Assignment 1

Introduction

Portugal has been long celebrated for its wine production, from port wine to *vino verde* from the Minho province. To address growing demand, the wine industry is interested in optimising its wine production. As wine is a food product, most of its prized features are taste and aroma, which are subjective measurements. Previous studies have tried to categorise wine by quality through combining human taste testers, physico-chemical analysis and statistical methods in attempts to introduce objectivity[1]. In this project, we are most concerned with which **particular variables** are essential for considering wine quality. By knowing which variables should be prioritised, this can motivate further study on optimising the wine according to essential attributes and enforce more efficient production.

Therefore, this report aims to address the following questions:

1. Which variables play a significant role in ascertaining the quality of red and white wine?
2. Are there any trends between wine attributes and its perceived quality?
3. Are there any differences between mean acidity values of wine?
4. Are there any differences between mean sulfate/sulfur dioxide values of wine?

The dataset employed in this study comprises data sourced from laboratory tests, providing an intricate look into the chemical composition of wines from Portugal's Minho region. It encompasses a comprehensive range of variables, including fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH levels, sulphates, alcohol content, and a subjective quality rating on a scale of 0 to 10, where 10 represents the highest quality. Additionally, a color indicator, as a dummy variable, distinguishes between red and white wines. - Data checked for outliers - Total size is 6497 - To account for outliers but also not to lose too much data, 5% was chosen (325) entries as max threshold to lose - Applied a IQR check. Normally, data less than Q1 - IQR*1.5 or more than Q3 + 1.5* IQR is common procedure as it does not assume normality - However, this lead to a large amount fo data being lost, so stricter threshold of 2.5 was chosen instead.

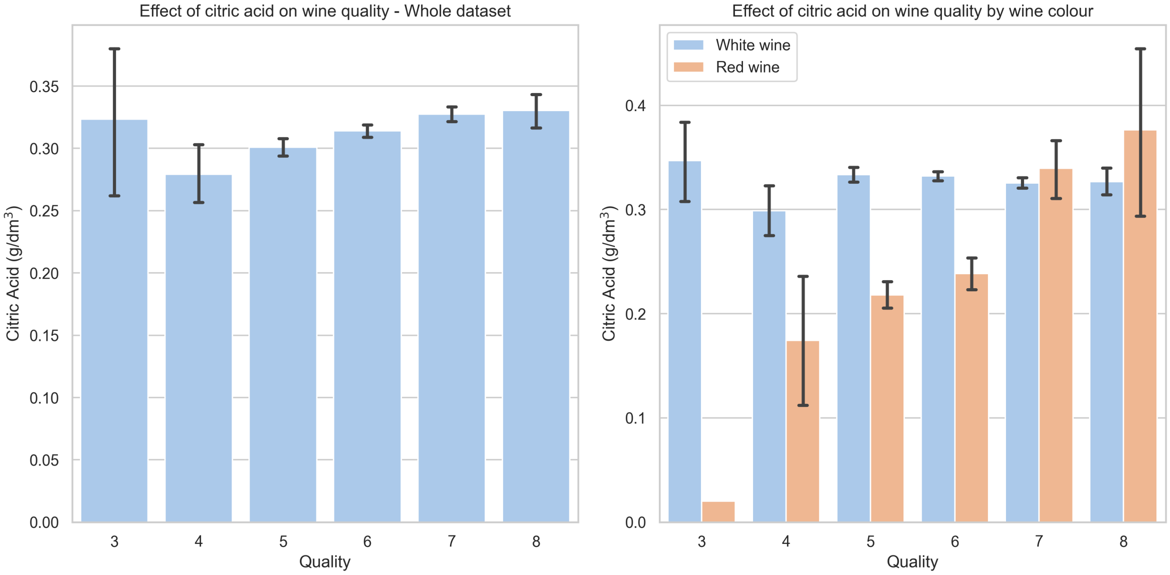
EDA - How does citric acid play a role in quality of wines?

- Citric acid plays a vital role in wine production
- It helps add freshness to the wine, allowing more lively and enjoyable tasting experience, but too much makes it harsh, difficult to drink[2]
- Therefore, we are interested in any trends between citric acid concentration and perceived wine quality

[1] Cortez et al. [1]

[2] **RN3**

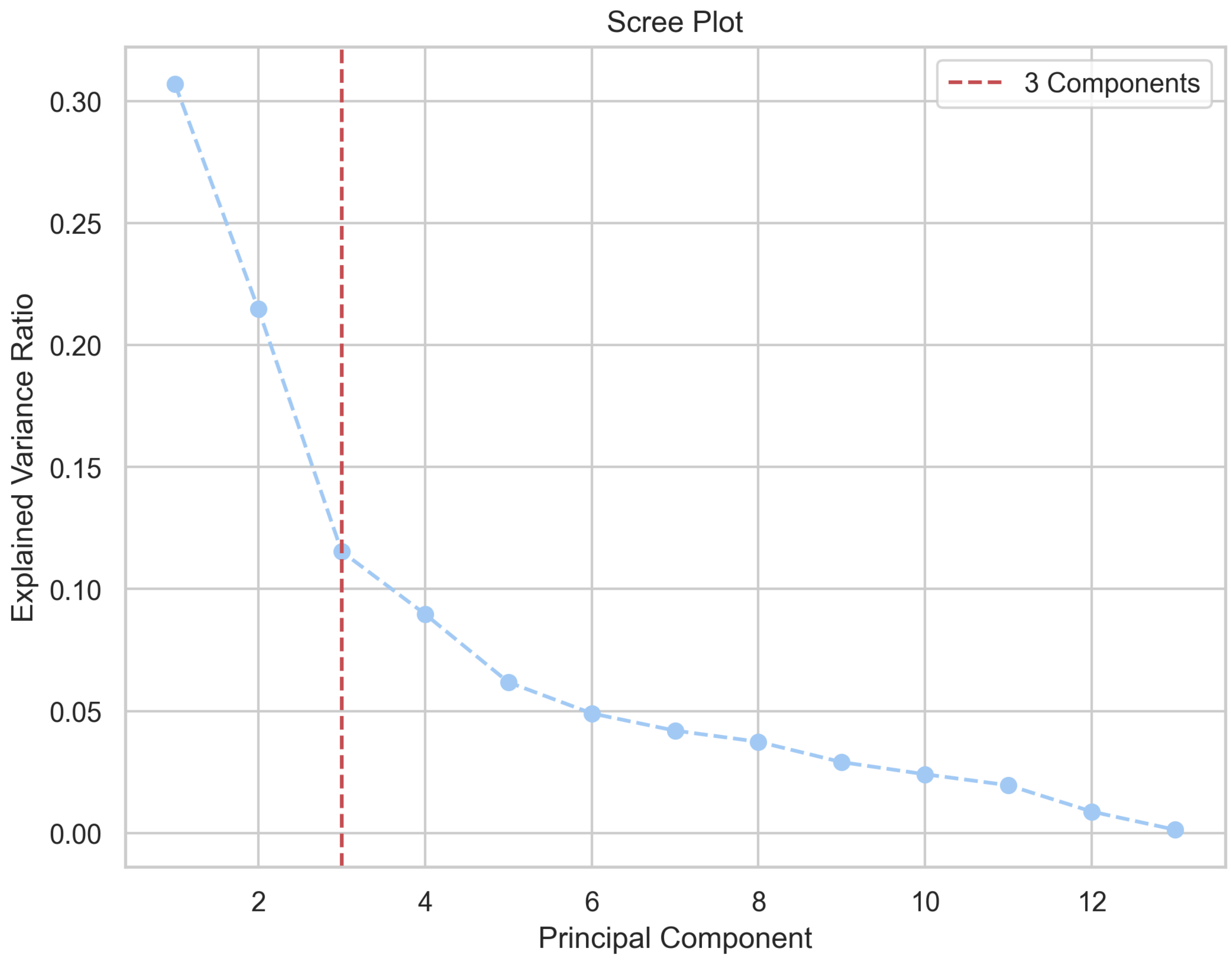
- Question: Specific to wines of the minho region, what ranges of concentrations is related to wine quality?



- Across dataset:
  - High citric acid for low quality (but not certain due to low numbers in category 3 and large error bar)
  - Steady increase from quality 4 to 8, but plateaus around 0.33 g/dm^3
  - Wines that are "high quality" tend to have citric acid concentrations between 0.30 g/dm^3 and 0.35 g/dm^3
- Between wine groups:
  - In general, citric acid concentration over higher quality white wine seems to be fairly consistent, around 0.30 g/dm^3 and 0.35 g/dm^3
  - Red wine much more drastic. Even after accounting for large error bars from smaller datapoints for red wine, there is a clear increase between higher quality wines have more citric acid
- Conclusion: It seems that higher quality red wines have more citric acid in them, but it is unclear whether red wine quality of 9 or higher will have more citric acid due to the large error bars. What is apparent is higher quality wines in general tend to have citric acid concentrations between 0.30 to 0.35 g/dm^3. This disparity could be explained by how white wines tend to have more residual sugar than red wines, where adding some freshness is more necessary to balance out the additional sweetness.[3]

[3] Cortez et al. [1]

PCA - Chemical differences between red and white wines



Looking at the scree plot, the elbow appears around n = 3 components, so we will use this when proceeding with our PCA model. When considering the key chemical differences between red and white wines, we need to identify which features produce large loadings for our model. These features will help maximumise the langrange multiplier, producing the largest variance which is essential in differentiating the chemical differences between red and white wines. !(biplots_combined)[biplots_combined.png] From the principal component plots, the key insights from the loadings we can observe are: - PC1: Chlorides - Moderate and positive, Volatile acidity - Large and positive, Colour - large and positive, Sulphates - moderate and positive, pH - moderate and positive, total sulfur dioxide - moderate and negative - PC2: Density - Large and positive, Alcohol - large and negative, Free sulfur dioxide - moderate and positive, Residual sugar - large and positive - PC3: Fixed acidity - large and positive, Citric acid - large and positive, colour - close to zero, pH - large and negative

Insights:

1. Colour is coded as 1 with red wine. Since colour is large and positive, red wines will score more highly for PC1. Therefore, we can determine that red wines are associated with higher volatile acidity, sulphates, pH and total sulfur dioxide. We can confirm this by looking through the dataset:

- Chlorides: Most of red wines (min: 0.012, Q1: 0.069, median: 0.078, Q3: 0.087, max: 0.132) g(sodium chloride)/dm^3 have higher chloride values than white wine (min: 0.009, Q1: 0.036, median: 0.043, Q3: 0.050, max: 0.132) g(sodium chloride)/dm^3

- Volatile acidity: Most of red wines (min: 0.12, Q1: 0.395, median: 0.52, Q3: 0.62, max: 0.825) g(acetic acid)/dm^3 have higher volatile acidity values than white wine (min: 0.08, Q1: 0.210, median: 0.26, Q3: 0.32, max: 0.815) g(acetic acid)/dm^3
- Sulphates: Most of red wines (min: 0.37, Q1: 0.55, median: 0.61, Q3: 0.71, max: 1.02) g(potassium sulphate)/dm^3 have higher sulphate values than white wine (min: 0.22, Q1: 0.41, median: 0.47, Q3: 0.55, max: 1.01) g(potassium sulphate)/dm^3
- pH: Most of the red wines (min: 2.88, Q1: 3.24, median: 3.33, Q3: 3.41, max: 3.78) have higher pH values than white wine (but marginally) (min: 2.72, Q1: 3.09, median: 3.18, Q3: 3.28, max: 3.82)
- Total sulfur dioxide: Most the red wines (min: 6.0, Q1: 23.0, median: 38.0, Q3: 63.0, max: 289.0) have much lower total sulfur dioxide values than white wines (min: 9.0, Q1: 108.0, median: 134.0, Q3: 167.0, max: 344.0)

2. Wine is produced by fermenting sugar and residual sugar decreases with more fermentation. Furthermore, adding sugar or salt to a liquid makes it denser. As the alcohol value is large and negative, this means wines with less alcohol will have higher PC2 scores. Therefore, this component is associated with the age of the wine. While this component is not used for chemical differences between red and white wines, this will be useful later when considering the quality of the wines.

3. Colour does not affect the PC3 score as it is close to zero. Furthermore, the group does not appear to be associated with a particular red/white wine group. Wines with higher citric acid have higher PC3 scores (tends to be white wine, (min: 0.0, Q1: 0.27, median: 0.315, Q3: 0.38, max: 0.74) g/dm^3 compared to red wine (min: 0.0, Q1: 0.09, median: 0.24, Q3: 0.38, max: 0.73) g/dm^3). In contrast, wines with high fixed acidity (tends to be red wine) and low pH also score highly (Mostly white wine). However, this group could be associated with grape harvest time, as studies have suggested a relationship between early/late harvest of grapes and grape acidity from citric acid and tartaric acid. More research would be needed to confirm this.[4]

Conclusion: The main chemical differences between red and whites are that red wines will have higher chloride, volatile acidity, sulphates, pH than white wines, but lower total sulfur dioxide and citric acid concentrations.

PCA - Attributes present in wines of high quality

To help with visu

1. Plots of principle components
2. Comment on the main chemical differences between red and white wines
3. Including quality variable what features are likely to be present in wines of good quality? Is it different for red and white?

Your research question show address the following: "What features are most influential on a particular type of wine of high quality?" You should also consider the main chemical differences between red and white wines (Use the PCA components for this)

One page - Hotelling T square test

1. Perform a Hotelling's T^2 -test to test the hypothesis that the red and while wines have the same acidity means (the variables fixed acidity, volatile acidity and pH)
2. Select some variables and compute μ_W of selected variables for white wine
3. Perform 1-sample T^2 test to check whether corresponding means for red wine dataset are equal to μ_W

[4] **RN4**

Approaching the Hotelling T square test

1. Give a sentence or two for motivation of test
2. Give a little math background
3. State the hypothesis clearly
4. Perform test
5. State the result with a confidence interval if applicable

Your report should have: 1. A question stated clearly 2. Explaining the statistical test used to address question 3. Give solution 4. Potentially visualisation

Other notes: 1. You must give references 2. Try to keep it to 4 pages

Things to keep in mind

- Citric acid and residual sugar levels are more important in white wine, where the equilibrium between the freshness and sweet taste is more appreciated
- volatile acidity has a negative impact on wine taste, as it introduces bitterness (cite this)
- Sulphastes might link to wine aroma
- Additional research into impact of what affects wine tastes could prove useful.

Sulphates formed from fermentation. More fermentation => more age => more quality?

References

[1] P. Cortez et al. "Modeling wine preferences by data mining from physicochemical properties". In: *Decis. Support Syst.* 47 (2009), pp. 547–553.