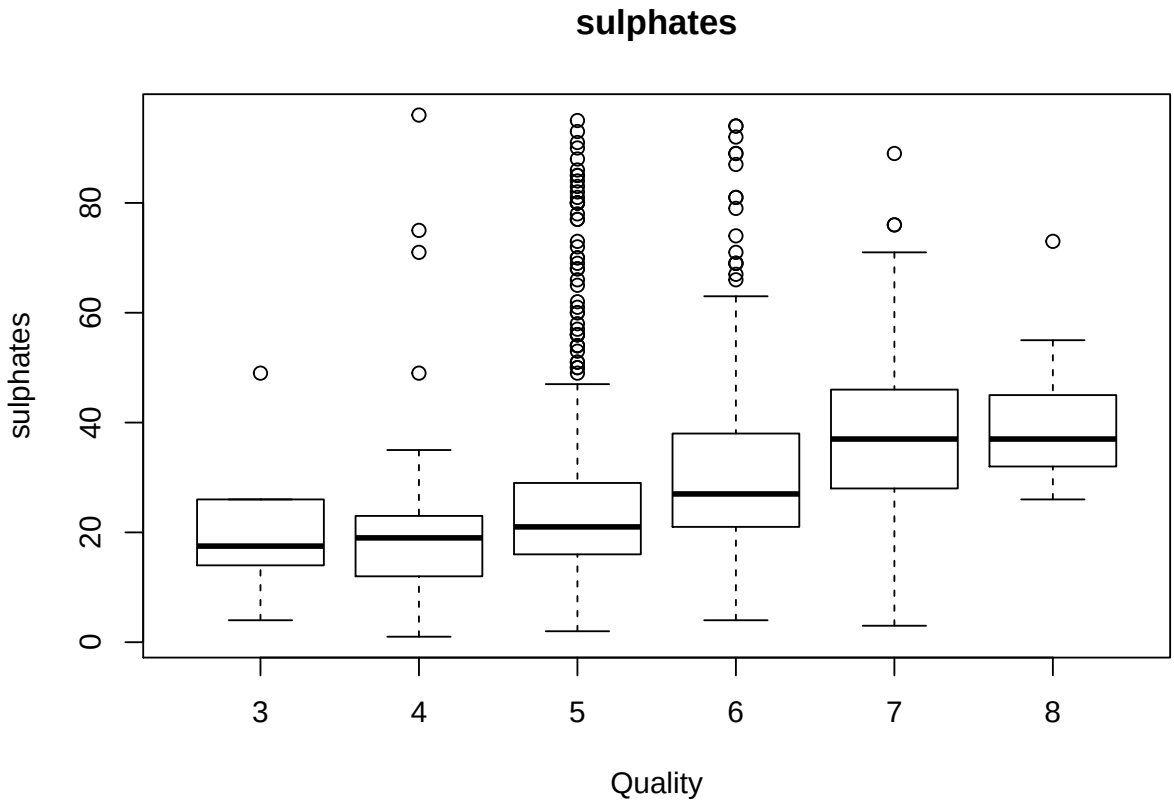

chlorides
chlorides
0
50
100
150
3
4
5
6
7
8
Quality

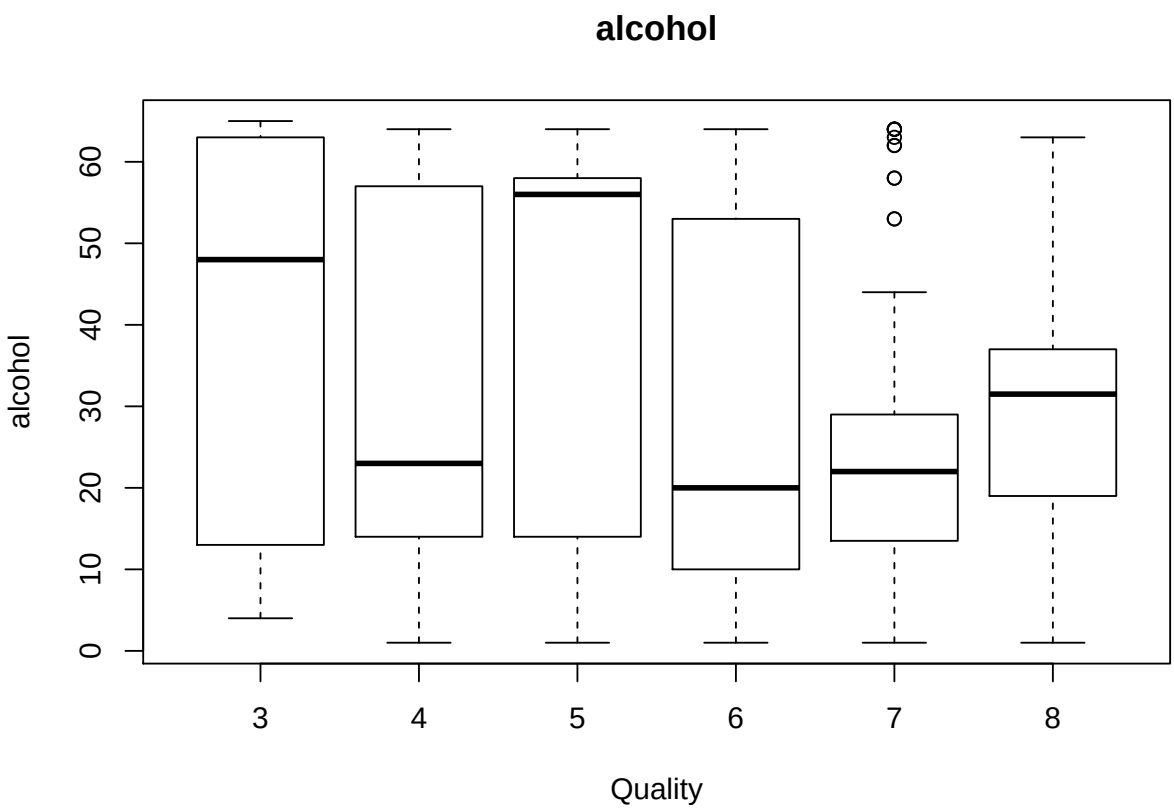

free.sulfur.dioxide
free.sulfur.dioxide
0
10
20
30
40
50
60
3
4
5
6
7
8
Quality


total.sulfur.dioxide
total.sulfur.dioxide
0
20
40
60
80
100
140
3
4
5
6
7
8
Quality


density
density
0
100
200
300
400
3
4
5
6
7
8
Quality


pH
0
20
40
60
80
pH
3
4
5
6
7
8
Quality

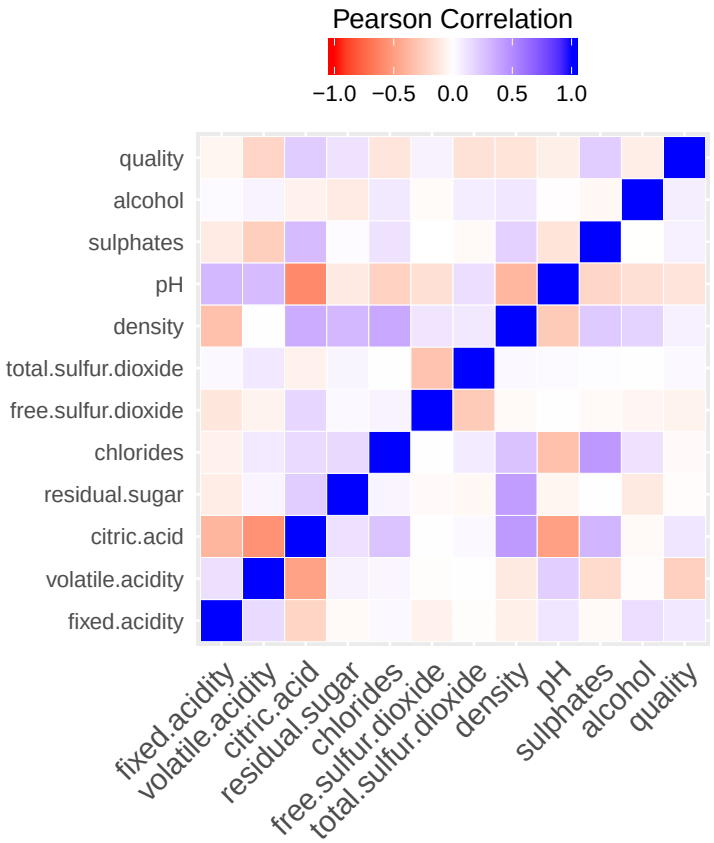

sulphates
sulphates
0
20
40
60
80
3
4
5
6
7
8
Quality



Experimental Plot of correlation between low and high quality wines. Upper triangular portion is high quality correlation. Lower trianglular portion is low quality correlation

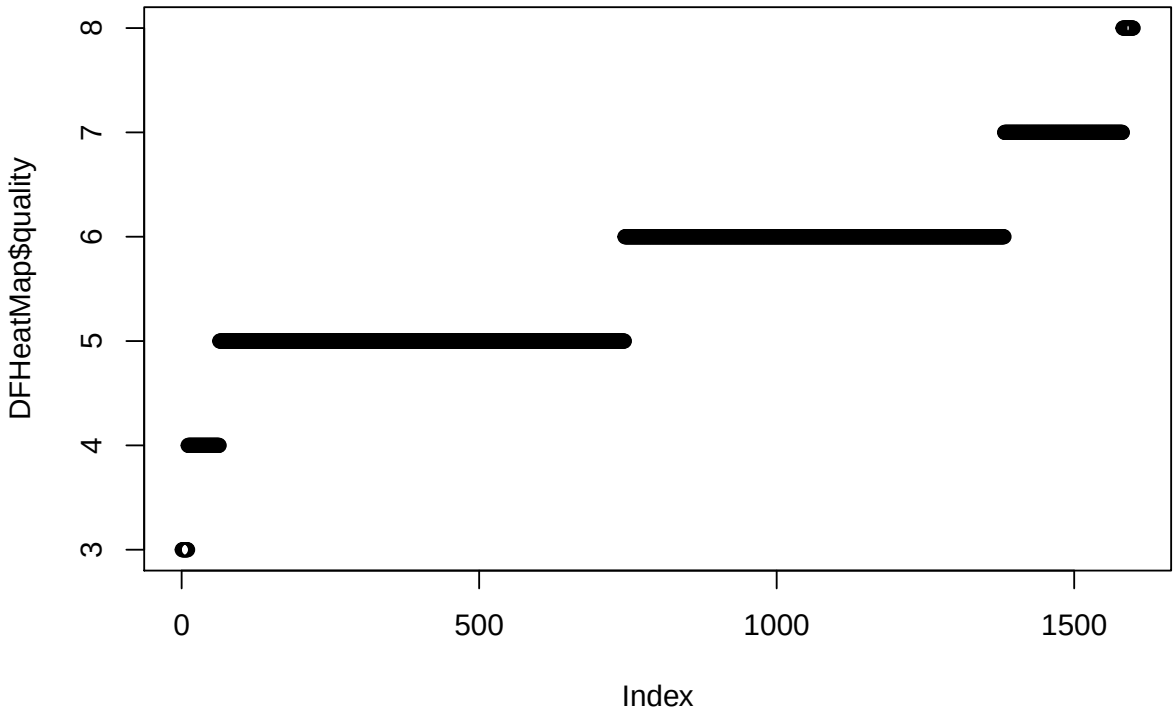
```
library(reshape2)

reorder_cormat <- function(cormat) {
    # Use correlation between variables as distance
    dd <- as.dist((1 - cormat)/2)
    hc <- hclust(dd)
    cormat <- cormat[hc$order, hc$order]
}

# Get upper triangle of the correlation matrix
get_upper_tri <- function(cormat) {
    cormat[lower.tri(cormat)] <- 0
    return(cormat)
}

# Get lower triangle of the correlation matrix
get_lower_tri <- function(cormat) {
    cormat[upper.tri(cormat)] <- 0
    diag(cormat) <- 0
    return(cormat)
```

```
}
cormat.high <- cor(DF[DF$quality >= 6, ])
cormat.low <- cor(DF[DF$quality < 6, ])

lower_tri <- get_lower_tri(cormat.high)
upper_tri <- get_upper_tri(cormat.low)

melted_cormat <- melt(lower_tri + upper_tri)

ggplot(melted_cormat, aes(Var2, Var1, fill = value)) + geom_tile(color = "white") +
    scale_fill_gradient2(low = "red", high = "blue", mid = "white", midpoint = 0,
        limit = c(-1, 1), space = "Lab", name = "Pearson Correlation") + theme(axis.title.x = element_bl
    axis.title.y = element_blank(), axis.ticks = element_blank(), legend.justification = c(1,
        0), legend.position = "top", legend.direction = "horizontal") + guides(fill = guide_colorbar(bar
    barheight = 1, title.position = "top", title.hjust = 0.5)) + theme(axis.text.x = element_text(angle
    vjust = 1, size = 12, hjust = 1)) + coord_fixed()
```

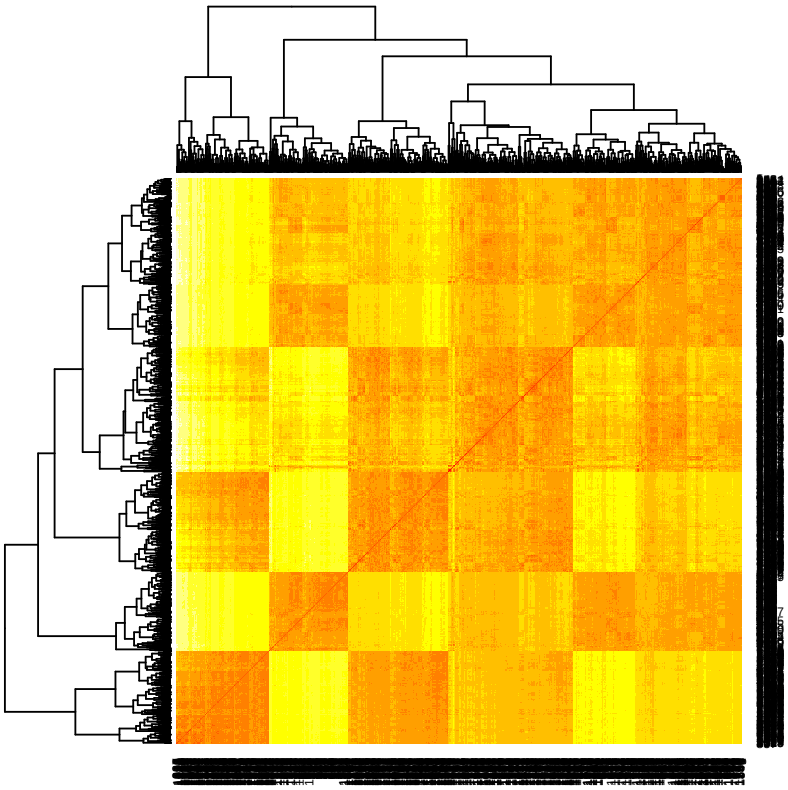


Heat Map - sorting by quality

```
DFHeatMap <- DF[order(DF$quality), ]
plot(DFHeatMap$quality)
```

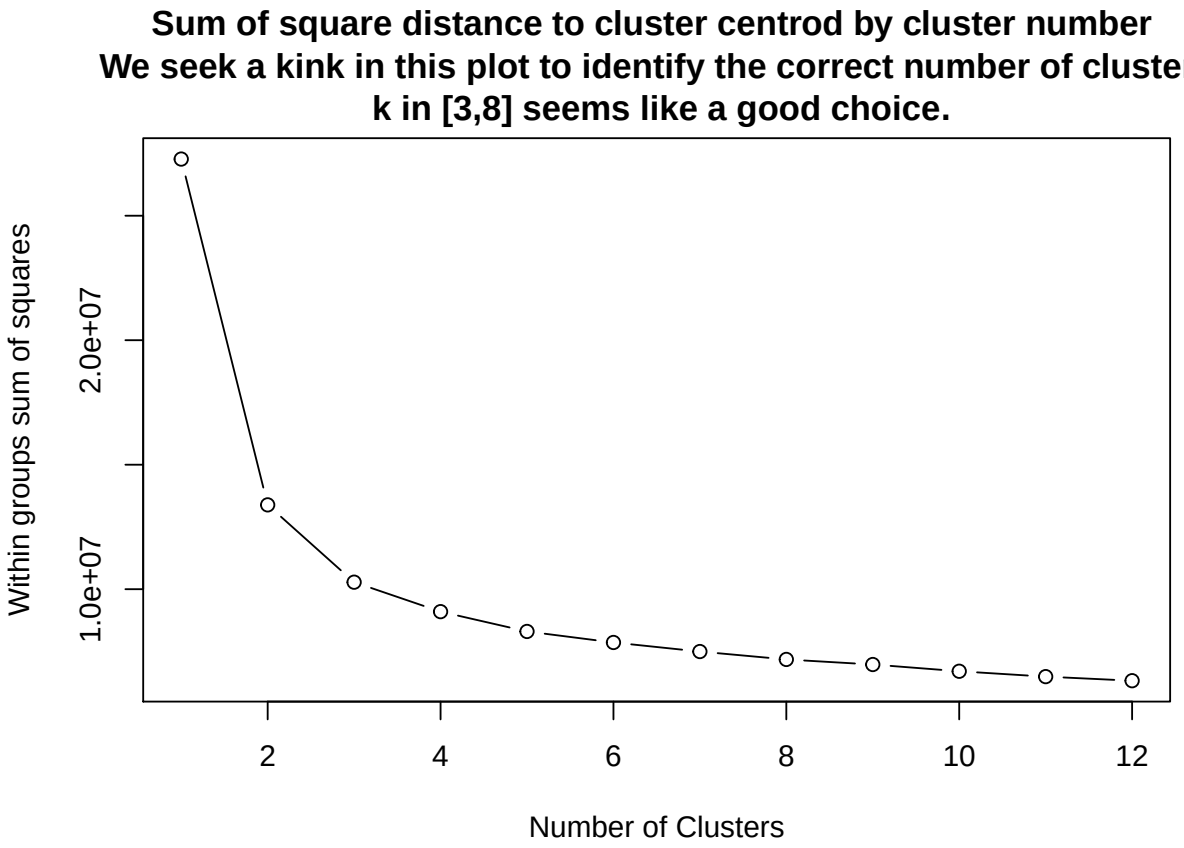



```
DFHeatMap$quality <- NULL
dist.mat <- as.matrix(dist(DFHeatMap, method = "euclidian"))

heatmap(dist.mat)
```

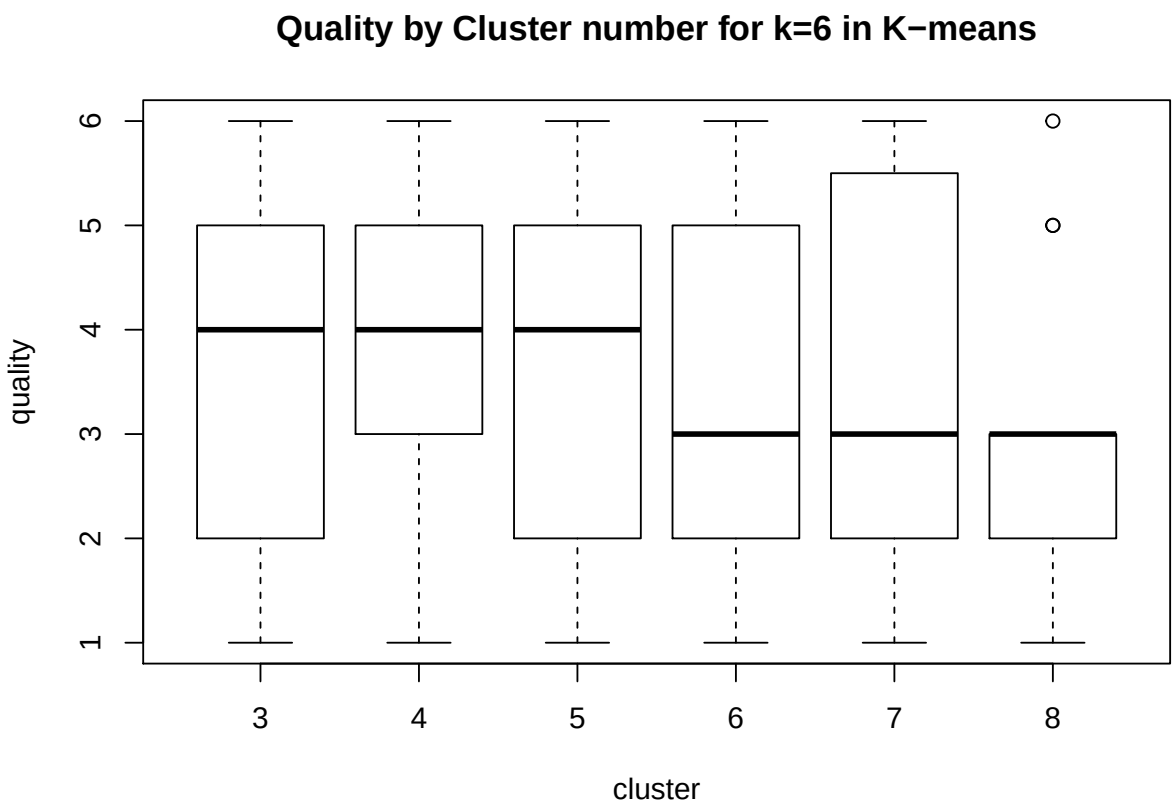


K-means clustering

```
DFOrdered <- DF[order(DF$quality), ]

# Determine number of clusters. Here we calculate the
wss <- (nrow(DFOrdered) - 1) * sum(apply(DFOrdered, 2, var))
for (i in 2:12) {
    wss[i] <- sum(kmeans(DFOrdered, centers = i)$withinss)
}

plot(1:12, wss, type = "b", xlab = "Number of Clusters", ylab = "Within groups sum of squares")
title("Sum of square distance to cluster centrod by cluster number \n We seek a kink in this plot to id
```




```r
# Run k-means with k=6
km.out = kmeans(DF, 6, nstart = 20)

cluster_kmean.label <- km.out$cluster

boxplot(cluster_kmean.label ~ DF$quality, xlab = "cluster", ylab = "quality",
    main = "Quality by Cluster number for k=6 in K-means")
```



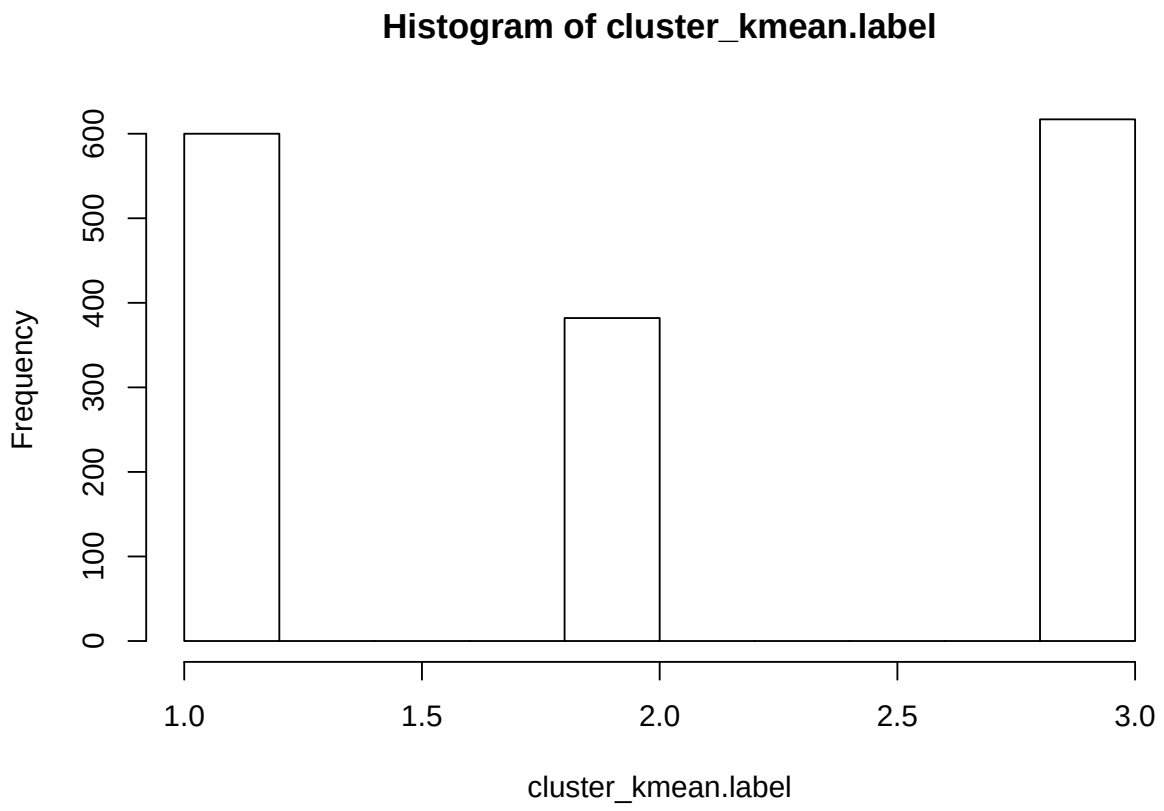

```
TB <- table(cluster_kmean.label, DF$quality)
library(pander)
pander(TB, caption = "Cluster matchup by quality for kmeans k=6.  This is NOT a confusion matrix.  The
```

Table 1: Cluster matchup by quality for kmeans k=6. This is NOT a confusion matrix. The cluster numbers are not indentified with quality.

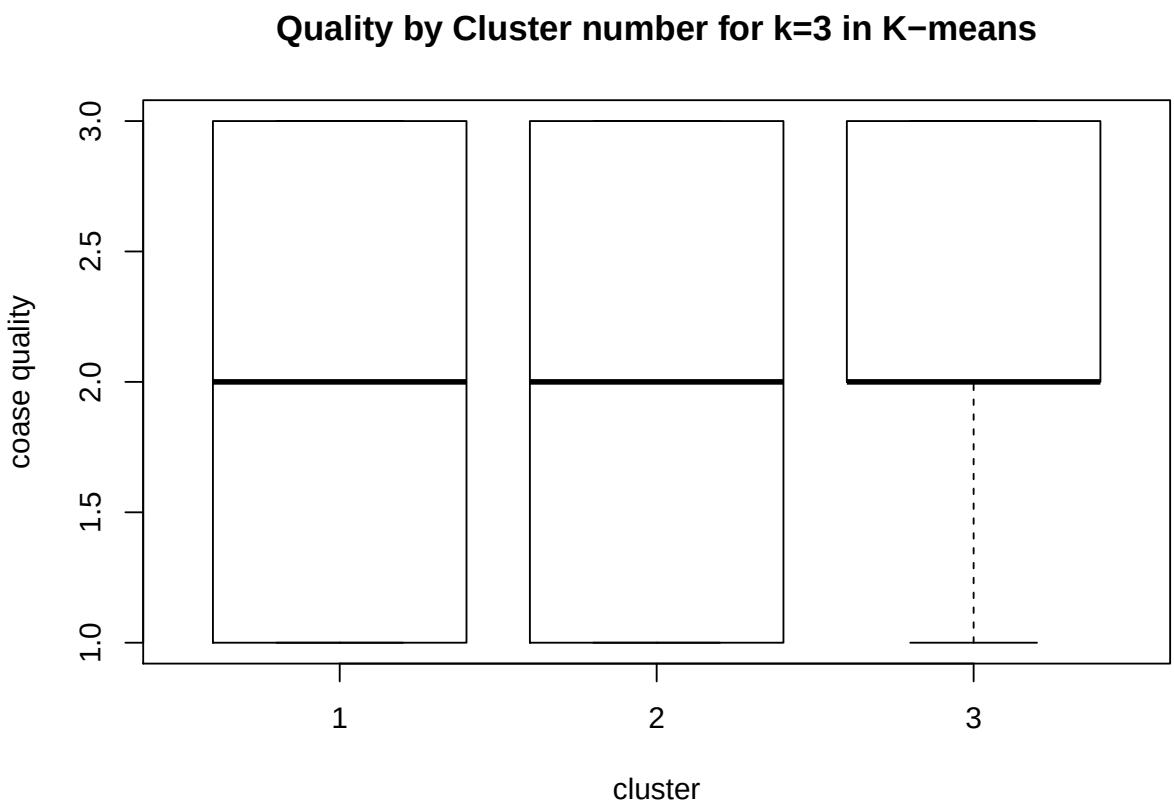
3	4	5	6	7	8
1	7	156	131	14	1
3	5	66	110	40	5
0	6	37	90	50	9
2	10	201	97	17	0
2	15	129	64	28	2
2	10	92	146	50	1

```
# Run k-means with k=3
km.out = kmeans(DF, 3, nstart = 20)

cluster_kmean.label <- km.out$cluster

quality_cat <- (ifelse(wine.data$quality < 5, 1, ifelse(wine.data$quality >
    6, 3, 2)))
```

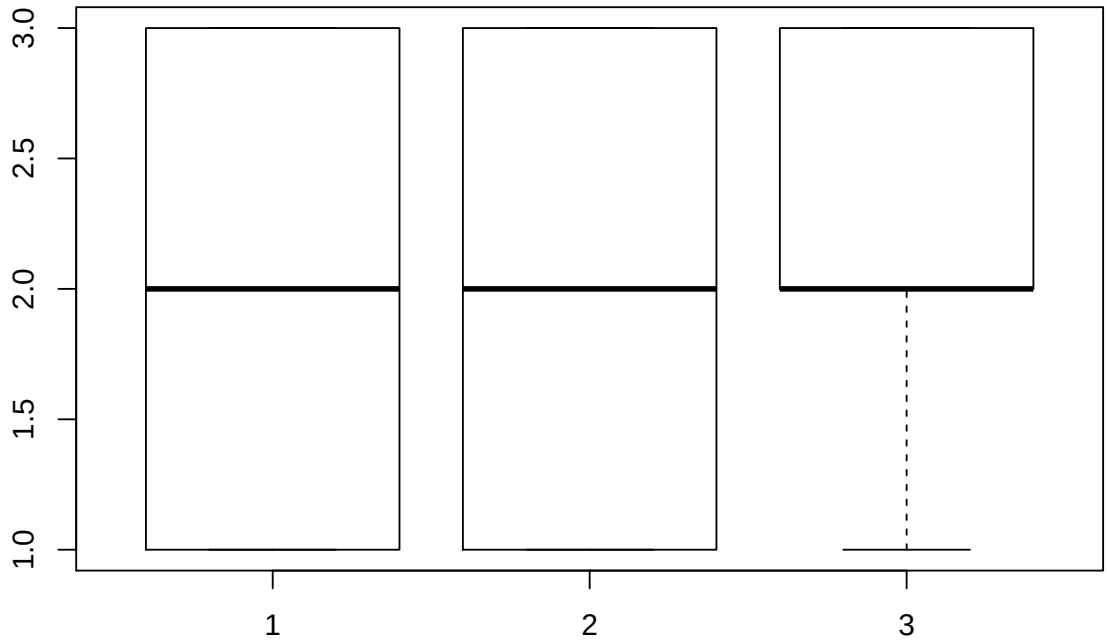
```r
hist(cluster_kmean.label)
```




```r
boxplot(cluster_kmean.label ~ quality_cat, xlab = "cluster", ylab = "coase quality",
    main = "Quality by Cluster number for k=3 in K-means")
```




```
boxplot(cluster_kmean.label ~ quality_cat)
```




```
TB <- table(cluster_kmean.label, quality_cat)
library(pander)
pander(TB, caption = "Cluster matchup by quality for kmeans k=3.  This is NOT a confusion matrix.  The
```

Table 2: Cluster matchup by quality for kmeans k=3. This is NOT a confusion matrix. The cluster numbers are not indentified with quality.

1	2	3
27	526	47
13	265	104
23	528	66

```
# Run k-means with k=4
km.out = kmeans(DF, 4, nstart = 20)

cluster_kmean.label <- km.out$cluster

TB <- table(cluster_kmean.label, DF$quality)
library(pander)
pander(TB, caption = "Cluster matchup by quality for kmeans k=4.  This is NOT a confusion matrix.  The
```

Table 3: Cluster matchup by quality for kmeans k=4. This is NOT a confusion matrix. The cluster numbers are not indentified with quality.

3	4	5	6	7	8
5	7	187	170	44	3
2	20	252	160	37	3
2	10	55	139	74	10
1	16	187	169	44	2

We split into training and test sets for now. Notice that there are very few points in the extremes of quality. There are arguments for and against splitting the extremes. The features for those sample points could help or hurt a classifyer in the middle ranges of quality. It's standard to split the data into training and test sets, but we'd like to reserve the right to revisit how we handle the classes with low counts at the end of the analysis.

```
# train <- sample(nrow(DF), floor(nrow(DF)* 2/3))

# write.csv(train,file = 'train.sample.csv',row.names = FALSE ,quote =
# FALSE)

# Check that it works
train <- as.integer(unlist(read.csv("train.sample.csv", header = TRUE)))

DFTrain <- DF[train, ]

DFTest <- DF[-train, ]

TDTrain <- table(DFTrain$quality)

TDTest <- table(DFTest$quality)

ratio.class <- TDTrain/TDTest

library(pander)
pander(TDTrain, caption = "Distribution of quality for training sample")
```

Table 4: Distribution of quality for training sample

3	4	5	6	7	8
8	35	453	415	142	13

```
pander(TDTest, caption = "Distribution of quality for test sample")
```

Table 5: Distribution of quality for test sample

3	4	5	6	7	8
2	18	228	223	57	5

LDA

```
library(MASS)
lda.fit = lda(quality ~ ., data = DFTrain)
lda.fit
```

```
## Call:
## lda(quality ~ ., data = DFTrain)
##
## Prior probabilities of groups:
##          3          4          5          6          7          8
## 0.00750469 0.03283302 0.42495310 0.38930582 0.13320826 0.01219512
##
## Group means:
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 3      48.00000         96.62500    21.50000       30.00000  79.62500
## 4      59.57143         79.25714    16.45714       25.34286  41.28571
## 5      68.14349         55.30905    25.81898       24.79249  49.98896
## 6      59.32289         42.92289    29.17349       23.46988  45.08434
## 7      57.04225         30.69014    38.30282       29.35211  39.23239
## 8      45.84615         35.23077    42.07692       27.69231  33.00000
##   free.sulfur.dioxide total.sulfur.dioxide  density       pH sulphates
## 3            31.25000             65.25000 302.3750 52.00000  19.62500
## 4            26.11429             72.88571 240.5714 52.57143  19.00000
## 5            24.68653             73.55188 276.2009 43.81015  24.44592
## 6            24.82892             77.34217 243.9494 44.47952  30.72289
## 7            25.52113             64.88732 213.9296 41.69014  36.61972
## 8            34.61538             64.76923 179.9231 40.38462  38.53846
##    alcohol
## 3 33.00000
## 4 34.94286
## 5 40.54967
## 6 27.27229
## 7 22.29577
## 8 26.53846
##
## Coefficients of linear discriminants:
##                                LD1          LD2          LD3           LD4
## fixed.acidity        -0.0065111404  0.024436828 -0.009532841 -0.0003469340
## volatile.acidity     -0.0185341165 -0.029053556 -0.014879177 -0.0074534741
## citric.acid           0.0038691850 -0.018829195 -0.034792127  0.0112188995
## residual.sugar        0.0163789540 -0.005783305 -0.032080721  0.0085494090
## chlorides            -0.0116658109 -0.004324411  0.011580919  0.0417800645
## free.sulfur.dioxide  -0.0010528827 -0.006144894  0.001009564 -0.0067156178
## total.sulfur.dioxide  0.0007387804  0.002609760  0.014328658 -0.0087314508
## density              -0.0048510299  0.003823320  0.004054947 -0.0001108575
## pH                   -0.0065916941 -0.029058850  0.007104401  0.0132065980
## sulphates             0.0377371174 -0.002838857 -0.004609353 -0.0058031310
## alcohol              -0.0156181508  0.009124249 -0.025642449 -0.0091778291
##                               LD5
## fixed.acidity        -0.010717349
## volatile.acidity      0.004507974
## citric.acid           0.012455231
```

```
## residual.sugar       -0.019135658
## chlorides             0.004926826
## free.sulfur.dioxide   0.030014077
## total.sulfur.dioxide  0.011513051
## density              -0.002456265
## pH                   -0.014776405
## sulphates             0.012575906
## alcohol               0.020559970
##
## Proportion of trace:
##    LD1    LD2    LD3    LD4    LD5
## 0.7608 0.1151 0.0848 0.0295 0.0098
```

```
lda.pred = predict(lda.fit, DFTest)
lda.class = lda.pred$class
TD <- table(lda.class, DFTest$quality)
pander(TD)
```

	3	4	5	6	7	8
3	0	1	4	0	1	0
4	0	0	2	4	0	0
5	2	9	163	90	6	0
6	0	7	54	119	31	4
7	0	1	5	10	19	1
8	0	0	0	0	0	0

```
ACC_lda = (sum(diag(as.array(TD))))/length(DFTest$quality)
```

The accuracy `0.564728` is not great - but we see that there is some good overall agreement in the 5-6 and 6-7 range. We also note that NO low quality wines were classified as high quality and that no high quality wines were classified as low quality. We might consider three level factor grouping quality {3,4}, {5,6}, {7,8}

```
DFCoarse <- DF
DFCoarse$quality_cat <- ifelse(wine.data$quality < 5, "LOW", ifelse(wine.data$quality >
    6, "HIGH", "MEDIUM"))
DFCoarse$quality <- NULL
DFCoarseTrain <- DFCoarse[train, ]
DFCoarseTest <- DFCoarse[-train, ]

lda.fit = lda(quality_cat ~ ., data = DFCoarseTrain)
lda.fit
```

```
## Call:
## lda(quality_cat ~ ., data = DFCoarseTrain)
##
## Prior probabilities of groups:
##       HIGH        LOW     MEDIUM
## 0.14540338 0.04033771 0.81425891
##
## Group means:
##        fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
```

```
## HIGH        56.10323         31.07097    38.61935       29.21290  38.70968
## LOW         57.41860         82.48837    17.39535       26.20930  48.41860
## MEDIUM      63.92627         49.38710    27.42281       24.16014  47.64401
##        free.sulfur.dioxide total.sulfur.dioxide  density       pH
## HIGH              26.28387             64.87742 211.0774 41.58065
## LOW               27.06977             71.46512 252.0698 52.46512
## MEDIUM            24.75461             75.36406 260.7811 44.13018
##        sulphates  alcohol
## HIGH    36.78065 22.65161
## LOW     19.11628 34.58140
## MEDIUM  27.44700 34.20161
##
## Coefficients of linear discriminants:
##                                 LD1          LD2
## fixed.acidity        -8.161248e-05  0.018938074
## volatile.acidity      1.614776e-02 -0.031574594
## citric.acid          -1.199469e-02 -0.026433335
## residual.sugar       -2.393399e-02 -0.017199071
## chlorides             1.194487e-02  0.003651235
## free.sulfur.dioxide   2.524600e-03 -0.002775764
## total.sulfur.dioxide  3.816477e-03  0.007441980
## density               5.038371e-03  0.004701649
## pH                    1.073514e-02 -0.025406808
## sulphates            -3.420472e-02 -0.004130855
## alcohol               5.812238e-03  0.002369115
##
## Proportion of trace:
##    LD1    LD2
## 0.8181 0.1819
```

```
lda.pred = predict(lda.fit, DFCoarseTest)
lda.class = lda.pred$class
TD <- table(lda.class, DFCoarseTest$quality)
pander(TD)
```

	HIGH	LOW	MEDIUM
HIGH	16	1	10
LOW	0	1	8
MEDIUM	46	18	433

```
ACC_lda_coarse = (sum(diag(as.array(TD))))/length(DFTest$quality)
```

We see the accuracy `0.8442777` has improved by coalescing the quality levels.

Fit a two class SVM classification model

```
# We do a logistic classification for comparison

DFCoarse <- DF
```

```r
DFCoarse$quality_cat <- ifelse(wine.data$quality <= 5, 0, 1)
DFCoarse$quality <- NULL
DFCoarseTrain <- DFCoarse[train, ]
DFCoarseTest <- DFCoarse[-train, ]

glm.fit <- glm(quality_cat ~ ., data = DFCoarseTrain, family = binomial)
summary(glm.fit)
```

```
##
## Call:
## glm(formula = quality_cat ~ ., family = binomial, data = DFCoarseTrain)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.5317  -0.8364   0.4104   0.8525   2.4000
##
## Coefficients:
##                        Estimate Std. Error z value Pr(>|z|)
## (Intercept)           2.7113203  0.5486222   4.942 7.73e-07 ***
## fixed.acidity        -0.0113550  0.0030596  -3.711 0.000206 ***
## volatile.acidity     -0.0216674  0.0034508  -6.279 3.41e-10 ***
## citric.acid          -0.0045903  0.0055387  -0.829 0.407231
## residual.sugar        0.0097113  0.0049915   1.946 0.051704 .
## chlorides            -0.0108621  0.0036092  -3.010 0.002616 **
## free.sulfur.dioxide   0.0003851  0.0037779   0.102 0.918807
## total.sulfur.dioxide  0.0049662  0.0023648   2.100 0.035724 *
## density              -0.0042597  0.0008244  -5.167 2.38e-07 ***
## pH                   -0.0036695  0.0059213  -0.620 0.535446
## sulphates             0.0424062  0.0056815   7.464 8.40e-14 ***
## alcohol              -0.0223319  0.0033278  -6.711 1.94e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 1472.6  on 1065  degrees of freedom
## Residual deviance: 1154.6  on 1054  degrees of freedom
## AIC: 1178.6
##
## Number of Fisher Scoring iterations: 4
```

```r
glm.probs = predict(glm.fit, DFCoarseTest, type = "response")

glm.pred = rep(0, nrow(DFCoarseTest))
glm.pred[glm.probs > 0.5] = 1
TB <- table(glm.pred, DFCoarseTest$quality_cat)
pander(TB, caption = "Logistic Regression")
```

Table 8: Logistic Regression

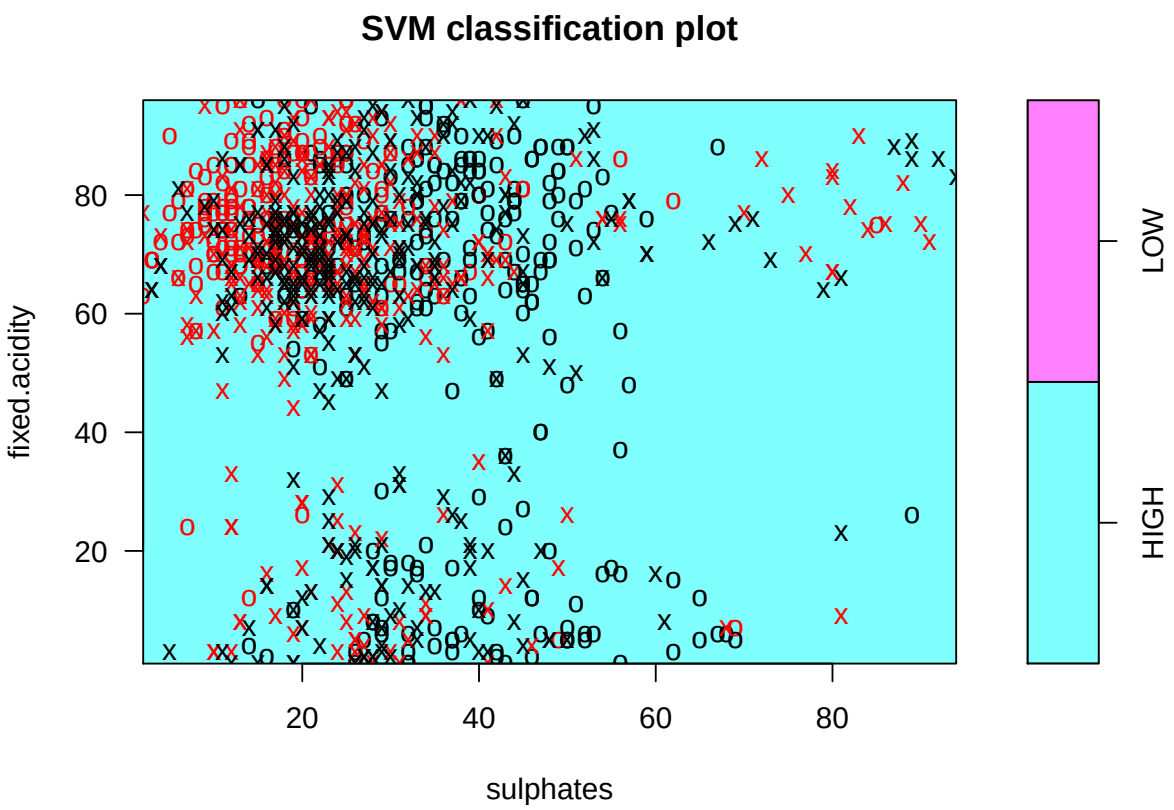
	0	1
0	176	94

	0	1
1	72	191

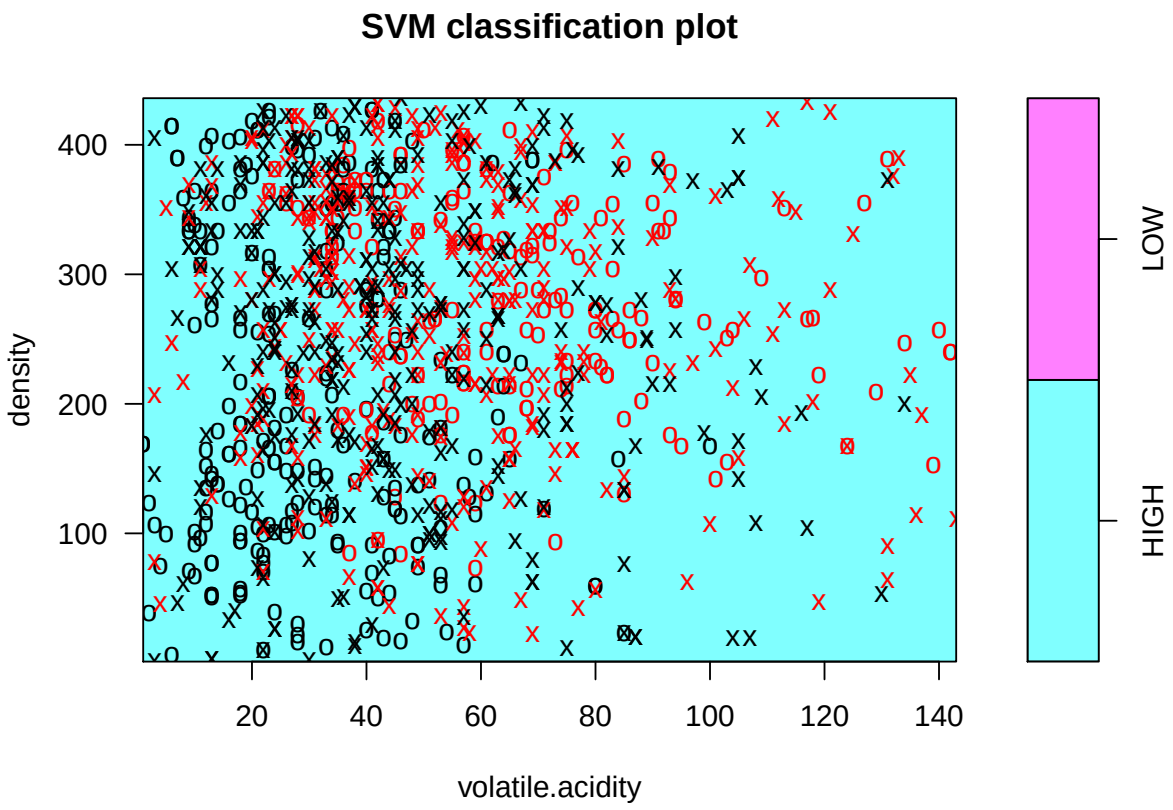
```
ACC_glm_binomial = (TB[1] + TB[4])/length(DFCoarseTest$quality_cat)
Specificity = TB[1]/sum(DFCoarseTest$quality_cat == 0)
Sensitivity = TB[4]/sum(DFCoarseTest$quality_cat == 1)

#### We require a categorical response for the e1071 package so the data frame
#### for the 2 class SVM is regenerated here

DFCoarse <- DF
DFCoarse$quality_cat <- as.factor(ifelse(wine.data$quality <= 5, "LOW", "HIGH"))
DFCoarse$quality <- NULL
DFCoarseTrain <- DFCoarse[train, ]
DFCoarseTest <- DFCoarse[-train, ]

library(e1071)

tune.svm = tune(svm, quality_cat ~ ., data = DFCoarseTrain, kernel = "radial",
    ranges = list(cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100)))

svm.fit <- tune.svm$best.model

svm.pred <- predict(svm.fit, DFCoarseTest)
TB <- table(svm.pred, DFCoarseTest$quality_cat)
pander(TB)
```

	HIGH	LOW
HIGH	202	60
LOW	83	188

```
ACC_Linear_SVM = (TB[1] + TB[4])/length(DFCoarseTest$quality_cat)

plot(svm.fit, DFCoarseTrain, fixed.acidity ~ sulphates)
```




```
plot(svm.fit, DFCoarseTrain, density ~ volatile.acidity)
```



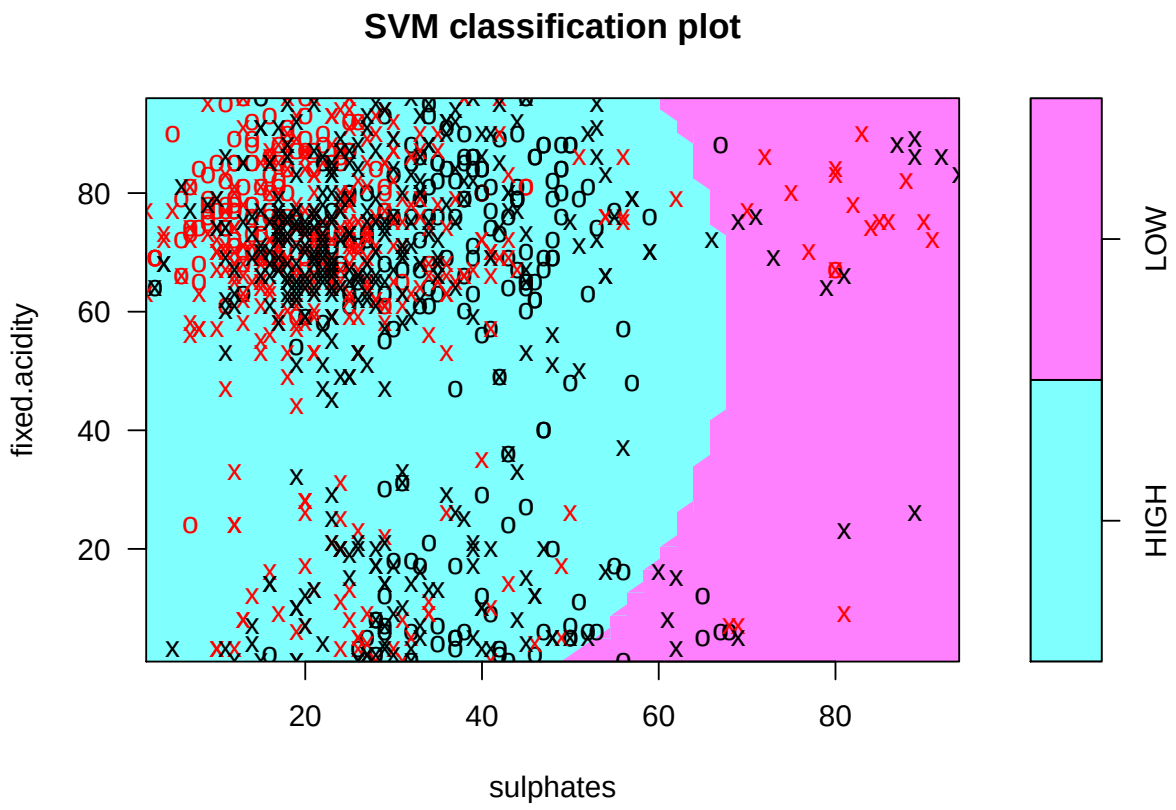
We see that we need to use a non linear kernel. We train a non linear SVM below using the built in cross validation method tune to optimize the cost and gamma hyper-parameters

```
gamma_default <- 1/(ncol(DFCoarseTrain) - 1)

gamma_list <- ((1:10)/5) * gamma_default

tune.svm = tune(svm, quality_cat ~ ., data = DFCoarseTrain, kernel = "radial",
    ranges = list(gamma = gamma_list, cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100)))


svm.fit <- tune.svm$best.model

svm.pred <- predict(svm.fit, DFCoarseTest)
TB <- table(svm.pred, DFCoarseTest$quality_cat)
pander(TB)
```

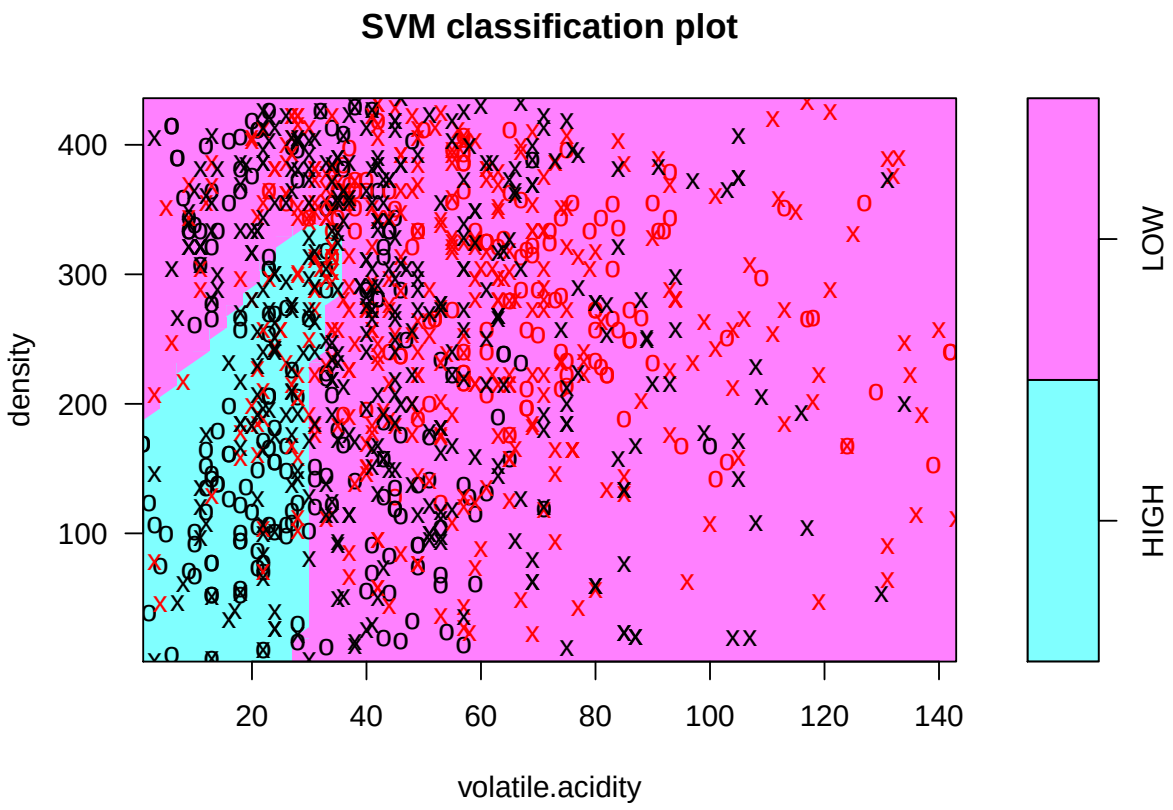
	HIGH	LOW
HIGH	208	57
LOW	77	191

```
ACC_Radial_SVM = (TB[1] + TB[4])/length(DFCoarseTest$quality_cat)
```

```
# Beware - these plots may have a bug for the non linear svm!

plot(svm.fit, DFCoarseTrain, fixed.acidity ~ sulphates)
```




```
plot(svm.fit, DFCoarseTrain, density ~ volatile.acidity)
```



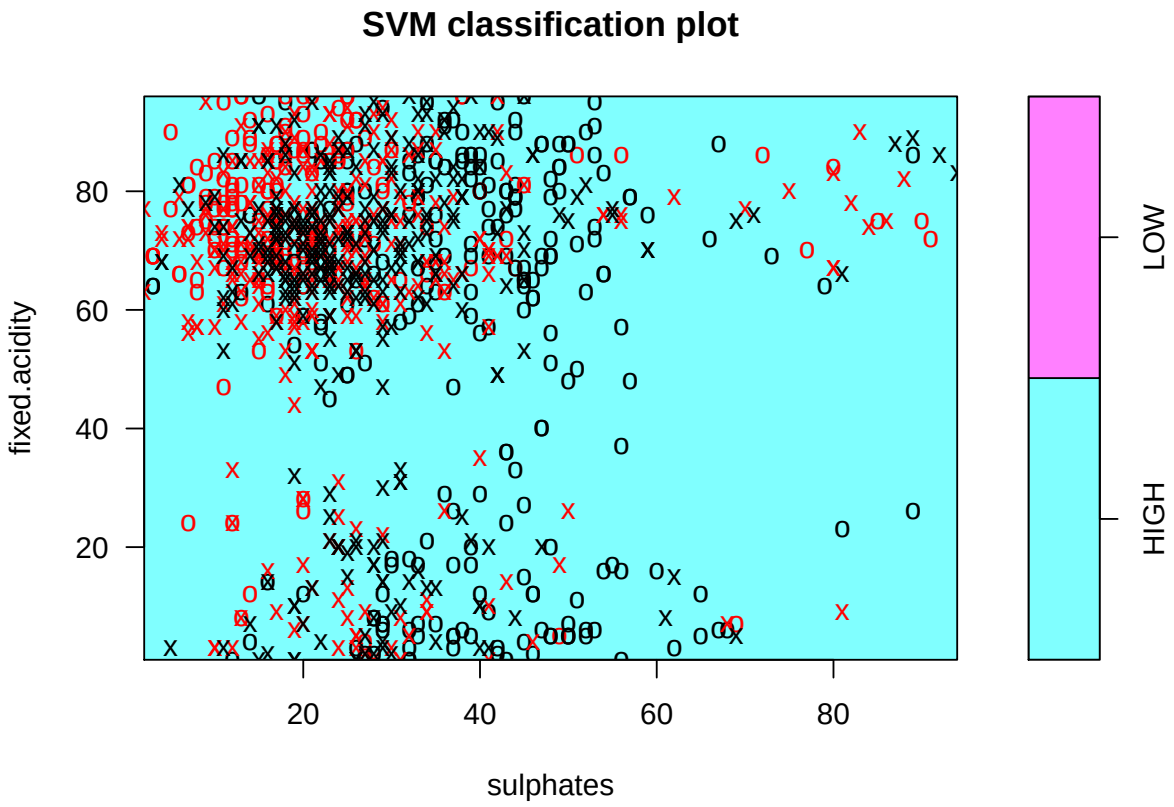
For the SVM trained with a kernel using the radial basis similarity function the accuracy has gone from 0.7317073 to 0.7485929.

```
gamma_default <- 1/(ncol(DFCoarseTrain) - 1)

gamma_list <- ((1:10)/5) * gamma_default

tune.svm = tune(svm, quality_cat ~ ., data = DFCoarseTrain, kernel = "polynomial",
    ranges = list(gamma = gamma_list, cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100),
        degree = c(2, 3, 4)))

svm.fit <- tune.svm$best.model

svm.pred <- predict(svm.fit, DFCoarseTest)
TB <- table(svm.pred, DFCoarseTest$quality_cat)
pander(TB)
```

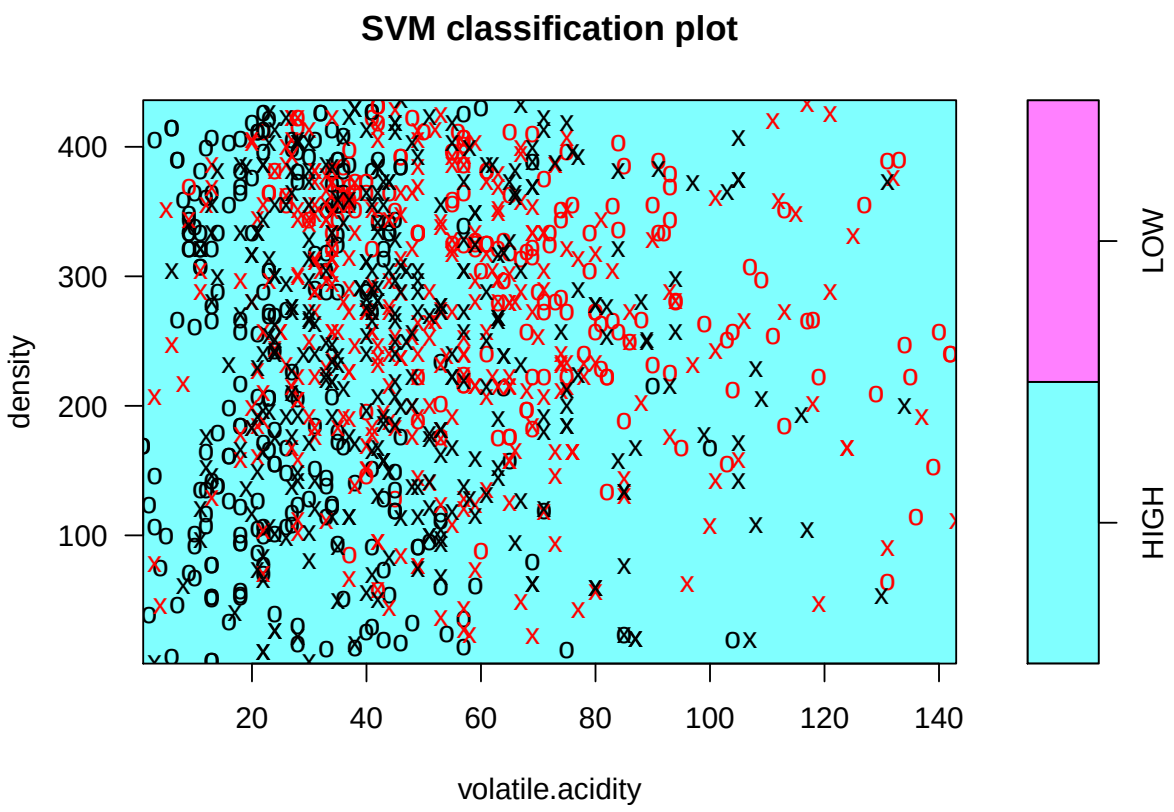
	HIGH	LOW
HIGH	203	79
LOW	82	169

```
ACC_Polynomial_SVM = (TB[1] + TB[4])/length(DFCoarseTest$quality_cat)
# Beware - these plots may have a bug for the non linear svm!
```

```
plot(svm.fit, DFCoarseTrain, fixed.acidity ~ sulphates)
```




```
plot(svm.fit, DFCoarseTrain, density ~ volatile.acidity)
```



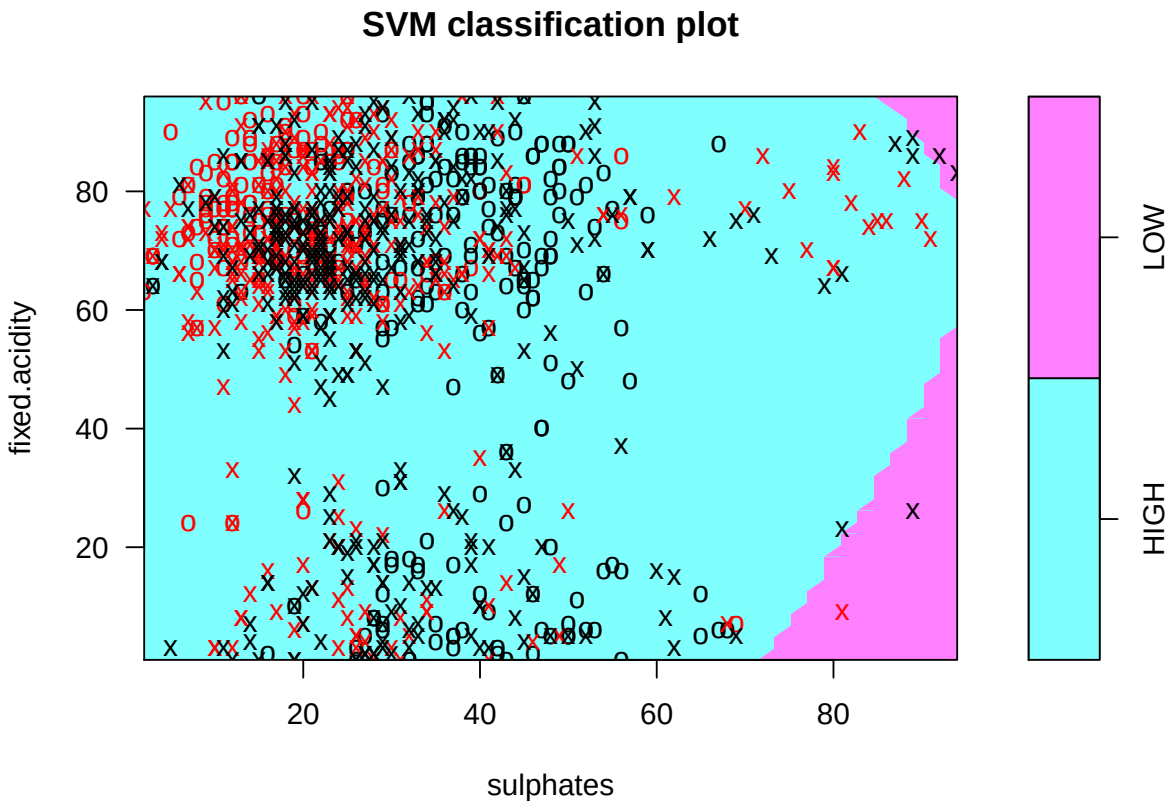
The ploynomial svm tuned to use the best degree,gamma, and cost yielded an accuracy of `0.6979362`

Now we try the nu-svm

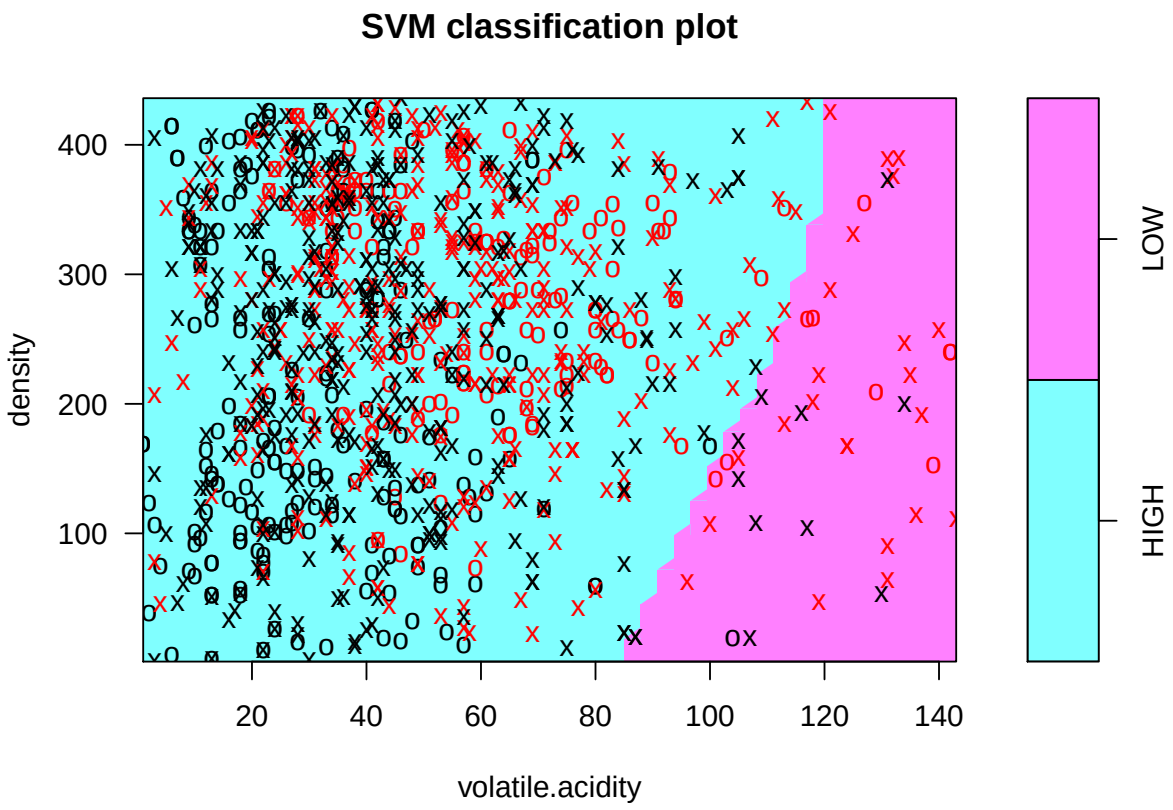
```
gamma_default <- 1/(ncol(DFCoarseTrain) - 1)

gamma_list <- ((1:10)/5) * gamma_default

tune.svm = tune(svm, quality_cat ~ ., data = DFCoarseTrain, kernel = "radial",
    type = "nu-classification", ranges = list(gamma = gamma_list, cost = c(0.001,
        0.01, 0.1, 1, 5, 10, 100)))

svm.fit <- tune.svm$best.model

svm.pred <- predict(svm.fit, DFCoarseTest)
TB <- table(svm.pred, DFCoarseTest$quality_cat)
pander(TB)
```

	HIGH	LOW
HIGH	209	57
LOW	76	191

```
ACC_Radial_nuSVM = (TB[1] + TB[4])/length(DFCoarseTest$quality_cat)

# Beware - these plots may have a bug for the non linear svm!

plot(svm.fit, DFCoarseTrain, fixed.acidity ~ sulphates)
```




```
plot(svm.fit, DFCoarseTrain, density ~ volatile.acidity)
```



One Versus All for three level classification. We learned that e1071 now provides direct multiclass classification. We leave the code here for now.

```
# DFCoarse <-DF DFCoarse$quality_cat_low_vs_med_high <-
# as.factor(ifelse(wine.data$quality<5,'LOW','MED_HIGH'))
# DFCoarse$quality_cat_high_vs_low_med <-
# as.factor(ifelse(wine.data$quality>6,'HIGH','LOW_MED'))
# DFCoarse$quality_cat_med_vs_low_high <- as.factor(ifelse((
# wine.data$quality==6 | wine.data$quality==5),'MED','LOW_HIGH'))
# DFCoarse$quality <-NULL DFCoarseTrain <-DFCoarse[train,] DFCoarseTest
# <-DFCoarse[-train,] gamma_default <- 1/(ncol(DFCoarseTrain)-1) gamma_list
# <-((1:10)/5)*gamma_default cost_list=c(0.001 , 0.01, 0.1, 1,5,10,100)
# #Overrides for fast development change back!  gamma_list<-c(.17)
# cost_list<-c(.1) #LOW VS REST
# tune.svm.quality_cat_low_vs_med_high=tune(svm,quality_cat_low_vs_med_high~.,
# data=DFCoarseTrain , kernel ='radial',ranges
# =list(gamma=gamma_list,cost=cost_list ),type='nu-classification')
# svm.fit.quality_cat_low_vs_med_high
# <-tune.svm.quality_cat_low_vs_med_high$best.model #MED VS REST
# tune.svm.quality_cat_med_vs_low_high=tune(svm,quality_cat_med_vs_low_high~.,
# data=DFCoarseTrain , kernel ='radial',ranges
# =list(gamma=gamma_list,cost=cost_list ),type='nu-classification')
# svm.fit.quality_cat_med_vs_low_high<-tune.svm.quality_cat_med_vs_low_high$best.model
# #HIGH VS REST
# tune.svm.quality_cat_high_vs_low_med=tune(svm,quality_cat_high_vs_low_med~.,
```

```
# data=DFCoarseTrain , kernel ='radial',ranges
# =list(gamma=gamma_list,cost=cost_list ),type='nu-classification')
# svm.fit.quality_cat_high_vs_low_med<-tune.svm.quality_cat_high_vs_low_med$best.model

# svm.pred.quality_cat_low_vs_med_high <-
# predict(svm.fit.quality_cat_low_vs_med_high, DFCoarseTest)
# svm.pred.quality_cat_med_vs_low_high <-
# predict(svm.fit.quality_cat_med_vs_low_high, DFCoarseTest)
# svm.pred.quality_cat_high_vs_low_med <-
# predict(svm.fit.quality_cat_high_vs_low_med, DFCoarseTest)
```

```
DFCoarse <- DF
DFCoarse$quality_cat <- factor(ifelse(wine.data$quality < 5, "LOW", ifelse(wine.data$quality >
    6, "HIGH", "MED")))
DFCoarse$quality <- NULL
DFCoarseTrain <- DFCoarse[train, ]
DFCoarseTest <- DFCoarse[-train, ]

gamma_default <- 1/(ncol(DFCoarseTrain) - 1)

gamma_list <- ((1:10)/5) * gamma_default
cost_list = c(0.001, 0.01, 0.1, 1, 5, 10, 100)

tune.svm.quality_cat = tune(svm, quality_cat ~ ., data = DFCoarseTrain, kernel = "polynomial",
    ranges = list(gamma = gamma_list, cost = cost_list))
svm.fit.quality_cat <- tune.svm.quality_cat$best.model

svm.pred.quality_cat <- predict(svm.fit.quality_cat, DFCoarseTest)
TB <- table(svm.pred.quality_cat, DFCoarseTest$quality_cat)
pander(TB)
```

	HIGH	LOW	MED
HIGH	21	2	22
LOW	0	5	13
MED	41	13	416

```
ACC_Multiclass = (sum(diag(TB)))/length(DFCoarseTest$quality_cat)
```

```
method.accuracy <- data.frame(method = c("Multiclass SVM 3 class", "svm rbf nu 2 class",
    "lda 3 class", "lda 6 class", "gml 2 class", "linear svm 2 class", "rbf svm 2 class",
    "polynomial svm 2 class"), accuracy = c(ACC_Multiclass, ACC_Radial_nuSVM,
    ACC_lda_coarse, ACC_lda, ACC_glm_binomial, ACC_Linear_SVM, ACC_Radial_SVM,
    ACC_Polynomial_SVM))

method.accuracy <- method.accuracy[order(method.accuracy$accuracy, decreasing = TRUE),
    ]

pander(method.accuracy, caption = "Accuracy by Method")
```

Table 14: Accuracy by Method

	method	accuracy
3	lda 3 class	0.8443
1	Multiclass SVM 3 class	0.8293
2	svm rbf nu 2 class	0.7505
7	rbf svm 2 class	0.7486
6	linear svm 2 class	0.7317
8	polynomial svm 2 class	0.6979
5	gml 2 class	0.6886
4	lda 6 class	0.5647

Now we train a reduced model choosing the significant variables from the glm

```
DFCoarse <- DF[, c("fixed.acidity", "volatile.acidity", "chlorides", "total.sulfur.dioxide",
    "density", "sulphates", "alcohol")]
DFCoarse$quality_cat <- factor(ifelse(wine.data$quality < 5, "LOW", ifelse(wine.data$quality >
    6, "HIGH", "MED")))
DFCoarse$quality <- NULL
DFCoarseTrain <- DFCoarse[train, ]
DFCoarseTest <- DFCoarse[-train, ]

gamma_default <- 1/(ncol(DFCoarseTrain) - 1)

gamma_list <- ((1:10)/5) * gamma_default
cost_list = c(0.001, 0.01, 0.1, 1, 5, 10, 100)

tune.svm.quality_cat = tune(svm, quality_cat ~ ., data = DFCoarseTrain, kernel = "polynomial",
    ranges = list(gamma = gamma_list, cost = cost_list))
svm.fit.quality_cat <- tune.svm.quality_cat$best.model

svm.pred.quality_cat <- predict(svm.fit.quality_cat, DFCoarseTest)
TB <- table(svm.pred.quality_cat, DFCoarseTest$quality_cat)
pander(TB)
```

	HIGH	LOW	MED
HIGH	15	0	8
LOW	0	2	3
MED	47	18	440

```
ACC_Multiclass_reduced = (sum(diag(TB)))/length(DFCoarseTest$quality_cat)

ACC_Class_HIGH = diag(TB)[1]/sum(DFCoarseTest$quality_cat == "HIGH")
ACC_Class_HIGH
```

```
##      HIGH
## 0.2419355
```

```
ACC_Class_LOW = diag(TB)[2]/sum(DFCoarseTest$quality_cat == "LOW")
ACC_Class_LOW
```

```
## LOW
## 0.1
```

```
ACC_Class_MED = diag(TB)[3]/sum(DFCoarseTest$quality_cat == "MED")
ACC_Class_MED
```

```
##       MED
## 0.9756098
```

Looking at the accuracy across the classes we see that a 2 class model may be preferrable.

There are ways to reduce the error introduced by class skew such as limiting the number of the over-represented class, or tuning the model to enhance the sensitivity or specificity of some classes. If there a string desire to have more than two classes - we'd consider applying these methods to the multiple classifyer one-versus all approach. We could train the 2 class classifiers for the classes with low representation to favor the underrepresented class and use a voting scheme for the final classification.

It's possible that we could build a generic classifier for the middle levels of quality and a separate classifier for the edge cases of very low and very high as an anomaly detection problem. In this case we would apply both classifiers in sucsession and use the result of the anomaly detector is there was a positive classification for low or high quality. The anomaly detector itself could be two separate classifiers - one for quality 3 and one for quality 8.