

Intelligent Data Analysis - Homework 1.2

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1 Basic exploration of a dataset

1.1 Introduction

We have chosen the wines dataset, this dataset has 11 variables based on physicochemical tests on different wines plus a categorical variable grading the wine quality by experts between 0 (very bad) and 10 (very excellent) and a binary variable, type: (1 = white wine and 2 = red wine). In order to understand better the dataset, we have research information about the different variables:

- Fixed acidity: a non-volatile acid (also known as a fixed acid or metabolic acid) is an acid produced from sources other than carbon dioxide. They are produced from e.g. an incomplete metabolism of carbohydrates, fats, and proteins.
- Volatile acidity: In the context of wine making, volatile acidity is a form of wine spoilage that is by-product of microbial metabolism that can occur during the wine making process with the introduction of harmful bacteria. Dimensionality not appreciated
- Citric acid has many uses in wine production. Citric acid is a weak organic acid, which is often used as a natural preservative or additive to food or drink to add a sour taste to food. It can also be used to neutralize surfaces that have been treated with basic substances. Dimensionality not appreciated
- Residual sugar, percentage of sugar not fermented (sugar fermented= alcohol)
- Chloride: Cl-, don't know too much but high concentrations makes the wine salty (pH >7)
- Free sulphur dioxide: Sulphur dioxide (SO₂) is used as a preservative and stabilizer in wine production to prevent undesired biochemical processes in the must and the final product. The concentration of SO₂ is restricted by national regulations. There are two main forms of SO₂ in wine-free (inorganic forms) and bound (fixed to organic compounds, e.g. aldehydes)

- Total sulphur dioxide
- Density: mass/volume
- pH(acid, salinity meter)
- Sulphates: turns into sulphur dioxide (S-)
- Alcohol percentage
- Quality: rated from 0 to 10
- Type (1= white wine or 2)

1.2 Descriptive statistics

1.2.1 Questions

- a) **Choose a quantitative variable and explore its distribution in terms of descriptive measures of center, dispersion, skewness and kurtosis. Is a normal model a plausible one for its distribution? If the answer is no, can you think of a transformation of the variable that improves normality. Are there any outliers?**

We have choose to explore the quantitative variable “Total Sulfur Dioxide”, and we have calculated the statistics related with center, dispersion, skewness and kurtosis.

The skewness is 0.2167518. This value implies that the distribution of the data is slightly skewed to the right or positive skewed. It is skewed to the right because the computed value is positive, and is slightly, because the value is close to zero. For the kurtosis, we have 2.073274 implying that the distribution of the data is platykurtic, since the computed value is less than 3. By checking the histogram of the variable, its easy to check that it seems to not follow a normal distribution because it shows two different peaks:

We also have tested normality with the Anscombe-Glynn Kurtosis-based test and D’Agostino skewness-based test. The kurtosis test rejects normality in part because of the two-peaks that we can see in the distribution, on the other hand, the skewness is closer to a normal distribution. Finally the jarque bera test has a p-value greater than 0.05 but still small (0.11). In order to improve the normality of the data, we have chosen to apply the the Box-Cox transformation:

After applying the transformation and reapplying the test, we can see that there is not significance improvement regarding normality. It could be because this variable is explained by others variables in the dataset. Finally, by using a boxplot graph, we have checked that there are not outliers in the data:

b) Choose two quantitative variables and describe its joint bivariate distribution. Does it seem to be Normal? Are there any outliers?

For this part, we have chosen the variables “Volatile acidity” and “Residual sugar”. As a first step we have tested if any of the variables by their own follow a normal distribution, after that we have applied the Shapiro Wilk test for bivariate data. We have seen that the data does not follow a normal distribution:

Then we have applied the box-cox transformation to the bivariate data (check shiny app), we can see that neither the transformation follows a normal distribution by following the fact that the mahalanobis distance of a bivariate normal distribution follows a Chi-Square distribution (mardia test):

In the qqplot for the original data we can appreciate that the distribution of the distance seems to be bimodal and right-light tailed compared with the chi-squared distribution. On the other hand, the transformed data seems to have heavier right tails.

Finally, we check for outliers by using also the mahalanobis distance and taking all and comparing the values that take the chi squared distribution with 2 degrees of freedom and 95% quantile.

We can see that it seems to be 8 outliers, with two pairs of two observations with the same Mahalanobis distance (and the same values), that is why in the scatterplot we can only see six red dots:

c) Choose a subset of 4 or 5 quantitative variables and explore linear relationships

We have chosen 5 quantitative variables which are *Residual sugar*, *Chlorides*, *Sulphites*, *pH* and *Alcohol percentage*.

2 Permutation tests

2.1 Choose a subset of 4 or 5 quantitative variables and explore linear relationships

a) R matrix of pairwise correlations

The following is the matrix of partial correlations:

Is it possible to appreciate:

- Moderate direct relation between Chlorides and Sulfites which makes sense as are used together for taste stabilizers.
- Negligible inverse relation between Residual sugar and pH levels, which tells us that the more sugar molecules rest in the wine, the pH will descent making the wine more acid. (The same happens in our mouth when we eat candies)
- Negligible direct relation between Alcohol percentage and pH, which can be explain with the logic of the point above, in the other words, more alcohol, less sugar so pH increases (less acidity).
- Negligible inver relation between chlorides and alcohol, as acyl chlorides consumes alcohols to produce esters.

b) Matrix of partial correlations

Partial conrrelation between 2 given variables, removes the external influences of the rest of the variables, by comparing this matrix with the R matrix we can reveal hidden relations between 2 variables alone , e.g. in our example we can see that the relations commented before are only enhanced so there are not hidden relations revealed. The Pearson coefficient between chlorides and alcohol percentage is still on the same value. The relationship between Chlorides and Sulfites has decreased, but Alcohol and Residual Sugar is enhanced which makes the most sense as the the fermentation of sugar molecules creates ethanol molecules that increase the Alcohol percentage.

c) Coefficient of determination (function `r2multv()` we define in R)

Chlorides (chlor) is the best linearly explained by the others ($R^2 = 0.372$), followed by Sulphates (S, $R^2 = 0.308$). The worst linearly explained by the others is pH (pH, $R^2 = 0.129$).

d) The determinant of R (correlation matrix) as an overall measure of linear relationships.

The determinant of R is:

A non-zero $|R|$ indicates that there are not strong correlations among the variables and so there are no possible linear combinations.

e) An eigenanalysis of matrix R , looking for really small eigenvalues.

Looking at the eigenvalues we observe that Sulfites, pH and Alcohol percentage have eigenvalues closer to zero.

Lets analyze their eigenvectors:

- [3] For Sulfites, assuming all values are close to 0 except the third -0,968 we can conclude that this variable has very small variance, it is almost constant through the observed data.
- [4] For pH, assuming all values are close to 0 except the forth -0,978 we can conclude that this variable has very small variance, it is almost constant through the observed data.
- [5] For Alcohol %, assuming all values are close to 0 except the second -0,989 we can conclude that this variable has very small variance, it is almost constant through the observed data.

2.2 Repeat the analysis deleting the values for three customers that left a tip greater than 30% of the bill. These generous customers seem to be outliers.