# Capstone Project: Wine Quality

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### Introduction

This project is part of the HarvardX:PH125.9x Data Science Capstone project. There are two datasets used that provide multiple physiochemical tests based on red and white wine samples that came from northern Portugal. The goal of this project is to develop machine learning algorithms based on all the physiochemical test results provided, in attempt to predict if a certain wine will be of high quality.

The datasets used can be found at the link below. (https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/).

### **Data Wrangling**

##

set.seed(42)

```
# Install any neccessary libraries
if(!require(caret)) install.packages("caret", repos = "http://cran.us.r-project.org")
if(!require(tidyverse)) install.packages("tidyverse", repos = "http://cran.us.r-project.org")
```

The following code was used to import the data and split it into test and training sets for later models.

```
# Import the Red and White datasets
url_red <- "https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv"
url_white <- "https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white.

red_data <- read.csv(url_red, sep=';')
white_data <- read.csv(url_white, sep=';')

# Merge the two separate red and white wine datasets into one dataset
wine <- rbind(red_data, white_data)

# Adding a column to classify an excellent wine quality
table(wine$quality)</pre>
```

```
## 3 4 5 6 7 8 9
## 30 216 2138 2836 1079 193 5

wine <- wine %>% mutate(Excellent = ifelse(quality > 6, 1, 0))
wine$Excellent <- as.factor(wine$Excellent)

# remove files no longer necessary
rm(url_red, url_white, red_data, white_data)

# Splitting data into test and train sets 80/20 split</pre>
```

#set.seed(1, sample.kind="Rounding") #if using R 3.5 or later

```
test_index <- createDataPartition(wine$Excellent, times = 1, p = 0.2, list = FALSE)
train_set <- wine[-test_index,]
test_set <- wine[test_index,]</pre>
```

### **Exploratory Analysis**

Once the data is available initial analysis and research the dataset can begin. Using the code below we can see that this dataset is in tidy format, and it contains 6497 rows and 13 columns.

```
# data is in tidy format
wine %>% as.tibble()
## # A tibble: 6,497 x 13
##
      fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
##
              <dbl>
                                           <dbl>
                               <dbl>
                                                          <dbl>
                                                                    <dbl>
##
   1
                7.4
                               0.7
                                            0
                                                            1.9
                                                                    0.076
                7.8
## 2
                               0.88
                                            0
                                                            2.6
                                                                    0.098
##
   3
                7.8
                               0.76
                                            0.04
                                                            2.3
                                                                    0.092
## 4
               11.2
                               0.28
                                            0.56
                                                            1.9
                                                                    0.075
## 5
                7.4
                               0.7
                                            0
                                                            1.9
                                                                    0.076
                7.4
## 6
                               0.66
                                                            1.8
                                                                    0.075
                                            0
   7
                7.9
                               0.6
##
                                            0.06
                                                            1.6
                                                                    0.069
## 8
                7.3
                               0.65
                                            0
                                                            1.2
                                                                    0.065
## 9
                7.8
                               0.580
                                            0.02
                                                            2
                                                                    0.073
                7.5
                               0.5
                                            0.36
                                                            6.1
                                                                    0.071
## 10
## # ... with 6,487 more rows, and 8 more variables: free.sulfur.dioxide <dbl>,
      total.sulfur.dioxide <dbl>, density <dbl>, pH <dbl>, sulphates <dbl>,
      alcohol <dbl>, quality <int>, Excellent <fct>
## #
# checking the structure of the data
str(wine)
## 'data.frame':
                    6497 obs. of 13 variables:
## $ fixed.acidity
                          : num 7.4 7.8 7.8 11.2 7.4 7.4 7.9 7.3 7.8 7.5 ...
## $ volatile.acidity
                                 0.7 0.88 0.76 0.28 0.7 0.66 0.6 0.65 0.58 0.5 ...
                          : num
                                0 0 0.04 0.56 0 0 0.06 0 0.02 0.36 ...
## $ citric.acid
                          : num
## $ residual.sugar
                          : num 1.9 2.6 2.3 1.9 1.9 1.8 1.6 1.2 2 6.1 ...
## $ chlorides
                                0.076 0.098 0.092 0.075 0.076 0.075 0.069 0.065 0.073 0.071 ...
                          : num
## $ free.sulfur.dioxide : num
                                 11 25 15 17 11 13 15 15 9 17 ...
## $ total.sulfur.dioxide: num
                                34 67 54 60 34 40 59 21 18 102 ...
## $ density
                                0.998 0.997 0.997 0.998 0.998 ...
                          : num
## $ pH
                                 3.51 3.2 3.26 3.16 3.51 3.51 3.3 3.39 3.36 3.35 ...
                          : num
                                0.56 0.68 0.65 0.58 0.56 0.56 0.46 0.47 0.57 0.8 ...
## $ sulphates
                          : num
                          : num 9.4 9.8 9.8 9.8 9.4 9.4 9.4 10 9.5 10.5 ...
## $ alcohol
## $ quality
                          : int 555655775 ...
   $ Excellent
                          : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 2 2 1 ...
# checking basic summary statistics
summary(wine)
```

```
Min.
           : 3.800
                            :0.0800
                                              :0.0000
                                                               : 0.600
##
                     Min.
                                      Min.
                                                        Min.
   1st Qu.: 6.400
##
                     1st Qu.:0.2300
                                      1st Qu.:0.2500
                                                        1st Qu.: 1.800
                                      Median :0.3100
   Median : 7.000
                     Median :0.2900
                                                        Median : 3.000
          : 7.215
                            :0.3397
                                                               : 5.443
##
  Mean
                     Mean
                                      Mean
                                              :0.3186
                                                        Mean
##
   3rd Qu.: 7.700
                     3rd Qu.:0.4000
                                      3rd Qu.:0.3900
                                                        3rd Qu.: 8.100
           :15.900
##
   Max.
                            :1.5800
                                      Max.
                                             :1.6600
                                                               :65.800
                     \mathtt{Max}.
                                                        Max.
                      free.sulfur.dioxide total.sulfur.dioxide
##
      chlorides
                                                                   density
##
  Min.
           :0.00900
                      Min. : 1.00
                                          Min.
                                                 : 6.0
                                                                Min.
                                                                       :0.9871
##
   1st Qu.:0.03800
                      1st Qu.: 17.00
                                          1st Qu.: 77.0
                                                                1st Qu.:0.9923
##
  Median :0.04700
                      Median : 29.00
                                          Median :118.0
                                                                Median :0.9949
  Mean
           :0.05603
                      Mean
                            : 30.53
                                          Mean
                                                 :115.7
                                                                Mean
                                                                       :0.9947
                      3rd Qu.: 41.00
                                           3rd Qu.:156.0
                                                                3rd Qu.:0.9970
##
   3rd Qu.:0.06500
           :0.61100
##
                      Max.
                             :289.00
                                          Max.
                                                 :440.0
                                                                Max.
                                                                       :1.0390
                                        alcohol
##
         pН
                      sulphates
                                                         quality
                                                                      Excellent
##
                                            : 8.00
                                                             :3.000
                                                                      0:5220
  Min.
         :2.720
                    Min.
                           :0.2200
                                     Min.
                                                     Min.
##
   1st Qu.:3.110
                    1st Qu.:0.4300
                                     1st Qu.: 9.50
                                                     1st Qu.:5.000
                                                                      1:1277
                    Median :0.5100
                                     Median :10.30
                                                     Median :6.000
##
  Median :3.210
##
  Mean
           :3.219
                           :0.5313
                                           :10.49
                                                      Mean
                                                             :5.818
                    Mean
                                     Mean
##
  3rd Qu.:3.320
                    3rd Qu.:0.6000
                                     3rd Qu.:11.30
                                                      3rd Qu.:6.000
## Max.
           :4.010
                    {\tt Max.}
                           :2.0000
                                     Max.
                                            :14.90
                                                      Max.
                                                             :9.000
# Number of rows and columns
nrow(wine)
## [1] 6497
ncol(wine)
## [1] 13
# Check for missing values
any(is.na(wine))
```

## [1] FALSE

Installing additional libraries which may be useful for analysis and modeling

```
if(!require(ggplot2)) install.packages("ggplot2", repos = "http://cran.us.r-project.org")
if(!require(reshape2)) install.packages("reshape2", repos = "http://cran.us.r-project.org")
if(!require(lubridate)) install.packages("lubridate", repos = "http://cran.us.r-project.org")
if(!require(randomForest)) install.packages("randomForest", repos = "http://cran.us.r-project.org")
if(!require(rpart)) install.packages("rpart", repos = "http://cran.us.r-project.org")
```

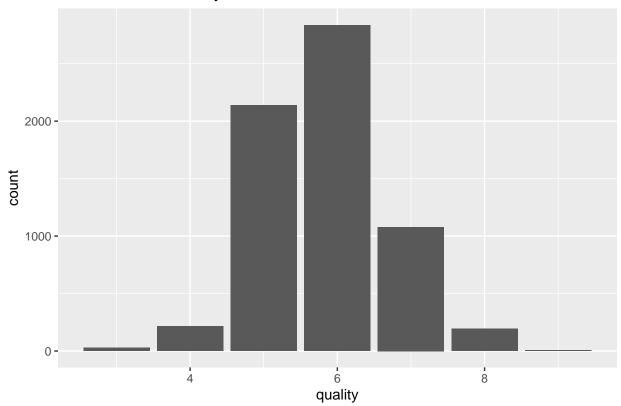
The first observation to check is the overall distribution of wines based on their quality.

```
# Overall Average Quality
mean(wine$quality)
```

## [1] 5.818378

```
# Distribution in Quality
wine %>%
    ggplot(aes(quality)) +
    geom_bar() +
    ggtitle("Distribution of Quality")
```

## Distribution of Quality



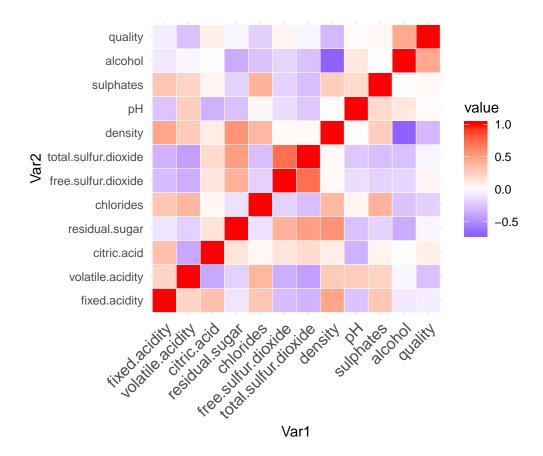
```
# Percentage of Excellent wines
mean(wine$Excellent == 1)
```

### ## [1] 0.1965523

Based on the following code creating a heatmap can allow for pin-pointing a few attributes that have higher correlations than others. These variables may play a bigger part in predictions later on, so it's good to take a further look. (alcohol, total.sulfur.dioxide, free.sulfur.dioxide, residual.sugar, and density)

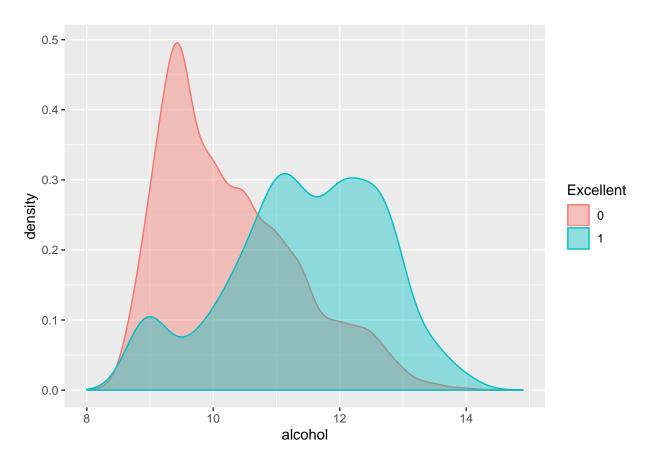
```
train.cor <- cor(subset(wine, select=-c(Excellent)))

ggplot(melt(train.cor), aes(Var1, Var2, fill=value)) +
    geom_tile(color = "white") + #color white is for border
    scale_fill_gradient2(low="blue", high="red", mid="white") +
    theme_minimal() + # minimal theme
    theme(axis.text.x = element_text(angle = 45, vjust = 1, size = 12, hjust = 1)) +
    coord_fixed()</pre>
```

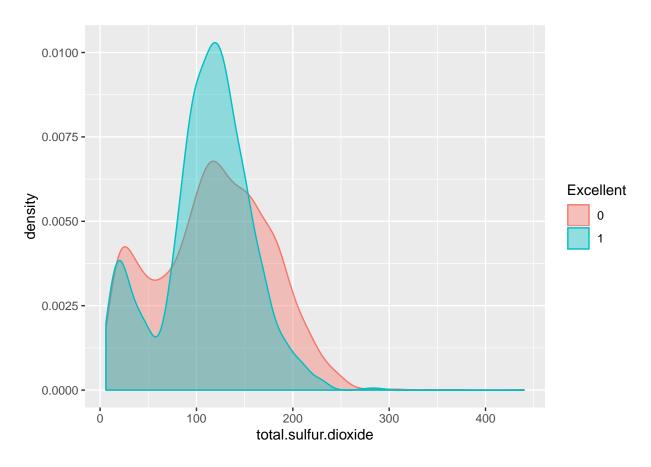


The below density plots check each of the physichemical tests to give a better understanding of their distributions. The flag created during data wrangling portion which specifies if a wine was considered excellent or not can also be added to give further insights.

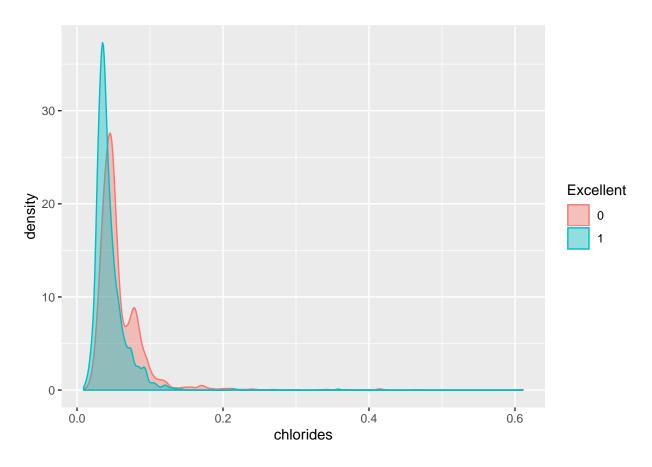
```
ggplot(wine, aes(alcohol, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



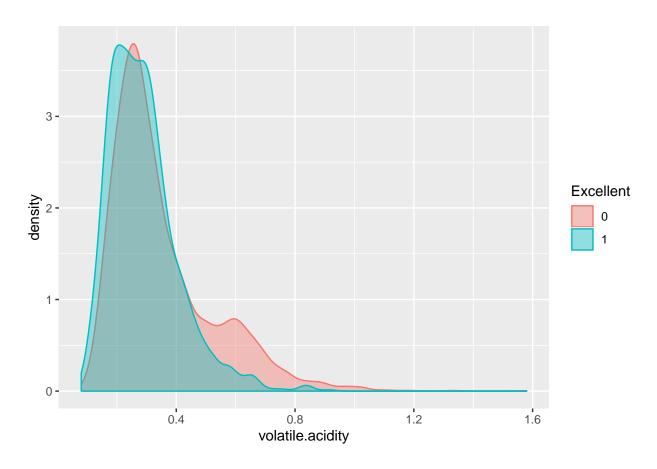
```
ggplot(wine, aes(total.sulfur.dioxide, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



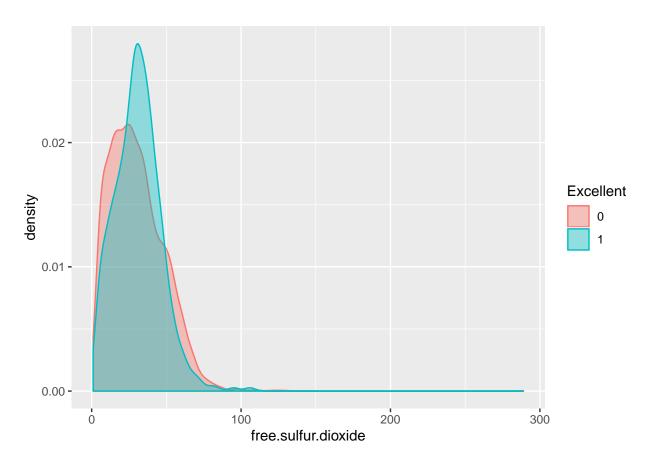
```
ggplot(wine, aes(chlorides, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



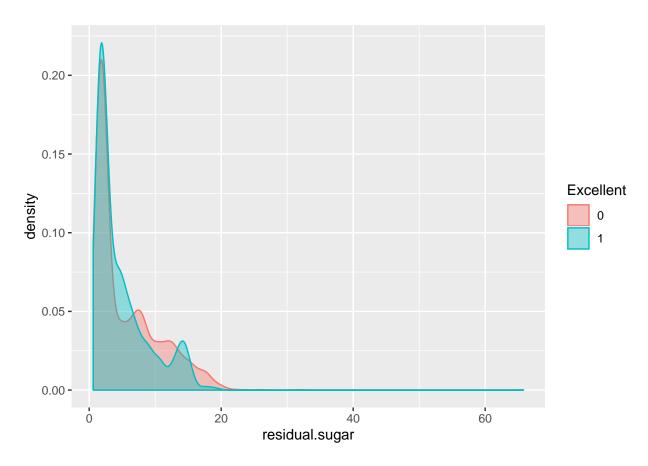
```
ggplot(wine, aes(volatile.acidity, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



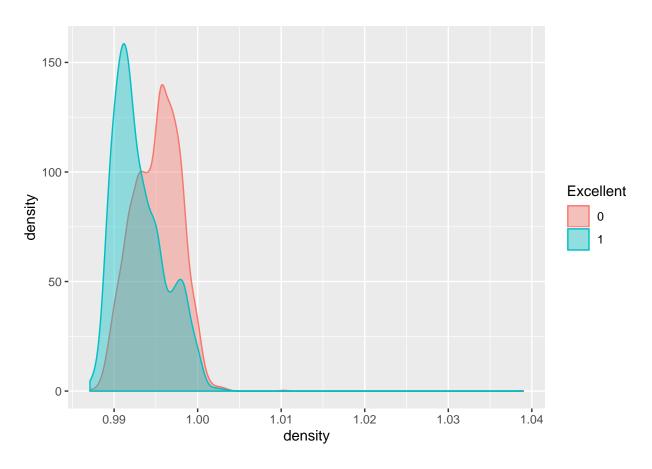
```
ggplot(wine, aes(free.sulfur.dioxide, color=Excellent, fill=Excellent)) +
  geom_density(alpha = 0.4)
```



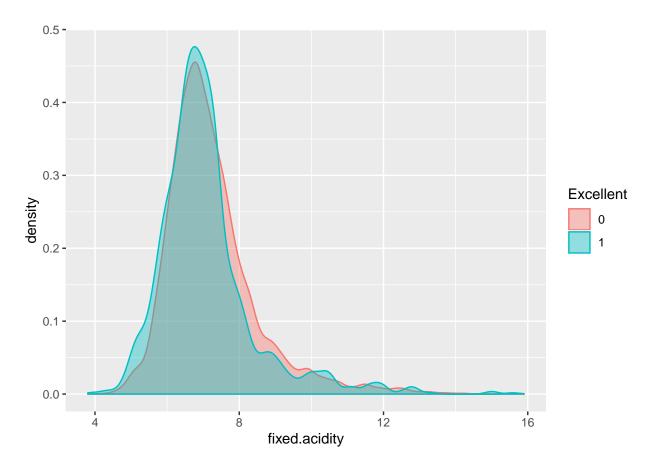
```
ggplot(wine, aes(residual.sugar, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



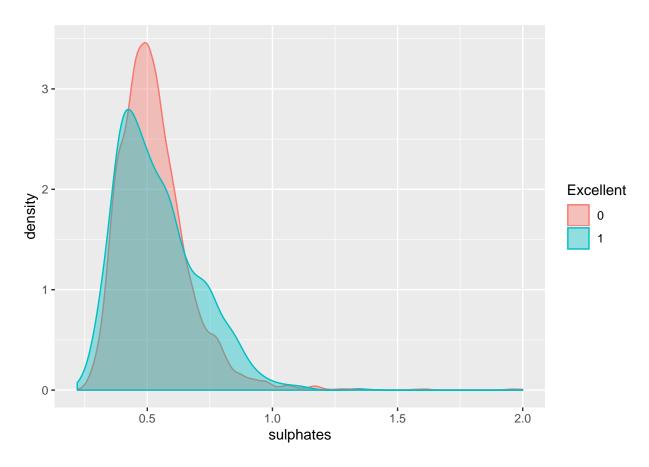
```
ggplot(wine, aes(density, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



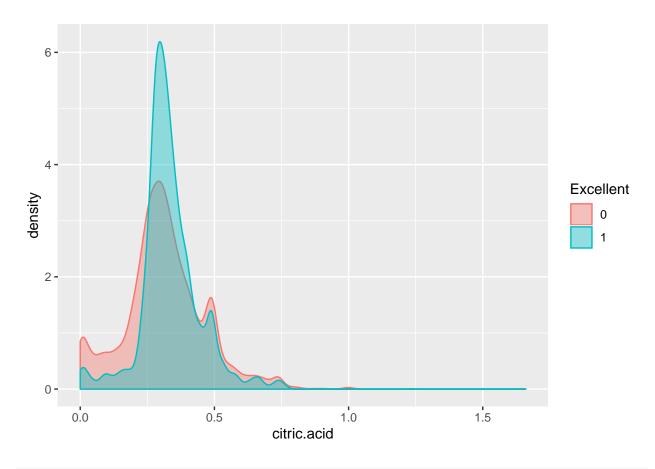
```
ggplot(wine, aes(fixed.acidity, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



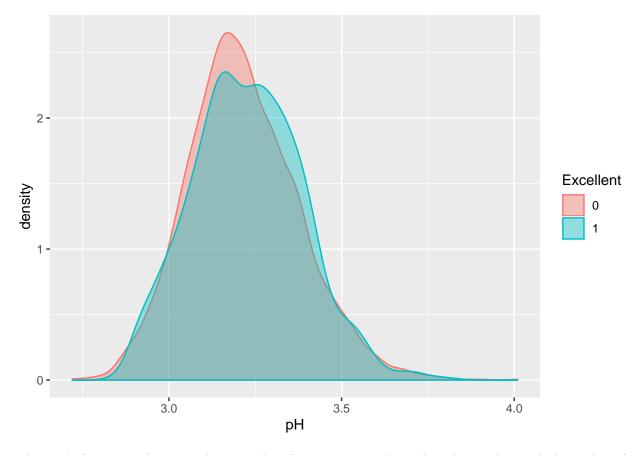
```
ggplot(wine, aes(sulphates, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



```
ggplot(wine, aes(citric.acid, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



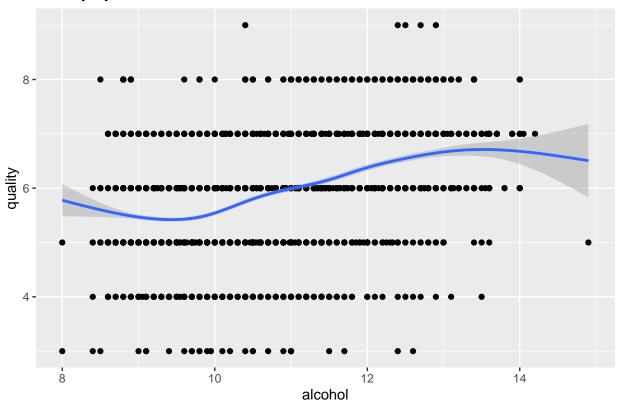
```
ggplot(wine, aes(pH, color=Excellent, fill=Excellent)) +
geom_density(alpha = 0.4)
```



Taking a look at a couple scatterplots may show how certain attributes directly correlate with the quality. As shown in the plots below, when the alcohol content increases the quality generally increases as well. Density however, the quality tends to decrease as density increases.

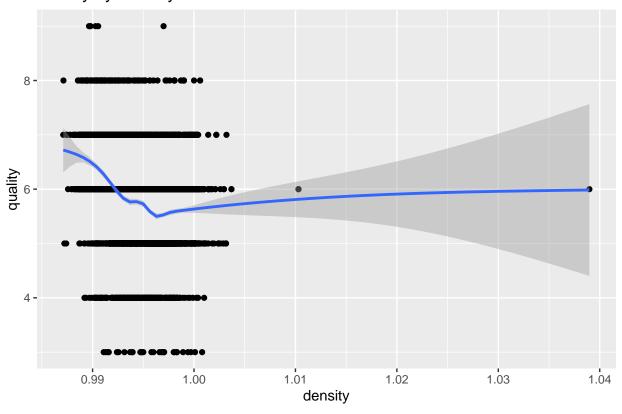
```
ggplot(wine, aes(alcohol, quality)) +
  geom_point() +
  geom_smooth() +
  ggtitle("Quality by Alcohol")
```

# Quality by Alcohol



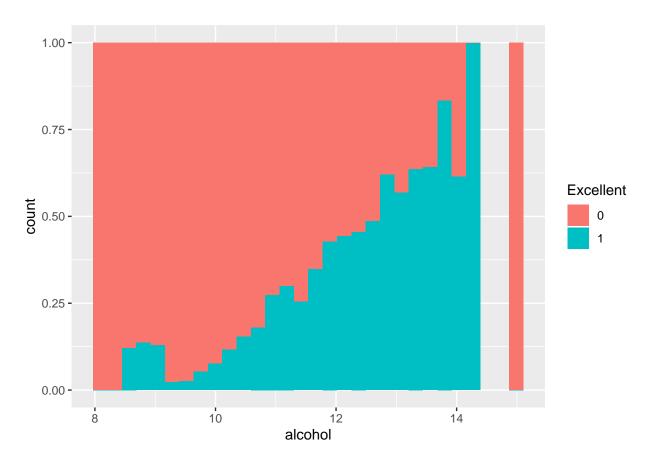
```
ggplot(wine, aes(density, quality)) +
  geom_point() +
  geom_smooth() +
  ggtitle("Quality by Density")
```

## Quality by Density

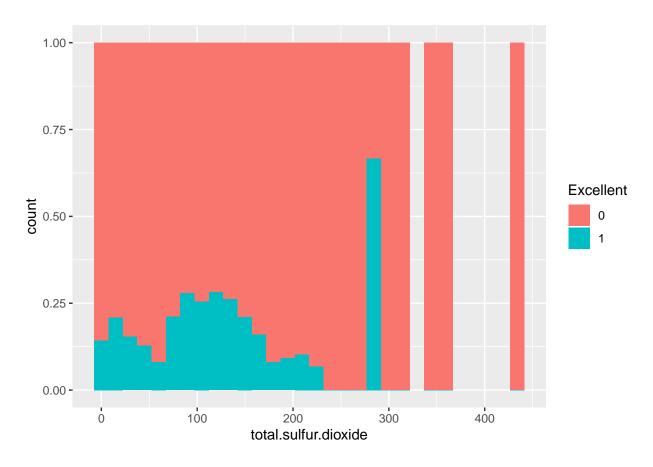


Stacked bar charts to easily show the percentage of excellent wines overall, based on particular variables. The images below continue to show similar results as previously mentioned, where higher quality wines tend to have higher alcohol content and lower densities.

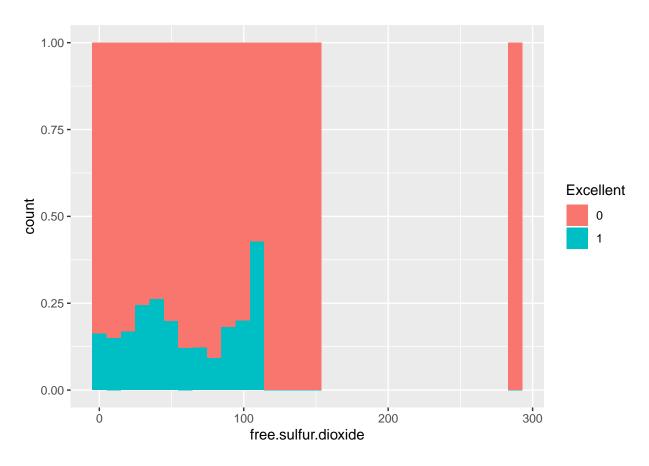
```
ggplot(wine, aes(alcohol, fill=Excellent)) +
  geom_histogram(bins=30, position="fill")
```



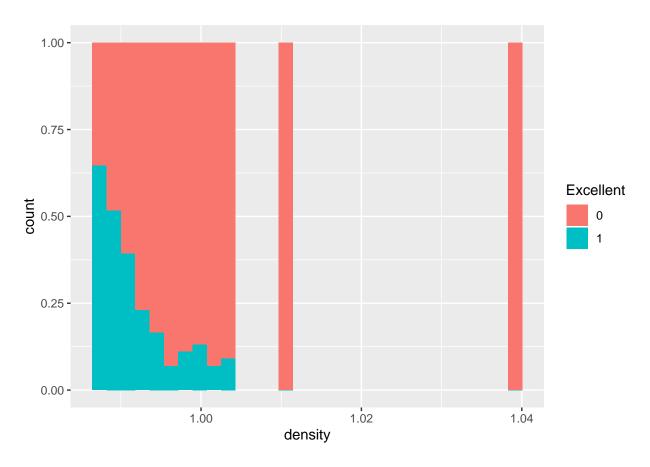
ggplot(wine, aes(total.sulfur.dioxide, fill=Excellent)) +
geom\_histogram(bins=30, position="fill")



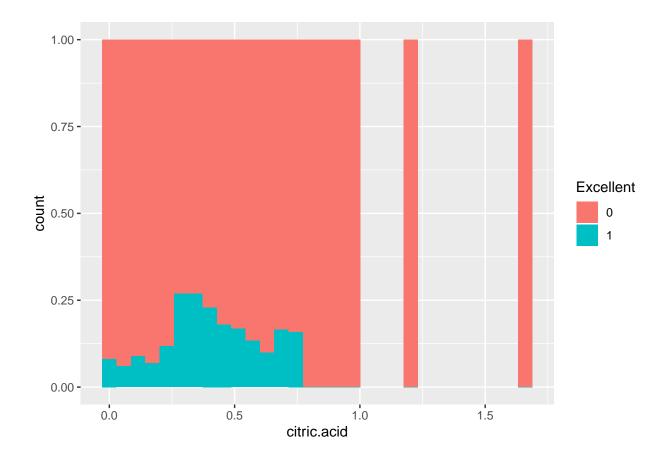
ggplot(wine, aes(free.sulfur.dioxide, fill=Excellent)) +
geom\_histogram(bins=30, position="fill")



```
ggplot(wine, aes(density, fill=Excellent)) +
geom_histogram(bins=30, position="fill")
```



ggplot(wine, aes(citric.acid, fill=Excellent)) +
 geom\_histogram(bins=30, position="fill")



### Modeling

Each of the models below are using all the physiochemical tests variables available to predict if a wine will be considered excellent. The quality column is not included as a predictor of Excellent since it was directly used to create the classification flags.

```
# Logistic Regression Model
set.seed(1)
train_glm <- train(Excellent ~ .-quality, method = "glm", data = train_set)
glm_pred <- predict(train_glm, test_set, type = "raw")
confusionMatrix(glm_pred, test_set$Excellent)$overall[["Accuracy"]]</pre>
```

## [1] 0.8323077

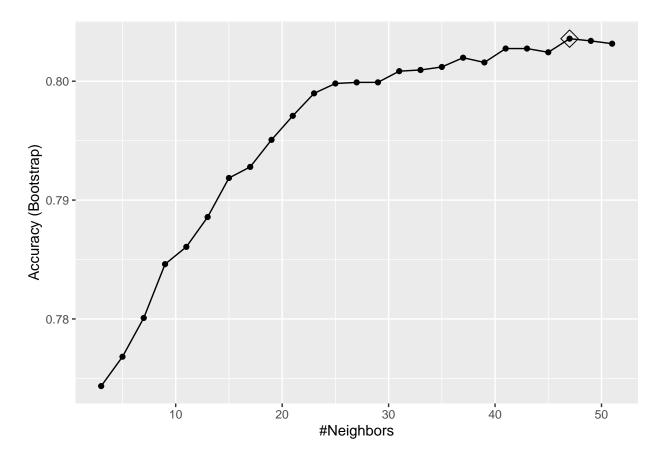
```
# LDA Model
set.seed(1)
train_lda <- train(Excellent ~ .-quality, method = "lda", data = train_set)
lda_pred <- predict(train_lda, test_set)
confusionMatrix(lda_pred, test_set$Excellent)$overall[["Accuracy"]]</pre>
```

## [1] 0.8323077

```
# QDA Model
set.seed(1)
train_lda <- train(Excellent ~ .-quality, method = "qda", data = train_set)
qda_pred <- predict(train_lda, test_set)
mean(lda_pred == test_set$Excellent)</pre>
```

### ## [1] 0.8323077

#### ## [1] 0.8376923

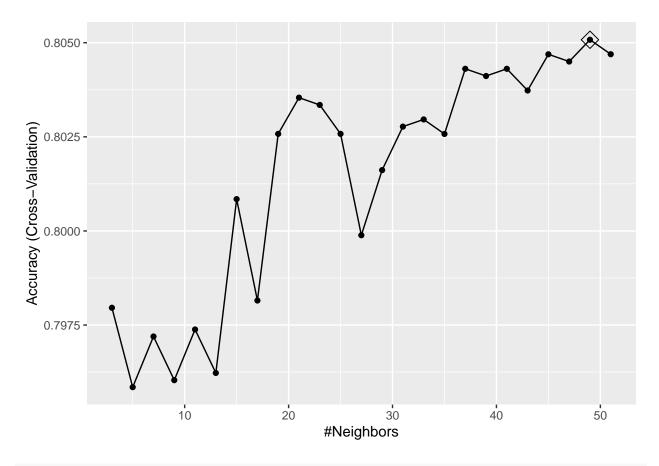


```
train_knn$bestTune
```

```
## k
## 23 47
```

```
knn_pred <- predict(train_knn, test_set, type = "raw")
confusionMatrix(knn_pred, test_set$Excellent)$overall["Accuracy"]</pre>
```

## Accuracy ## 0.8030769

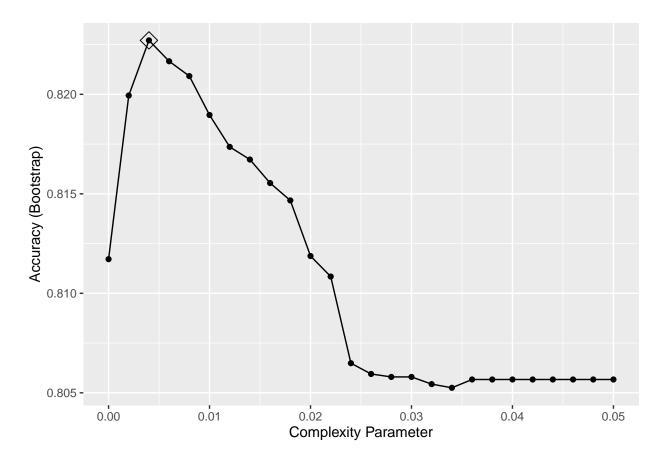


train\_knn\_cross\$bestTune

## k ## 24 49

```
knn_cross_pred <- predict(train_knn_cross, test_set, type = "raw")
confusionMatrix(knn_cross_pred, test_set$Excellent)$overall["Accuracy"]</pre>
```

```
## Accuracy
## 0.8038462
```



```
train_tree$bestTune
```

```
## cp
## 3 0.004

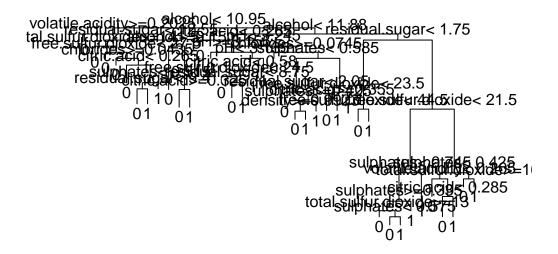
rpart_pred <- predict(train_tree, test_set, type = "raw")
confusionMatrix(rpart_pred,test_set$Excellent)$overall["Accuracy"]</pre>
```

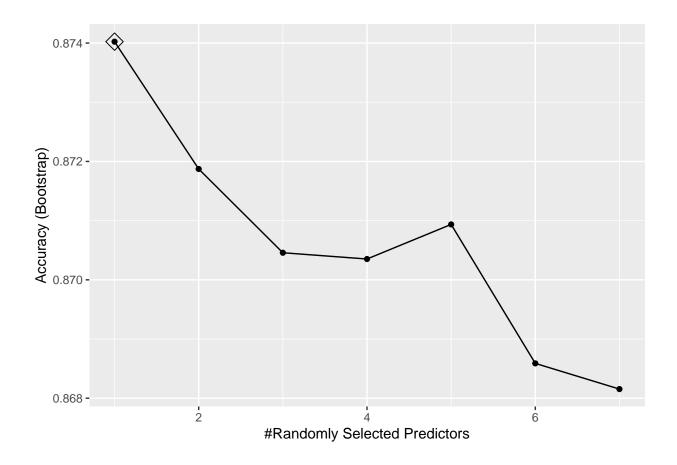
## Accuracy ## 0.8346154

```
## n= 5197
  node), split, n, loss, yval, (yprob)
##
         * denotes terminal node
##
##
     1) root 5197 1021 0 (0.80354050 0.19645950)
##
       2) alcohol< 10.95 3453 329 0 (0.90472053 0.09527947)
##
         4) volatile.acidity>=0.2025 2838 176 0 (0.93798450 0.06201550) *
##
         5) volatile.acidity< 0.2025 615 153 0 (0.75121951 0.24878049)
##
          10) residual.sugar< 12.55 486
                                          91 0 (0.81275720 0.18724280)
            20) total.sulfur.dioxide>=141.5 164
                                                 9 0 (0.94512195 0.05487805) *
##
            21) total.sulfur.dioxide< 141.5 322
##
                                                82 0 (0.74534161 0.25465839)
              42) free.sulfur.dioxide< 27.5 165
                                                  25 0 (0.84848485 0.15151515) *
##
              43) free.sulfur.dioxide>=27.5 157
                                                  57 0 (0.63694268 0.36305732)
##
                86) chlorides>=0.0435 74
                                          13 0 (0.82432432 0.17567568) *
##
##
                87) chlorides< 0.0435 83
                                           39 1 (0.46987952 0.53012048)
##
                 174) citric.acid< 0.265 15
                                               1 0 (0.93333333 0.06666667) *
                 175) citric.acid>=0.265 68
##
                                              25 1 (0.36764706 0.63235294)
##
                   350) sulphates< 0.515 45
                                              22 0 (0.51111111 0.48888889)
##
                     700) residual.sugar< 9.4 28
                                                    8 0 (0.71428571 0.28571429) *
##
                     701) residual.sugar>=9.4 17
                                                    3 1 (0.17647059 0.82352941) *
##
                   351) sulphates>=0.515 23
                                               2 1 (0.08695652 0.91304348) *
##
          11) residual.sugar>=12.55 129
                                          62 0 (0.51937984 0.48062016)
            22) alcohol>=9.15 57
##
                                  10 0 (0.82456140 0.17543860) *
##
            23) alcohol< 9.15 72
                                   20 1 (0.27777778 0.72222222)
##
              46) citric.acid>=0.325 21
                                           4 0 (0.80952381 0.19047619) *
##
              47) citric.acid< 0.325 51
                                           3 1 (0.05882353 0.94117647) *
##
       3) alcohol>=10.95 1744 692 0 (0.60321101 0.39678899)
##
         6) alcohol< 11.875 897 274 0 (0.69453735 0.30546265)
##
          12) citric.acid< 0.265 220
                                       35 0 (0.84090909 0.15909091) *
##
          13) citric.acid>=0.265 677 239 0 (0.64697194 0.35302806)
##
            26) pH< 3.245 413 119 0 (0.71186441 0.28813559)
##
              52) pH>=3.155 155
                                  28 0 (0.81935484 0.18064516) *
##
              53) pH< 3.155 258
                                  91 0 (0.64728682 0.35271318)
                                    66 0 (0.69585253 0.30414747)
##
               106) pH< 3.135 217
                 212) citric.acid< 0.58 209
                                              60 0 (0.71291866 0.28708134)
##
##
                   424) free.sulfur.dioxide< 24.5 79
                                                      13 0 (0.83544304 0.16455696) *
##
                   425) free.sulfur.dioxide>=24.5 130 47 0 (0.63846154 0.36153846)
                                                     31 0 (0.71559633 0.28440367) *
##
                     850) residual.sugar< 8.75 109
##
                     851) residual.sugar>=8.75 21
                                                     5 1 (0.23809524 0.76190476) *
##
                 213) citric.acid>=0.58 8
                                             2 1 (0.25000000 0.75000000) *
                                   16 1 (0.39024390 0.60975610) *
##
               107) pH>=3.135 41
##
            27) pH>=3.245 264 120 0 (0.54545455 0.45454545)
              54) chlorides>=0.0745 37
##
                                          5 0 (0.86486486 0.13513514) *
##
              55) chlorides< 0.0745 227 112 1 (0.49339207 0.50660793)
##
               110) sulphates< 0.585 151
                                           63 0 (0.58278146 0.41721854)
                 220) residual.sugar< 2.05 76
                                                22 0 (0.71052632 0.28947368) *
##
                 221) residual.sugar>=2.05 75
##
                                                34 1 (0.45333333 0.54666667)
##
                   442) sulphates>=0.425 47
                                             20 0 (0.57446809 0.42553191)
##
                     884) density>=0.9923 29
                                                8 0 (0.72413793 0.27586207) *
                     885) density< 0.9923 18
##
                                                6 1 (0.33333333 0.66666667) *
```

```
##
                   443) sulphates< 0.425 28
                                               7 1 (0.25000000 0.75000000) *
##
               111) sulphates>=0.585 76
                                         24 1 (0.31578947 0.68421053)
                 222) free.sulfur.dioxide< 23.5 31
##
                                                     15 0 (0.51612903 0.48387097)
##
                   444) citric.acid>=0.355 18
                                                 4 0 (0.77777778 0.22222222) *
##
                   445) citric.acid< 0.355 13
                                                 2 1 (0.15384615 0.84615385) *
##
                 223) free.sulfur.dioxide>=23.5 45
                                                      8 1 (0.17777778 0.82222222) *
##
         7) alcohol>=11.875 847 418 0 (0.50649351 0.49350649)
##
          14) residual.sugar< 1.75 198 68 0 (0.65656566 0.34343434)
##
            28) free.sulfur.dioxide< 44.5 183
                                              56 0 (0.69398907 0.30601093) *
##
            29) free.sulfur.dioxide>=44.5 15
                                                3 1 (0.20000000 0.80000000) *
##
          15) residual.sugar>=1.75 649 299 1 (0.46070878 0.53929122)
            30) free.sulfur.dioxide< 21.5 239
##
                                                96 0 (0.59832636 0.40167364)
              60) sulphates< 0.745 196
##
                                       64 0 (0.67346939 0.32653061)
##
               120) sulphates>=0.335 187
                                           56 0 (0.70053476 0.29946524)
##
                 240) total.sulfur.dioxide>=13 164
                                                     43 0 (0.73780488 0.26219512) *
##
                 241) total.sulfur.dioxide< 13 23
                                                    10 1 (0.43478261 0.56521739)
##
                   482) sulphates< 0.575 10
                                               2 0 (0.80000000 0.20000000) *
##
                   483) sulphates>=0.575 13
                                               2 1 (0.15384615 0.84615385) *
##
               121) sulphates< 0.335 9
                                          1 1 (0.11111111 0.88888889) *
##
              61) sulphates>=0.745 43
                                        11 1 (0.25581395 0.74418605) *
##
            31) free.sulfur.dioxide>=21.5 410 156 1 (0.38048780 0.61951220)
##
              62) sulphates< 0.425 168
                                        82 1 (0.48809524 0.51190476)
##
               124) volatile.acidity< 0.205 19
                                                  3 0 (0.84210526 0.15789474) *
               125) volatile.acidity>=0.205 149
                                                  66 1 (0.44295302 0.55704698)
##
##
                 250) citric.acid< 0.285 45
                                              15 0 (0.66666667 0.333333333) *
##
                 251) citric.acid>=0.285 104
                                               36 1 (0.34615385 0.65384615) *
##
              63) sulphates>=0.425 242
                                       74 1 (0.30578512 0.69421488)
               126) total.sulfur.dioxide>=168.5 16
                                                    5 0 (0.68750000 0.31250000) *
##
##
               127) total.sulfur.dioxide< 168.5 226
                                                      63 1 (0.27876106 0.72123894) *
```

plot(train\_tree\$finalModel, margin = 0.1)
text(train\_tree\$finalModel)





```
train_rf$bestTune

## mtry
## 1 1

rf_pred <- predict(train_rf, test_set, type = "raw")
confusionMatrix(rf_pred,test_set$Excellent)$overall["Accuracy"]

## Accuracy
## 0.9053846</pre>
```

```
#importance of variables
varImp(train_rf)
```

```
## rf variable importance
##
##
                       Overall
## alcohol
                       100.000
                        76.208
## density
## chlorides
                        39.376
## volatile.acidity
                       19.975
## total.sulfur.dioxide 17.175
## sulphates
                     14.729
## residual.sugar
                       13.334
```

```
## free.sulfur.dioxide 12.734
## citric.acid 11.799
## pH 9.679
## fixed.acidity 0.000
```

### Results

```
## Model Accuracy
## 1 Logistic Regression 0.8323077
## 2 LDA 0.8323077
## 3 QDA 0.7792308
## 4 Loess 0.8376923
## 5 K nearest neighbors 0.8030769
## 6 Cross Validation 0.8038462
## 7 Rpart 0.8346154
## 8 Random forest 0.9053846
```

When comparing the results from all the different models performance it is clear that the highest performing model was the Random Forest which had a 90.5% accuracy. This is large improvement from the lowest performing model which was QDA at 77.9%.

#### Conclusion

Through our analysis we were able to interpret the visualizations and determine a few variables that play a higher role in predicting the outcome. These variables were later confirmed with the random forest model which showed both alcohol and density as having the highest importance for predictions. Since this data didn't contain every aspect of wine data, things like brand name, age, sell price could all potentially improve these models and make it easier to classify an excellent wine from a mediocre.