HDSDA
SEP2

Data mining project

Wine Quality Analysis using Machine Learning Techniques

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Abstract

White Wines are very specific goods. The quality depends on many factors like barrels, type of grapes, location and ingredients. All that makes attributes of wine. Very important are activities carried over production process. The level of preservatives, level of alcohol and ph ratio and many other attributes depend on the production process.

The level of preservatives, level of alcohol and ph ratio and many other attributes can determine if the manufacturer of the wine will get desired certification and will not loose on quality of wine.

We used the classification technique – clustering to find the similarities between attributes and Decision Tree, Naïve Bayes, Generalised Linear Regression, Random Forest, Gradient Boosted Tree to find dependencies between physiochemical qualities of wine and the target attributes and to predict the target attributes.

Keywords: wine quality, data mining, classification, clustering, k-means, x-means, decision tree, gradient boosted tree, random forest, generalised linear regression

Problem Statement

Preservatives in wines are necessary ingredient but they might be a problem also. How much is too much?

What level of preservatives influences the other attributes of wine? Is that wine still balanced and healthy for us? How about level of alcohol in wine?

How about answering these questions by studying the properties of already made wines? It will certainly cost less than a process of developing a new quality wines. There is literature about manufacturing wines and this expertise is necessary, but we would like to show just small scope for improvement.

The quality management is very important in many industries. Data mining is a nowadays a necessary tool in this field. This project will focus on physiochemical properties of wine and connections and dependencies between them.

And hopefully it will help a little bit more in understanding the dependencies between different attributes. In this project we will take a holistic approach to quality of wine understood not just as a single attribute but an overall blend of various ingredients and attributes.

We decided to use sugar /pH ratio as the wine should not be either too sweet or too dry. We expect to find some correlation between the ratio and quality.

There are two main preservatives in wine: sulphates and chlorides. We want to test whether the level of preservatives has any correlation to quality. Sulfur dioxide (SO_2) is widely used in winemaking mainly because of its anti-oxidative and anti-microbial properties in wine. It is also used for cleaning purposes at the wineries (Carel, 2011). We suspect that too much of preservatives will have negative impact on quality.

For the alcohol content, we wanted to group wines into three categories based on their alcohol level.

Balanced wine – we wanted to created perfect balanced wine, with balanced and healthy ratios of ingredients. Wine which will pass the certification of organic wine (low artificial preservatives) etc.

On the market there are many certificates available for wine merchants. Some of regulations are compulsory like European Union regulations about percentage of alcohol and remaining sugar content. Some are voluntary like for example CCOF (Organic Vineyards), USDA (USDA Organic –wines and others. (Organicvineyardalliance, 2017). For organic certificates you need to pass many regulations including level of preservatives and amount of other chemicals allowed.

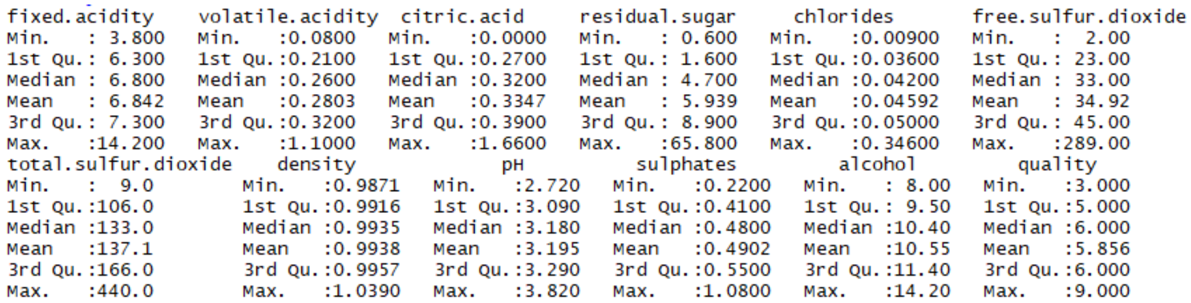
Data set description and pre-processing

We chose “Wine quality - white” as a data set for our project. Data set contains a samples wine testing of Portuguese *vinho verde*. Data set is available to download as a .csv file on http://www3.dsi.uminho.pt/pcortez/wine/ (Cortez, Cerderira, Almeida, Matos, Reis, 2009). Original data set consists of 4899 rows and the following 12 columns:

fixed acidity	-	real number	-	measure of tartaric acid [g/dm3]
volatile acidity	-	real number	-	amount of acetic acid [g/dm3]
citric acid	-	real number	-	amount of citric acid [g/dm3]
residual sugar	-	real number	-	amount of residual sugar [g/dm3]
Chlorides	-	real number	-	amount of sodium chloride {g/dm3]
free sulfur dioxide	-	real number	-	measure of sulfur dioxide [mg/dm3]
total sulfur dioxide	-	real number	-	measure of sulfur dioxide [mg/dm3]
Density	-	real number	-	[g/cm3]
pH	-	real number	-	potential of hydrogen of wine [mole]
sulphates	-	real number	-	potassium sulphate [g/dm3]
Alcohol	-	real number	-	[vol.%]
Quality	-	ordinal	-	number from range 0 -10

First 11 attributes are the input and 12th - “quality” is an output attribute. There is no missing attributes. All are numeric. There were 898 duplicates in the data set which we removed and that left us with 4000 of rows of data.

We ran some descriptive statistics in R to see how the data is structured and to get a better understanding of it.



```
 fixed.acidity    volatile.acidity  citric.acid      residual.sugar     chlorides         free.sulfur.dioxide
 Min.   : 3.800   Min.   :0.0800   Min.   :0.0000   Min.   : 0.600   Min.   :0.00900   Min.   :  2.00
 1st Qu.: 6.300   1st Qu.:0.2100   1st Qu.:0.2700   1st Qu.: 1.600   1st Qu.:0.03600   1st Qu.: 23.00
 Median : 6.800   Median :0.2600   Median :0.3200   Median : 4.700   Median :0.04200   Median : 33.00
 Mean   : 6.842   Mean   :0.2803   Mean   :0.3347   Mean   : 5.939   Mean   :0.04592   Mean   : 34.92
 3rd Qu.: 7.300   3rd Qu.:0.3200   3rd Qu.:0.3900   3rd Qu.: 8.900   3rd Qu.:0.05000   3rd Qu.: 45.00
 Max.   :14.200   Max.   :1.1000   Max.   :1.6600   Max.   :65.800   Max.   :0.34600   Max.   :289.00
 total.sulfur.dioxide    density             pH            sulphates         alcohol          quality
 Min.   :  9.0         Min.   :0.9871   Min.   :2.720   Min.   :0.2200   Min.   : 8.00   Min.   :3.000
 1st Qu.:106.0         1st Qu.:0.9916   1st Qu.:3.090   1st Qu.:0.4100   1st Qu.: 9.50   1st Qu.:5.000
 Median :133.0         Median :0.9935   Median :3.180   Median :0.4800   Median :10.40   Median :6.000
 Mean   :137.1         Mean   :0.9938   Mean   :3.195   Mean   :0.4902   Mean   :10.55   Mean   :5.856
 3rd Qu.:166.0         3rd Qu.:0.9957   3rd Qu.:3.290   3rd Qu.:0.5500   3rd Qu.:11.40   3rd Qu.:6.000
 Max.   :440.0         Max.   :1.0390   Max.   :3.820   Max.   :1.0800   Max.   :14.20   Max.   :9.000
```

Acids (fixed, citric and volatile) – important components of wine, occurring in grapes and during the winemaking process. Acids control level of pH and are also antibacterial.

Residual sugar – natural grape sugar used in winemaking that is left after the fermentation process. It determines sweetness of the wine. Our wines have from 0.600 to 65.800 mg/dm3.

Chlorides – group of preservatives used for different purposes in wine making.

Sulphates (including total and free sulphur oxide – preservative and also a cleaning product. Although it is not a desirable ingredient, it is not possible to make a wine without it as some amount is produced during the winemaking process and some amount is required because of their antioxidant and antibacterial properties. It is a common allergen. In tested wines the amount of total sulphur dioxide has a big range – it varies from 9 to 440 mg/dm3.

Density - represents the concentration of dissolved sugar.

pH - potential of hydrogen value measures acidity in wine. It ranges from 2.720 to 3.820 in our data set. The lower pH value is the higher acidity level is observed.

Alcohol – percentage of alcohol content is an important factor for potential customer, in our dataset alcohol level is from 8 to 14.20 % with a mean of 10.55%.

Quality – the only original output in our database and only attribute that is based on sensory assessor's' rating (each wine was tested by a minimum of three assessors using blind tests and quality final quality score is a median of these tests) (Cortez et al., 2009). Scale available to assessors was 0 (very bad) to 10 (excellent) but in the data set quality varies from 3 to 9.

For the purpose of this project we created three more output attributes:

sugar /PH ratio	-	real number	-	ratio between sugar and pH
level of preservatives	-	polynomial	-	low, medium, high
alcohol content	-	polynomial	-	low, medium, high
balanced wine	-	binomial	-	balanced, unbalanced

We used the following classification rules to establish our output attributes:

For sugar /pH ratio:

Sugar/PH ratio

For level of preservatives

Low – If sulphates <=0.45 and chlorides <= 0.045

Medium – If sulphates <=0.6 and chlorides <= 0.06

High – Others

For alcohol content:

High – above - 11%

Medium – 9-11%

Low – 9% and less

Balanced wine:

Balanced - If total sulfur dioxide <=200 and ph ratio<=3 and level of alcohol = medium

Unbalanced - others

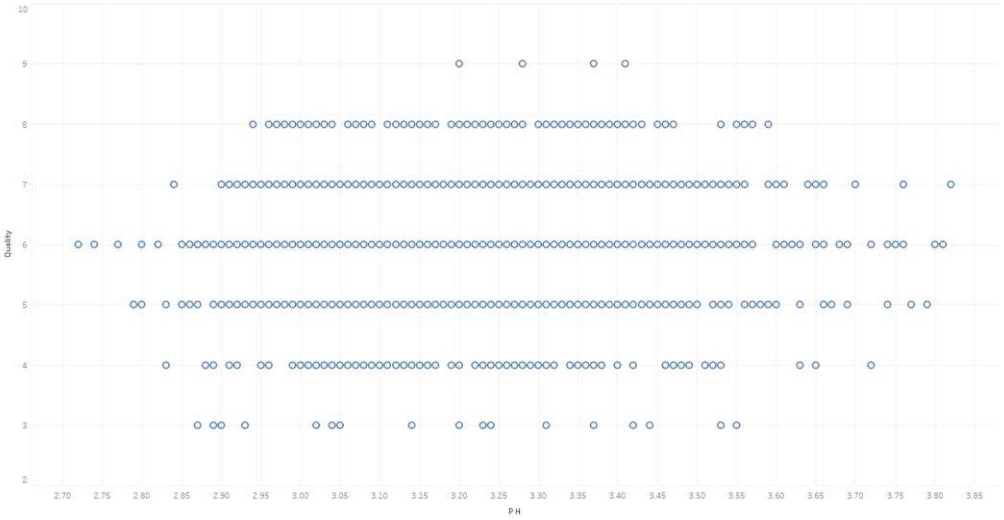


Figure 1.1. PH to quality scatter plot

Tools used and data overview

We used Tableau, Excel, Weka, RapidMiner, R and Python in our project.

First, we have run some visualisations to see how data is distributed and checked for outliers and possible correlations.

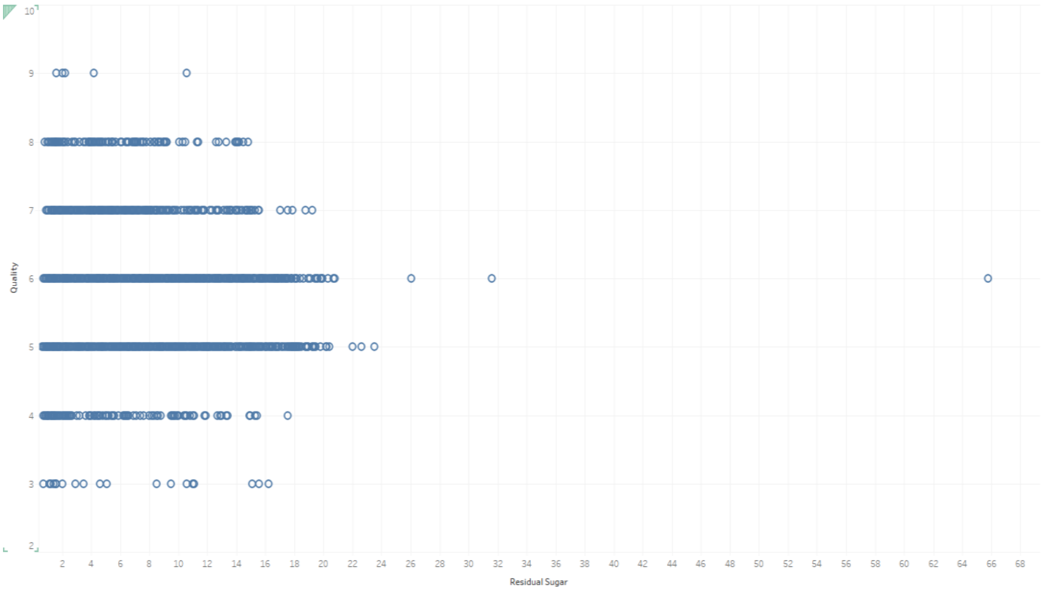


Figure 1.2. Sugar to quality scatter plot

There is an outlier on this graph - a sugar at level of 65.8. We decided to leave that outlier in our model as the amount of sugar in white wines can vary from 0 to 220 grams per litre (WineFolly, 2015). It is possible that one of the tested wines had that amount of sugar.

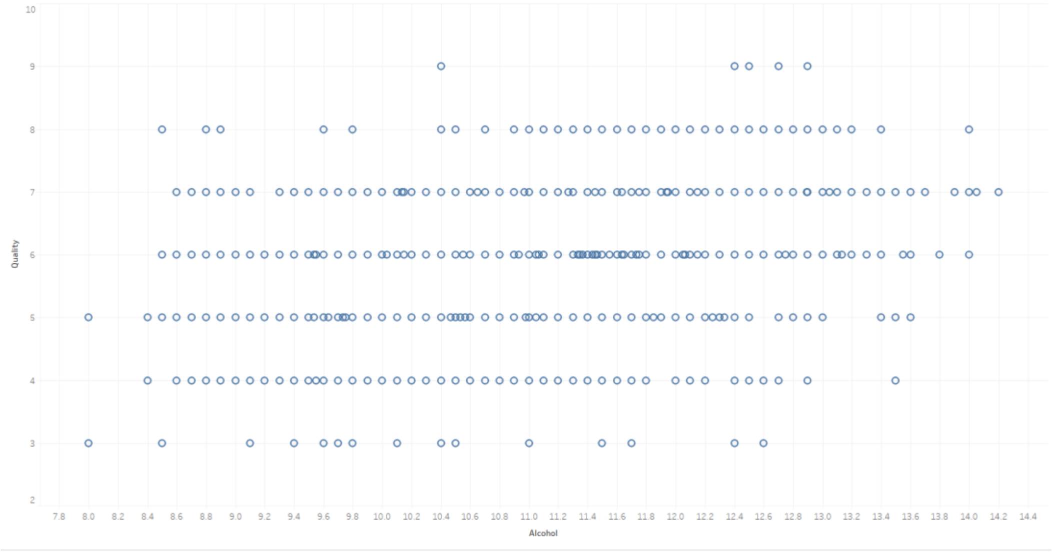


Figure 1.3. Alcohol to Quality Scatter plot

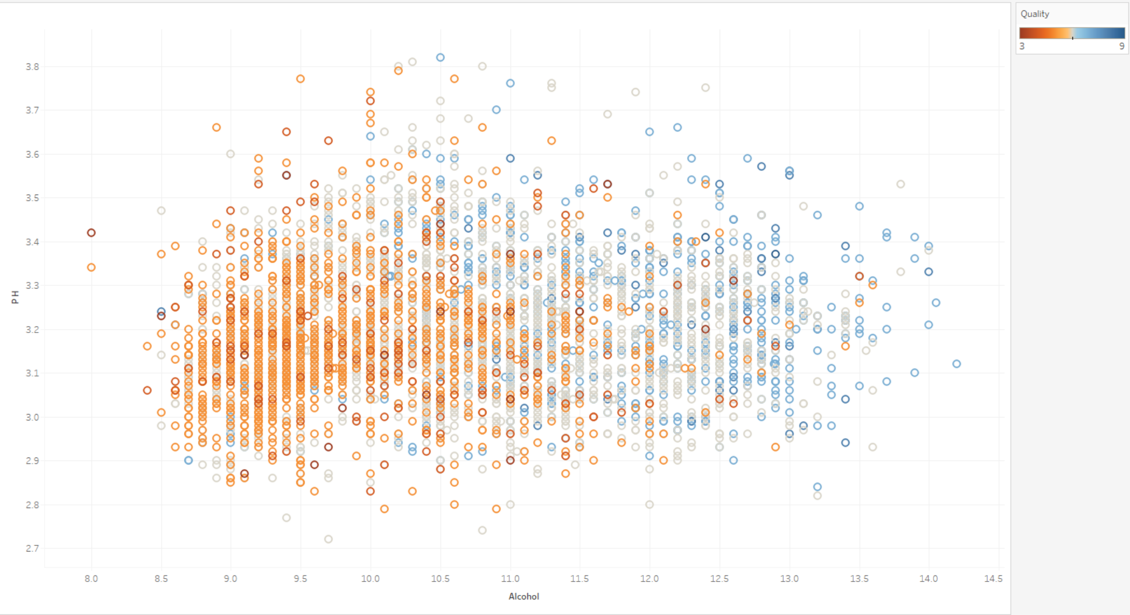


Figure 1.4. Alcohol to pH with quality as a factor scatter plot

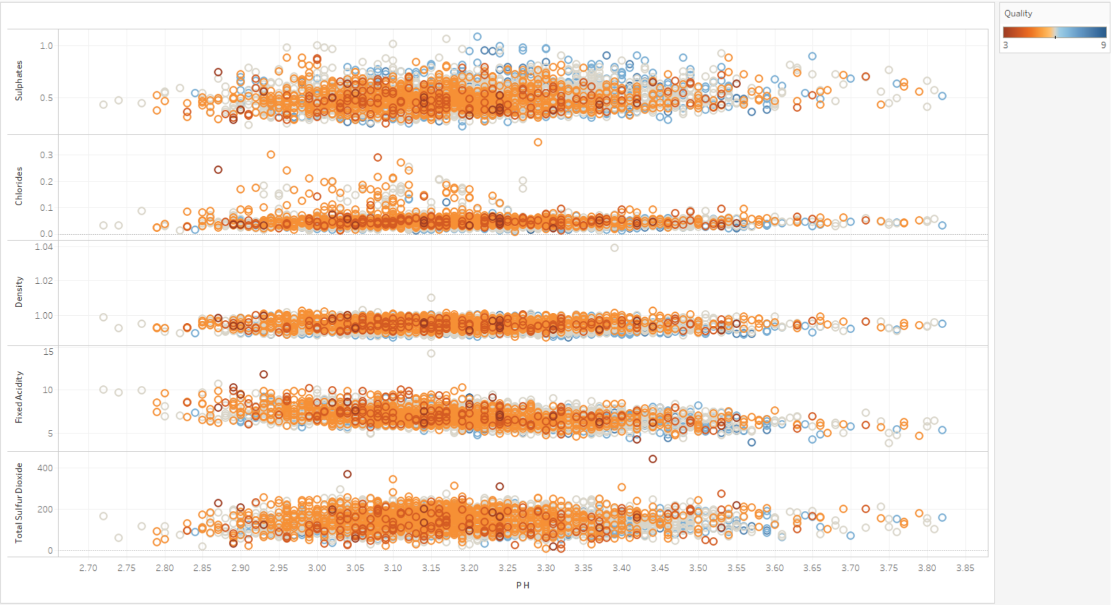


Figure1.5. Sulfur dioxide, fixed acidity, density, chlorides and sulphates to pH scatter plots

From the scatter plots we learn that any deviation from the mean is taking points from wine quality (excluding alcohol content – if less alcohol in wine, then it is less probable that it will good quality wine).

Unsupervised learning – cluster analysis

Clustering is a descriptive method of data mining used to find groups of observations (clusters) that share similar characteristics in a data set. In our project we decided to use cluster analysis to group together attributes of white wine. We wanted to find similarities between attributes as a step to build a good model.

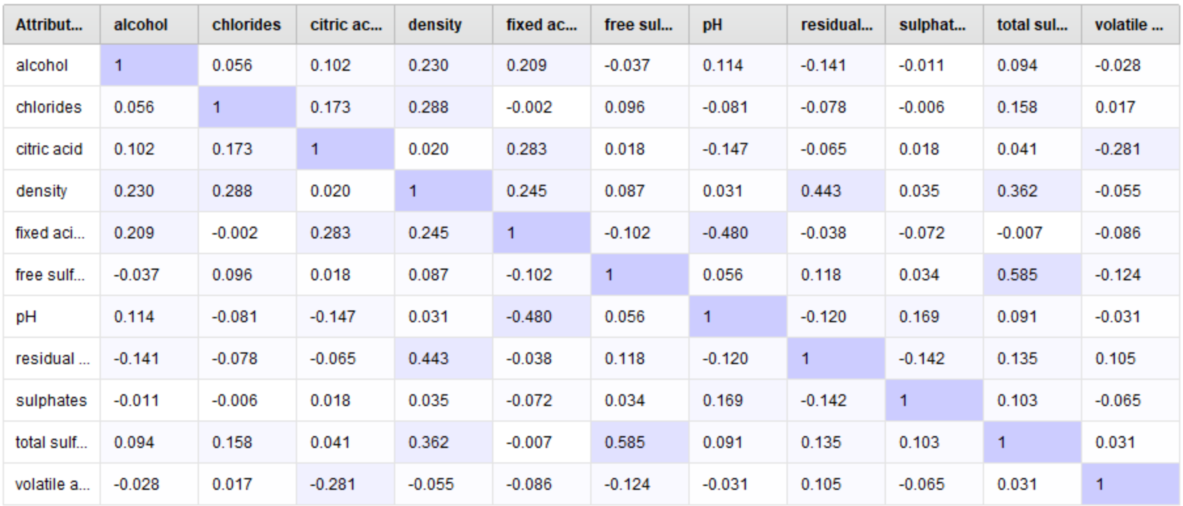
It is a form of unsupervised learning – that means machine is learning from a raw data. All target attributes have been removed for the moment of training (Han, Kamber, Pei, 2011).

In that particular case we decided to use partitioning approach. We have used k-means and x-means and a variation of k-means to compare these two methods. K-means is the best known method in data science. We also chose x-means as in x-means we do not need to specify the number of clusters.

K-means calculating again the centroid after every assignment and repeat that step until there is no change. That is why it is sensitive for changes.

In clustering we have be very careful with outliers. That is why we were extremely careful when pre-processing data. We took the following steps:

1. Correlations for clustering purposes



Attribut...	alcohol	chlorides	citric ac...	density	fixed ac...	free sul...	pH	residual...	sulphat...	total sul...	volatile ...
alcohol	1	0.056	0.102	0.230	0.209	-0.037	0.114	-0.141	-0.011	0.094	-0.028
chlorides	0.056	1	0.173	0.288	-0.002	0.096	-0.081	-0.078	-0.006	0.158	0.017
citric acid	0.102	0.173	1	0.020	0.283	0.018	-0.147	-0.065	0.018	0.041	-0.281
density	0.230	0.288	0.020	1	0.245	0.087	0.031	0.443	0.035	0.362	-0.055
fixed aci...	0.209	-0.002	0.283	0.245	1	-0.102	-0.480	-0.038	-0.072	-0.007	-0.086
free sulf...	-0.037	0.096	0.018	0.087	-0.102	1	0.056	0.118	0.034	0.585	-0.124
pH	0.114	-0.081	-0.147	0.031	-0.480	0.056	1	-0.120	0.169	0.091	-0.031
residual ...	-0.141	-0.078	-0.065	0.443	-0.038	0.118	-0.120	1	-0.142	0.135	0.105
sulphates	-0.011	-0.006	0.018	0.035	-0.072	0.034	0.169	-0.142	1	0.103	-0.065
total sulf...	0.094	0.158	0.041	0.362	-0.007	0.585	0.091	0.135	0.103	1	0.031
volatile a...	-0.028	0.017	-0.281	-0.055	-0.086	-0.124	-0.031	0.105	-0.065	0.031	1

Table 1.1. Correlation table – RapidMiner – white wines

Highest correlations between the attributes in our data set are:

- Total sulfur dioxide and free sulfur dioxide - 0.585
- Fixed acid and pH - 0.480
- Residual sugar and density - 0.443

This information can be very helpful in later stage of project when building a prediction model. This is also a basis for clustering analysis. That is also our basis for choosing the right number of clusters in k-means cluster analysis.

2. K-means clustering for white wine

We started that part by examining the scatter plots from data exploration part of project, and we decided to use 4 clusters. We did analysis in RapidMiner:

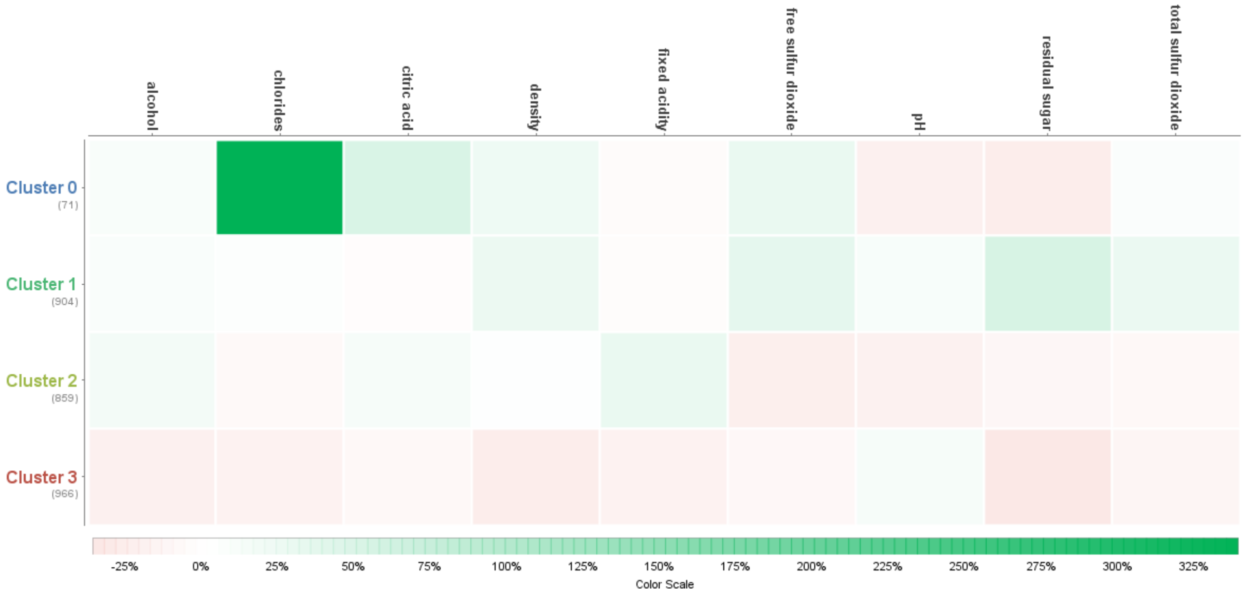
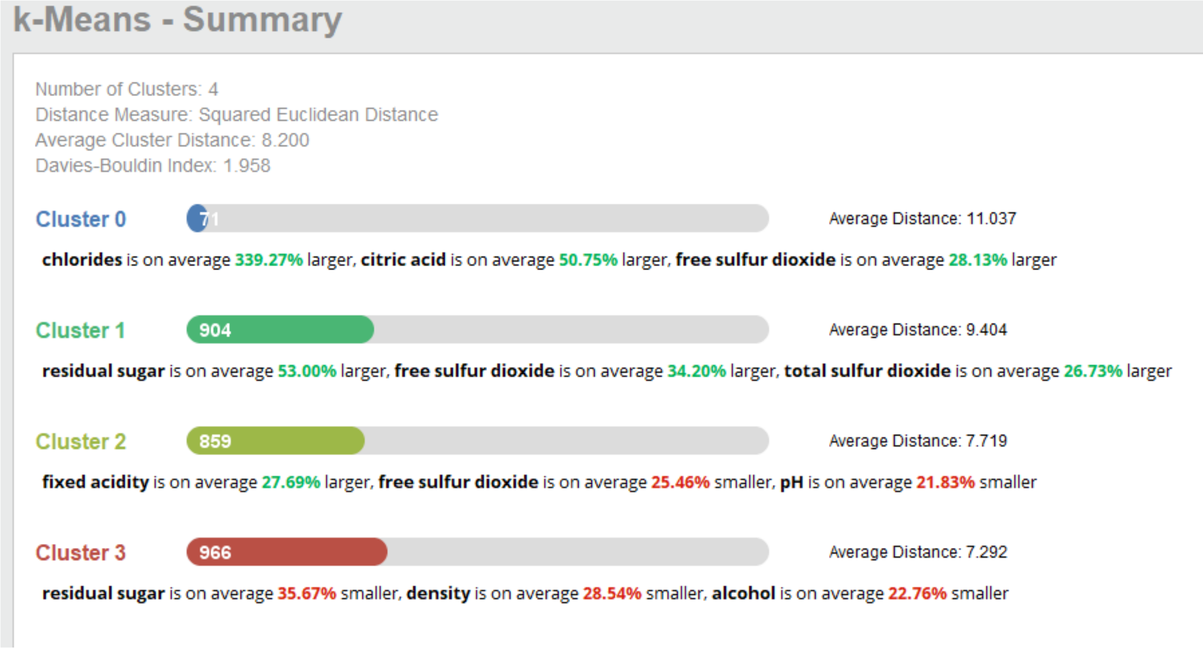


Figure 1.6. Heat map 1 – Rapidminer studio k-means– White wines attributes

Chlorides could look here as outliers as we can see very intensive green. But in reality, there chlorides in wine depends on the kind of grapes. There are types of grapes with very high natural volume of chlorides.



k-Means - Summary

Number of Clusters: 4
Distance Measure: Squared Euclidean Distance
Average Cluster Distance: 8.200
Davies-Bouldin Index: 1.958

Cluster 0 71 Average Distance: 11.037

chlorides is on average 339.27% larger, **citric acid** is on average 50.75% larger, **free sulfur dioxide** is on average 28.13% larger

Cluster 1 904 Average Distance: 9.404

residual sugar is on average 53.00% larger, **free sulfur dioxide** is on average 34.20% larger, **total sulfur dioxide** is on average 26.73% larger

Cluster 2 859 Average Distance: 7.719

fixed acidity is on average 27.69% larger, **free sulfur dioxide** is on average 25.46% smaller, **pH** is on average 21.83% smaller

Cluster 3 966 Average Distance: 7.292

residual sugar is on average 35.67% smaller, **density** is on average 28.54% smaller, **alcohol** is on average 22.76% smaller

Figure 1.7. Summary 1 – K-means RapidMiner studio – white wines

In above outcome it is clearly visible that 4 clusters were a good choice. Although it is still not perfect distribution.

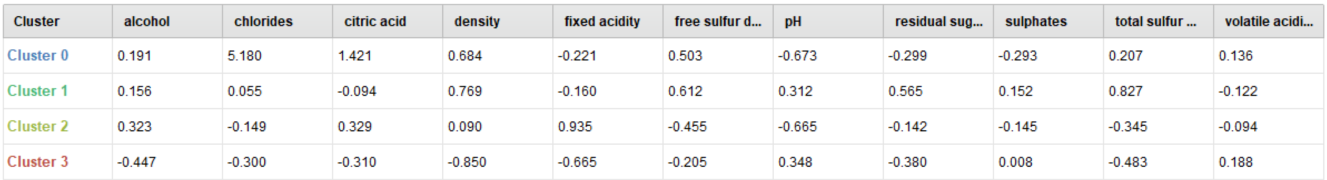
By Davis Bouldin Index we got only 1.958. It is an index for evaluation of cluster algorithms. As closer to zero than the clusters have been better assigned and they are closer to each other.

In cluster 0 we can see that chlorides are on average 339.27% larger than others, citric acid is on average 50.75% larger and free sulfur dioxide is on average 28.13% larger then in others. There are only 71 entries in this category, but average distance here is 11.

In cluster 1 we can see that residual sugar is on average 53% larger, free sulfur dioxide is on average 34.20% larger and total sulfur dioxide is on average 26.73% larger. There are 904 entries in this cluster but average distance here is 9.4.

In cluster 2 fixed acidity is on average 27.69% larger free sulfur dioxide is on average 25.46% smaller and pH is on average 21.83% smaller. There are 859 entries and average distance here is 7.7

In cluster 3 residual sugar is on average 35.67% smaller, density is on average 28.54% smaller, alcohol is on average 22.76% smaller. That is the biggest cluster with 966 entries and average distance here is 7.2.



Cluster	alcohol	chlorides	citric acid	density	fixed acidity	free sulfur d...	pH	residual sug...	sulphates	total sulfur ...	volatile acidi...
Cluster 0	0.191	5.180	1.421	0.684	-0.221	0.503	-0.673	-0.299	-0.293	0.207	0.136
Cluster 1	0.156	0.055	-0.094	0.769	-0.160	0.612	0.312	0.565	0.152	0.827	-0.122
Cluster 2	0.323	-0.149	0.329	0.090	0.935	-0.455	-0.665	-0.142	-0.145	-0.345	-0.094
Cluster 3	-0.447	-0.300	-0.310	-0.850	-0.665	-0.205	0.348	-0.380	0.008	-0.483	0.188

Table 1.2. Rapidminer, k-means white wine

In tables we can see the differences between clusters. Below there is line plot with 4 clusters and scatter plots for all 4 clusters separately (Fig. 1.8).

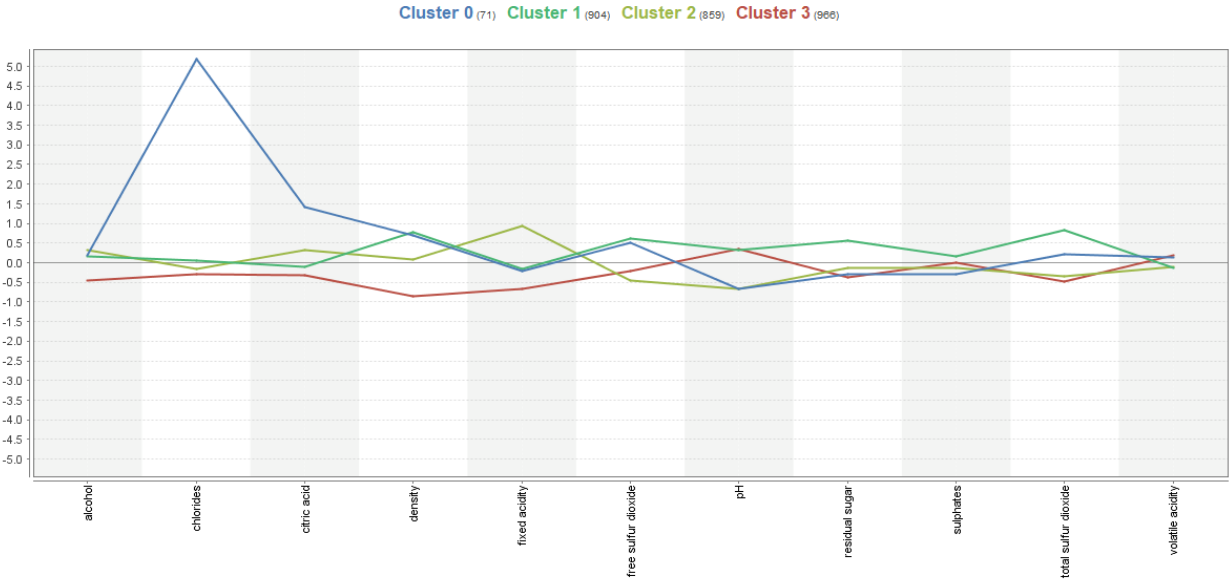


Figure 1.8. Line plot – Rapid miner k-means – White wine

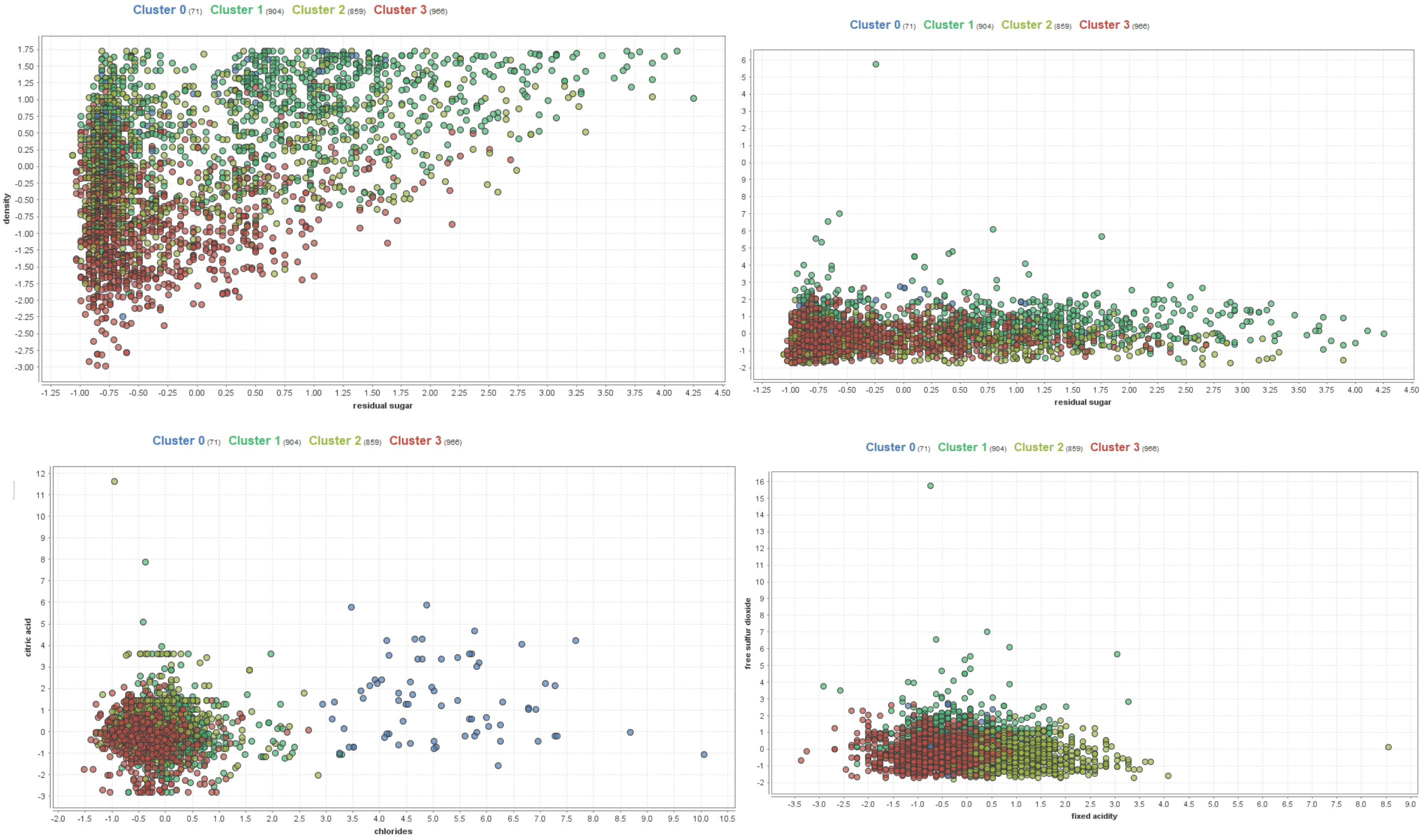


Figure 1.9. Scatterplots RapidMiner X-mean white wine

3. X- means clustering for white wine

In this analysis we did not need to choose number of clusters. The algorithm did it itself. X-means it is a variation of K-means. The results are:

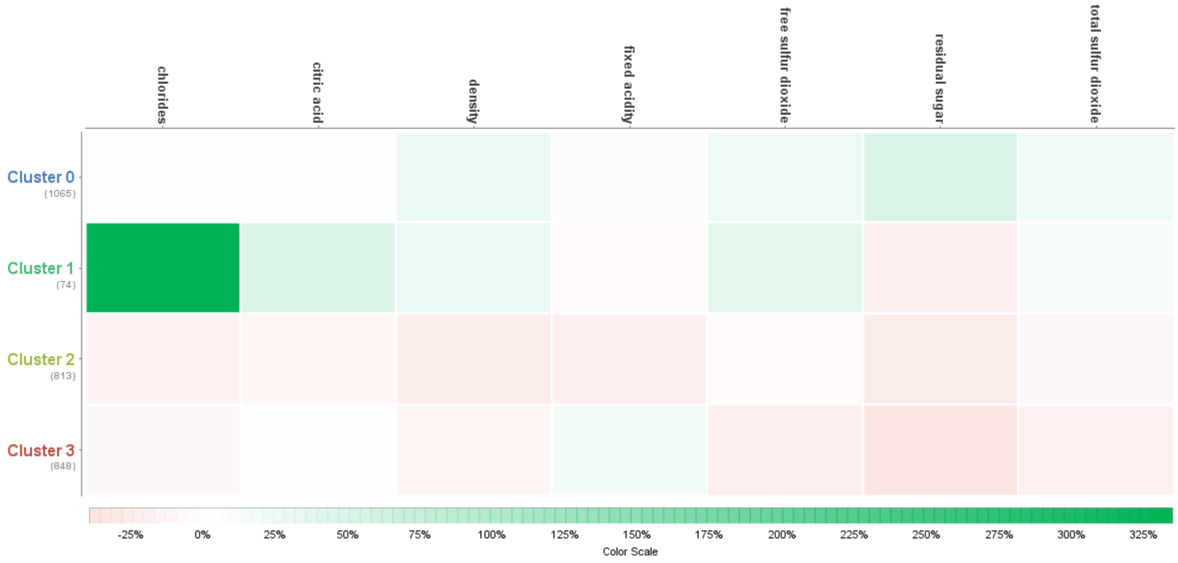
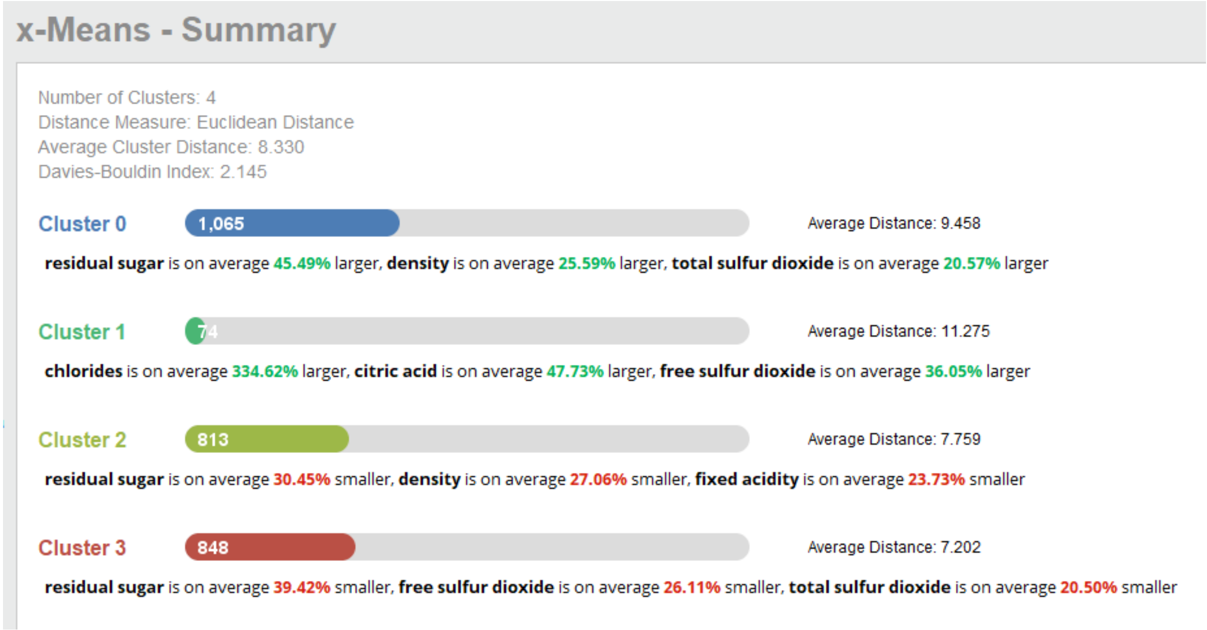


Figure 1.10. Heatmap 2 – Rapidminer X-means White wines

In this algorithm we can see that chlorides have been associated in different cluster than the previous k-means algorithm. Interesting fact is those algorithms also choose doing 4 clusters. That means we made similar assumptions.



x-Means - Summary

Number of Clusters: 4
Distance Measure: Euclidean Distance
Average Cluster Distance: 8.330
Davies-Bouldin Index: 2.145

Cluster 0 1,065 Average Distance: 9.458

residual sugar is on average 45.49% larger, **density** is on average 25.59% larger, **total sulfur dioxide** is on average 20.57% larger

Cluster 1 74 Average Distance: 11.275

chlorides is on average 334.62% larger, **citric acid** is on average 47.73% larger, **free sulfur dioxide** is on average 36.05% larger

Cluster 2 813 Average Distance: 7.759

residual sugar is on average 30.45% smaller, **density** is on average 27.06% smaller, **fixed acidity** is on average 23.73% smaller

Cluster 3 848 Average Distance: 7.202

residual sugar is on average 39.42% smaller, **free sulfur dioxide** is on average 26.11% smaller, **total sulfur dioxide** is on average 20.50% smaller

Figure 1.11. Summary Rapidminer X-means – white wines

By Davis Bouldin Index we got only 2.145. So, its means that k-means was better choice in that case.

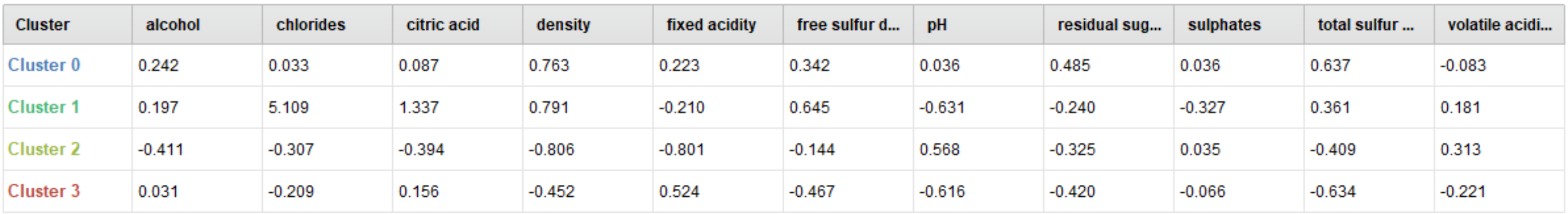
We can see that we have 4 clusters too.

In cluster 0 we can see that residual sugar are on average 45.49% larger than others, density is on average 25.59% larger and total sulfur dioxide is on average 20.57% larger then in others. It has large number of entries 1065 and average distance here is 9.45.

In cluster 1 we can see that chlorides is on average 334.62% larger, citric acid is on average 47.73% larger and free sulfur dioxide is on average 36.05% larger. There are only 74 entries here but average distance here is 11.27.

In cluster 2 residual sugar is on average 30.45% smaller density is on average 27.06% smaller and fixed acidity is on average 23.73% smaller. There are 813 entries in this cluster and average distance here is 7.7

In cluster 3 residual sugar is on average 39.42% smaller, free sulfur dioxide is on average 26.11% smaller, total sulfur dioxide is on average 20.5% smaller. There are 848 entries and average distance here is 7.2.



Cluster	alcohol	chlorides	citric acid	density	fixed acidity	free sulfur d...	pH	residual sug...	sulphates	total sulfur ...	volatile acidi...
Cluster 0	0.242	0.033	0.087	0.763	0.223	0.342	0.036	0.485	0.036	0.637	-0.083
Cluster 1	0.197	5.109	1.337	0.791	-0.210	0.645	-0.631	-0.240	-0.327	0.361	0.181
Cluster 2	-0.411	-0.307	-0.394	-0.806	-0.801	-0.144	0.568	-0.325	0.035	-0.409	0.313
Cluster 3	0.031	-0.209	0.156	-0.452	0.524	-0.467	-0.616	-0.420	-0.066	-0.634	-0.221

Table 1.3. Rapidminer – Table of clusters

In tables we can see the differences between clusters. Below there is line plot with 4 clusters and scatter plots for all 4 clusters separately.

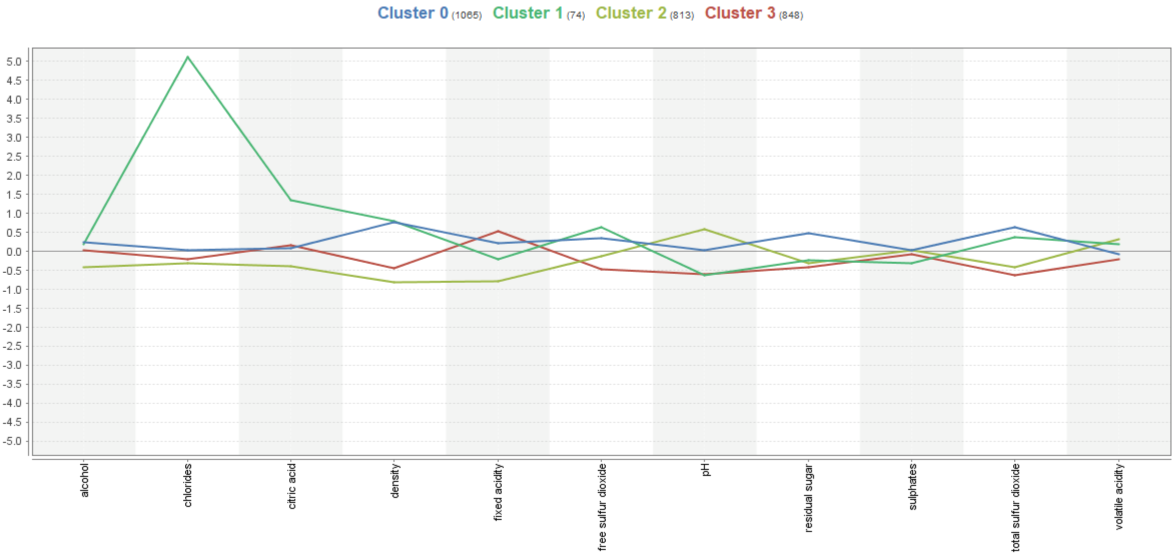


Figure 1.12. Rapidminer – Lineplot – X-means

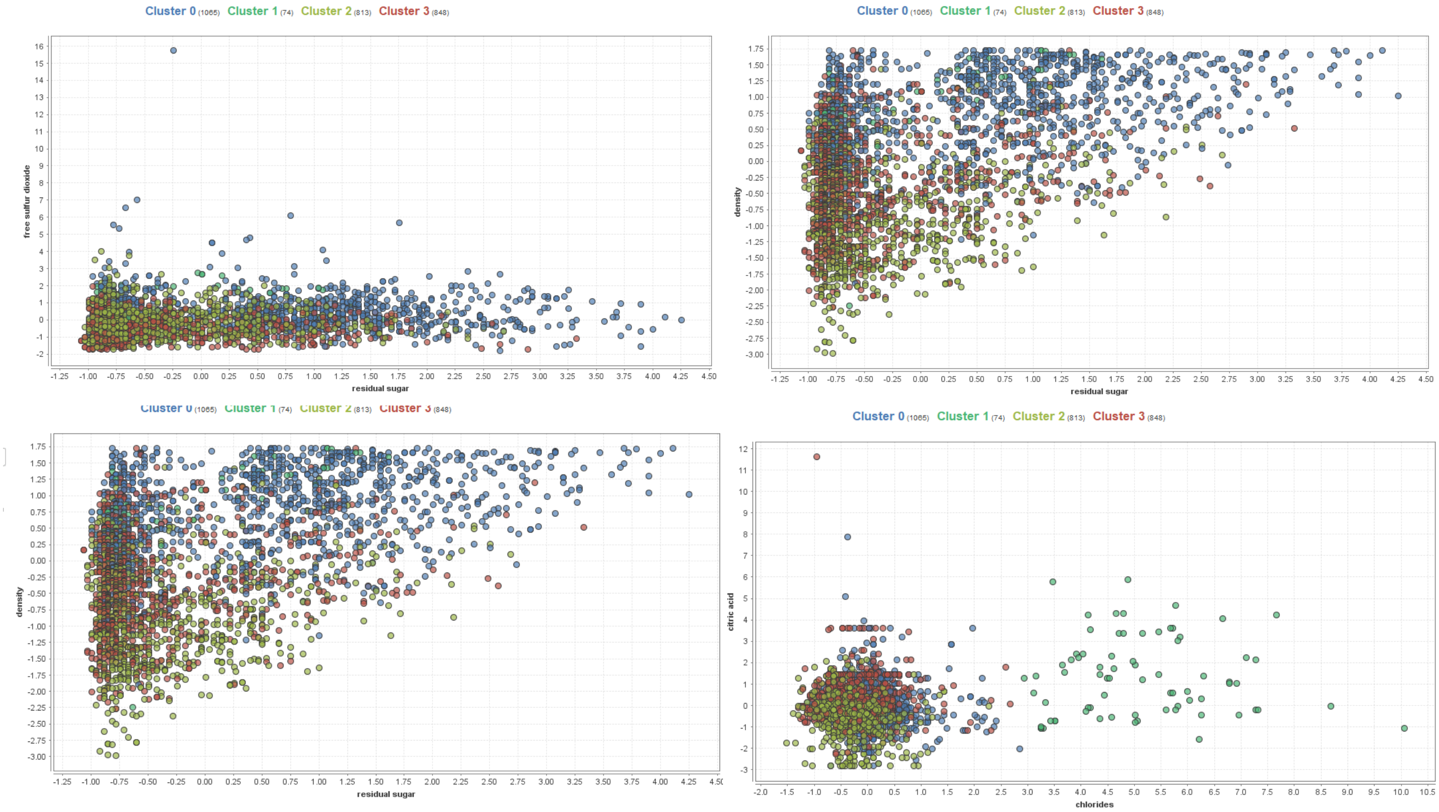


Figure 1.13. Scatter plots of 4 clusters of white wines x-means – Rapidminer

We found the following weaknesses in clustering:

- We cannot use it for categorical data as it applicable for continuous attributes only.
- In k-means we need to specify number of clusters
- We need to remove outliers.
- Only standard shape of clusters
- X-means seems to be variation of k-means but as in our example k-means was better choice in this particular case.

Quality analysis

We will use classification models including decision trees and naïve Bayes and clustering.

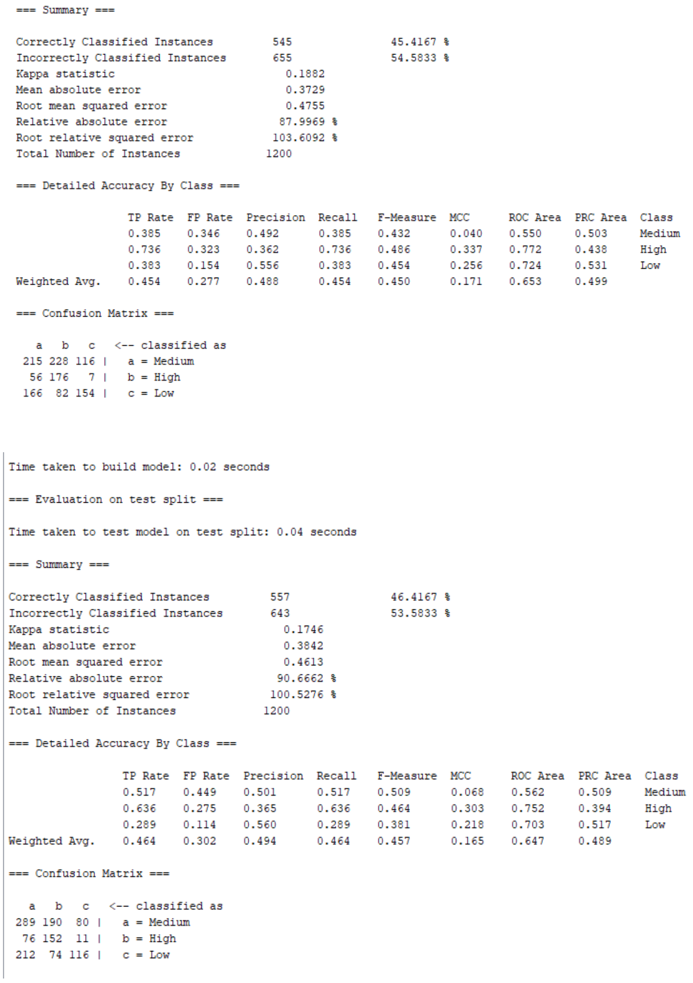
Decision tree is a classification method and a predictive technique. Classification methods use existing data to create a model that will allow to classify new data. In our project we will use decision tree to predict quality and classify alcohol content and sugar/ pH ratio, level of preservatives and wine balance.

Clustering is a descriptive technique that finds groups of observations (clusters) that share similar characteristics in a data set.

Naïve Bayes

Naïve Bayes model was run in Weka using the dataset with 4,000 instances (split 70 /30 - 70.0% of data is for training, remaining 30% is for testing purposes) and 12 attributes (fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, Quality and Alcohol content).

The accuracy of that model was only 45.4% (Fig 1.14).



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=== Summary ===

Correctly Classified Instances         545               45.4167 %
Incorrectly Classified Instances       655               54.5833 %
Kappa statistic                          0.1882
Mean absolute error                      0.3729
Root mean squared error                  0.4755
Relative absolute error                 87.9969 %
Root relative squared error            103.6092 %
Total Number of Instances             1200

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.385    0.346    0.492      0.385    0.432      0.040    0.550     0.503     Medium
                 0.736    0.323    0.362      0.736    0.486      0.337    0.772     0.438     High
                 0.383    0.154    0.556      0.383    0.454      0.256    0.724     0.531     Low
Weighted Avg.    0.454    0.277    0.488      0.454    0.450      0.171    0.653     0.499

=== Confusion Matrix ===

   a   b   c   <-- classified as
 215 228 116 |   a = Medium
  56 176   7 |   b = High
 166  82 154 |   c = Low
```

```
Time taken to build model: 0.02 seconds

=== Evaluation on test split ===

Time taken to test model on test split: 0.04 seconds

=== Summary ===

Correctly Classified Instances         557               46.4167 %
Incorrectly Classified Instances       643               53.5833 %
Kappa statistic                          0.1746
Mean absolute error                      0.3842
Root mean squared error                  0.4613
Relative absolute error                 90.6662 %
Root relative squared error            100.5276 %
Total Number of Instances             1200

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.517    0.449    0.501      0.517    0.509      0.068    0.562     0.509     Medium
                 0.636    0.275    0.365      0.636    0.464      0.303    0.752     0.394     High
                 0.289    0.114    0.560      0.289    0.381      0.218    0.703     0.517     Low
Weighted Avg.    0.464    0.302    0.494      0.464    0.457      0.165    0.647     0.489

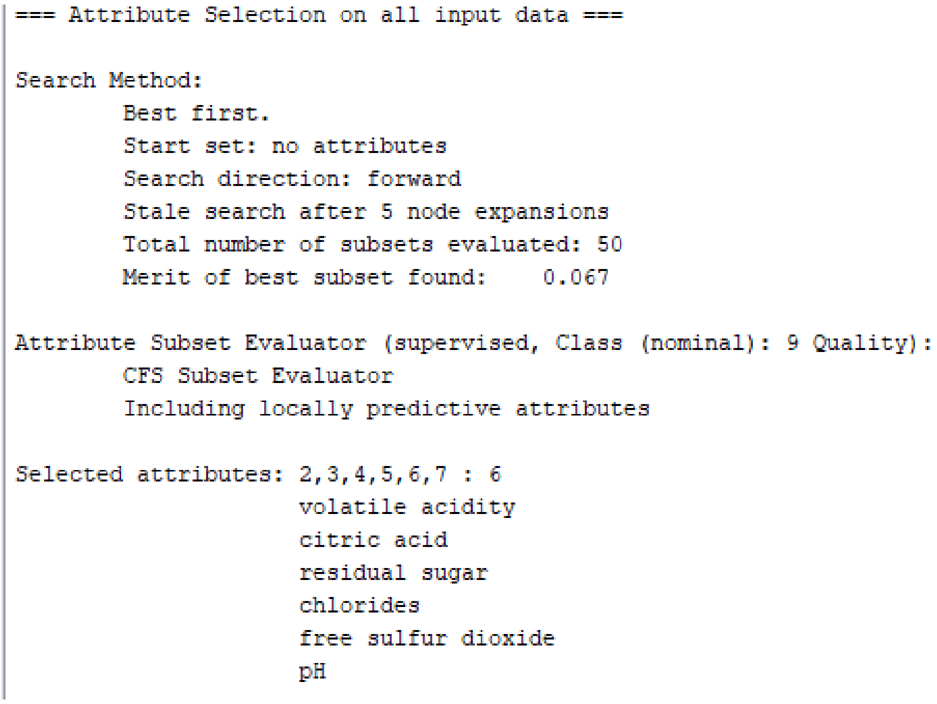
=== Confusion Matrix ===

   a   b   c   <-- classified as
 289 190  80 |   a = Medium
  76 152  11 |   b = High
 212  74 116 |   c = Low
```

Figure 1.14. Naïve Bayes classifiers' output comparison

The same model was run after removing total sulfur dioxide attribute (correlated to free sulfur dioxide) and slight improvement in accuracy level was observed – 46.4%.

In the next step we used the correlation-based feature selection (CFS) algorithm in Weka to further eliminate the correlated redundant features from the dataset (Fig. 1.15).



```
=== Attribute Selection on all input data ===

Search Method:
        Best first.
        Start set: no attributes
        Search direction: forward
        Stale search after 5 node expansions
        Total number of subsets evaluated: 50
        Merit of best subset found:    0.067

Attribute Subset Evaluator (supervised, Class (nominal): 9 Quality):
        CFS Subset Evaluator
        Including locally predictive attributes

Selected attributes: 2,3,4,5,6,7 : 6
                     volatile acidity
                     citric acid
                     residual sugar
                     chlorides
                     free sulfur dioxide
                     pH
```

Figure 1.15. Attributes selected by applying the CFS algorithm in Weka

However, after executing the Naïve Bayes model in Weka using only attributes selected by CFS algorithm (volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, pH and Quality) we did not observe any major improvement in accuracy. The accuracy for this model was 45.5%.

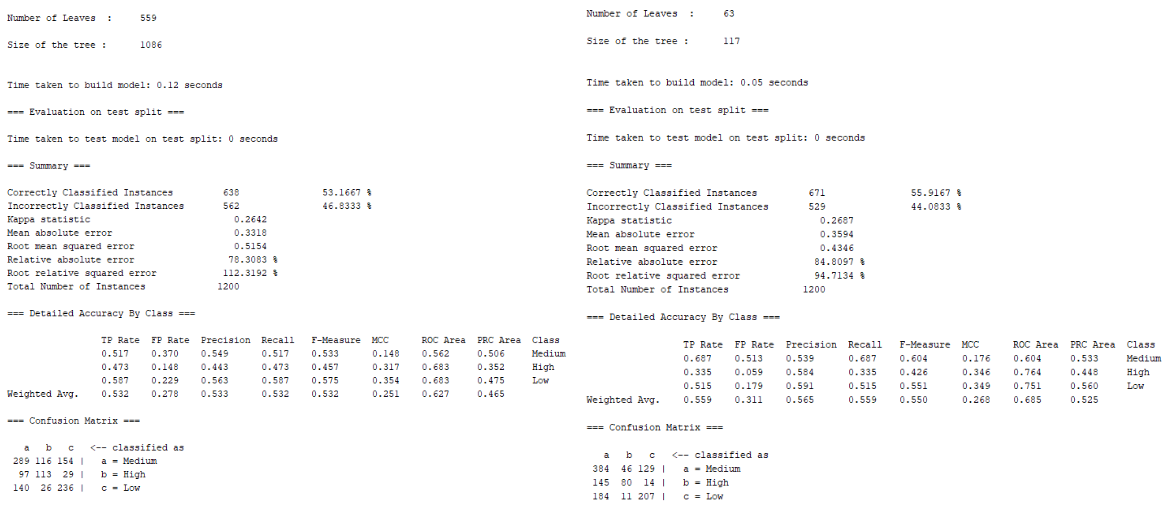
	Class		
Attribute	High	Medium	Low
	0.21	0.45	0.34
fixed acidity			
Mean	6.6968	6.8267	6.9602
std. dev.	0.7846	0.8485	0.9121
weight sum	834	1806	1360
Precision	0.1552	0.1552	0.1552
volatile acidity			
Mean	0.2689	0.2615	0.3121
std. dev.	0.0946	0.0895	0.1167
weight sum	834	1806	1360
Precision	0.0082	0.0082	0.0082
citric acid			
Mean	0.3306	0.3394	0.3329
std. dev.	0.0828	0.1206	0.1436
weight sum	834	1806	1360
Precision	0.0193	0.0193	0.0193
residual sugar			
Mean	4.6206	6.0033	6.6776
std. dev.	3.7365	4.9864	5.1673
weight sum	834	1806	1360
Precision	0.211	0.211	0.211
Chlorides			
Mean	0.0374	0.0452	0.0522
std. dev.	0.0108	0.0209	0.0288
weight sum	834	1806	1360
Precision	0.0021	0.0021	0.0021
free sulfur dioxide			
Mean	34.1524	35.313	34.7731
std. dev.	14.2492	15.7009	20.5611
weight sum	834	1806	1360
Precision	2.1908	2.1908	2.1908
pH			
Mean	3.2288	3.1951	3.1728
std. dev.	0.1536	0.1512	0.147
weight sum	834	1806	1360
Precision	0.0108	0.0108	0.0108
Sulphates			
Mean	0.5	0.4921	0.4816
std. dev.	0.1345	0.1118	0.1008
weight sum	834	1806	1360
Precision	0.011	0.011	0.011
Alcohol content			
High	300	564	473
Medium	467	1008	777
Low	70	237	113
[total]	837	1809	1363

Table 1.4. Naïve Bayes classifier model

It would appear that the quality is decreasing with higher level of fixed acidity, residual sugar and chlorides and it is improved with higher pH level.

Decision Tree

Decision Tree J48 model was executed in Weka using the dataset with 4,000 instances (split 70/30) and 12 attributes (fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, Quality and Alcohol content) to predict Quality attribute. The first Decision Tree model was executed with default settings in Weka (batch size 100, confidence factor 0.25, minimum number of instances per leaf 2). The accuracy of that model was 53.2%. The model was simplified by increasing the minimum number of instances per leaf to 28 and it improved its accuracy to 55.9%.



```
Number of Leaves  :     559

Size of the tree :      1086


Time taken to build model: 0.12 seconds

=== Evaluation on test split ===

Time taken to test model on test split: 0 seconds

=== Summary ===

Correctly Classified Instances         638               53.1667 %
Incorrectly Classified Instances       562               46.8333 %
Kappa statistic                          0.2642
Mean absolute error                      0.3318
Root mean squared error                  0.5154
Relative absolute error                 78.3083 %
Root relative squared error            112.3192 %
Total Number of Instances             1200

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.517    0.370    0.549      0.517    0.533      0.148    0.562     0.506     Medium
                 0.473    0.148    0.443      0.473    0.457      0.317    0.683     0.352     High
                 0.587    0.229    0.563      0.587    0.575      0.354    0.683     0.475     Low
Weighted Avg.    0.532    0.278    0.533      0.532    0.532      0.251    0.627     0.465

=== Confusion Matrix ===

   a   b   c   <-- classified as
 289 116 154 |   a = Medium
  97 113  29 |   b = High
 140  26 236 |   c = Low
```

```
Number of Leaves  :     63

Size of the tree :      117


Time taken to build model: 0.05 seconds

=== Evaluation on test split ===

Time taken to test model on test split: 0 seconds

=== Summary ===

Correctly Classified Instances         671               55.9167 %
Incorrectly Classified Instances       529               44.0833 %
Kappa statistic                          0.2687
Mean absolute error                      0.3594
Root mean squared error                  0.4346
Relative absolute error                 84.8097 %
Root relative squared error             94.7134 %
Total Number of Instances             1200

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.687    0.513    0.539      0.687    0.604      0.176    0.604     0.533     Medium
                 0.335    0.059    0.584      0.335    0.426      0.346    0.764     0.448     High
                 0.515    0.179    0.591      0.515    0.551      0.349    0.751     0.560     Low
Weighted Avg.    0.559    0.311    0.565      0.559    0.550      0.268    0.685     0.525

=== Confusion Matrix ===

   a   b   c   <-- classified as
 384  46 129 |   a = Medium
 145  80  14 |   b = High
 184  11 207 |   c = Low
```

Figure 1.16. Decision Tree J48 models' comparison

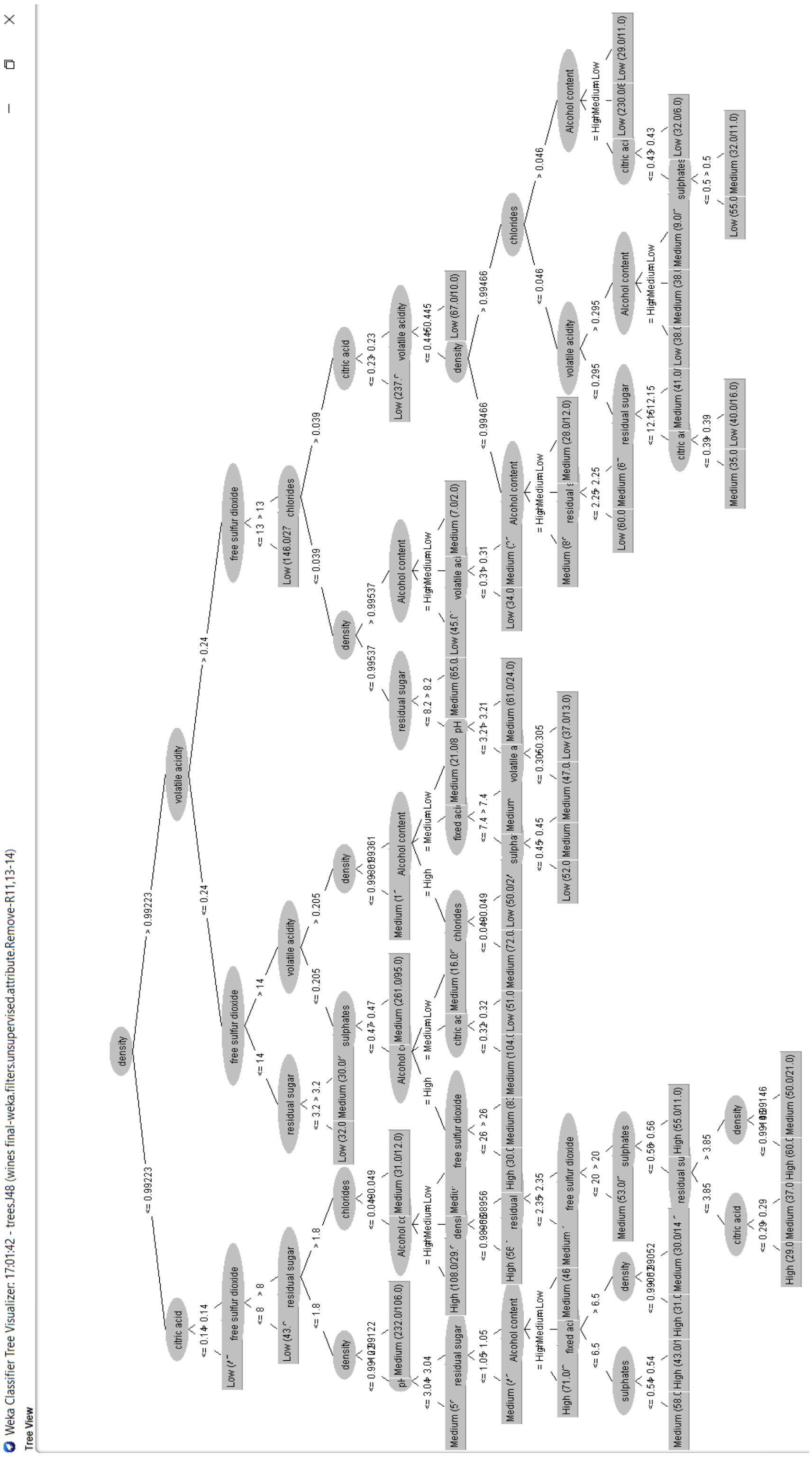
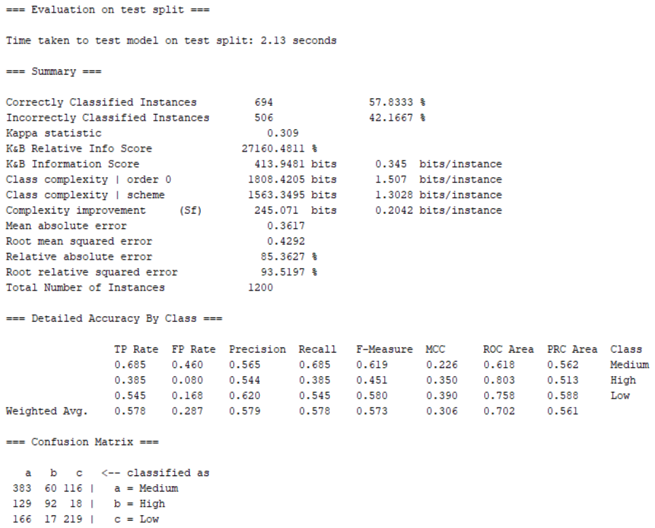


Figure 1.17. Decision Tree J48 model - Weka

We also used Support Vector Machine model in Weka – SMO to predict the quality attribute. The accuracy of that model was 57.8% (Fig. 1.18).

Support vector machine algorithm transforms training data into a higher dimension, where it searches for “decision boundary” (linear optimal separating hyperplane) that separates the data from one class from another. To find this hyperplane SVM model uses support vectors (“essential” training tuples) and margins (defined by the support vectors).



```
=== Evaluation on test split ===

Time taken to test model on test split: 2.13 seconds

=== Summary ===

Correctly Classified Instances         694               57.8333 %
Incorrectly Classified Instances       506               42.1667 %
Kappa statistic                          0.309
K&B Relative Info Score              27160.4811 %
K&B Information Score                  413.9481 bits      0.345  bits/instance
Class complexity | order 0            1808.4205 bits      1.507  bits/instance
Class complexity | scheme             1563.3495 bits      1.3028 bits/instance
Complexity improvement     (Sf)        245.071  bits      0.2042 bits/instance
Mean absolute error                      0.3617
Root mean squared error                  0.4292
Relative absolute error                 85.3627 %
Root relative squared error             93.5197 %
Total Number of Instances             1200

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.685    0.460    0.565      0.685    0.619      0.226    0.618     0.562     Medium
                 0.385    0.080    0.544      0.385    0.451      0.350    0.803     0.513     High
                 0.545    0.168    0.620      0.545    0.580      0.390    0.758     0.588     Low
Weighted Avg.    0.578    0.287    0.579      0.578    0.573      0.306    0.702     0.561

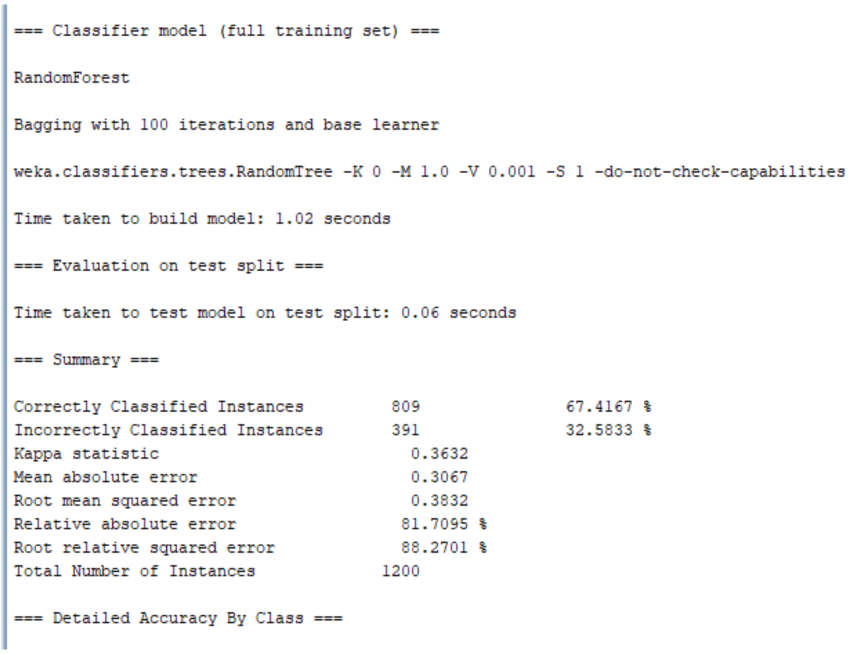
=== Confusion Matrix ===

   a   b   c   <-- classified as
 383  60 116 |   a = Medium
 129  92  18 |   b = High
 166  17 219 |   c = Low
```

Figure 1.18. SMO model Weka – evaluation output

The best accuracy level 67.4% (Fig. 1.19) was achieved using the Random Forest model using the dataset with 4,000 instances (split 70.0% train, remainder test) and 11 attributes (fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, density, pH, sulphates, Quality and Alcohol content).

This is not surprising as Random Forest is an ensemble method where the decision is based on the outcome of a number (forest) of decision tree classifiers. The individual decision trees are generated using a random selection of attributes at each node to determine the split. During classification, each tree votes and the most popular class is returned.



```
=== Classifier model (full training set) ===

RandomForest

Bagging with 100 iterations and base learner

weka.classifiers.trees.RandomTree -K 0 -M 1.0 -V 0.001 -S 1 -do-not-check-capabilities

Time taken to build model: 1.02 seconds

=== Evaluation on test split ===

Time taken to test model on test split: 0.06 seconds

=== Summary ===

Correctly Classified Instances         809               67.4167 %
Incorrectly Classified Instances       391               32.5833 %
Kappa statistic                          0.3632
Mean absolute error                      0.3067
Root mean squared error                  0.3832
Relative absolute error                 81.7095 %
Root relative squared error             88.2701 %
Total Number of Instances             1200

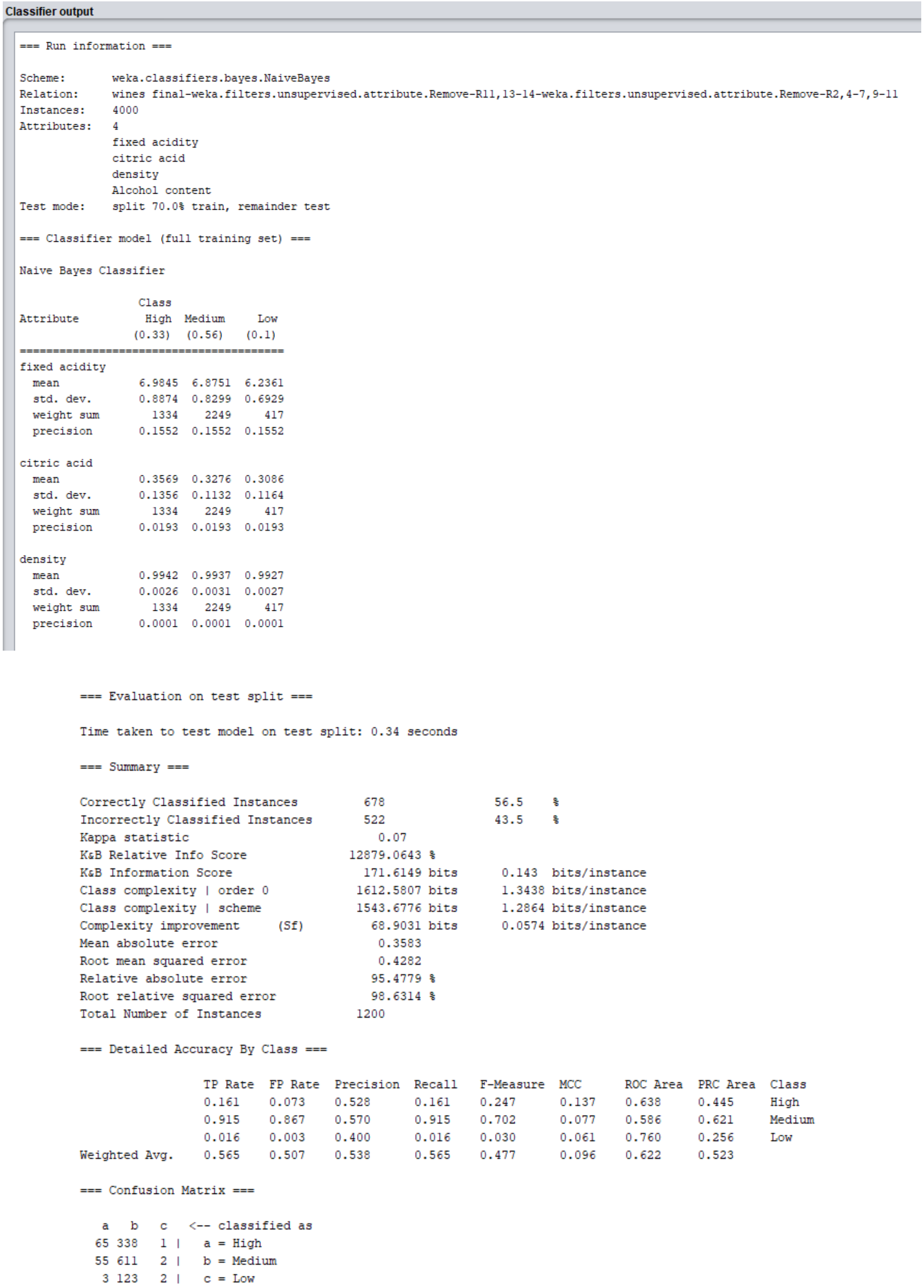
=== Detailed Accuracy By Class ===
```

Figure 1.19. Random Forest model in Weka

Classification Models – alcohol content

We also used **Naïve Bayes and Decision Tree** models to review alcohol content. The original alcohol values were discretised: values lower than 9% were classed as low, 9 to 11% as medium and above 11% as high.   After running the correlation-based feature selection (CFS) algorithm in Weka to we eliminated all attributes but fixed acidity, citric acid and density to classify alcohol content. The accuracy of the model was 56.5% (Fig. 1.20). An interesting insight learnt from this model is that alcohol content seems to be higher in wines with higher fixed acidity levels and amount of citric acid and higher density.

Decision Tree (pruned J48) model was also executed using 12 attributes (fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, Quality and Alcohol content) with minimum number of instances per leaf 28. The accuracy of that model was 61.7% (Fig. 1.21).



```
=== Run information ===

Scheme:       weka.classifiers.bayes.NaiveBayes
Relation:     wines final-weka.filters.unsupervised.attribute.Remove-R11,13-14-weka.filters.unsupervised.attribute.Remove-R2,4-7,9-11
Instances:    4000
Attributes:   4
              fixed acidity
              citric acid
              density
              Alcohol content
Test mode:    split 70.0% train, remainder test

=== Classifier model (full training set) ===

Naive Bayes Classifier

                  Class
Attribute          High  Medium     Low
                 (0.33)  (0.56)   (0.1)
========================================
fixed acidity
  mean            6.9845  6.8751  6.2361
  std. dev.       0.8874  0.8299  0.6929
  weight sum        1334    2249     417
  precision       0.1552  0.1552  0.1552

citric acid
  mean            0.3569  0.3276  0.3086
  std. dev.       0.1356  0.1132  0.1164
  weight sum        1334    2249     417
  precision       0.0193  0.0193  0.0193

density
  mean            0.9942  0.9937  0.9927
  std. dev.       0.0026  0.0031  0.0027
  weight sum        1334    2249     417
  precision       0.0001  0.0001  0.0001
```

```
=== Evaluation on test split ===

Time taken to test model on test split: 0.34 seconds

=== Summary ===

Correctly Classified Instances         678               56.5    %
Incorrectly Classified Instances       522               43.5    %
Kappa statistic                          0.07
K&B Relative Info Score              12879.0643 %
K&B Information Score                  171.6149 bits      0.143  bits/instance
Class complexity | order 0            1612.5807 bits      1.3438 bits/instance
Class complexity | scheme             1543.6776 bits      1.2864 bits/instance
Complexity improvement     (Sf)         68.9031 bits      0.0574 bits/instance
Mean absolute error                      0.3583
Root mean squared error                  0.4282
Relative absolute error                 95.4779 %
Root relative squared error             98.6314 %
Total Number of Instances             1200

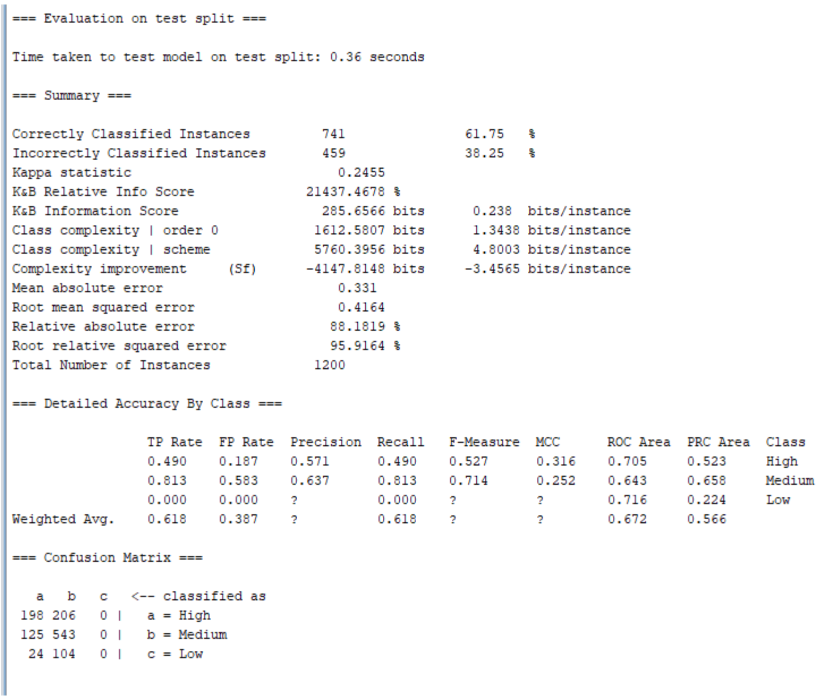
=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.161    0.073    0.528      0.161    0.247      0.137    0.638     0.445     High
                 0.915    0.867    0.570      0.915    0.702      0.077    0.586     0.621     Medium
                 0.016    0.003    0.400      0.016    0.030      0.061    0.760     0.256     Low
Weighted Avg.    0.565    0.507    0.538      0.565    0.477      0.096    0.622     0.523

=== Confusion Matrix ===

   a   b   c   <-- classified as
  65 338   1 |   a = High
  55 611   2 |   b = Medium
   3 123   2 |   c = Low
```

Figure 1.20. Naïve Bayes model – alcohol content



```
=== Evaluation on test split ===

Time taken to test model on test split: 0.36 seconds

=== Summary ===

Correctly Classified Instances         741               61.75   %
Incorrectly Classified Instances       459               38.25   %
Kappa statistic                          0.2455
K&B Relative Info Score              21437.4678 %
K&B Information Score                  285.6566 bits      0.238  bits/instance
Class complexity | order 0            1612.5807 bits      1.3438 bits/instance
Class complexity | scheme             5760.3956 bits      4.8003 bits/instance
Complexity improvement     (Sf)      -4147.8148 bits     -3.4565 bits/instance
Mean absolute error                      0.331
Root mean squared error                  0.4164
Relative absolute error                 88.1819 %
Root relative squared error             95.9164 %
Total Number of Instances             1200

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
                 0.490    0.187    0.571      0.490    0.527      0.316    0.705     0.523     High
                 0.813    0.583    0.637      0.813    0.714      0.252    0.643     0.658     Medium
                 0.000    0.000    ?          0.000    ?          ?        0.716     0.224     Low
Weighted Avg.    0.618    0.387    ?          0.618    ?          ?        0.672     0.566

=== Confusion Matrix ===

   a   b   c   <-- classified as
 198 206   0 |   a = High
 125 543   0 |   b = Medium
  24 104   0 |   c = Low
```

Figure 1.21. Decision Tree J48 – alcohol content prediction – evaluation output Weka

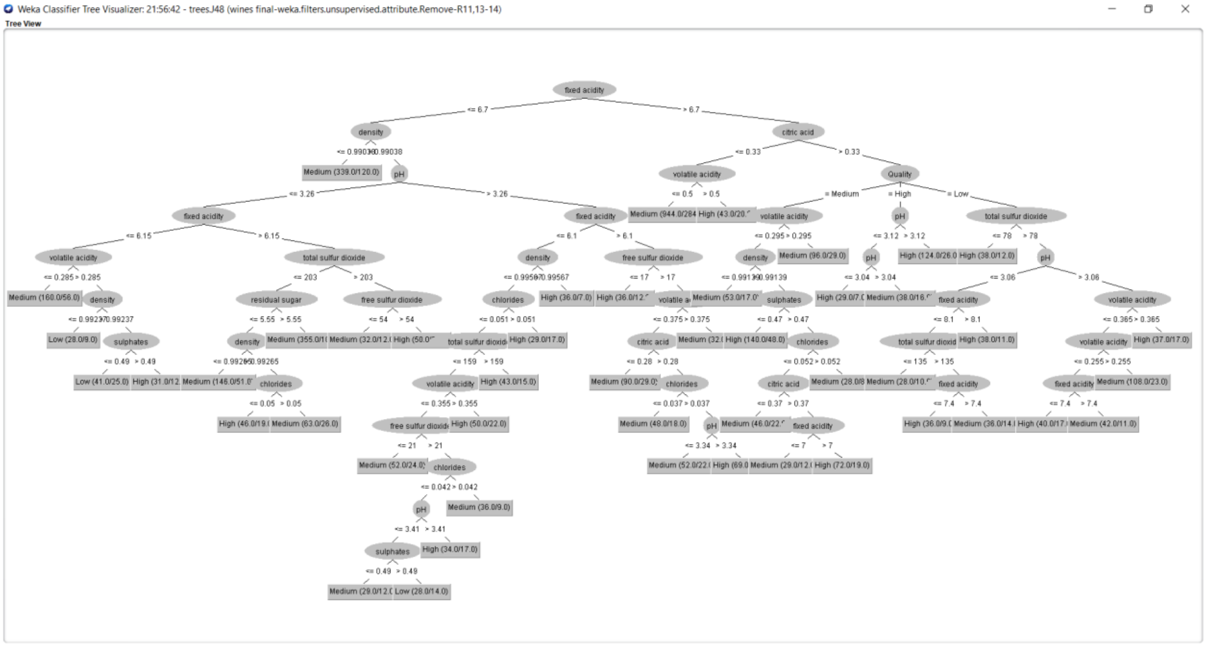


Figure 1.22. Decision Tree J48 model – alcohol content prediction (Weka)

Quality analysis of white wines – comparison of accuracy

Methods used:

- Naïve Bayes
- Generalised Linear model
- Decision Tree
- Random Forest
- Gradient Boosted Trees

Target variable – level of preservatives

In this particular exercise we are doing analysis to figure out how changing the average of one of measurement affects another.

These attributes has been created for this purposes – Level of preservatives in white wine. It is categorical attribute.

Rule:

=IF(AND(J44<=0.45,E44<=0.045),"Low",IF(AND(J44<=0.6,E44<=0.06),"Medium","High"))

There are 3 types of output Low, Medium and High (Ordinal Polynomial attributes).

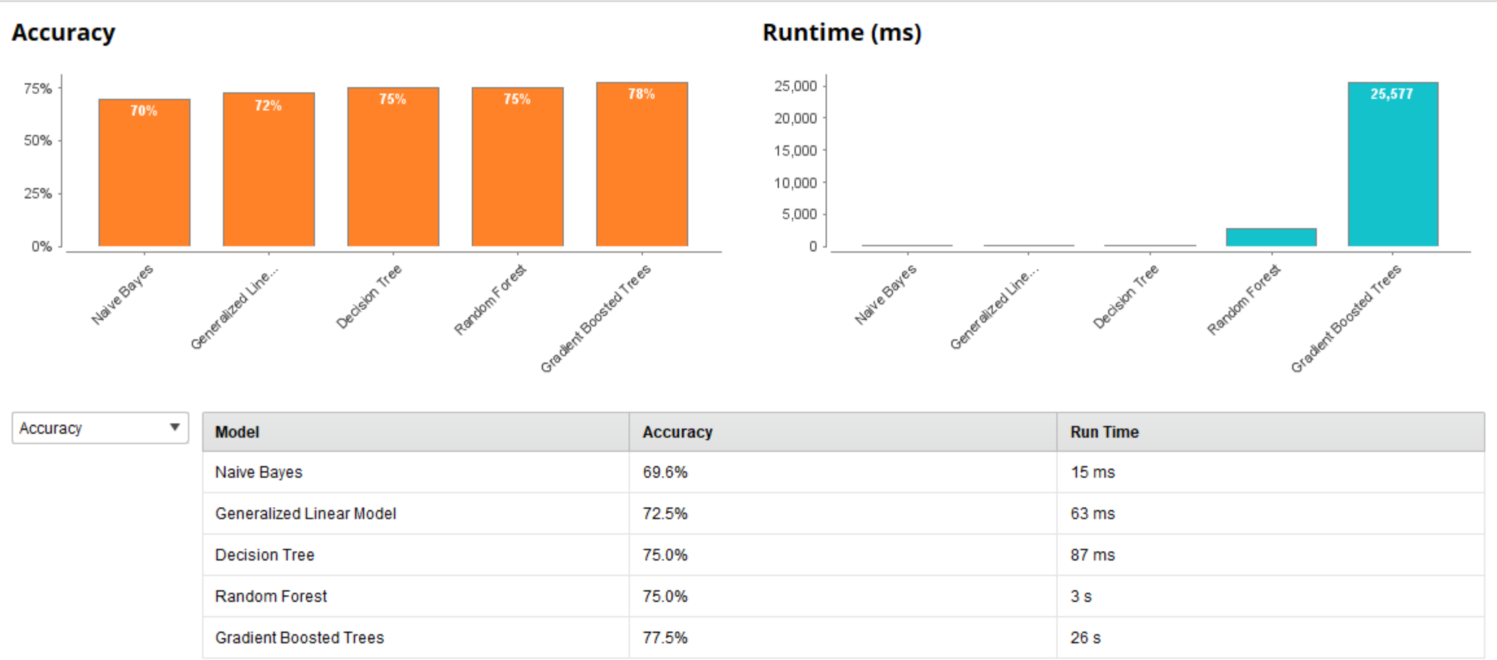
The aim of this analysis is to check what will happen with one variable if we will change or delete the other. In that case we have deleted chlorides.

Training set was extracted at 70% of dataset and 30% was a test set.

Summary of model outputs.

In test set we have deleted chloride attribute and then tried to predict the outcome of target variables based only on other attributes.

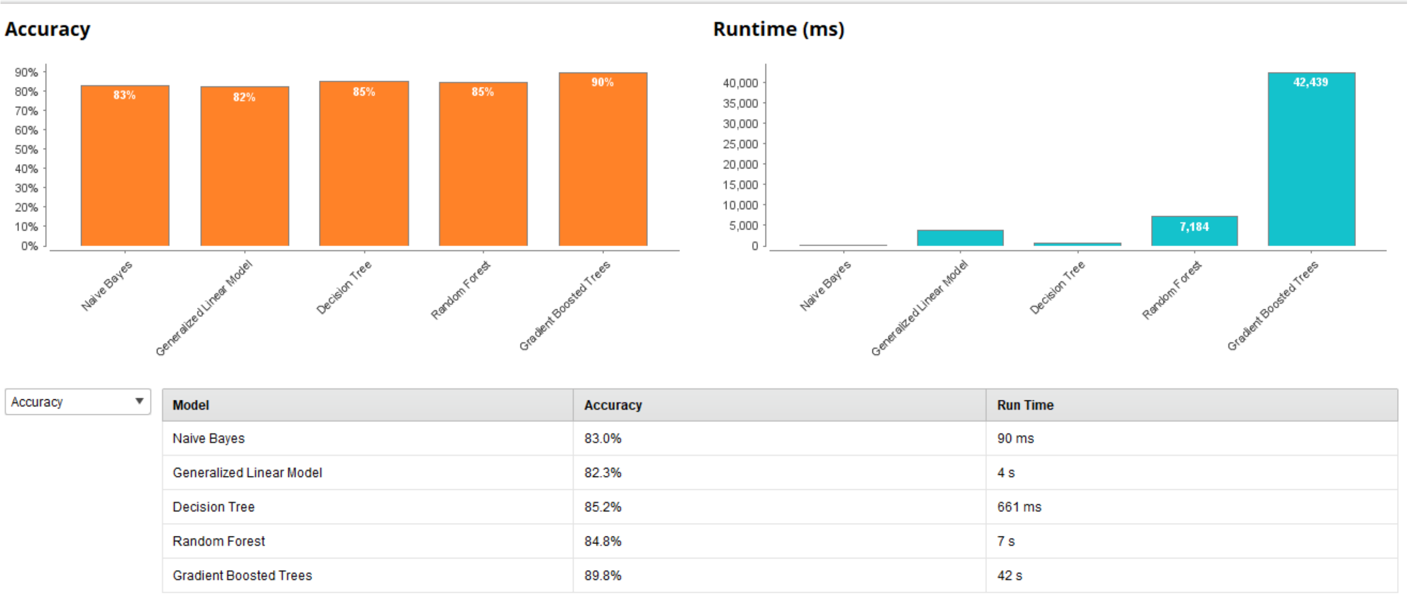
Training:



Model	Accuracy	Run Time
Naive Bayes	69.6%	15 ms
Generalized Linear Model	72.5%	63 ms
Decision Tree	75.0%	87 ms
Random Forest	75.0%	3 s
Gradient Boosted Trees	77.5%	26 s

Figure 1.23. Training set – level of preservatives – Rapidminer output

Test:



Model	Accuracy	Run Time
Naive Bayes	83.0%	90 ms
Generalized Linear Model	82.3%	4 s
Decision Tree	85.2%	661 ms
Random Forest	84.8%	7 s
Gradient Boosted Trees	89.8%	42 s

Figure 1.24. Test set - Cross – validation – level of preservatives – Rapidminer output

Summary of models' outputs

As we can see the Gradient Boosted Trees method had the highest accuracy at 77.5%. But it was the slow as it takes 26 seconds compared to others.

That's mean that even without chloride attribute the other attributes of white wines can give us information about level of preservatives at 77.5% chances that we are correct.

Training set had higher score of 89%, but still model is quite good.

We can see that model had no problem with medium level of preservatives but had problem with the High and Low level.

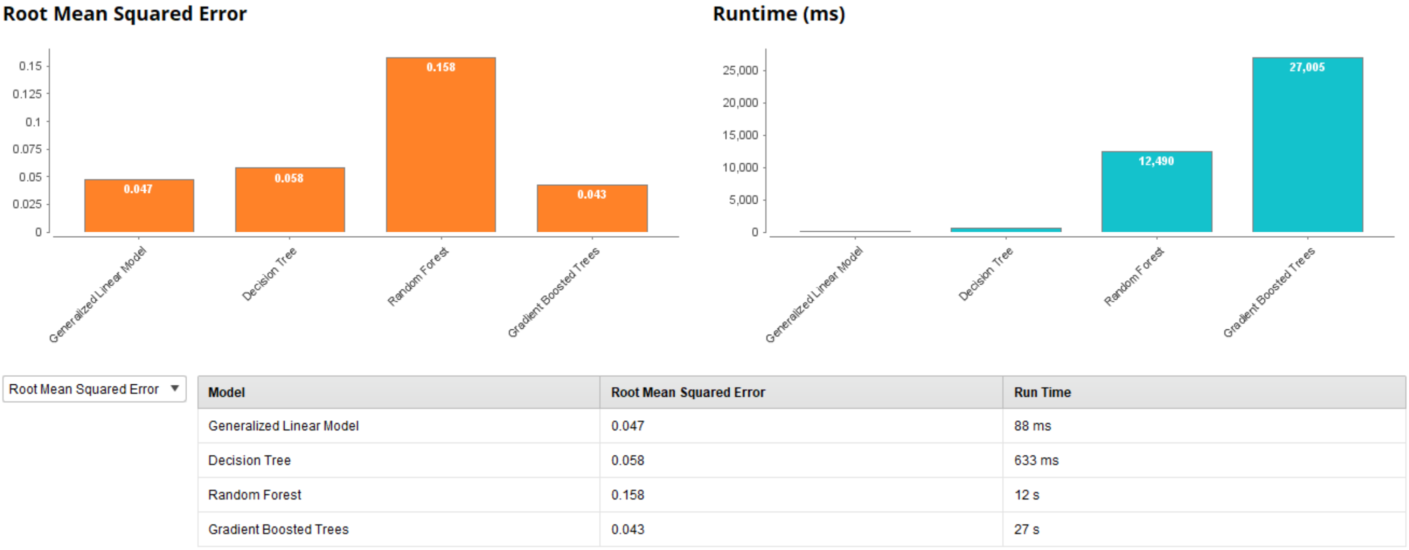
Target attribute Sugar/PH ratio

This ratio was picked not without discussion and further research. It is proven that this ratio should be the lowest to make sure that wine will be tasty.

Are we able to prove it with our sample of wines?

Methodology used as in previous example: training 70%, test 30% and we have deleted PH attribute.

Training:

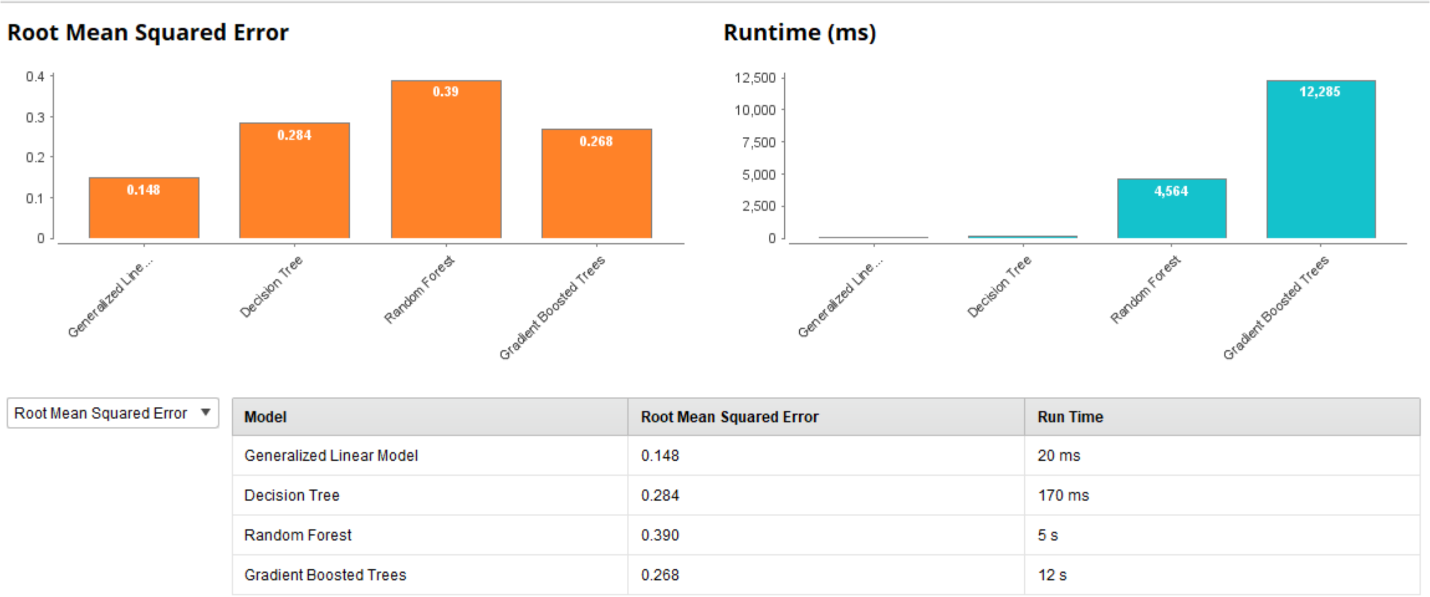


Model	Root Mean Squared Error	Run Time
Generalized Linear Model	0.047	88 ms
Decision Tree	0.058	633 ms
Random Forest	0.158	12 s
Gradient Boosted Trees	0.043	27 s

Figure 1.25. Summary of model outputs with given attribute – root mean squared error

Cross -validation:

Test:



Root Mean Squared Error ▼

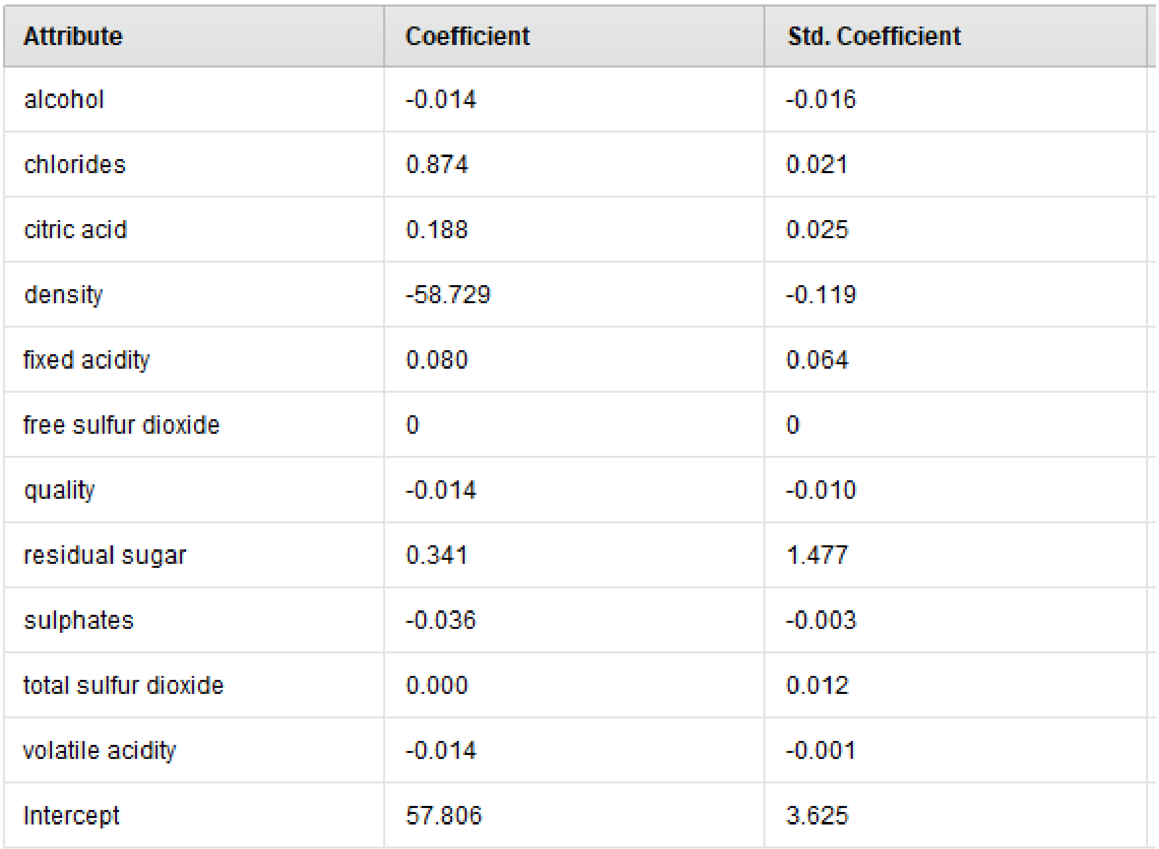
Model	Root Mean Squared Error	Run Time
Generalized Linear Model	0.148	20 ms
Decision Tree	0.284	170 ms
Random Forest	0.390	5 s
Gradient Boosted Trees	0.268	12 s

Figure 1.26. Summary of model outputs with deleted attribute – Ph

In this case the best was simple Generalised Linear Model with the smallest error.

Error in both training 0.043 and test 0.268 is quite small. We can assume that model is quite good.

Output below:



Attribute	Coefficient	Std. Coefficient
alcohol	-0.014	-0.016
chlorides	0.874	0.021
citric acid	0.188	0.025
density	-58.729	-0.119
fixed acidity	0.080	0.064
free sulfur dioxide	0	0
quality	-0.014	-0.010
residual sugar	0.341	1.477
sulphates	-0.036	-0.003
total sulfur dioxide	0.000	0.012
volatile acidity	-0.014	-0.001
Intercept	57.806	3.625

That's is very interesting finding. We can see here that even without given PH of wine we are able to predict sugar/Ph ratio in almost 90% accuracy.

The biggest impact on that ratio will have density -58.72. But few others are also very important like chlorides or residual sugar.

Target attributes - level of alcohol

That is a very interesting one. Are we able to predict level of alcohol without given alcohol content?

Level of alcohol was set up under rule:

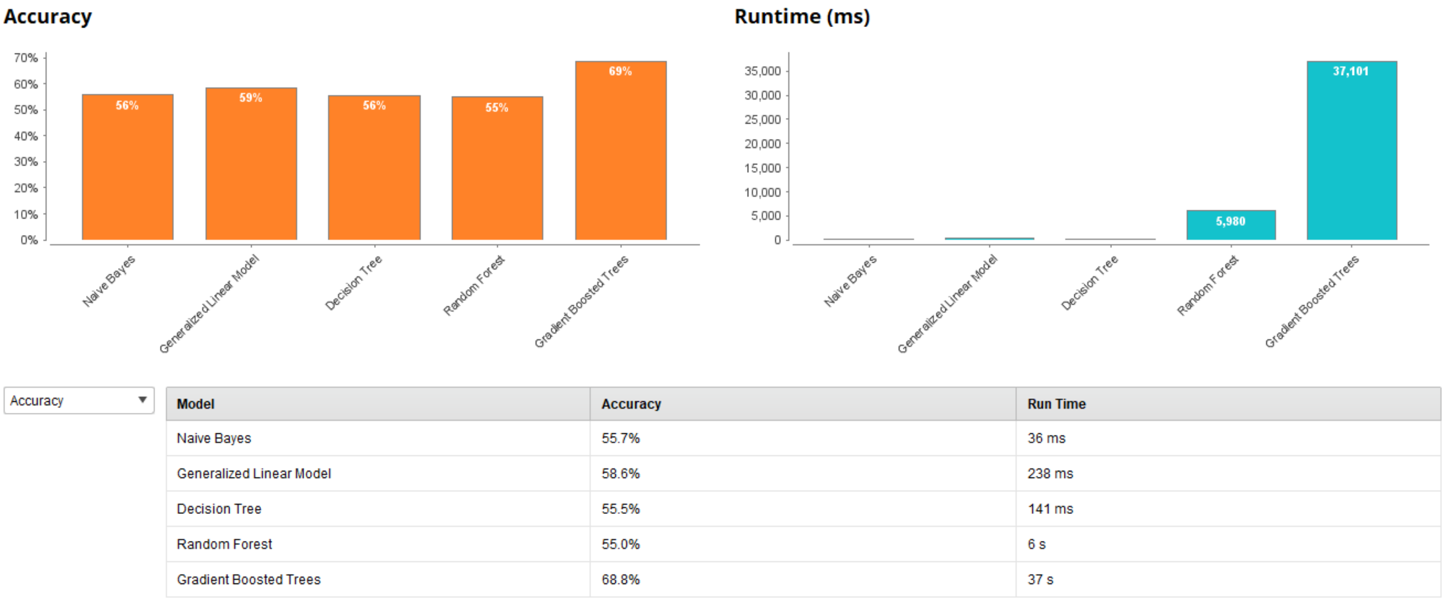
=IF(K2<=9,"Low",IF(K2<=11,"Medium","High"))

There are 3 types of output Low, Medium and High (Ordinal Polynomial attributes).

Methodology used as in previous example: training 70%, test 30% and we have deleted alcohol content attribute.

Training:

Summary of model outputs with given attribute.

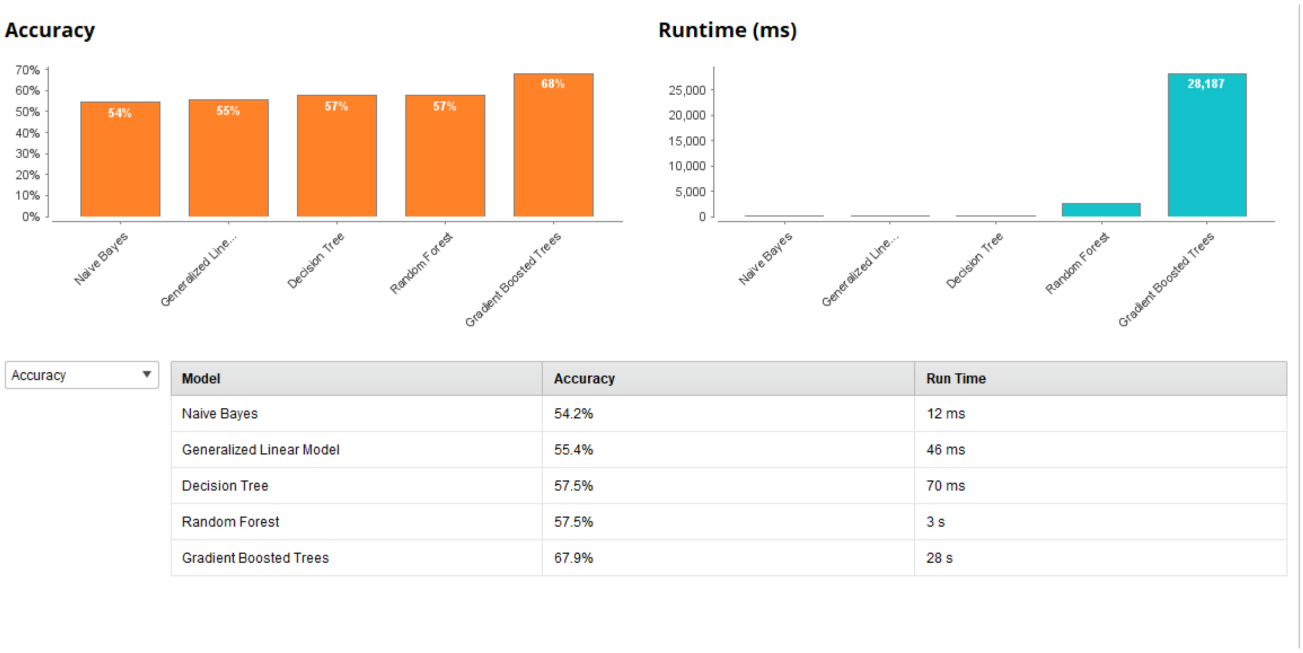


Model	Accuracy	Run Time
Naive Bayes	55.7%	36 ms
Generalized Linear Model	58.6%	238 ms
Decision Tree	55.5%	141 ms
Random Forest	55.0%	6 s
Gradient Boosted Trees	68.8%	37 s

Figure 1.27. Summary of model outputs with deleted attribute – alcohol content

Test:

Cross-validation:



Model	Accuracy	Run Time
Naive Bayes	54.2%	12 ms
Generalized Linear Model	55.4%	46 ms
Decision Tree	57.5%	70 ms
Random Forest	57.5%	3 s
Gradient Boosted Trees	67.9%	28 s

Figure 1.28. Summary of model outputs with deleted attribute – alcohol content

Only Gradient Boosted Trees could give us 68% of accuracy in both training and test set. The conclusion is that even without knowing the alcohol content we still can predict alcohol level in wines when other attributes are known in 68%.

Target variable – Balanced wine

The aim was to classify wines under label balanced and unbalanced. So that is binominal attribute.

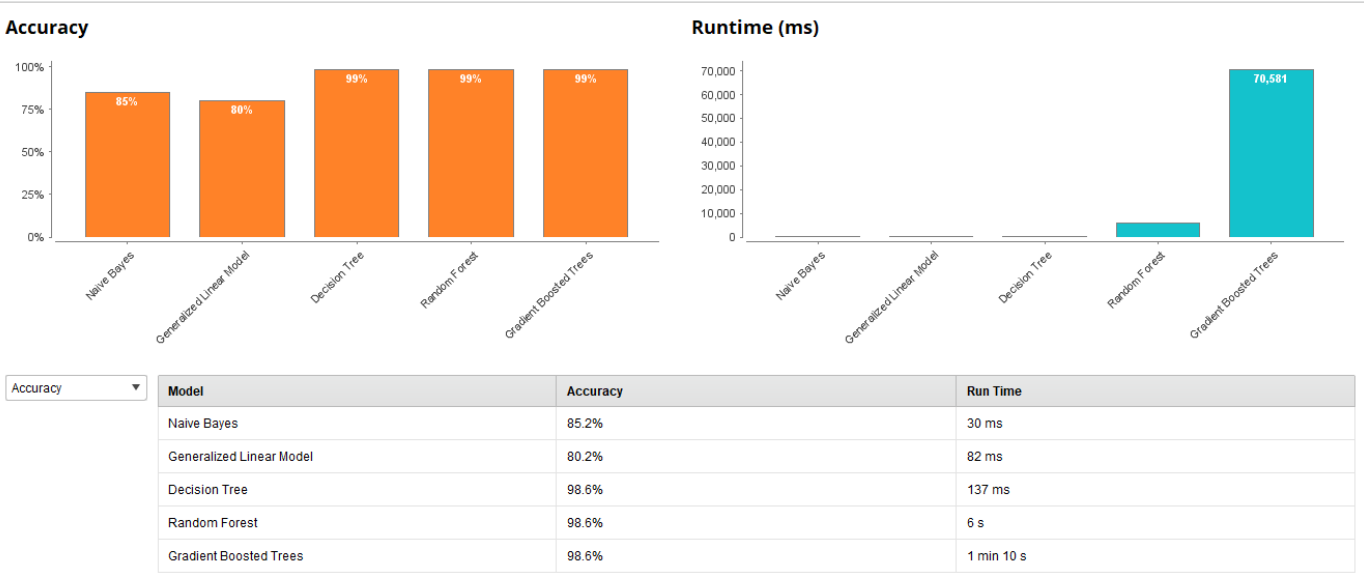
Classification rule:

If total sulfur dioxide <=200, and sugar/ph ratio<=3, and level of alcohol = medium

The unknown here is free and total sulfur dioxide.

Is machine able to correctly classify wines with given attributes but unknown total sulfur dioxide?

Methodology used as in previous example: training 70%, test 30%.



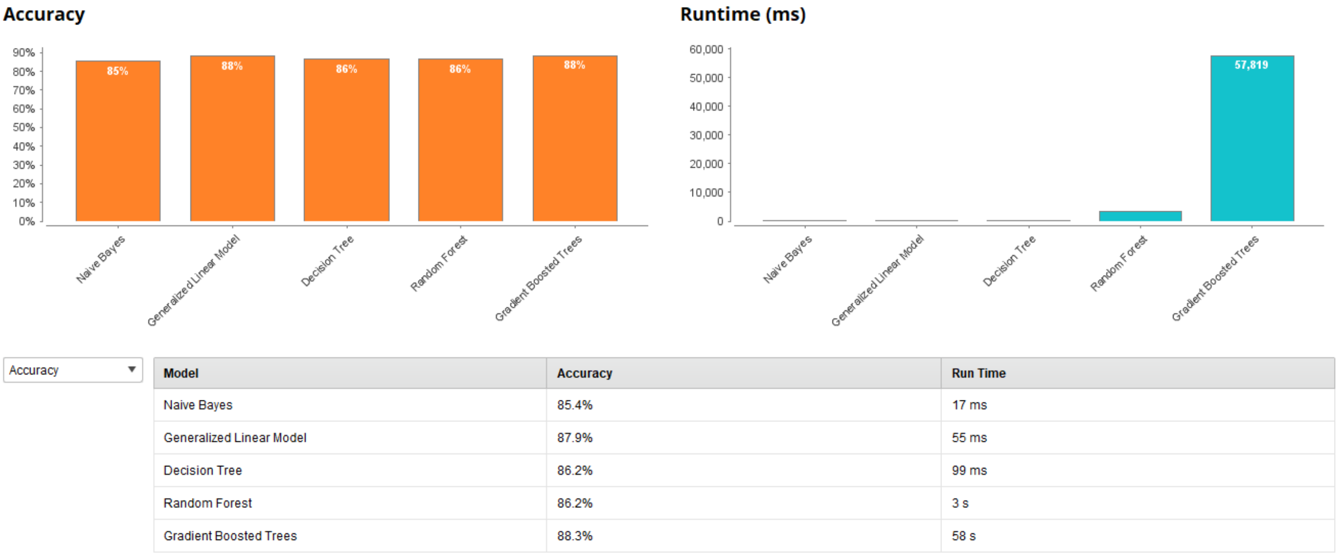
Model	Accuracy	Run Time
Naive Bayes	85.2%	30 ms
Generalized Linear Model	80.2%	82 ms
Decision Tree	98.6%	137 ms
Random Forest	98.6%	6 s
Gradient Boosted Trees	98.6%	1 min 10 s

Training:

Figure 1.29. Rapidminer – accuracy of training model – balanced wine

Test

Cross – validation:



Model	Accuracy	Run Time
Naive Bayes	85.4%	17 ms
Generalized Linear Model	87.9%	55 ms
Decision Tree	86.2%	99 ms
Random Forest	86.2%	3 s
Gradient Boosted Trees	88.3%	58 s

Figure 1.30. Rapidminer – Accuracy of test – balances wine

The highest accuracy of models we can see in Gradient Boosted Tree and Generalised Linear model in test set– 88% and 98% in training set. It is quite good classification model.

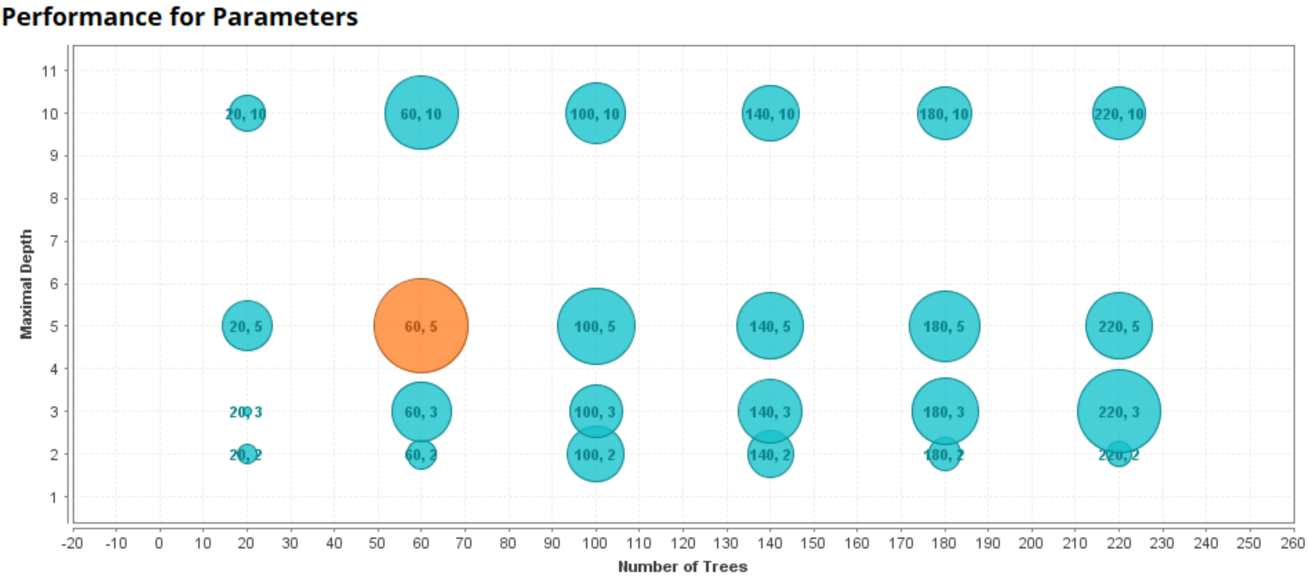
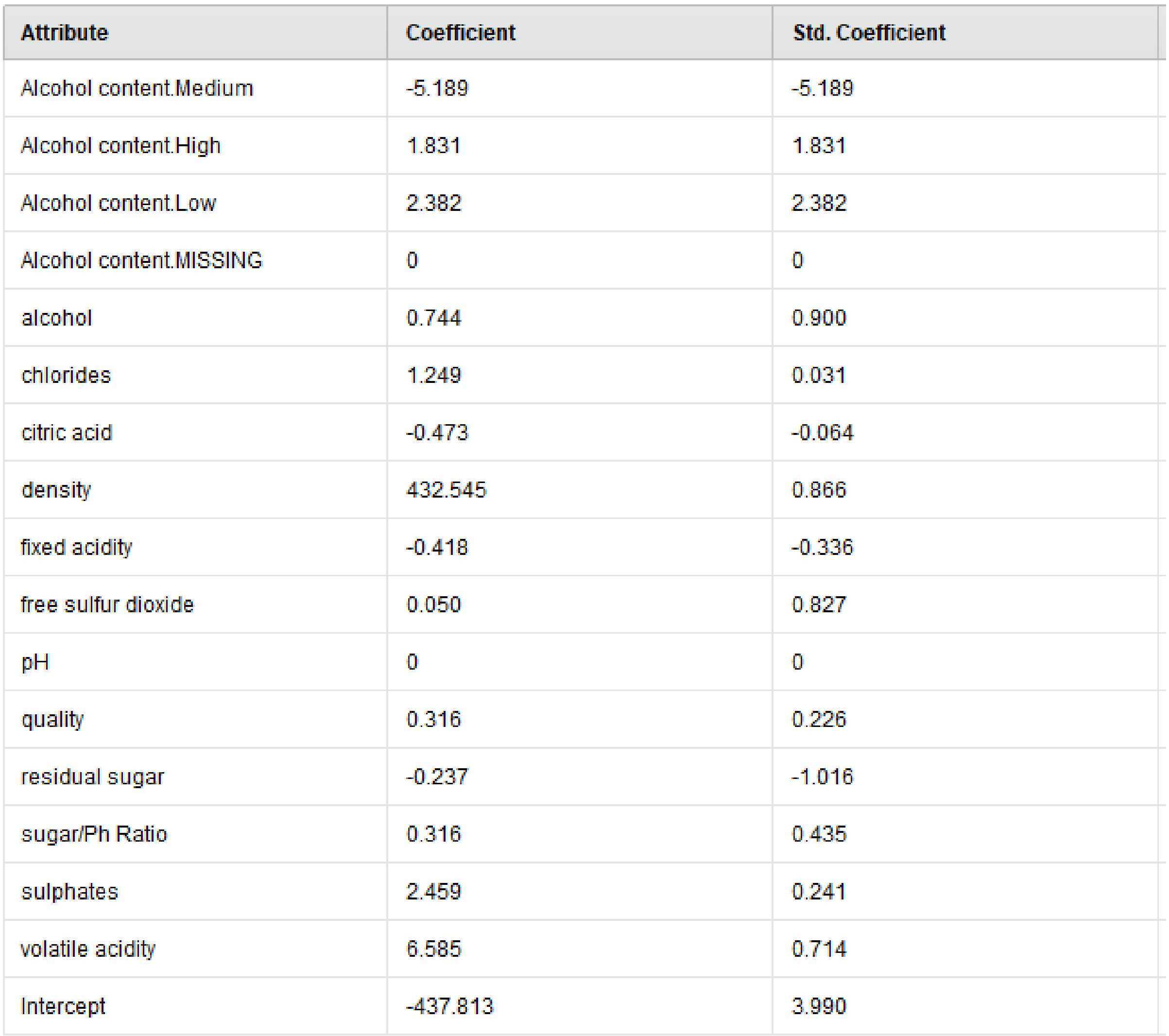


Figure 1.31. Rapidminer – GBT – balanced wine – performance for parameters

Model also shows us that the best result was achieved with 60 trees and 5 level of depth (Fig. 1.31).

Generalised linear model:



Attribute	Coefficient	Std. Coefficient
Alcohol content.Medium	-5.189	-5.189
Alcohol content.High	1.831	1.831
Alcohol content.Low	2.382	2.382
Alcohol content.MISSING	0	0
alcohol	0.744	0.900
chlorides	1.249	0.031
citric acid	-0.473	-0.064
density	432.545	0.866
fixed acidity	-0.418	-0.336
free sulfur dioxide	0.050	0.827
pH	0	0
quality	0.316	0.226
residual sugar	-0.237	-1.016
sugar/Ph Ratio	0.316	0.435
sulphates	2.459	0.241
volatile acidity	6.585	0.714
Intercept	-437.813	3.990

Figure 1.32. Rapidminer - Generalised Linear model outcome – balanced wine

Results of Generalised Linear models are much clearer for us to understand but it’s not mean it is better even if accuracy is high. We can see many drawbacks of this technique.

As it can see data only in linear position, it can classify wines even with dummy variables.

But overall information which we can take from this model that:

Even without known free and total sulfur dioxide we can classify wines with 88% accuracy. Very important attributes which affects balance of wine will be density, volatile acidity and sulphates.

Some visualisation of findings:

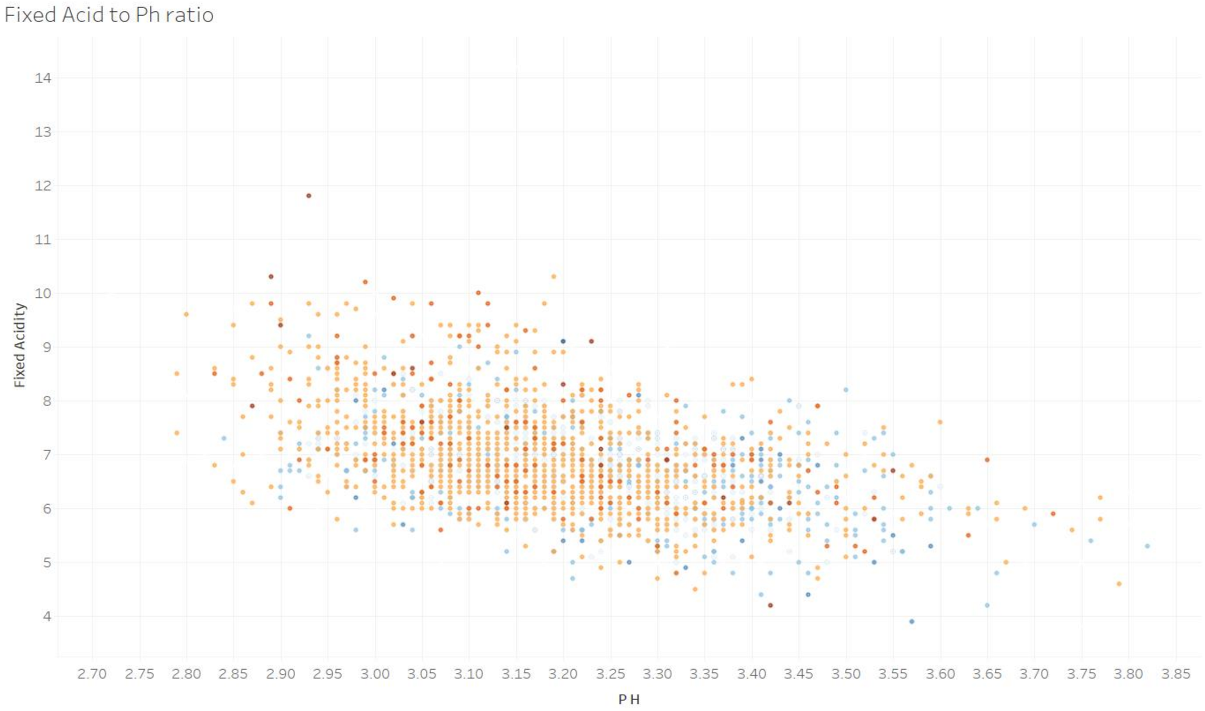


Figure 1.33. Tabelau – Ph to Fixed Acid scatter plot (high blue – low orange quality of wine)

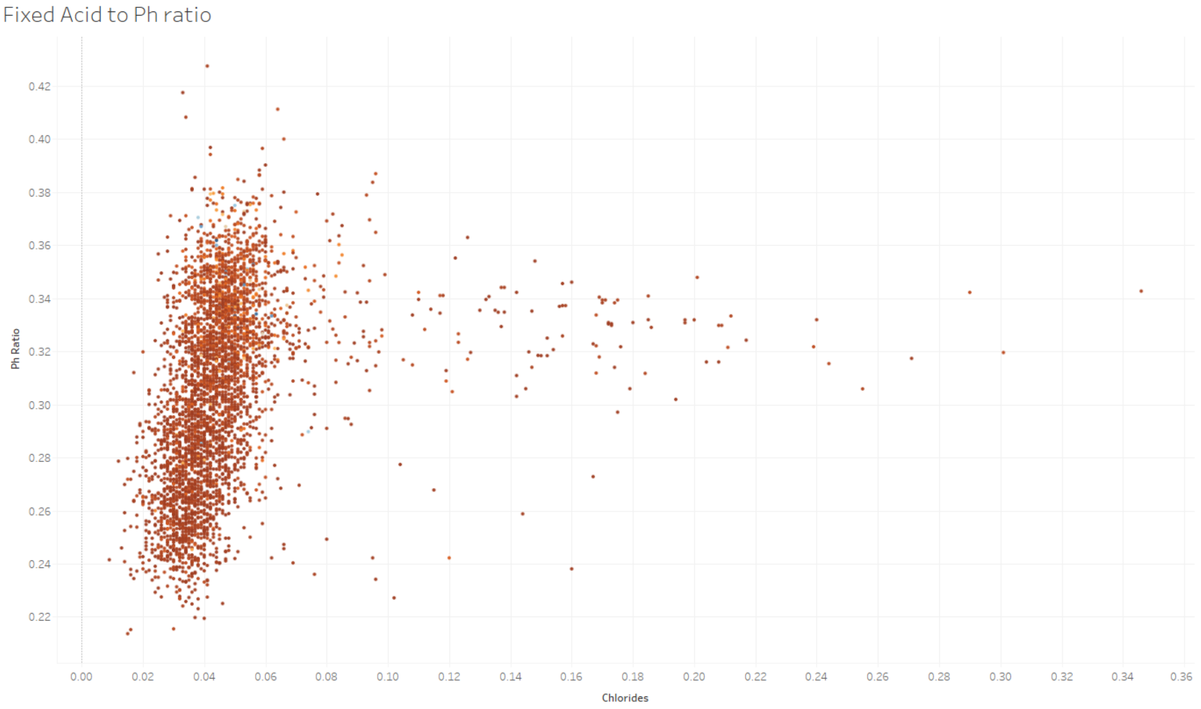


Figure 1.34. Tableau – Ph ratio to chlorides scatter plot

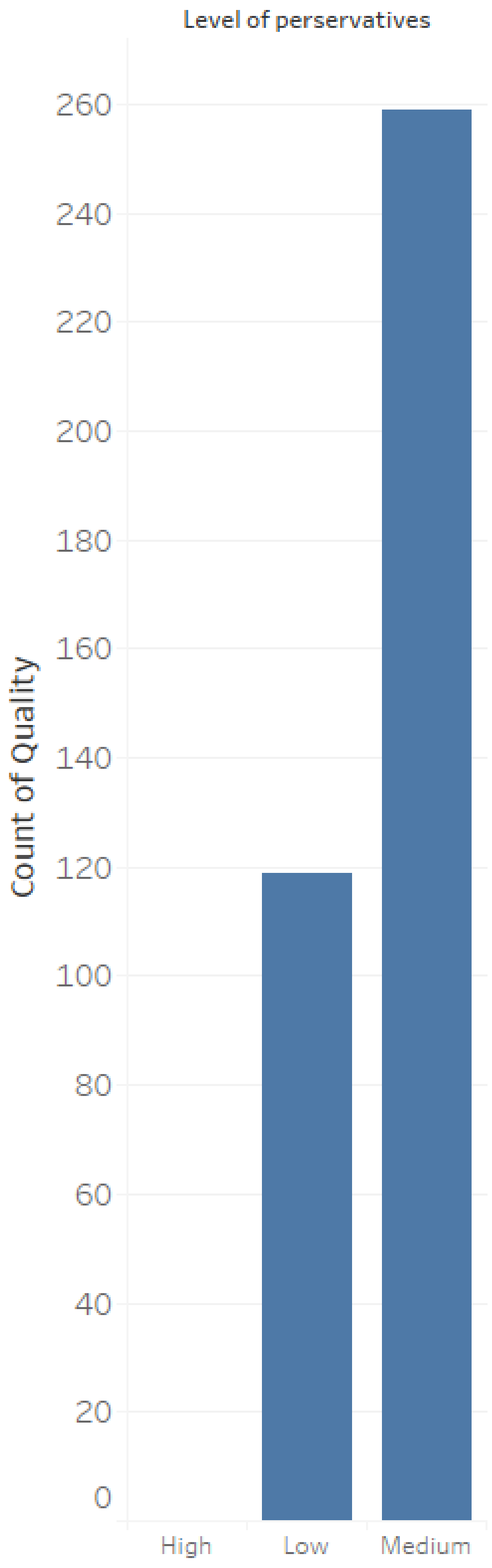


Figure 1.35. Tableau – Bar graph showing number of highest scored wines grouped by level of preservatives (7-9).

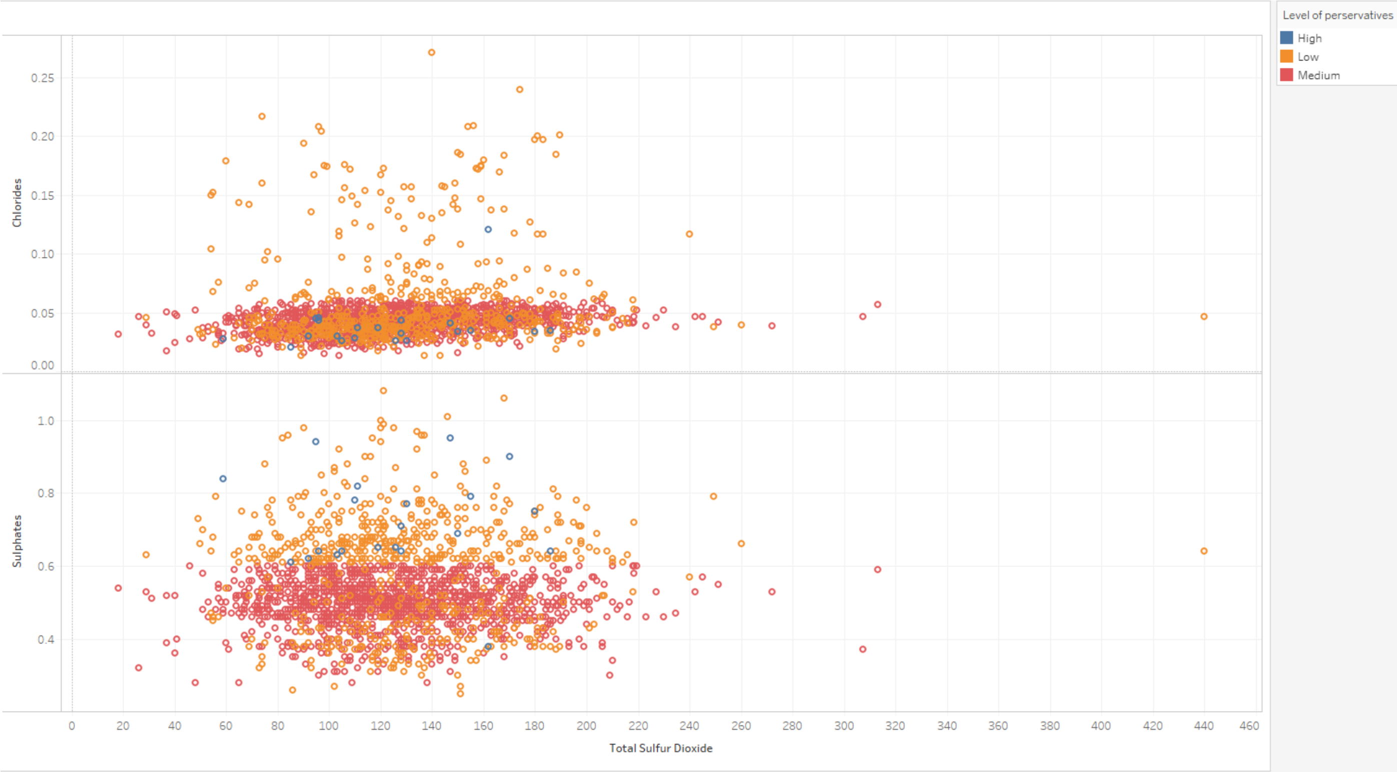


Figure 1.36. Tableau – scatter plot showing number of wines grouped by preservatives and colour determining level of preservatives (red – Medium, Orange – Low, Blue – High).

Conclusions

We can see from the work above that all the ingredients in wine are connected. All of them impact each other.

Although it is still hard to predict the taste of wine and quality. We have to remember that attribute quality it is a subjective attribute. Others in our dataset are purely scientific.

The Clustering analysis showed us that we can deal with 4 groups of clusters, showed us dependencies and correlations for example between Total sulfur dioxide and free sulfur dioxide, Fixed acid and PH, Residual sugar and density.

Target attributes analysis of targets such us level of alcohol, sugar/Ph ratio, level of preservatives and Key Performance Indicator – Balanced wine prove that other ingredients of wine influence the important attribute and they cannot be tested in isolation.

By eliminating some attributes, we just made our model weaker. They are all necessary.

In two cases Gradient Boosted Trees (GBTs) were the best choice and gave us the best accuracy, and in 2 cases simple generalised linear model gave us the best accuracy.
It is not a surprising that GBT is better than Random forest. As in Random forest the trees are built randomly and in GBT the trees are build one by one when next one fixes problems of previous one. But unfortunately, GBT is time consuming for training and expensive technique.
About Generalised Linear models we would have more concerns.
It is built based on linear regression. It is very sensitive to outliers; the outliers can change the model a lot. Accuracy was good in our predictions but still if we will choose something outside of range that prediction could be not accurate. We are also not sure that we have linear correlations between these attributes. What if the relationships have different shape? Giving these weaknesses we would be sceptical choosing this model without more tests.

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