Wine Quality Prediction

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Project and Dataset Presentation

In this notebook we will use the data from the Kaggle Repository (https://www.kaggle.com/rajyellow46/wine-quality) by P. Cortez, A. Cerdeira, F. Almeida, T. Matos, and J. Reis. The data include examples of red and white wines from Portugal-one of the world's leading wine-producing countries.

For each wine, a laboratory analysis measured characteristics such as acidity, sugar content, chlorides, sulfur, alcohol, pH, and density. The samples were then rated in a blind tasting by panels of no less than three judges on a quality scale ranging from zero (very bad) to 10 (excellent). In the case of judges disagreeing on the rating, the median value was used.

Objective of this notebook The objective that we want to achieve throw this notebook is to build a machine learning model of classification type, that will predict if a wine is considered as good or note. The model takes as input some wine characteristics (alcohol content, acidity, sugar proportion, etc), and gives as output a binary variable that describes the quality of the wine ("Good" or "Bad"). We'll use a decision tree as our classification model.

Dataset description The wine dataset is composed by a total of 14 different variables :

1- fixed acidity (tartaric acid - g/dm3) : most acids involved with wine or fixed or nonvolatile (do not evaporate readily)

2- volatile acidity (acetic acid - g/dm3): the amount of acetic acid in wine, which at too high of levels can lead to an unpleasant, vinegar taste

3- citric acid (g/dm3) : found in small quantities, citric acid can add 'freshness' and flavor to wines

4- residual sugar (g/dm3) : the amount of sugar remaining after fermentation stops, it's rare to find wines with less than 1 gram/liter and wines with greater than 45 grams/liter are considered sweet

5- chlorides (sodium chloride - g/dm3) : the amount of salt in the wine

6- free sulfur dioxide (mg/dm3) : the free form of SO2 exists in equilibrium between molecular SO2 (as a dissolved gas) and bisulfite ion; it prevents microbial growth and the oxidation of wine

7- total sulfur dioxide (mg/dm3) : amount of free and bound forms of S02; in low concentrations, SO2 is mostly undetectable in wine, but at free SO2 concentrations over 50 ppm, SO2 becomes evident in the nose and taste of wine

8- density (g/cm3) : the density of water is close to that of water depending on the percent alcohol and sugar content

9- pH : describes how acidic or basic a wine is on a scale from 0 (very acidic) to 14 (very basic); most wines are between 3-4 on the pH scale

10- sulphates (potassium sulphate - g/dm3) : a wine additive which can contribute to sulfur dioxide gas (S02) levels, wich acts as an antimicrobial and antioxidant

11- alcohol (% by volume) : the percent alcohol content of the wine Output variable (based on sensory data):

12- quality: score between 0 and 10 that describes the quality of the wine.

13- good: boolean variable related to the quality variable, is true when quality > 7 else the variable is false.

14- color: color of the wine. There are two type wine, red wine and white wine.

Exploratory Data Analysis on the wine dataset

Load the wine dataset We start by reading the data which is stored in the csv file `winequality.csv`. The file is loaded using the `read.csv` command, along with the `as.data.frame` command which store our data inside a structure of dataframe type.

```
# Load the data
df_wine <- as.data.frame( read.csv(file = './data/winequality.csv', sep=',', stringsAsFactors=F))
head(df_wine)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.4             0.70        0.00            1.9     0.076
## 2           7.8             0.88        0.00            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             0.70        0.00            1.9     0.076
## 6           7.4             0.66        0.00            1.8     0.075
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  11                   34  0.9978 3.51      0.56     9.4
## 2                  25                   67  0.9968 3.20      0.68     9.8
## 3                  15                   54  0.9970 3.26      0.65     9.8
## 4                  17                   60  0.9980 3.16      0.58     9.8
## 5                  11                   34  0.9978 3.51      0.56     9.4
## 6                  13                   40  0.9978 3.51      0.56     9.4
##   quality color
## 1       5   red
## 2       5   red
## 3       5   red
## 4       6   red
## 5       5   red
## 6       5   red
```

```
tail(df_wine)
```

```
##      fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 6492           6.5             0.23        0.38            1.3     0.032
## 6493           6.2             0.21        0.29            1.6     0.039
## 6494           6.6             0.32        0.36            8.0     0.047
## 6495           6.5             0.24        0.19            1.2     0.041
## 6496           5.5             0.29        0.30            1.1     0.022
## 6497           6.0             0.21        0.38            0.8     0.020
##      free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 6492                  29                  112 0.99298 3.29      0.54     9.7
## 6493                  24                   92 0.99114 3.27      0.50    11.2
## 6494                  57                  168 0.99490 3.15      0.46     9.6
## 6495                  30                  111 0.99254 2.99      0.46     9.4
## 6496                  20                  110 0.98869 3.34      0.38    12.8
## 6497                  22                   98 0.98941 3.26      0.32    11.8
```

```
##      quality color
## 6492       5 white
## 6493       6 white
## 6494       5 white
## 6495       6 white
## 6496       7 white
## 6497       6 white
```

Basic analysis on the dataset

Now we're gonna achieve some basic analysis on our wine dataset to get a better understanding of its contents, size and structure.

Dimension of our wine Dataset :

```
cat('The number of rows inside the dataset is : ', dim(df_wine)[1])
```

```
## The number of rows inside the dataset is :  6497
```

```
cat('The number of columns/features inside the dataset is : ', dim(df_wine)[2])
```

```
## The number of columns/features inside the dataset is :  13
```

Structure and distribution of the variables :

We use the `str` and `summary` functions to display some basic statistics about our dataset. The `str` function shows the nature (type) of each variable (feature) of our dateset, and some values that the feature can take. The `summary` function in other hand give us some statistics metrics (min, max, median, etc) for each feature of the dataset.

```
str(df_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    : num  0.7 0.88 0.76 0.28 0.7 0.66 0.6 0.65 0.58 0.5 ...
##  $ citric.acid         : num  0 0 0.04 0.56 0 0 0.06 0 0.02 0.36 ...
##  $ residual.sugar      : num  1.9 2.6 2.3 1.9 1.9 1.8 1.6 1.2 2 6.1 ...
##  $ chlorides           : num  0.076 0.098 0.092 0.075 0.076 0.075 0.069 0.065 0.073 0.071 ...
##  $ free.sulfur.dioxide : num  11 25 15 17 11 13 15 15 9 17 ...
##  $ total.sulfur.dioxide: num  34 67 54 60 34 40 59 21 18 102 ...
##  $ density             : num  0.998 0.997 0.997 0.998 0.998 ...
##  $ pH                  : num  3.51 3.2 3.26 3.16 3.51 3.51 3.3 3.39 3.36 3.35 ...
##  $ sulphates           : num  0.56 0.68 0.65 0.58 0.56 0.56 0.46 0.47 0.57 0.8 ...
##  $ alcohol             : num  9.4 9.8 9.8 9.8 9.4 9.4 9.4 10 9.5 10.5 ...
##  $ quality             : int  5 5 5 6 5 5 5 7 7 5 ...
##  $ color               : chr  "red" "red" "red" "red" ...
```

```
summary(df_wine)
```

```
##  fixed.acidity    volatile.acidity  citric.acid     residual.sugar
##  Min.   : 3.800   Min.   :0.0800   Min.   :0.0000   Min.   : 0.600
##  1st Qu.: 6.400   1st Qu.:0.2300   1st Qu.:0.2500   1st Qu.: 1.800
##  Median : 7.000   Median :0.2900   Median :0.3100   Median : 3.000
##  Mean   : 7.215   Mean   :0.3397   Mean   :0.3186   Mean   : 5.443
##  3rd Qu.: 7.700   3rd Qu.:0.4000   3rd Qu.:0.3900   3rd Qu.: 8.100
##  Max.   :15.900   Max.   :1.5800   Max.   :1.6600   Max.   :65.800
##    chlorides       free.sulfur.dioxide total.sulfur.dioxide    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.:0.06500   3rd Qu.: 41.00      3rd Qu.:156.0        3rd Qu.:0.9970
##  Max.   :0.61100   Max.   :289.00      Max.   :440.0        Max.   :1.0390
##        pH          sulphates         alcohol         quality
##  Min.   :2.720   Min.   :0.2200   Min.   : 8.00   Min.   :3.000
##  1st Qu.:3.110   1st Qu.:0.4300   1st Qu.: 9.50   1st Qu.:5.000
##  Median :3.210   Median :0.5100   Median :10.30   Median :6.000
##  Mean   :3.219   Mean   :0.5313   Mean   :10.49   Mean   :5.818
##  3rd Qu.:3.320   3rd Qu.:0.6000   3rd Qu.:11.30   3rd Qu.:6.000
##  Max.   :4.010   Max.   :2.0000   Max.   :14.90   Max.   :9.000
##     color
##  Length:6497
##  Class :character
##  Mode  :character
##
##
##
```

Correlation between the variables :

```
as.data.frame( cor(df_wine[c(-13, -14)]))
```

```
##                       fixed.acidity volatile.acidity citric.acid residual.sugar
## fixed.acidity           1.00000000       0.21900826  0.32443573    -0.11198128
## volatile.acidity        0.21900826       1.00000000 -0.37798132    -0.19601117
## citric.acid             0.32443573      -0.37798132  1.00000000     0.14245123
## residual.sugar         -0.11198128      -0.19601117  0.14245123     1.00000000
## chlorides               0.29819477       0.37712428  0.03899801    -0.12894050
## free.sulfur.dioxide    -0.28273543      -0.35255731  0.13312581     0.40287064
## total.sulfur.dioxide   -0.32905390      -0.41447619  0.19524198     0.49548159
## density                 0.45890998       0.27129565  0.09615393     0.55251695
## pH                     -0.25270047       0.26145440 -0.32980819    -0.26731984
## sulphates               0.29956774       0.22598368  0.05619730    -0.18592741
## alcohol                -0.09545152      -0.03764039 -0.01049349    -0.35941477
## quality                -0.07674321      -0.26569948  0.08553172    -0.03698048
##                        chlorides free.sulfur.dioxide total.sulfur.dioxide
## fixed.acidity         0.29819477         -0.28273543          -0.32905390
## volatile.acidity      0.37712428         -0.35255731          -0.41447619
## citric.acid           0.03899801          0.13312581           0.19524198
## residual.sugar       -0.12894050          0.40287064           0.49548159
## chlorides             1.00000000         -0.19504479          -0.27963045
## free.sulfur.dioxide  -0.19504479          1.00000000           0.72093408
## total.sulfur.dioxide -0.27963045          0.72093408           1.00000000
## density               0.36261466          0.02571684           0.03239451
## pH                    0.04470798         -0.14585390          -0.23841310
## sulphates             0.39559331         -0.18845725          -0.27572682
## alcohol              -0.25691558         -0.17983843          -0.26573964
## quality              -0.20066550          0.05546306          -0.04138545
##                          density          pH    sulphates      alcohol
## fixed.acidity         0.45890998 -0.25270047  0.299567744 -0.095451523
## volatile.acidity      0.27129565  0.26145440  0.225983680 -0.037640386
## citric.acid           0.09615393 -0.32980819  0.056197300 -0.010493492
## residual.sugar        0.55251695 -0.26731984 -0.185927405 -0.359414771
## chlorides             0.36261466  0.04470798  0.395593307 -0.256915580
```

```
## free.sulfur.dioxide   0.02571684 -0.14585390 -0.188457249 -0.179838435
## total.sulfur.dioxide  0.03239451 -0.23841310 -0.275726820 -0.265739639
## density               1.00000000  0.01168608  0.259478495 -0.686745422
## pH                    0.01168608  1.00000000  0.192123407  0.121248467
## sulphates             0.25947850  0.19212341  1.000000000 -0.003029195
## alcohol              -0.68674542  0.12124847 -0.003029195  1.000000000
## quality              -0.30585791  0.01950570  0.038485446  0.444318520
##                          quality
## fixed.acidity        -0.07674321
## volatile.acidity     -0.26569948
## citric.acid           0.08553172
## residual.sugar       -0.03698048
## chlorides            -0.20066550
## free.sulfur.dioxide   0.05546306
## total.sulfur.dioxide -0.04138545
## density              -0.30585791
## pH                    0.01950570
## sulphates             0.03848545
## alcohol               0.44431852
## quality               1.00000000
```

Number of NAN values for each variables :

```
cat('Number of NAN values for each variable :', colSums(is.na(df_wine)))
```

```
## Number of NAN values for each variable : 0 0 0 0 0 0 0 0 0 0 0 0 0
```

Preparing the data

We want to predict the quality of the wine (score between 1 and 10) by using the rest of the feature variables. Here, wine quality is the variable we want to predict (Y variable).

Inspect the wine quality score feature Let's take a look at the distribution of the wine quality score in our dataset. We see that Wine quality appear to follow a bell shaped distribution (Gaussian/Normal distribution). This implies most wines are of average quality and few are good or bad

```
# Simple Bar Plot
hist(df_wine$quality, main="Wine Quality Score Distribution",ylab="Count", xlab="Wine Quality Score", b
```

Now let's check the frequency of each wine quality score. From the above table, we see that an approximate 45% of the wine quality scores have a 6 score value.

```
table(df_wine$quality)
```

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

Binning the Wine Quality Score Variable We want to predict the quality of the wine based on the rest of the variables present in our dataset. We see from the above table that the wine quality score variable takes 7 different values (3, 4, 5, 6, 7, 8, 9) inside our dataset. If we want to build a machine learning model to predict this variable, we'll use a classification model that will achieve a multiclass classification, in our case we have 7 distinct classes (7 possible values).

The question we want to answer through this notebook is whatever a wine is good or bad ? In our case, the output variable (Y) that we want to get is a binary variable True => "Good" and False => "Bad".

We transform our win quality score variable to a binary variable by achieving a binning on its values, i.e we fix a specific threshold and associate each score to a unique class, the class "Bad" for the lower quality wines and the class "Good" for the best wines.

Threshold : - Good : scores from 7 to 9. - Bad : scores from 1 to 6.

```
cat('Threshold  distribution :', table(ifelse(df_wine$quality<=6,'Bad', ifelse(df_wine$quality>=7, "Goo
```

```
## Threshold  distribution : 5220 1277
```

```r
# We drop the quality column and replace it with the new qualityClass variable.
qualityClass <- as.factor(ifelse(df_wine$quality<=6,'Bad', ifelse(df_wine$quality>=7, 'Good','')))
df_wine <- data.frame(subset (df_wine, select = -quality), qualityClass)
```

Build a Decision Tree Model

Splitting the data into training and testing sets We split our data into two different sets :

- Training set for the model fitting (learning the patterns)
- Testing set for estimating the model's accuracy

```r
# we set the seed to get reproducible results
set.seed(10)

# get the training dataset indexes
dataset_size <- dim(df_wine)[1]
train_set_size <- round(0.8*dataset_size)
train_index <- sample(dataset_size, train_set_size, replace=FALSE)

# split into train and test sets
training_data <- df_wine[train_index, ]
test_data <- df_wine[-train_index,]
```

Instantiate and train the decision tree model We will begin by training a classification tree model. Although almost any implementation of decision trees can be used to perform classification tree modeling, the `rpart` (recursive partitioning) package offers the most faithful implementation of classification trees as they were described by the CART team. As the classic R implementation of CART, the rpart package is also well-documented and supported with functions for visualizing and evaluating the rpart models.

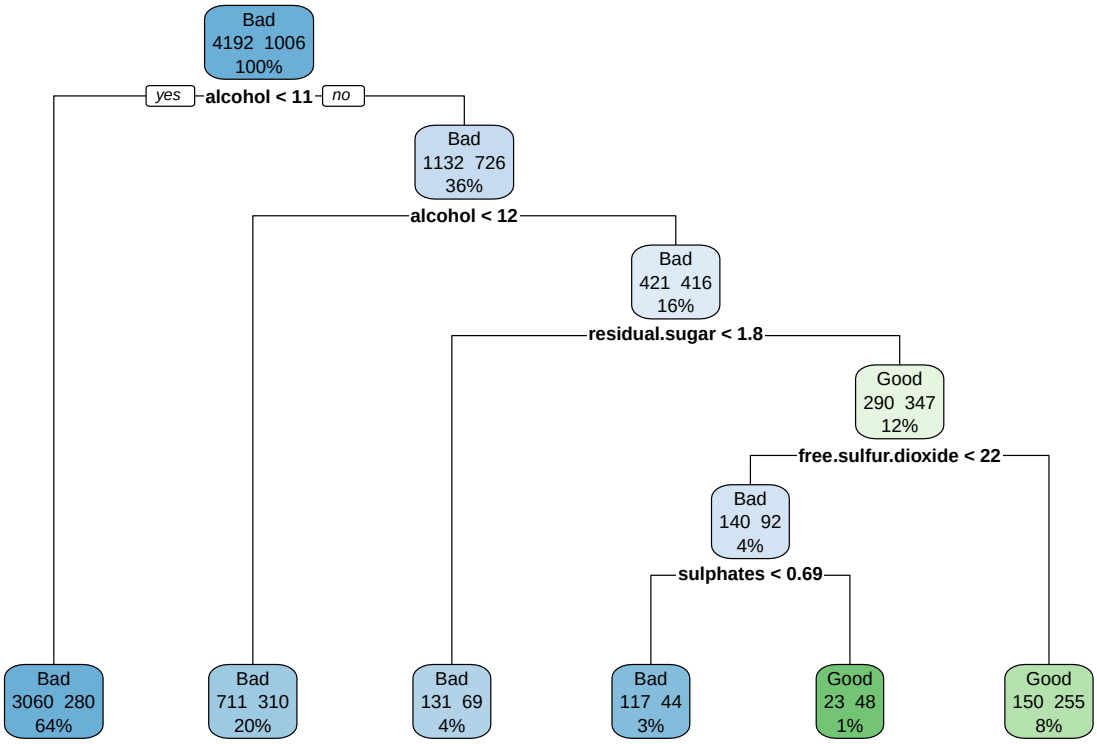
Using the R formula interface, we can specify `qualityClass` as the outcome variable and use the dot notation to allow all the other columns in the training_data data frame to be used as predictors.

```r
rpart_model <- rpart(qualityClass~., data=training_data, method="class")

# choosing the best complexity parameter "cp" to prune the tree
cp.optim <- rpart_model$cptable[which.min(rpart_model$cptable[,"xerror"]),"CP"]

# tree prunning using the best complexity parameter. For more in
tree <- prune(rpart_model, cp=cp.optim)
```

Visualization of the decision tree model The tree can be understood using only the preceding output, it is often more readable using visualization. After installing the package using the install.packages("rpart.plot") command, the rpart.plot() function produces a tree diagram from any rpart model object. The following commands plot the classification tree we built earlier which produces a tree diagram is as follows:

For each node in the tree, the number of examples reaching the decision point is listed. For instance, all 5198 examples (100% of the examples) begin at the root node, of which 64% have alcohol < 11. Because alcohol was used first in the tree, it is the single most important predictor of wine quality class.

```r
# Visualise the decision tree model graphically
rpart.plot(rpart_model, extra=101)
```



Model Evaluation

```
library(caret,quietly = TRUE)
predict_rpart <- predict(rpart_model,  test_data[, -13], type="class")
t <- table(test_data[, 13], predict_rpart)
confusionMatrix(t)
```

Prediction on the test set

```
## Confusion Matrix and Statistics
##
##       predict_rpart
##        Bad Good
##   Bad  987   41
##   Good 202   69
##
##                Accuracy : 0.8129
##                  95% CI : (0.7906, 0.8338)
##     No Information Rate : 0.9153
##     P-Value [Acc > NIR] : 1
##
##                   Kappa : 0.2749
##
##  Mcnemar's Test P-Value : <2e-16
##
```

```
##             Sensitivity : 0.8301
##             Specificity : 0.6273
##          Pos Pred Value : 0.9601
##          Neg Pred Value : 0.2546
##              Prevalence : 0.9153
##          Detection Rate : 0.7598
##    Detection Prevalence : 0.7914
##       Balanced Accuracy : 0.7287
##
##        'Positive' Class : Bad
##
```

```
#
#mean(predict_rpart != test_data[, 13])
```