Alcohol Content in Portuguese Red Wine

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Abstract:

There are several attributes that can be analyzed in wine, such as acidity and concentration of sulphates. Our raw data set included 12 attributes, including the response variable (k=11) and 1,599 observations (n=1,599). The main research question we looked to answer was of the 11 predictors which were significant predictors for determining alcohol content in Portuguese Red Wine. We hypothesized that all 11 of the given predictors would be best suited for predicting the attribute and response variable, alcohol content. To test this hypothesis, we analyzed Anova type III tables, stepwise AIC functions, partial F-tests, residual graphs, and Box-Cox methods. From our findings, the model with predictors fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, total sulfur dioxide, density, pH, sulphates, and quality is the best model to determine alcohol content in Portuguese red wine.

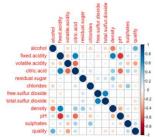
Introduction:

For our project, we are analyzing the red wine variant of the Portuguese "Vinho Verde" red wine and its attributes. Out of the 12 attributes, we chose alcohol as our response variable because it is a continuous numerical variable. The other 11 attributes act as predictors to best predict because alcohol content is a continuous numerical value. Our research question is to find out which predictors provide the most information about the wine's alcoholic content. Our predictors include fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, total sulfur dioxide, density, pH, sulphates, and quality. We made quality a dummy variable since it is a categorical variable.

[1] 1599 12											
alcohol	fixed.acidity	volatile.acidit	y citric.acid	residual.sugar	chlorides	free.sulfur.dioxid	e total.sulfur.dioxid	e density	pН	sulphates	quality
Min. : 8.40	Min. : 4.60	Min. :0.1200	Min. :0.000	Min. : 0.900	Min. :0.01200	Min. : 1.00	Min. : 6.00	Min. :0.9901	Min. :2.740	Min. :0.3300	Min. :3.000
1st Qu.: 9.50	1st Qu.: 7.10	1st Qu.:0.3900	1st Qu.:0.090	1st Qu.: 1.900	1st Qu.:0.07000	1st Qu.: 7.00	1st Qu.: 22.00	1st Qu.:0.9956	1st Qu.:3.210	1st Qu.:0.5500	1st Qu.:5.000
Median :10.20	Median : 7.90	Median :0.5200	Median :0.260	Median : 2.200	Median :0.07900	Median :14.00	Median : 38.00	Median :0.9968	Median :3.310	Median :0.6200	Median :6.000
Mean :10.42	Mean : 8.32	Mean :0.5278	Mean :0.271	Mean : 2.539	Mean :0.08747	Mean :15.87	Mean : 46.47	Mean :0.9967	Mean :3.311	Mean :0.6581	Mean :5.636
3rd Qu.:11.10	3rd Qu.: 9.20	3rd Qu.:0.6400	3rd Qu.:0.420	3rd Qu.: 2.600	3rd Qu.:0.09000	3rd Qu.:21.00	3rd Qu.: 62.00	3rd Qu.:0.9978	3rd Qu.:3.400	3rd Qu.:0.7300	3rd Qu.:6.000
Max. :14.90	Max. :15.90	Max. :1.5800	Max. :1.000	Max. :15.500	Max. :0.61100	Max. :72.00	Max. :289.00	Max. :1.0037	Max. :4.010	Max. :2.0000	Max. :8.000

Above is a table of all our attributes and their minimums, 1st quartiles, medians, means, 3rd quartiles, and maximums. We note that free sulfur dioxide and total sulfur dioxide have very high maximums. In turn, free sulfur dioxide and total sulfur dioxide also had very high standard deviations

as well. When we look at the summary output for our model f, we note that free sulfur dioxide has the highest p-value. We will use this



information to help us create our new model. To the left we have our correlation plot. The predictors that have the best linear relationship out of all the other ones with alcohol are quality and density. Just about all of

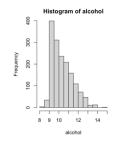
	0.11	01	0.11	
fixed.acidity	5.749245	1		2.397758
volatile.acidity	1.842350	1		1.357332
citric.acid	2.996653	1		1.731084
residual.sugar	1.326675	1		1.151814
chlorides	1.492344	1		1.221615
total.sulfur.dioxide	1.267179	1		1.125691
density	3.130913	1		1.769439
pH	2.457958	1		1.567788
sulphates	1.429858	1		1.195767
factor(quality)	1.687309	5		1.053706

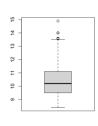
GVIE Df GVIE^(1/(2*Df))

the other predictors have a light coloration, meaning they do not have much of a linear relationship with alcohol. To the right we have our variance inflation factor output. We use this to determine if there is severe multicollinearity within our data.

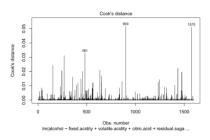
Since none of these values are greater than 10, we conclude that there is no severe multicollinearity within our model.

On the right we have a histogram and box plot of alcohol. As we can see the histogram is skewed to the left, meaning that we do not have normal distribution. Furthermore, with the boxplot we can see that we have a few distinct outliers that we will have to be aware of.



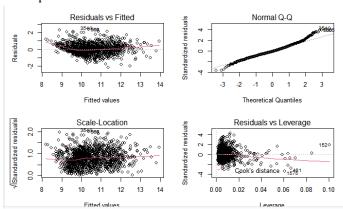


Next, we tested for potential outliers and influential points. First, we checked studentized residuals for outliers, there were a few points that had a value greater than 3 but were not deemed influential. When testing Cook's distance, data point 900 had a value greater than 0.5, but because the value did not exceed 1, it was deemed that the point was not influential.



Methods & Analysis:

For our project to use multiple linear regression, we are naming attribute alcohol content as the response variable because this is a continuous, numerical value. We will also only consider a subset of the other attributes to use as predictor variables.



We can note from the plots that the Normal Q-Q plot has a significant S-shaped curve. Since they do not follow the Y = X line, the normality assumption is not met. Likewise, from the bottom left graph, the red line is slightly curved, especially as the fitted values increase. Although the line does not have a large curvature, we should be cautious of the linearity assumption. From Residuals vs. Fitted, the left side of the graph closely resembles a megaphone shaped, leading to the conclusion that the constant variance assumption is not met

either. From the Residuals vs. Leverage, it looks like some points are past or very close to the \pm 3.5 range. We should be cautious of and further investigate all possible outliers and influential points.

Using the Anova Type III function and testing predictor significance, we found that predictor free sulfur dioxide has a p-value of .1178 that we can use in a hypothesis test where H0: Beta (free.sulfur.dioxide) = 0 Ha: Beta (free.sulfur.dioxide) != 0. The p-value is greater than alpha of .05, so we fail to reject null and conclude that there is not enough evidence that this predictor is significant to Y if all other predictors are included. We have concluded to eliminate this predictor from the model because of the hypothesis testing and the presence of

predictor total.sulfur.dioxide that we chose to keep instead.

```
lm(formula = alcohol ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar + chlorides + total.sulfur.dioxide + density + pH + sulphates + factor(quality), data = d
Min 1Q Median 3Q Max
-2.13482 -0.36894 -0.04298 0.33494 2.53012
Coefficients:
                                                                                                 d. Error
.359e+01
.048e-02
.127e-01
.322e-01
.215e-02
.860e-01
                                                                                                                         t value
41.100
23.698
5.272
6.402
21.210
-2.504
-3.756
(Intercept)
fixed.acidity
volatile.acidity
citric.acid
residual.sugar
chlorides
                                                             -9.664e-01

-1.912e-03

-5.678e+02

3.554e+00

9.302e-01

1.889e-01

2.972e-01

5.627e-01

7.778e-01

1.108e+00
 total.sulfur.dioxide
density
                                                                                                   089e-04
394e+01
pH
sulphates
factor(quality)4
factor(quality)5
factor(quality)6
factor(quality)7
factor(quality)8
                                                                                                                              23.532
8.866
0.915
1.540
                                                                                                  510e-01
049e-01
064e-01
                                                                                             1.930e-01
1.939e-01
Signif, codes: 0 '***' 0.001 '**' 0.01 '*'
                                                                                                                          0.05 '.' 0.1 ' ' 1
Residual standard error: 0.5945 on 1584 degrees of freedo
Multiple R-squared: 0.6915, Adjusted R-squared: 0.68
F-statistic: 253.6 on 14 and 1584 DF, p-value: < 2.2e-16
```

The model f2, introduced to the left, is the original f model with the removal of the free sulfur dioxide predictor. Looking at the coefficients in the model summary, we can conclude that chlorides, total sulfur dioxide, and density negatively affect alcohol content, whereas the rest of the predictors are positively correlated. Density has the largest estimated coefficient meaning this predictor changes alcohol content the most (a decrease of 571.9) when it is increased one by 1 unit. This seems like a surprisingly steep slope, but density varies only slightly when since all examples are liquids of relative thickness. pH is the largest positive coefficient and will change the response variable by 5.59 for every increase in one unit. Both of these increments

given by the coefficients table imply that the rest of the predictors are held constant.

We think that model f2 seems like a possible valid model to use for our project. The p-values are all less

than alpha now and the r squared is .6915 which is the proportion of the variance of Y that can be explained through the predictors. However, we are going to use the partial F-test to see if a reduced model could be a better option.

```
Analysis of Variance Table
Model 1: alcohol ~ fixed.acidity + volatile.acidity + residual.sugar + total.sulfur.dioxide + density + pH + factor(quality)
Model 2: alcohol ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar + chlorides + total.sulfur.dioxide + density + pH + sulphates + factor(quality)
Res.DF RSS DF Sum of Sq F Pr(>F)
       1587 607.52
1584 559.89 3 47.629 44.916 < 2.2e-16 ***
 Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We think that a reduced model could simplify

the project and still be a significant model to predict Y. To test this hypothesis, we performed a partial F-test with f2 and a reduced model of our choosing. Looking at the anova table image shown above, the p-value is less than alpha of .05 so we can reject null and conclude there is enough evidence that the full model (f2) is significantly better.

```
Initial Model:
alcohol ~ 1
 Final Model:
alcohol ~ factor(quality) + density + fixed.acidity + pH + residual.sugar
sulphates + citric.acid + volatile.acidity + total.sulfur.dioxide +
chlorides
                                           Step Df Deviance Resid. Df Resid. Dev
                                                                                                       1814.7645
1330.8266
1036.0002
940.7527
765.7050
608.5128
                                                                                                                               204.3971
-281.5416
-679.9838
-832.1949
                 + factor(quality)
                                                           483.937982
                     + density
+ fixed.acidity
                                                           175.047758
157.192137
                   + pH
+ residual.sugar
                                                                                                                             -1159.4025
-1524.8190
          + residual.sugar
+ sulphates
+ citric.acid
+ volatile.acidity
total.sulfur.dioxide
+ chlorides
                                                                                            1588
                                                             29.904908
                                                                                                           578.6079
573.6467
                                                                                             1587
                                                               4.961212
                                                                                                                             -1615.1668
```

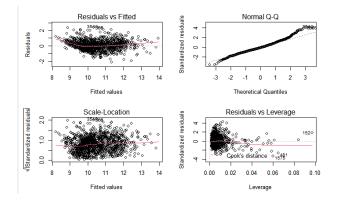
We performed a step AIC function (stepwise selection) to compare all alternative models. Note that the final model, which includes all predictors has the lowest AIC value. Using (step3\$anova) allows us to consolidate all the AIC values and compare them side-by-side.

When our group considered this data set more, we realized that we should possibly exclude 'quality' from the predictors because this may be an opinion predictor and not have much relation to alcohol content. We are using another partial F test to test this hypothesis. f2 is the model with

```
quality and f3 is excluding this variable. With the small p-
value, we conclude that there is evidence that the full model
with quality is significant for predicting alcohol content.
```

```
Analysis of Variance Table
Model 1: alcohol ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar + chlorides + total.sulfur.dioxide + density + pH + sulphates + factor(quality)
Model 2: alcohol ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar + chlorides + total.sulfur.dioxide + density + pH + sulphates
Res.Df RSS pf Sum of Sq F Pr(>F)
1 18M 550 80
      1584 559.89
1589 599.11 -5 -39.225 22.194 < 2.2e-16 ***
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

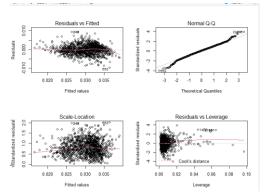
These residuals graphs show that even with our best model (f2) the variance assumption is not met because it has a megaphone shape. Although the Normal Q-Q plot follows an S-shape (the normality assumption is not met), we can still pass this assumption since the data set is very large.



The assumptions are not met using the various hypothesis tests because the p-value are less than the alpha of .05 (original test shown on the next page). We will check to see if the Box-Cox method will provide any solution. Using the Box-Cox method, we found lambda should equal -1.5 based on the log-likelihood graph.

The residual plots below represent the new transformed model. The normality s-shaped and the megaphone-shape of the top two plots have significantly decreased.

The two images on the next page show a comparison of the numeric diagnostic tests for the normality, constant variance, and independence assumptions using the Breusch-Pagan and Anderson-Darling, Shapiro-Wilk, and Durbin-Watson tests, respectively. The original model f2 is on the left, while the transformed model is on the right. While the p-values are still less than alpha of .05, they have significantly increased from the transformation.



```
studentized Breusch-Pagan test
                                                                                studentized Breusch-Pagan test
                                                                        data: f2_bc
BP = 198.13, df = 14, p-value < 2.2e-16
BP = 179.96, df = 14, p-value < 2.2e-16
        Anderson-Darling normality test
                                                                                Anderson-Darling normality test
      f2$residuals
data:
                                                                               f2_bc$residuals
                                                                        A = 1.7547, p-value = 0.0001714
A = 5.8559, p-value = 2.057e-14
                                                                                Shapiro-Wilk normality test
        Shapiro-Wilk normality test
                                                                         lata: f2_bc$residuals
/= 0.99246, p-value = 2.704e-07
data: f2$residuals
  = 0.98276, p-value = 6.306e-13
```

From the results of the Box-Cox method, we predict that the Weighted Least Squares method of transformation may be a better option to relieve the constant variance and normality assumption violations. In future research, we recommend trying this method.

Results:

```
> # Confidence Interval
> confint(f2, level=.95)
                               2.5 %
                                             97.5 %
                                                                    This first confidence interval tests the coefficients of each
(Intercept)
                       5.318561e+02 5.851645e+02
fixed.acidity
                       4.451947e-01
                                      5.255431e-01
                                                        predictor Beta(i) = 0 with i = [1, 10].
volatile.acidity
                       3.732494e-01
                                      8.155147e-01
citric.acid
                       5.869299e-01 1.105397e+00
                                                                    We are 95% confident that the slope for the regression line of
residual.sugar
                       2.338712e-01
                                      2.815340e-01
                      -1.723624e+00 -2.092670e-01
chlorides
                                                        alcohol content on fixed acidity, volatile acidity, citric acid, residual
total.sulfur.dioxide -2.909732e-03 -9.131852e-04
                                                        sugar, chlorides, total sulfur dioxide, density, pH, sulphates,
                      -5.951932e+02 -5.404940e+02
density
рΗ
                       3.257867e+00
                                      3.850345e+00
                                                        factor(quality)6, factor(quality)7, and factor(quality)8 do not include 0,
sulphates
                       7.244250e-01
                                      1.136004e+00
factor(quality)4
                      -2.158904e-01
                                      5.937793e-01
                                                        so we can reject the null hypothesis that H 0: Beta(i)=0 and conclude
                      -8.139546e-02
                                      6.757697e-01
factor(auality)5
                                                        that the coefficients are non-zero.
                       1.823095e-01
                                      9.431101e-01
factor(quality)6
                       3.864852e-01
                                      1.169053e+00
factor(auality)7
                                                                       Using our transformed model, the predictors that have the
                                                           best linear relationship out of all the other ones with alcohol content
                                                           is density and quality because they are closest to +/-1. Quality has a
                                                            negative correlation, while density is positively correlated. Since the
                                                            alcohol bc response is the original response variable raised to the -
                                                            1.5 power, we noted how the correlations are opposite from the
                                                           original. For example, quality was originally positively correlated
                                                            with the response alcohol content.
                                                                         > #Prediction for means, Quality = 6
> pred3 = predict(f2, data.frame(fixed.atdes), total.sulfur.dioxide = mean(total
> pred3
Sfit
                                                                                                                fit lwr upr
1 10.73413 9.564312 11.90395
fit lwr upr
1 10.14531 8.967737 11.32288
                                                                          fit lwr upr
1 10.51907 9.351974 11.68617
                                     fit Twr upr
1 10.25355 9.086373 11.42072
$se.fit
[1] 0.08341888
                                                                                                                $se.fit
[1] 0.04722329
                                     $se.fit
[1] 0.0249869
                                                                          $se.fit
[1] 0.02402432
$df
[1] 1584
                                                                          $df
[1] 1584
                                                                                                                $df
[1] 1584
                                     $df
[1] 1584
                                     $residual.scale
[1] 0.5945289
                                                                                                                $residual.scale
[1] 0.5945289
                                                                          $residual.scale
[1] 0.5945289
```

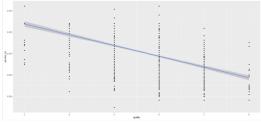
Above are the prediction intervals for quality fixed at 4, 5, 6, and 7, while all other variables are held at their mean values. We are 95% confident that, the alcohol content for red wine with a quality of 4 is somewhere between 8.97 and 11.32. We are 95% confident that, the alcohol content for red wine with a quality of 5 is somewhere between 9.07 and 11.42. We are 95% confident that, the alcohol content for red wine with a quality of 6 is somewhere between 9.35 and 11.69. We are 95% confident that, the alcohol content for red wine with a quality of 7 is somewhere between 9.56 and 11.90.

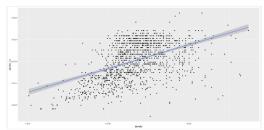
```
> COI
                                                                                                                                                                                                                                                   fit lwr upr
1 10.73413 10.6415 10.82676
fit lwr upr
1 10.14531 9.981683 10.30893
                                                                           fit 1wr upr
1 10.25355 10.20454 10.30256
                                                                                                                                                            $se.fit
[1] 0.02402432
                                                                                                                                                                                                                                                   $se.fit
[1] 0.04722329
                                                                            $se.fit
[1] 0.0249869
$se.fit
[1] 0.08341888
                                                                                                                                                                                                                                                   $df
[1] 1584
$df
[1] 1584
                                                                            $df
[1] 1584
                                                                                                                                                            $df
[1] 1584
                                                                                                                                                                                                                                                   $residual.scale
[1] 0.5945289
$residual.scale
[1] 0.5945289
                                                                            $residual.scale
[1] 0.5945289
                                                                                                                                                            $residual.scale
[1] 0.5945289
```

Above are the confidence intervals for quality fixed at 4, 5, 6, and 7, while all other variables are held at their mean values. We are 95% confident that, for all wine with a quality of 4, the alcohol content on average is somewhere between 9.98 and 10.31. We are 95% confident that, for all wine with a quality of 5, the alcohol content on average is somewhere between 10.20 and 10.30. We are 95% confident that, for all wine with a quality of 6, the alcohol content on average is somewhere between 10.47 and 10.57. We are 95% confident that, for all wine with a quality of 7, the alcohol content on average is somewhere between 10.64 and 10.83. We found it interesting that as quality increases, both the prediction and confidence intervals slightly increase their lower and upper bounds.

All these values VIF<10 indicate that there is no multicollinearity issue in our best fit model.

> vif(f2_bc)			
	GVIF	Df	GVIF^(1/(2°Df))
fixed.acidity	5.749245	1	2.397758
volatile.acidity	1.842350	1	1.357332
citric.acid	2.996653	1	1.731084
residual.sugar	1.326675	1	1.151814
chlorides	1.492344	1	1.221615
total.sulfur.dioxide	1.267179	1	1.125691
density	3.130913	1	1.769439
рн	2.457958	1	1.567788
sulphates	1.429858	1	1.195767
factor(quality)	1.687309	5	1.053706





After determining the predictors that were most correlated to alcohol content (quality and density), ggplots were constructed to create a prediction bond, about the most correlation predictor by holding other predictions constant. The plot on the left is for quality, and it shows the negative correlation because we are comparing quality to the transformed response, alcohol_bc. The plot on the right shows density's positive correlation. As density increases, the predicted value for alcohol content also increases. This is also using the transformed response variable, alcohol_bc, showing the opposite correlation as the matrices above.

Conclusion and Discussion:

Based on all the findings above, the model with predictors fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, total sulfur dioxide, density, pH, sulphates, and quality is the best model to determine alcohol content in Portuguese red wine. Our hypothesis that all predictors should be included in the model were wrong when we determined that free sulfur dioxide did not need to be included in the model. Our other hypothesis, that a smaller subset of the model, would increase the R^2 value and be more significant when predicting also proved to be wrong. While we used the original f2 for the confidence and prediction intervals, we used the transformed model for the plots and visualizations in order to investigate and explore the effects of the transformed model. Since we did not perform many visuals for the transformation models in class, we aimed to incorporate this piece in our project. We advise further researchers to explore other transformation methods to remediate the transformation limitations we faced as a group.

A potential follow-up question from this work would be to determine if this model can be applied to other types of wine, like white wines or other brands of red wine. This could be accomplished by collecting data for the same predictors as this study and interpreting the results through a regression analysis.

References:

Learning, UCI Machine. "Red Wine Quality." Kaggle, 27 Nov. 2017, www.kaggle.com/uciml/red-wine-quality-cortez-et-al-2009.

Mir, Ferran Rodriguez. "2019, Aug 07." Red Wine Quality - Data UAB, 19 Aug. 2019, datauab.github.io/red_wine_quality/.

Onukogu, Chinwendu. "Red Wine Quality Prediction Using Classification and Regression Model."

Medium, Dev Genius, 9 July 2020, medium.com/dev-genius/red-wine-quality-prediction-using-classification-and-\ regression-model-

f19337821b71#: ``: text = The %20 main %20 a im %20 of %20 the %20 red %20 wine %20 quality, are %20 non-volatile %20 acids %20 that %20 do %20 not %20 evaporate %20 readily.

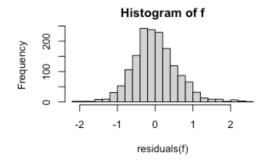
Individual Contributions:

Isabel Heard: "Introduction" code, analysis, and presentation slides.

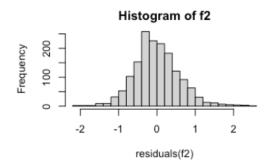
Corinne Steuk: "Methods & Analysis" code, analysis, presentation slides.; edited and ran "Results" code Taylor Hartman: wrote "Results" code, analysis, and presentation slides

Appendix:

Histogram of f

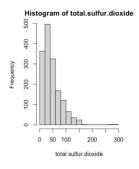


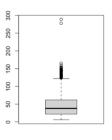
Histogram of f2



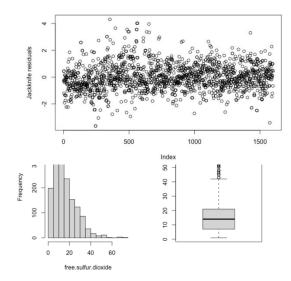
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Histogram and boxplot of total sulfur dioxide





Jackknife residual plot

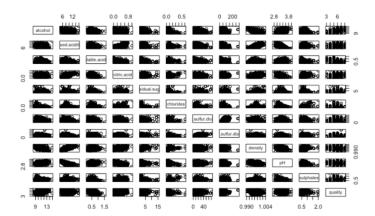


Histogram and boxplot of free sulfur dioxide

Summary table of f

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Scatter matrix plot



Standard deviations

```
Standard deviations
```{r}
sd(alcohol)
sd(fixed.acidity)
sd(volatile.acidity)
sd(citric.acid)
sd(residual.sugar)
sd(chlorides)
sd(free.sulfur.dioxide)
sd(total.sulfur.dioxide)
sd(density)
sd(pH)
sd(sulphates)
sd(quality)
```

- [1] 1.065668
- [1] 1.741096
- [1] 0.1790597
- [1] 0.1948011
- [1] 1.409928
- [1] 0.0470653
- [1] 10.46016
- [1] 32.89532
- [1] 0.001887334
- [1] 0.1543865
- [1] 0.169507
- [1] 0.8075694