White Wines Quality

 $\operatorname{HarvardX:\ PH125.9x\ Capstone,\ CYO\ Project}$

Andres Gomez June, 2020

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Introduction

In this project, we are going to use the white wines data set (only the white one) which is part of the study done by [Cortez et al., 2009], and you can find at the UCI list of curated datasets.

The dataset has the following *input* variables (based on physicochemical tests):

- 1. fixed acidity
- 2. volatile acidity
- 3. citric acid
- 4. residual sugar
- 5. chlorides
- 6. free sulfur dioxide
- 7. total sulfur dioxide
- 8. density
- 9. pH
- 10. sulphates
- 11. alcohol

And one *output* variable (based on sensory data):

12. quality (score between 0 and 10)

Our **goal** is to build some models that predict the white wines quality and help deciding whether to "buy" or "avoid" a wine. We will reduce the quality of wines to these two categories. We will explain how we define these categories in the Modeling approach section.

First, in the **Method/Analysis** section we import the data and clean it, preparing it for analysis. We perform some exploratory data analysis, variables distributions, box-plots, correlation matrix, etc. Finally, we expose the *modeling approach* which will consist of two techniques: KNN and Random Forests, and the corresponding performance measures.

Secondly, in the **Results** section, we share the results of the models, interpreting the results and evaluating the models.

Third, in the **Conclusions** section, we summarize the work done, and share thoughts on possible improvements and next steps.

Method/Analysis

In this section, we will do:

- 1. Data import and cleaning.
- 2. Exploratory data analysis.
- 3. The modeling approach, using KNN and Random Forest.

Data import and cleaning.

We start by downloading the white wines data used by [Cortez et al., 2009], which you can find at the UCI list of curated datasets https://archive.ics.uci.edu/ml/datasets/Wine+Quality. Keep in mind that we are just using the white wines dataset, and not the red wines. We narrow our goal just for simplicity.

```
# Download data to be used and create a DF (actually a spec_tbl_df type of file)
if(!require(readr)) install.packages("readr", repos = "http://cran.us.r-project.org")
if(!file.exists("winequality-white.csv"))
download.file("https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white
wines <- read delim("winequality-white.csv",
                    delim = ";",
                    locale = locale(decimal mark = ".",
                                     grouping_mark = ","),
                    col names = TRUE)
# Set column names
cnames <- c("fixed_acidity", "volatile_acidity", "citric_acid", "residual_sugar", "chlorides",</pre>
            "free_sulfur_dioxide", "total_sulfur_dioxide", "density", "pH", "sulphates",
            "alcohol", "quality")
# Rename columns to make it friendlier for R (at least for me)
colnames(wines) <- cnames</pre>
# Quality is numeric,
# let's create a variable "rating" that will be quality as factor with convenient format
if(!require(tidyverse)) install.packages("tidyverse", repos = "http://cran.us.r-project.org")
## package 'tidyverse' successfully unpacked and MD5 sums checked
## The downloaded binary packages are in
## C:\Users\andre\AppData\Local\Temp\RtmpC4tLME\downloaded_packages
if(!require(dplyr)) install.packages("dplyr", repos = "http://cran.us.r-project.org")
wines <- mutate(wines,</pre>
               rating = as.factor(quality))
levels(wines$rating) <- paste0("R_", levels(wines$rating))</pre>
```

Exporatory data analysis

First of all, let's get some high level stats, on the complete dataset, to understand how the looks like. I avoid doing the exploratory data analysis on partitioned datasets because we might lose some outliers, for example.

Summary Statistics

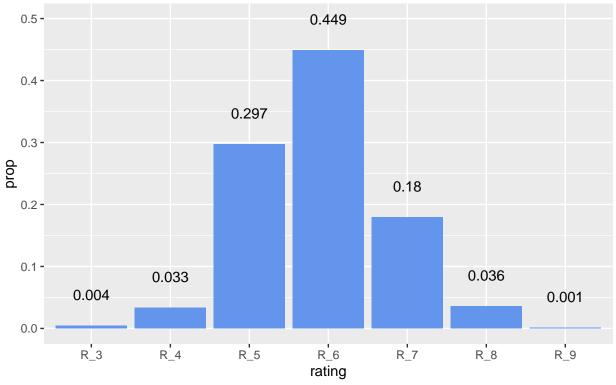
```
summary(wines)
```

```
## fixed_acidity
                  volatile_acidity citric_acid
                                                 residual_sugar
## Min. : 3.800
                        :0.0800 Min. :0.0000
                                                 Min. : 0.600
                  Min.
## 1st Qu.: 6.300
                  1st Qu.:0.2100 1st Qu.:0.2700
                                                 1st Qu.: 1.700
## Median : 6.800
                  Median :0.2600 Median :0.3200
                                                 Median : 5.200
## Mean : 6.855
                  Mean :0.2782 Mean :0.3342
                                                 Mean : 6.391
## 3rd Qu.: 7.300
                  3rd Qu.:0.3200 3rd Qu.:0.3900
                                                 3rd Qu.: 9.900
## Max. :14.200
                                       :1.6600
                  Max. :1.1000 Max.
                                                 Max.
                                                       :65.800
```

```
##
                     free_sulfur_dioxide total_sulfur_dioxide
##
     chlorides
                     Min. : 2.00
                                        Min. : 9.0
##
  Min. :0.00900
   1st Qu.:0.03600
                     1st Qu.: 23.00
                                        1st Qu.:108.0
                     Median : 34.00
##
   Median :0.04300
                                        Median :134.0
##
   Mean
         :0.04577
                     Mean : 35.31
                                        Mean :138.4
   3rd Qu.:0.05000
                     3rd Qu.: 46.00
                                        3rd Qu.:167.0
          :0.34600
                     Max. :289.00
##
   Max.
                                        Max.
                                               :440.0
##
##
                                     sulphates
                                                      alcohol
      density
                         рΗ
   Min.
          :0.9871
                    Min. :2.720
                                   Min. :0.2200
                                                   Min. : 8.00
   1st Qu.:0.9917
                    1st Qu.:3.090
                                   1st Qu.:0.4100
                                                    1st Qu.: 9.50
##
##
   Median :0.9937
                    Median :3.180
                                   Median :0.4700
                                                   Median :10.40
##
  Mean :0.9940
                    Mean :3.188
                                   Mean :0.4898
                                                   Mean :10.51
   3rd Qu.:0.9961
##
                    3rd Qu.:3.280
                                   3rd Qu.:0.5500
                                                   3rd Qu.:11.40
##
   Max. :1.0390
                    Max. :3.820
                                   Max.
                                        :1.0800
                                                   Max.
                                                         :14.20
##
##
      quality
                   rating
                   R_3: 20
##
  Min. :3.000
   1st Qu.:5.000
                   R 4: 163
##
##
  Median :6.000
                  R_5:1457
  Mean :5.878
                   R_6:2198
   3rd Qu.:6.000
                   R_7: 880
##
##
   Max. :9.000
                   R 8: 175
##
                   R_9: 5
```

Quality of wines distribution

Distribution of quality (rating) for white wines



data: entire white whines dataset

We see that most of wines have ratings between 5 and 7, being extreme ratings very rare.

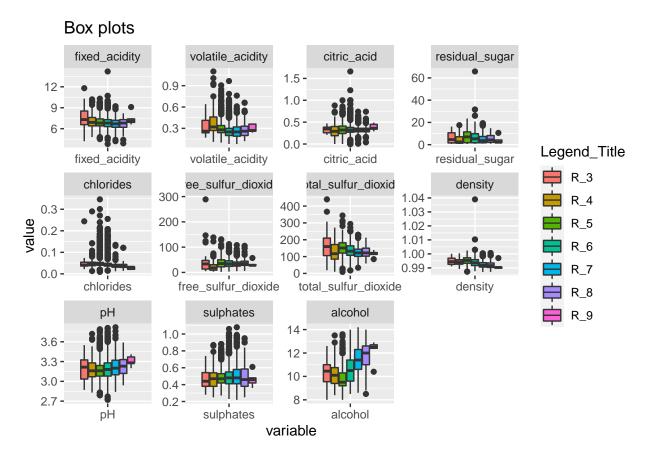
Box plots

Let's get box plots (quantiles, min and max, etc) for all variables.

Box plots volatile_acidity fixed_acidity citric_acid residual_sugar 60 **-**1.5 -0.9 -12 -40 **-**1.0 -9 -0.6 -0.5 -20 -6 -0.3 -0.0 -0 residual_sugar fixed_acidity volatile_acidity citric_acid chlorides free_sulfur_dioxide total_sulfur_dioxide density 300 -1.04 -400 -0.3 -1.03 -0.2 -0.1 -200 -300 -1.02 -200 -1.01 -0.1 -100 -1.00 -100 -0.99 -0 -0.0 -0 chlorides free_sulfur_dioxide total_sulfur_dioxide density рΗ sulphates alcohol 14 -1.0 -3.6 -0.8 -12 **-**3.3 -0.6 -10-3.0 -0.4 -8 -2.7 -0.2 alcohol sulphates рΗ

variable

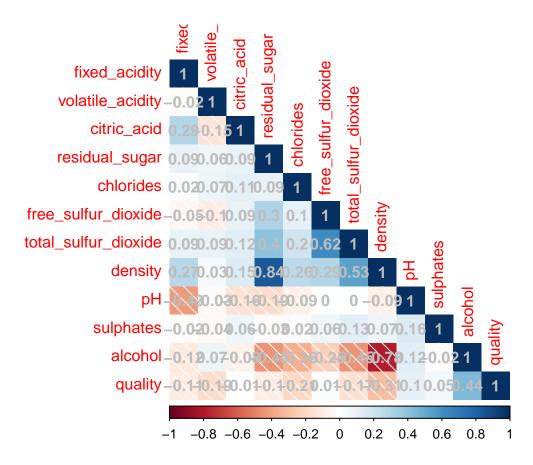
And now let's replicate it by wine rating:



We can see that the higher the rating, higher alcohol. Also there is some similar pattern for pH.

Correlation Matrix

Other than density & residual sugar, and alcohol & dennsity, it seems that the variables are not correlated, as it is shown in the correlation matrix:



Modeling approach

Let's start by preparing the data for modeling. First, we need to define what the category "buy/avoid" is. Using the descriptive statistics obtained earlier, we will define "avoid" as wines with ratings 3, 4 and 5, and "buy" was wines with ratings 6, 7, 8 and 9. "avoid" will represent 33.4% of the white wines sample, while "buy" 66.6%. Let's create this variable:

```
wines_m <- wines %>%
  mutate(recom = factor(case_when(
    rating %in% c("R_3", "R_4","R_5") ~ "avoid",
    rating %in% c("R_6", "R_7","R_8","R_9") ~ "buy",
    TRUE ~ "other"
    )))
```

Now, let's create training and test sets to build our models. We will keep 10% of the sample as test, given that our inicial dataset consists of 4898 observations, this should be sufficient.

```
# Train and test sets for wine type
training <- wines_m[indxTrain,]
testing <- wines_m[-indxTrain,]</pre>
```

Let's check the basic stats for both *train_set* and *test_test* to see if they are consistent with the entire dataset (which should be).

summary(training)

```
fixed_acidity
                      volatile acidity citric acid
                                                          residual_sugar
           : 3.800
##
    Min.
                      Min.
                             :0.0800
                                        Min.
                                               :0.0000
                                                          Min.
                                                                 : 0.600
                      1st Qu.:0.2100
##
    1st Qu.: 6.300
                                        1st Qu.:0.2700
                                                          1st Qu.: 1.700
    Median : 6.800
                      Median :0.2600
                                        Median :0.3200
                                                          Median : 5.100
##
    Mean
           : 6.851
                             :0.2773
                                                                 : 6.393
                      Mean
                                        Mean
                                               :0.3345
                                                          Mean
##
    3rd Qu.: 7.300
                      3rd Qu.:0.3200
                                        3rd Qu.:0.3900
                                                          3rd Qu.: 9.900
##
    Max.
           :14.200
                      Max.
                             :1.0050
                                        Max.
                                               :1.6600
                                                          Max.
                                                                 :65.800
##
##
      chlorides
                       free_sulfur_dioxide total_sulfur_dioxide
##
                       Min. : 2.00
                                                 : 9.0
    Min.
           :0.00900
                                            Min.
    1st Qu.:0.03600
                       1st Qu.: 23.00
                                            1st Qu.:108.0
##
    Median :0.04300
                       Median : 34.00
                                            Median :134.0
##
    Mean
           :0.04583
                       Mean
                             : 35.33
                                            Mean
                                                   :138.3
    3rd Qu.:0.05000
                       3rd Qu.: 46.00
                                            3rd Qu.:167.0
##
##
    Max.
           :0.29000
                       Max.
                              :289.00
                                            Max.
                                                    :440.0
##
##
                                         sulphates
                                                            alcohol
       density
                            Нq
##
    Min.
           :0.9871
                             :2.720
                                       Min.
                                              :0.2200
                                                         Min.
                                                                : 8.00
                      Min.
    1st Qu.:0.9917
                      1st Qu.:3.090
                                       1st Qu.:0.4100
                                                         1st Qu.: 9.50
##
    Median :0.9938
                      Median :3.180
                                       Median :0.4700
                                                         Median :10.40
##
    Mean
           :0.9940
                      Mean
                             :3.188
                                       Mean
                                              :0.4889
                                                         Mean
                                                                :10.51
##
    3rd Qu.:0.9961
                      3rd Qu.:3.280
                                       3rd Qu.:0.5500
                                                         3rd Qu.:11.40
##
    Max.
           :1.0390
                      Max.
                             :3.820
                                       Max.
                                              :1.0800
                                                         Max.
                                                                :14.20
##
##
                     rating
       quality
                                  recom
##
    Min.
           :3.000
                     R_3: 19
                                avoid:1476
    1st Qu.:5.000
                     R_4: 148
                                buy :2933
##
    Median :6.000
                     R_5:1309
##
    Mean
           :5.874
                    R_6:1984
    3rd Qu.:6.000
                     R 7: 795
##
    Max.
           :9.000
                     R_8: 149
##
                     R 9:
```

summary(testing)

```
fixed_acidity
                    volatile_acidity
                                       citric_acid
                                                        residual_sugar
##
                            :0.100
##
           :4.600
                                              :0.0000
                                                               : 0.700
    Min.
                    Min.
                                      Min.
                                                        Min.
    1st Qu.:6.300
                    1st Qu.:0.220
                                      1st Qu.:0.2700
                                                        1st Qu.: 1.900
##
  Median :6.800
                    Median :0.270
                                      Median :0.3100
                                                        Median : 5.600
##
   Mean
           :6.888
                            :0.287
                                              :0.3313
                                                                : 6.381
                    Mean
                                      Mean
                                                        Mean
##
    3rd Qu.:7.400
                    3rd Qu.:0.330
                                      3rd Qu.:0.3800
                                                        3rd Qu.:10.000
                                              :0.7900
   Max.
           :9.900
                    Max.
                            :1.100
                                      Max.
                                                        Max.
                                                                :19.800
##
```

```
##
      chlorides
                       free sulfur dioxide total sulfur dioxide
                               : 5.00
                                                     : 40.0
##
    Min.
            :0.01700
                       Min.
                                             Min.
    1st Qu.:0.03600
                                             1st Qu.:109.0
##
                        1st Qu.: 23.00
    Median :0.04300
                       Median : 33.00
                                             Median :135.0
##
##
    Mean
            :0.04528
                       Mean
                               : 35.09
                                             Mean
                                                     :138.7
##
    3rd Qu.:0.05000
                        3rd Qu.: 45.00
                                             3rd Qu.:166.0
##
    Max.
            :0.34600
                       Max.
                               :131.00
                                             Max.
                                                     :344.0
##
       density
                             рΗ
##
                                          sulphates
                                                              alcohol
            :0.9889
##
    Min.
                      Min.
                              :2.770
                                        Min.
                                                :0.2500
                                                          Min.
                                                                  : 8.70
##
    1st Qu.:0.9917
                      1st Qu.:3.090
                                        1st Qu.:0.4100
                                                          1st Qu.: 9.50
    Median :0.9936
                      Median :3.180
                                        Median :0.4900
                                                          Median :10.40
##
                                                                  :10.56
##
    Mean
            :0.9940
                              :3.187
                                                :0.4985
                                                          Mean
                      Mean
                                        Mean
                      3rd Qu.:3.280
                                                          3rd Qu.:11.50
##
    3rd Qu.:0.9962
                                        3rd Qu.:0.5600
##
                              :3.790
                                                                  :13.70
    Max.
            :1.0012
                      Max.
                                        Max.
                                                :1.0600
                                                          Max.
##
##
       quality
                    rating
                                 recom
##
    Min.
            :3.00
                    R 3: 1
                               avoid:164
                    R_4: 15
##
    1st Qu.:5.00
                               buy :325
##
    Median:6.00
                    R 5:148
##
    Mean
            :5.91
                    R_6:214
    3rd Qu.:6.00
                    R_7: 85
##
                    R_8: 26
##
    Max.
            :8.00
                    R 9: 0
##
```

Results are as expected (both datasets share the same estructure).

Now we are ready to develop a model using the *training set* and evaluate it using the *testing set*. Please note that in the moment that the model requires tuning, we will further partition the *training set* so we keep the *testing set* "pure" and use it just for the final evaluation.

The models that we will try are the following:

(1) KNN (k-nearest neighbors)

The k-nearest neighbors algorithm estimates the conditional probability:

$$p(x_1,..,x_p) = Pr(Y = k|X_1 = x_1,..,X_p = x_p)$$

The algorithm calculates the euclidean distance of all predictors, then for any point $(x_1, ..., x_p)$ in the multidimensional space that we want to predict, the algorithm determines the distance to k points. The k nearest points is referred as neighborhood.

For k = 1 the algorithm finds the distance to a single neighbor. For k equals to the number of samples, the algorithm uses all points. Hence, k is a tuning parameter that can be calculated running the algorithm for several values of k and picking the result with highest accuracy.

(2) Random Forest

Random forests improve prediction performance over classification trees by averaging multiple decision trees. The algorithm creates several random subsets of the original data, in this case the training set, and calculates the classification trees, then the final result is the average of all trees. A tree is basically a flow chart of yes or no questions.

The name random forest derives from the random process of splitting the data and creating many trees, or a forest.

(3) Performance Measures

There are several measures to consider when evaluating the performance of a classification model as we have.

It's very important to define and understand what the *confusion matrix* is: a simple table with the cross tabulation of the predicted values with the actual observed values.

	Actual Positive	Actual Negative
Predicted Positive	True Positive (TP)	False Positive (FP)
Predicted Negative	False Negative (FN)	True Negative (TN)

All values are in absolute numbers of observations and predictions, so for example the *True Positive* is the number of predicted values that are exactly the same as the actual values.

The meaning of the values in the table are:

True Positive (TP): Predicted positive for an actual positive value.

True Negative (TN): Predicted negative for an actual negative value.

False Positive (FP) or Type 1 Error: Predicted positive for an actual negative value.

False Negative (FN) or Type 2 Error: Predicted negative for an actual positive value.

Some useful statistic metrics can be calculated from the confusion matrix.

Accuracy: the proportion of correct predictions for both *positive* and *negative* outcomes, i.e. the ability to correctly predict a *positive* and *negative*. High accuracy with a large difference in the number of positives and negatives becomes less meaningful, since the algorithm loses the ability to predict the less common class. In this case, other metrics complements the analysis.

$$Accuracy = \frac{TP + TN}{TP + FP + TN + FN}$$

Sensitivity: the proportion of *positive* values when they are actually *positive*, i.e. the ability to predict *positive* values.

$$Sensitivity = \frac{TP}{TP + FN}$$

Specificity: is the probability of a predicted *negative* value conditioned to a *negative* outcome.

$$Specificity = Pr(\hat{Y} = Negative | Y = Negative)$$

In other words, specificity is the proportion of negative values when they are actually negative, i.e. the ability to predict negative values.

$$Specificity = \frac{TN}{TN + FP}$$

Prevalence: how often the *positive* value appears in the sample. Low prevalence may lead to statistically incorrect conclusions.

$$Prevalence = \frac{TP + FN}{TP + FP + TN + FN}$$

Precision: is the probability of an actual *positive* occurs conditioned to a predicted *positive* result.

$$Precision = Pr(Y = Positive | \hat{Y} = Positive)$$

Precision can be written as the proportion of positive values that are actually positive.

$$Precision = \frac{TP}{TP + FP}$$

Recall: is the same as sensitivity and is the probability of a predicted *positive* value conditioned to an actual *positive* value.

$$Recall = Sensitivity = Pr(\hat{Y} = Positive | Y = Positive)$$

$$Recall = \frac{TP}{TP + FN}$$

Results

Let's start by:

KNN

We'll use all features to predict the variable "recom" (our "recommendation" or "buy/avoid")

We also *center* and *scale* the variables since is a requirement for the technique:

```
trainX <- training[,names(training) != "recom"]
preProcValues <- preProcess(x = trainX,method = c("center", "scale"))
preProcValues

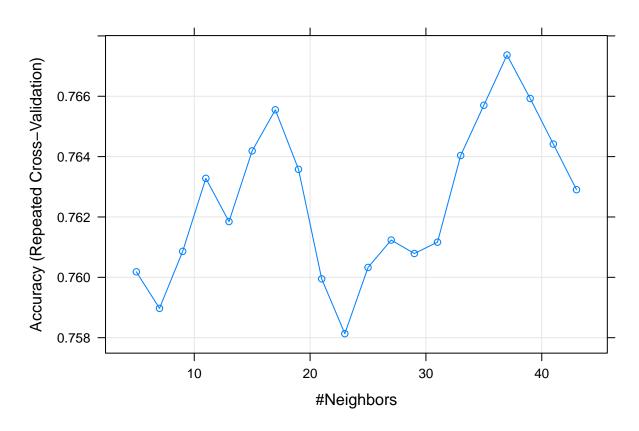
## Created from 4409 samples and 13 variables
##
## Pre-processing:
## - centered (12)
## - ignored (1)
## - scaled (12)</pre>
```

We will use the caret package to run KNN

```
if(!require(caret)) install.packages("caret", repos = "http://cran.us.r-project.org")
if(!require(ISLR)) install.packages("ISLR", repos = "http://cran.us.r-project.org")
trainX <- training[,names(training) != "recom"]
trainX_Rel <-trainX[,-c(12,13)]
preProcValues <- preProcess(x = trainX_Rel,method = c("center", "scale"))
preProcValues</pre>
```

```
## Created from 4409 samples and 11 variables
##
## Pre-processing:
##
    - centered (11)
##
     - ignored (0)
##
    - scaled (11)
#training and training control
set.seed(229, sample.kind = "Rounding")
ctrl <- trainControl(method="repeatedcv",repeats = 3)</pre>
knnFit <- train(recom ~ ., data = training[,-c(12,13)], method = "knn", trControl = ctrl, preProcess =
We can check the output of our model:
#Output of kNN fit
knnFit
## k-Nearest Neighbors
##
## 4409 samples
##
     11 predictor
##
      2 classes: 'avoid', 'buy'
##
## Pre-processing: centered (11), scaled (11)
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 3967, 3968, 3969, 3969, 3968, 3969, ...
## Resampling results across tuning parameters:
##
##
     k
        Accuracy
                    Kappa
##
     5 0.7601829 0.4465257
     7 0.7589727 0.4381366
##
##
     9 0.7608604 0.4411401
##
     11 0.7632793 0.4468791
##
     13 0.7618470 0.4425077
##
     15 0.7641901 0.4473107
     17 0.7655512 0.4481227
##
##
     19 0.7635796 0.4426478
##
     21 0.7599496 0.4333646
##
     23 0.7581342 0.4268754
##
     25 0.7603265 0.4312630
##
     27 0.7612354 0.4321200
##
     29 0.7607893 0.4305794
     31 0.7611659 0.4302653
##
##
     33 0.7640367 0.4369986
##
     35 0.7657014 0.4411798
##
     37 0.7673653 0.4457811
##
     39 0.7659271 0.4414698
##
     41 0.7644161 0.4371673
##
     43 0.7629045 0.4327092
## Accuracy was used to select the optimal model using the largest value.
```

The final value used for the model was k = 37.



We can see that the final k value used for our model was k=37.

Confusion matrix is as follows:

```
knnPredict <- predict(knnFit,newdata = testing[,-c(12,13)] )
#Get the confusion matrix to see accuracy value and other parameter values
confusionMatrix(knnPredict, testing$recom )</pre>
```

```
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction avoid buy
                 91 31
        avoid
##
        buy
                 73 294
##
##
##
                  Accuracy: 0.7873
##
                    95% CI: (0.7483, 0.8228)
       No Information Rate: 0.6646
##
       P-Value [Acc > NIR] : 1.637e-09
##
##
##
                     Kappa: 0.4906
##
    Mcnemar's Test P-Value : 5.810e-05
##
```

```
##
##
               Sensitivity: 0.5549
##
               Specificity: 0.9046
            Pos Pred Value: 0.7459
##
##
            Neg Pred Value: 0.8011
                Prevalence: 0.3354
##
##
            Detection Rate: 0.1861
      Detection Prevalence: 0.2495
##
##
         Balanced Accuracy: 0.7297
##
##
          'Positive' Class : avoid
##
```

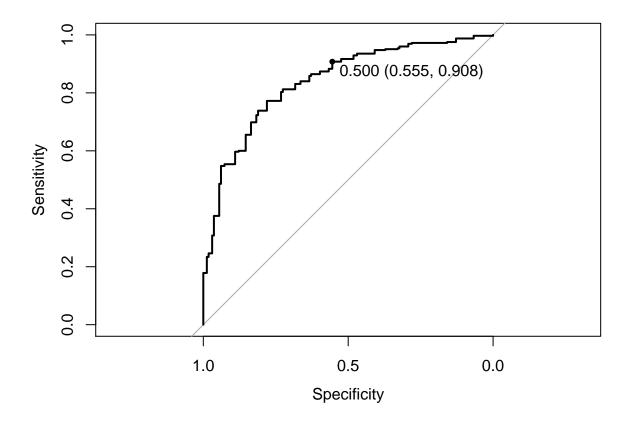
We see our accuracy is about 78%, but our prevalence is about 33%. Ideally we would like a greater prevalence. Also notice that in 73 cases we are telling "buy" while actually we should have suggested to "avoid", which is still high. We consider this like the worst error, since it's not that bad when you suggest to "avoid" and actually should be a "buy" (you would not have a bad experience).

And the ROC with respective AUC is:

```
if(!require(pROC)) install.packages("pROC", repos = "http://cran.us.r-project.org")
knnPredict <- predict(knnFit,newdata = testing , type="prob")
knnROC <- roc(testing$recom,knnPredict[,"avoid"])
knnROC

##
## Call:
## roc.default(response = testing$recom, predictor = knnPredict[, "avoid"])
##
## Data: knnPredict[, "avoid"] in 164 controls (testing$recom avoid) > 325 cases (testing$recom buy).
## Area under the curve: 0.8454

plot(knnROC, type="S", print.thres= 0.5)
```



So AUC is 0.8454... not terrible but could be improved, which we will try to do using Random Forest.

Random Forest

We have already installed the packages to use (caret and pROC)... let's start by training:

```
set.seed(229, sample.kind = "Rounding")
ctrl <- trainControl(method="repeatedcv",repeats = 3)
# Random forrest
rfFit <- train(recom~., data=training[,-c(12,13)],method="rf",trControl= ctrl,preProcess=c("center","sc</pre>
```

note: only 10 unique complexity parameters in default grid. Truncating the grid to 10 .

The trained model looks like:

```
rfFit
```

```
## Random Forest
##
## 4409 samples
## 11 predictor
## 2 classes: 'avoid', 'buy'
##
## Pre-processing: centered (11), scaled (11)
```

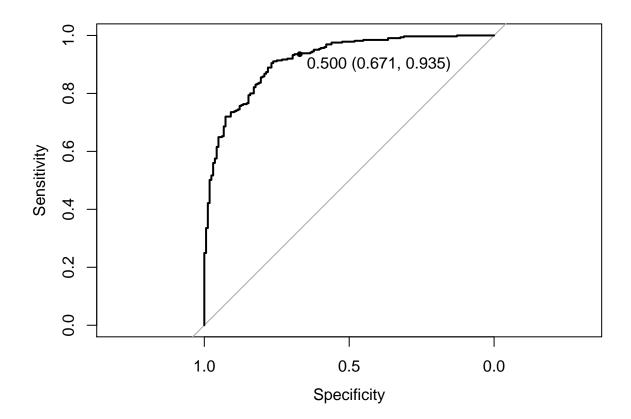
```
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 3967, 3968, 3969, 3969, 3968, 3969, ...
## Resampling results across tuning parameters:
##
##
     mtry
           Accuracy
                      Kappa
      2
           0.8438727
##
                      0.6376775
      3
           0.8412280 0.6326579
##
##
      4
           0.8413766 0.6335405
##
      5
           0.8397139 0.6303019
##
      6
           0.8390334 0.6287024
##
      7
           0.8392602 0.6301242
           0.8378229 0.6265734
##
      8
##
      9
           0.8394119 0.6305751
##
     10
           0.8383515 0.6283889
##
           0.8372931 0.6264728
     11
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 2.
Confusion matrix:
rfPredict <- predict(rfFit,newdata = testing[,-c(12,13)] )
confusionMatrix(rfPredict, testing$recom )
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction avoid buy
##
        avoid
                110 21
                 54 304
        buy
##
##
                  Accuracy : 0.8466
##
##
                    95% CI: (0.8116, 0.8774)
##
       No Information Rate: 0.6646
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 0.6379
##
   Mcnemar's Test P-Value: 0.0002199
##
##
               Sensitivity: 0.6707
##
##
               Specificity: 0.9354
            Pos Pred Value: 0.8397
##
##
            Neg Pred Value: 0.8492
                Prevalence: 0.3354
##
##
            Detection Rate: 0.2249
##
      Detection Prevalence: 0.2679
##
         Balanced Accuracy: 0.8031
##
##
          'Positive' Class: avoid
##
```

We improved accuracy, sensitivity and specificity... we have less number of false positives. Let's see how ROC and AUC look like:

```
rfPredict <- predict(rfFit,newdata = testing[,-c(12,13)] , type="prob")
rfROC <- roc(testing$recom,rfPredict[,"avoid"])
rfROC

##
## Call:
## roc.default(response = testing$recom, predictor = rfPredict[, "avoid"])
##
## Data: rfPredict[, "avoid"] in 164 controls (testing$recom avoid) > 325 cases (testing$recom buy).
## Area under the curve: 0.9156

plot(rfROC, type="S", print.thres= 0.5)
```



Now the AUC is 0.9156, which is much better.

Conclusions

In this report we have shown how to use the caret package to perform classification techniques in R, more especifically KNN and Random Forest, in order to predict white wines quality.

First we have explored the data, providing statistic summaries like quantiles, distributions, correlation, etc. Then we have shown how to perform KNN and Random Forest using the caret package.

We showed that we improve the KNN results by running Random Forest and obtaining an AUC = 0.9156. So we could say we have a model to "recommend" whether to "buy" or "avoid" a white wine based on variables generated by physicochemical tests.

As limitations we could highlight:

- 1. Personally I run into hardward limitations when running Random Forest, which limited my capacity to run several iterations with different parameters for example.
- 2. This model only uses features created by physicochemical tests, so we don't count with other information that could be valuable like market price, or customer experience.

Some next steps would be:

- 1. Enhance the models running different iterations with different parameters.
- 2. Use other models like LDA, QDA, Logistic Regression, etc... and even some clustering techniques (maybe with a modified goal, but still classifying).

References

• P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis. Modeling wine preferences by data mining from physicochemical properties. In Decision Support Systems, Elsevier, 47(4):547-553, 2009.