Project: Wine Quality

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Introduction

Wine testing is important to both sellers and consumers. By testing wine samples, vineyards are able to ensure that their wines are safe for consumers, and that the taste of each type of wine stays consistent. It is even used to help set pricing scales. This project will be comparing different physiochemical (chemical properties) and sensory elements of wine in order to see what elements impact quality.

The chemical composition of wine can impact both the quality of the wine and our bodies. This study will be looking at 11 different physiochemical properties: fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol content. We will specifically look to see if there is an interaction between volatile acidity and citric acidity. Volatile acidity is how wine spoilage is measured (Neeley, 2004). Typically, wine makers attempt to keep volatile acidity to a minimum to improve the quality of wine (MoreFlavor, n.d.). Citric acid keeps wine tasting fresh, while imparting a slight citric taste to the wine (University of California Davis, n.d.).

Hypotheses

This project answers the following research questions:

- Are variances of quality of red wines equal to variances of quality of white wines?
- Are mean quality of red wines equal to mean quality of white wines?
- Do physiochemical attributes significantly affect quality?
- If so which physiochemical attributes significantly affect quality?
- Is there an interaction between citric acid and volatile acidity for red wines?
- What physiochemical attribute differences might lead to better quality?

Methods

All tests are run at the 95% confidence level unless otherwise noted.

Below, you will find the tests for each hypothesis and a brief explanation and justification for each test.

Variances of quality

We used the F test because this test allows us to compare the variances of each data set to see if they are equal. We used this to guide us in determining which tests to use along the way.

Mean quality

Provided that the data met the assumptions, we used t-tests because the two sets of data are independent and this test allows us to compare means.

Do any physiochemical attributes affect quality?

We used multivariable regression and a multivariable ANOVA because this allowed us to create a model and analyze this model that will showed if there is any relationship between any of the attributes and the quality of the wine. We created pairwise scatterplots which give us a visual idea of what the data looks like.

Which physiochemical attributes affect quality?

We used the results from the multivariable ANOVA from the previous hypothesis to determine which attributes were significant predictors of quality.

Is there an interaction between citric acid and volatile acidity?

We created a regression model to determine if there is an interaction between citric acid and volatile acidity.

Physiochemical attributes potentially improving quality

We ran t-tests after testing assumptions to compare physiochemical attributes between red and white wine to determine the kind of difference.

Results

This project will compares different physiochemical and sensory elements of wine. The wine in this data set are Vinho Verde wines, which comes from Minho region of Portugal. The data was collected between May 2004 and February 2007 and includes 1599 red wine samples and 4898 white wine samples. This study looked at 11 different physiochemical variables: fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol content. This data also contains a sensory score variable called "quality." Each wine sample was tasted by at least 3 judges, each of whom scored the wine from 0 (very bad) to 10 (excellent). The quality variable was the median of the scores (Cortez, Cerdeira, Almeida, Matos, & Reis, 2009).

The first research question asked if the variance of quality was the same for both red and white wines. There is sufficient evidence to suggest that the variability of the quality scores of red and white wines is significantly different, with ($p < .001$) at the $\alpha = .05$ level. Because there is a difference in variability, it impacted which tests were run in the following hypothesis tests.

The next research question was to determine if the mean quality of the two types of wines were different. There is sufficient evidence to suggest that the mean quality is different, with ($p < .001$) at the $\alpha = .05$ level.

The natural follow-up question is, "Which wine has a greater mean quality" From several t-tests, it was determined that there is sufficient evidence to suggest that the mean quality of red wine is less than the mean quality of white wine at the $\alpha = .05$ level ($p < .001$).

The next research question was to see if physiochemical properties affect the quality of wine. The resulting multivariable regression line is The resulting regression model is

$\hat{y} = 55.76 + 0.07$ fixed acidity $f + -1.33$ volatile acidity $+ - 0.11$ citric acid $+0.04$ residual sugar $+ - 0.48$ chlorides $+0.01$ free sulfur dioxide $+0$ tota sulfur dioxide $+ - 54.97$ density $+0.44$ pH $+0.77$ sulphates $+0.27$ alcohol

The multivariable ANOVA test (results shown below, along with pairwise comparisons of the different physiochemical attributes) shows that there is sufficient evidence to suggest that wine quality scores are significantly affected by fixed acidity, volatile acidity, residual sugar, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. Quality scores are not dependent on citric acid or chlorides.

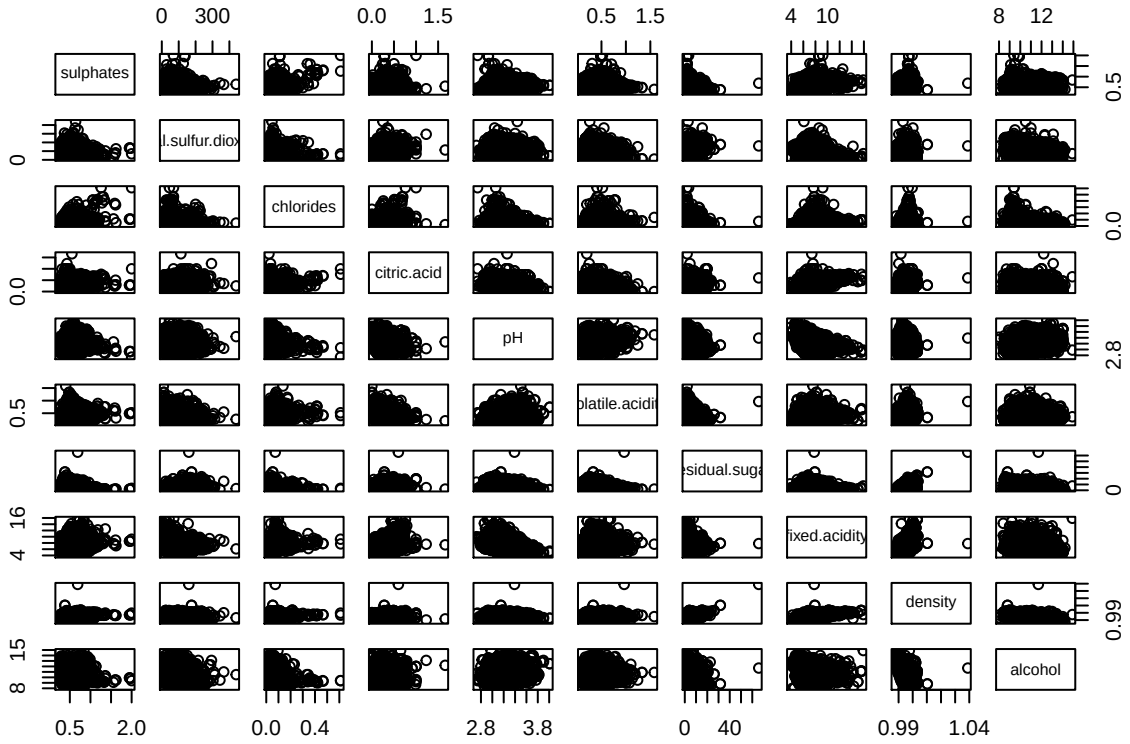
```
kable(h3_anova, digits = 3, format = "pandoc", caption = "ANOVA table",
      align=c('l', rep('r', 5))) # Output ANOVA table
```

Table 1: ANOVA table

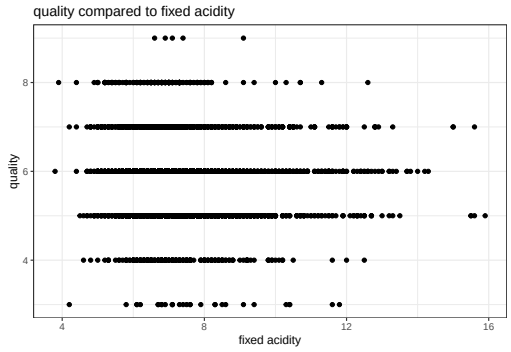
	SS	df	MS	F	p
Fixed acidity	10.214	1	10.214	18.890	< 0.0001
Volatile acidity	159.265	1	159.265	294.545	< 0.0001
Citric acid	1.026	1	1.026	1.897	0.1685
Residual sugar	38.595	1	38.595	71.378	< 0.0001
Chlorides	1.143	1	1.143	2.114	0.1460

	SS	df	MS	F	p
Free sulfur dioxide	34.155	1	34.155	63.166	< 0.0001
Total sulfur dioxide	43.495	1	43.495	80.441	< 0.0001
Density	11.090	1	11.090	20.509	< 0.0001
pH	12.777	1	12.777	23.630	< 0.0001
Sulphates	55.073	1	55.073	101.853	< 0.0001
Alcohol	137.789	1	137.789	254.829	< 0.0001
Error	3506.531	6485	0.541		
Total	4011.154	6496	505.163		

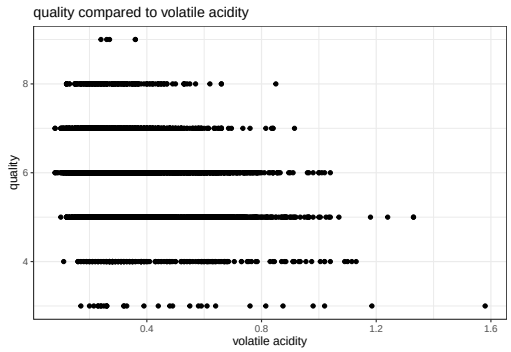
```
pairs(~ sulphates + total.sulfur.dioxide +
        chlorides + citric.acid + pH +
        volatile.acidity + residual.sugar +
        fixed.acidity + density +
        alcohol, data=wine)
```



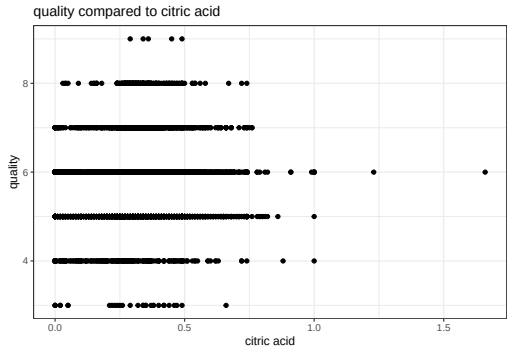

```
wine %>%
  ggplot(aes(x=wine$fixed.acidity, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to fixed acidity")+
  xlab("fixed acidity")+
  ylab("quality")+
  theme_bw()
```




```
wine %>%
  ggplot(aes(x=wine$volatile.acidity, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to volatile acidity")+
  xlab("volatile acidity")+
  ylab("quality")+
  theme_bw()
```

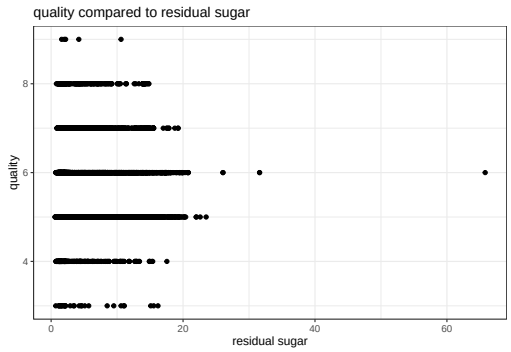



```
wine %>%
  ggplot(aes(x=wine$citric.acid, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to citric acid")+
  xlab("citric acid")+
  ylab("quality")+
  theme_bw()
```

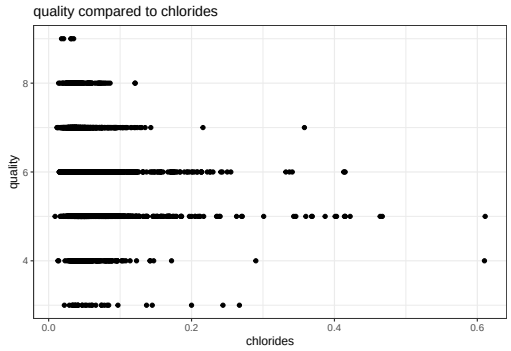



```
wine %>%
  ggplot(aes(x=wine$residual.sugar, y=wine$quality
```

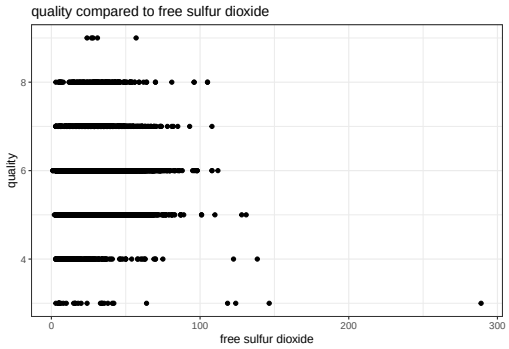
```
            )) +
    geom_point() +
  labs(title="quality compared to residual sugar")+
  xlab("residual sugar")+
  ylab("quality")+
  theme_bw()
```



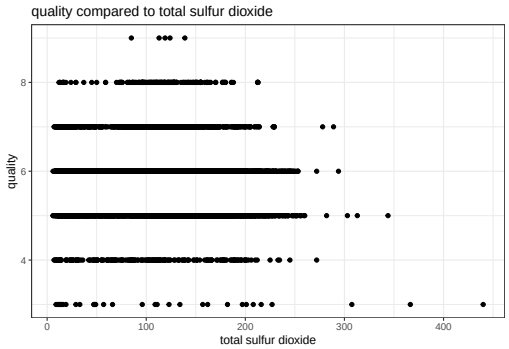

```
wine %>%
  ggplot(aes(x=wine$chlorides, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to chlorides")+
  xlab("chlorides")+
  ylab("quality")+
  theme_bw()
```



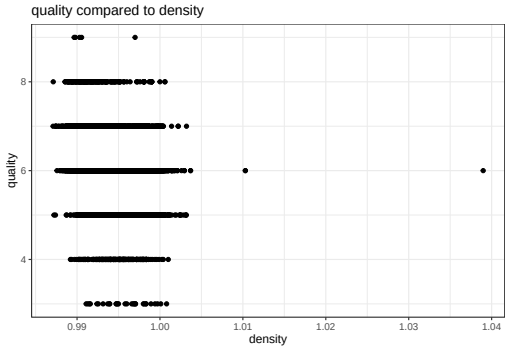

```
wine %>%
  ggplot(aes(x=wine$free.sulfur.dioxide, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to free sulfur dioxide")+
  xlab("free sulfur dioxide")+
  ylab("quality")+
  theme_bw()
```




```
wine %>%
  ggplot(aes(x=total.sulfur.dioxide, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to total sulfur dioxide")+
  xlab("total sulfur dioxide")+
  ylab("quality")+
  theme_bw()
```

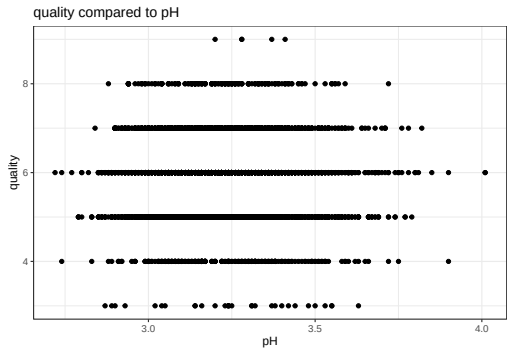



```
wine %>%
  ggplot(aes(x=wine$density, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to density")+
  xlab("density")+
  ylab("quality")+
  theme_bw()
```

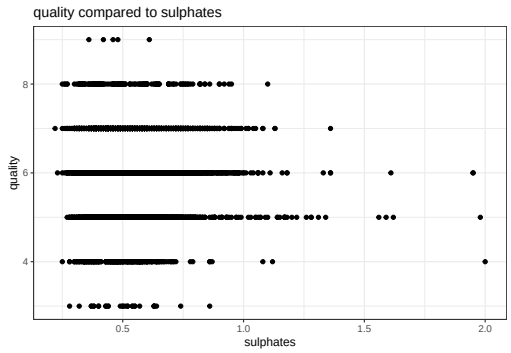



```
wine %>%
  ggplot(aes(x=wine$pH, y=wine$quality
```

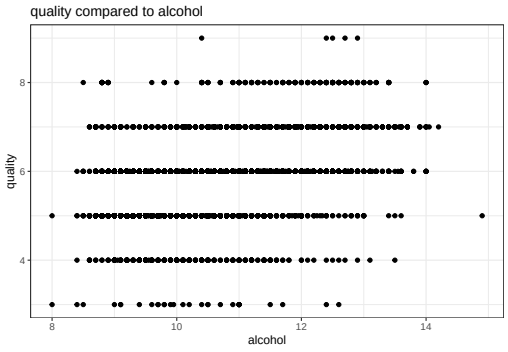
```
            )) +
    geom_point() +
  labs(title="quality compared to pH")+
  xlab("pH")+
  ylab("quality")+
  theme_bw()
```




```
wine %>%
  ggplot(aes(x=wine$sulphates, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to sulphates")+
  xlab("sulphates")+
  ylab("quality")+
  theme_bw()
```




```
wine %>%
  ggplot(aes(x=wine$alcohol, y=wine$quality
             )) +
    geom_point() +
  labs(title="quality compared to alcohol")+
  xlab("alcohol")+
  ylab("quality")+
  theme_bw()
```



Winemakers use citric acid to sterilize equipment between batches, and it is found in fruitier wines. However, citric acid can contribute to volatile acidity which leads to wine spoilage. Even though citric acid is not a significant predictor of quality, we want to see if there is an interaction between citric acid and volatile acidity.There is sufficient evidence to suggest that there is an interaction between citric acid and volatile acidity because $p = 0.0495$.

Knowing that all the physiochemical properties except for citric acid or chlorides these are all significant predictors of quality and that white wine has the higher quality, the last research question was to see how the physiochemical composition differs between white and red wines. There is sufficient evidence to suggest that white wine has less fixed acidity ($p < .001$), less volatile acidity (spoilage) ($p < .001$), more residual sugar ($p < .001$), greater free sulfur dioxide ($p < .001$), greater total sulfur dioxide ($p < .001$), less dense ($p < .001$), lower pH ($p < .001$), fewer sulphates ($p < .001$), and more alcohol ($p = 0.0021$).

Conclusion

This study of Portuguese wines shows that winemaking is both an art and a science. As vineyards strive to develop better tasting wines, they need to consider the physiochemical make-up of their product. The study found that the physiochemical properties of wine play an important part in the quality. Out of the eleven physiochemical properties studied, all but two, citric acid and chlorides, significantly predicted the quality of the wine. The data from this study showed that the white wine quality was better than red wine quality. When we looked at how the red and white wines differed in physiochemical properties, we found that white wine has less fixed acidity, less volatile acidity (spoilage), more residual sugar, greater free sulfur dioxide, greater total sulfur dioxide, less dense, lower pH, fewer sulphates, and more alcohol. Another notable find is that these physiochemical properties don't just impact the quality of the wines–they also impact each other, as seen by the interaction between citric acid and volatile acidity. These are important concepts to keep in mind for large vineyards all the way to those who want to try making their own wine at home.

One of the limitations of this study was that all the wine was from the same region of Portugal. Another limitation was that the quality variable was based on a score of small groups of judges–only 3 judges in some cases. Something important to keep in mind when considering the quality score is that the score is based on the median, rather than the average, of the judges' scores. Future studies could be done to include wines from different parts of the globe and to include a larger panel of judges.

Session Info

```
sessionInfo()
```

```
## R version 3.6.1 (2019-07-05)
## Platform: x86_64-apple-darwin19.0.0 (64-bit)
## Running under: macOS Catalina 10.15.2
##
## Matrix products: default
## BLAS/LAPACK: /usr/local/Cellar/openblas/0.3.7/lib/libopenblasp-r0.3.7.dylib
##
## locale:
```

```
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
##
## other attached packages:
##  [1] knitr_1.26      alr3_2.0.8      car_3.0-3       carData_3.0-2
##  [5] pander_0.6.3    BSDA_1.2.0      lattice_0.20-38 forcats_0.4.0
##  [9] stringr_1.4.0   dplyr_0.8.3     purrr_0.3.2     readr_1.3.1
## [13] tidyr_0.8.3     tibble_2.1.3    ggplot2_3.2.1   tidyverse_1.2.1
##
## loaded via a namespace (and not attached):
##  [1] tidyselect_0.2.5  xfun_0.11         haven_2.1.1       colorspace_1.4-1
##  [5] generics_0.0.2    vctrs_0.2.0       htmltools_0.4.0   yaml_2.2.0
##  [9] rlang_0.4.0       e1071_1.7-2       pillar_1.4.2      foreign_0.8-71
## [13] glue_1.3.1        withr_2.1.2       modelr_0.1.5      readxl_1.3.1
## [17] munsell_0.5.0     gtable_0.3.0      cellranger_1.1.0  zip_2.0.4
## [21] rvest_0.3.4       evaluate_0.14     labeling_0.3      rio_0.5.16
## [25] curl_4.0          class_7.3-15      highr_0.8         broom_0.5.2
## [29] Rcpp_1.0.2        scales_1.0.0      backports_1.1.4   jsonlite_1.6
## [33] abind_1.4-5       hms_0.5.1         digest_0.6.20     openxlsx_4.1.0.1
## [37] stringi_1.4.3     grid_3.6.1        cli_1.1.0         tools_3.6.1
## [41] magrittr_1.5      lazyeval_0.2.2    crayon_1.3.4      pkgconfig_2.0.2
## [45] zeallot_0.1.0     data.table_1.12.6 xml2_1.2.1        lubridate_1.7.4
## [49] assertthat_0.2.1  rmarkdown_1.14    httr_1.4.1        rstudioapi_0.10
## [53] R6_2.4.0          nlme_3.1-140      compiler_3.6.1
```

References

Cortez, P., Cerdeira, A., Almeida, F., Matos, T., & Reis, J. (2009). Modeling wine preferences by data mining from physicochemical properties. *Decision Support Systems*, *47*(4), 547–553. doi:10.1016/j.dss.2009.05.016

MoreFlavor. (n.d.). Citric acid. Retrieved from https://morewinemaking.com/products/citric-acid.html

Neeley, E. (2004). Wine spoilage is legally defined by volatile acidity, largely composed of acetic acid. Retrieved from https://waterhouse.ucdavis.edu/whats-in-wine/volatile-acidity

University of California Davis. (n.d.). Citric acid. Retrieved from https://wineserver.ucdavis.edu/industry-info/enology/methods-and-techniques/common-chemical-reagents/citric-acid