Assignment 3

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Introduction

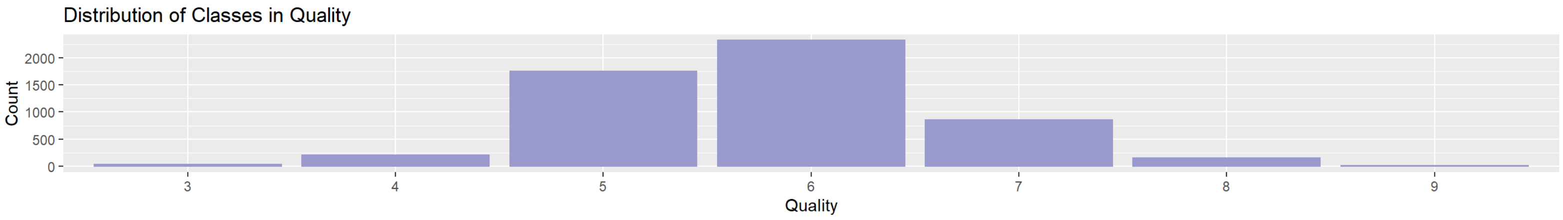
For the love of wine, and data science,
we attempt to explore, what makes it fine.

Objective

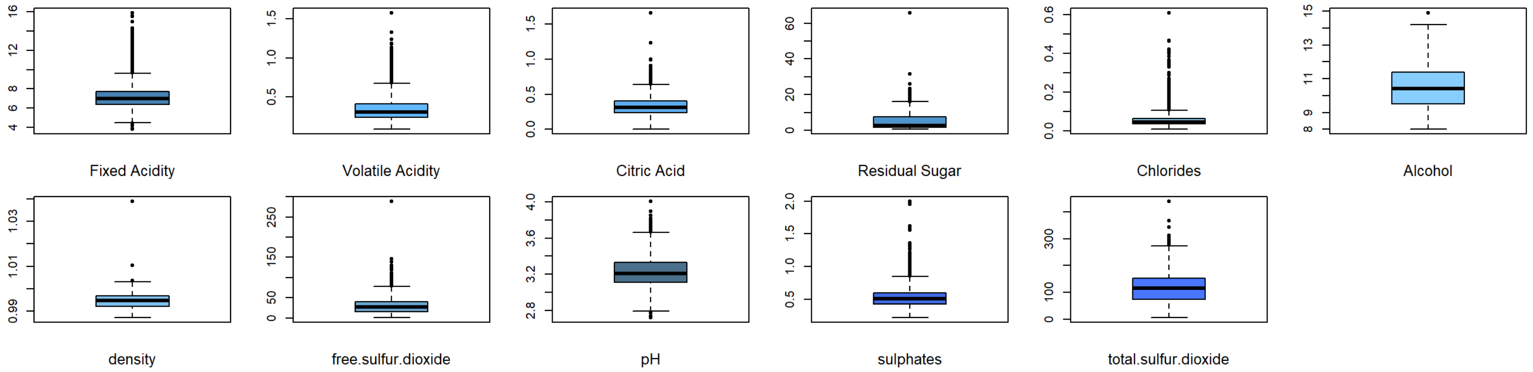
After analyzing several physiochemical properties, we aim to build a model that can predict quality of a wine based on its constituents. The two datasets employed contain information on red and white variants of the Portuguese “Vinho Verde” wine. Initially, the combined dataset had `6497` rows with all columns as integers apart from `color` which was coded as factor. For a reason to be discussed later, duplicate rows were excluded from our analysis leaving beind `5320` rows. With this aim in mind, we test the **hypothesis** that whether the chosen properties significantly determine wine’s quality.

Data Cleaning and Exploration

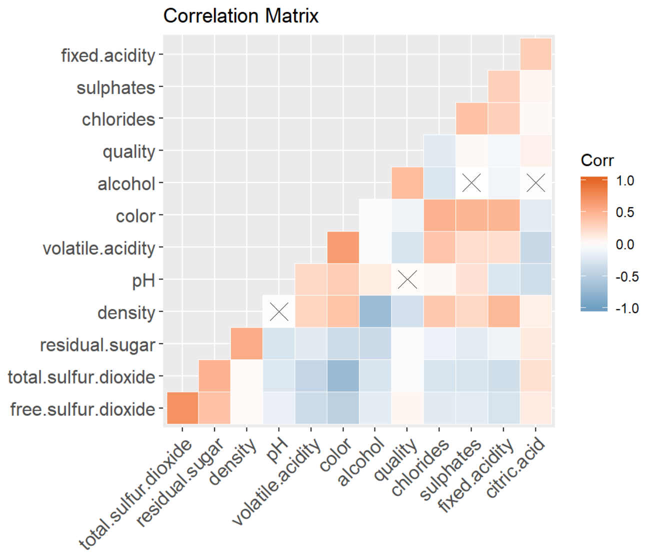
To quickly begin with the EDA process, we explore the class distribution of our outcome variable `quality` and find that the classes are imbalanced (unfortunately). Furthermore, the dataset has `0` NAs (fortunately).



To dig deeper and explore the spread of variables, we plot boxplots and find that apart from `alcohol` almost all variables have quite a large number of outliers. This, along with the fact that our classes are imbalanced, indicates the possibility that some ingredients are found in excessive quantity in low-quality and some in high-quality wines. Anyways, to ensure our model is not influenced by outliers, we removed all the outliers that had a less than 1% chance of occurring as a non-outlier.



To explore correlations in our data, we plot a **heatmap** and find that the highest postive correlation exists between `alcohol` and `quality`. `Citric.acid` and some other variables have apparently no correlation with `quality`. We ’ll keep this in mind while developing our model.



Model Building

As `quality` is an integer, we treat it as an ordinal categorical variable and employ **ordinal logistic regression** to build a prediction model. We will use `polr()` as it fits a logistic or probit regression model to an ordered factor response. But before diving into modelling, we first take a look at some of the underlying assumptions below.

Assumptions of Logistic Regression

1. **Categorical Predictor:** Quality is ordinal so this assumption holds.
2. **Large sample size:** We have `5320` rows so we are good to go!
3. **Independent Observations:** We have independent observations with all duplicates removed.
4. **No or Less Multicollinearity:** We'll come to that in a while.
5. **Linearity of predictors and logit of outcome variable:** We'll come to that in a while as well.
6. **Complete Information:** As mentioned earlier, we have `0` NAs.
7. **Incomplete Separation:** We can clearly see that there is no complete separation in the scatterplots. `Appendix (i)`

To check Multicollinearity, we calculate **Variance Inflation Factors** (VIF) `Appendix (ii)`. Based on this, we exclude 'density' as it has a VIF = 10.17 > 10 (a well-established no-go area). We removed color as well because it is really not a "determinant" of quality.

We now move on to testing the last assumption: Log-Linearity! To do this, we regress our model with log(predictor)*predictor interaction terms. When we do this `Appendix (iii)`, all the interaction variables except those of `free.sulphur.dioxide` and `pH`, are found non-signficant indicating that the assumption of linearity is met for all the other variables. ~~We have not yet discarded these two variables.~~

Feature Selection

For selecting predictors, we use **Backwards Step-wise Logistic Regression** using the `step()` function. For evaluation, we use **Akaike Information Criteria** that depends on model deviance (which is twice the **log-likelihood**) and number of predictor variables employed (thus penalizing the increase in number of predictors). Bottom-line: the smaller the AIC, the better the model.

Using this method, we find that by removing `citric.acid` from the model, we can achieve a lower AIC (`11716` in this case). `Appendix (iv)`

Evaluating Significance

Ho: We observe that p-value for `fixed.acidity` is greater than `0.05 Appendix (v)`. So, it is statistically insignifcant but when we tried removing it, it slightly increases the AIC (not good). To get a third opinion on this, we make another model with `fixed.acidity` removed and then apply **ANOVA** to see there's any improvement:

```
##   Resid. df Resid. Dev   Test    Df LR stat. Pr(Chi)
## 1      5308   11692.53                              
## 2      5308   11692.53 1 vs 2     0        0       1
```

By ANOVA, we get to know that removing `fixed.acidity` doesn't make a statistical difference. So, we keep the new model that requires less predictors.

Hypothesis Testing

Ho: Co-efficients of selected predictors are zero

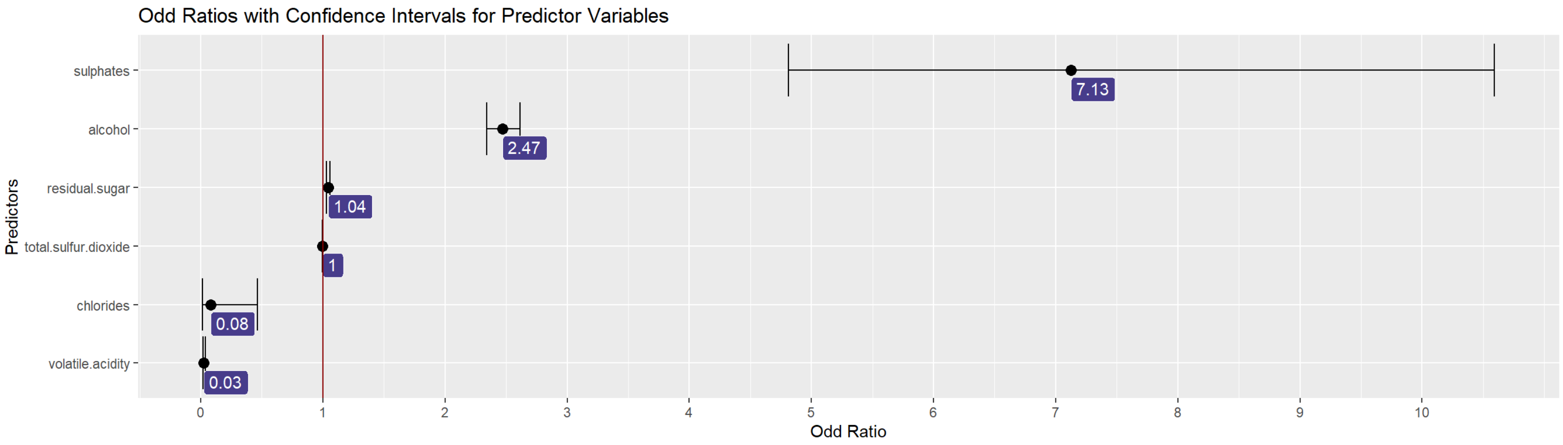
Ha: Co-efficients of selected predictors are non-zero

Based on the calculated co-efficients and their p-values, we reject Null Hypothesis and conclude that our model is significant. Our final model gives a **Hosmer and Lemeshow's R^2 for Goodness-of-Fit** of `0.14` and is summarised below.

```
## Coefficients:
##                         Value Std. Error t value
## volatile.acidity     -3.68059  0.1920681 -19.163
## residual.sugar        0.04394  0.0069213   6.349
## chlorides            -2.50068  0.8868677  -2.820
## total.sulfur.dioxide -0.00262  0.0006063  -4.322
## sulphates             1.96379  0.2012844   9.756
## alcohol               0.90526  0.0285225  31.738
## 
## Intercepts:
##     Value    Std. Error t value
## 3|4   3.1930   0.4002     7.9793
## 4|5   5.3482   0.3619    14.7778
## 5|6   8.3780   0.3628    23.0921
## 6|7  11.0028   0.3797    28.9798
## 7|8  13.3455   0.3960    33.6996
## 8|9  16.8420   0.5930    28.4002
## 
## Residual Deviance: 11692.53 
## AIC: 11716.53
```

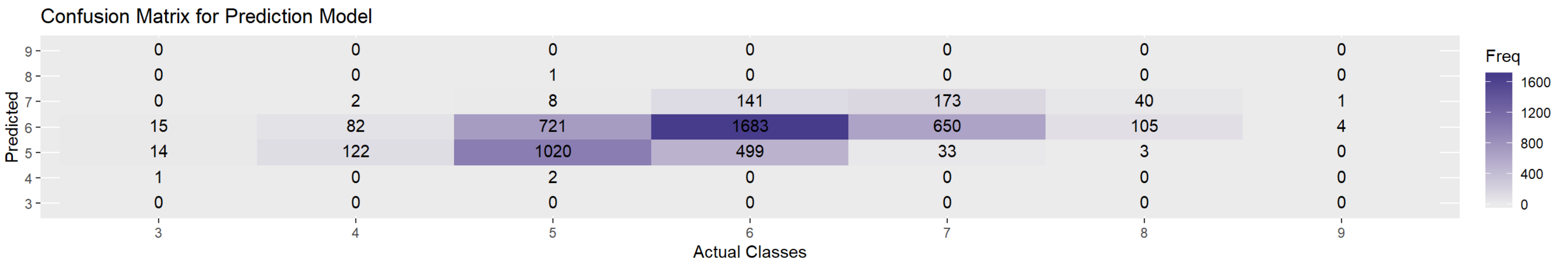
Model Interpretation and Insights

To interpret the co-efficients, we converted them to **odd-ratio** using exponentials, which are plotted below. For example, we would say that by keeping all other variables constant, when `residual.sugar` increases one unit, it is `1.04` times more likely to be in a higher category of `quality`. Furthermore, using confidence intervals, we can conclude that none of the intervals cross `1`, indicating that the direction of odd-ratios of all co-efficients is reliable. Thus, `sulphates` and `alcohol` have a high-positive impact on `quality` and, `chlorides` and `volatile.acidity` have a high-negative impact.



Testing Prediction Accuracy

For evaluating in-sample accuracy of our prediction model, we form a **confusion matrix** by `predict()` -ing using our original dataset. **Residual Plot** was also visualized and homoscedasticity was observed `Appendix (vi)` .



Predicted \ Actual	3	4	5	6	7	8	9
9	0	0	0	0	0	0	0
8	0	0	1	0	0	0	0
7	0	2	8	141	173	40	1
6	15	82	721	1683	650	105	4
5	14	122	1020	499	33	3	0
4	1	0	2	0	0	0	0
3	0	0	0	0	0	0	0

We can observe from above that accuracy for our model is `54.06` %. The low accuracy can be well-understood from the confusion matrix that classes with low frequency `(3,4,8,9)` were rarely predicted. This was due to the imbalance in the distribution of our classes.

Gap Analysis and Future Work

Class Imbalance: As already exhibited, the imbalance in our classes had a very negative impact on the accuracy of our model. Methods such as clustering or re-sampling may be be evaluated for improved accuracy (other than collecting more data for low-quality and high-quality wines, of course).

Conclusion

We conclude that quality of a wine can be significantly predicted by `sulphates` , `alohol` , `chlorides` , `volatile.acidity` and along with some impact by other variables as well that were included in our final model. The direction of odd-ratios is reliable because none of the confidence intervals cross `1` . The overall fit of the model as determined by Hosmer and Lemeshow’s R^2 for Goodness-of-Fit is `0.14` . The prediction accuracy is found to be `54.06` %.

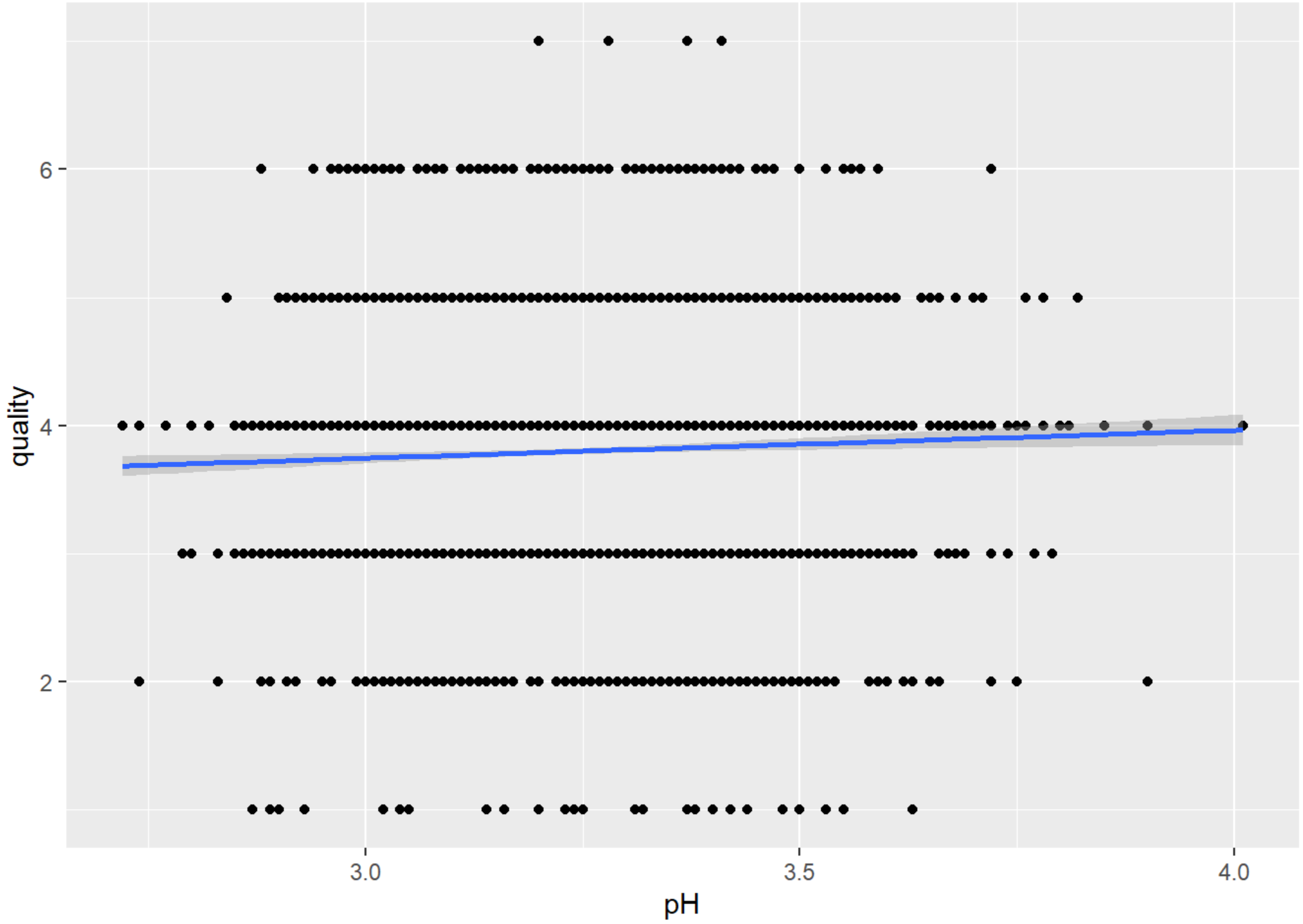
The outliers in our ingredients, along with the fact that our classes are imbalanced, indicates the possibility that some ingredients are found in excessive quantity in low-quality wine and some in high-quality wines. Also, there are not as many high-quality wines and low-quality wines as there are medium-quality wines.

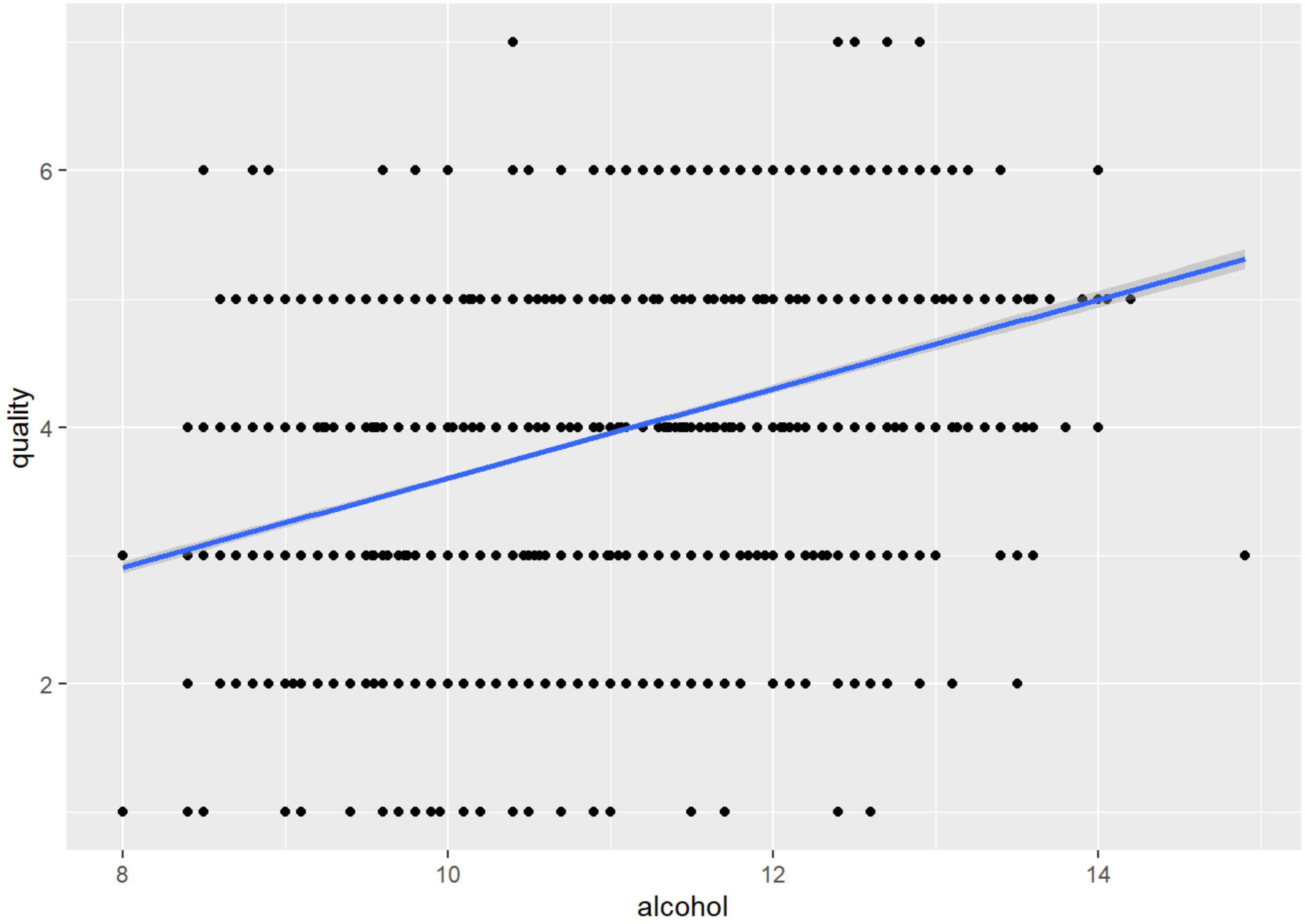
Appendix

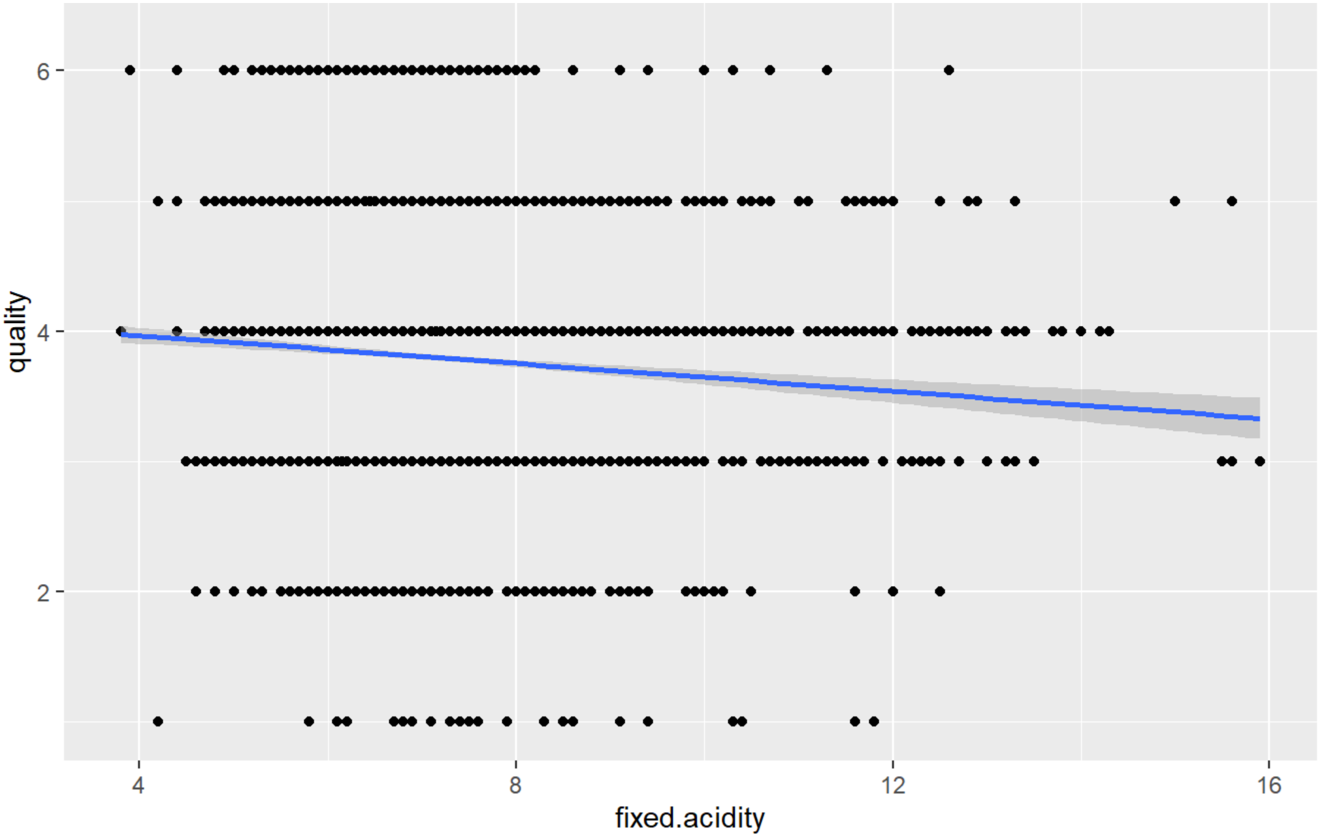
Work Distribution

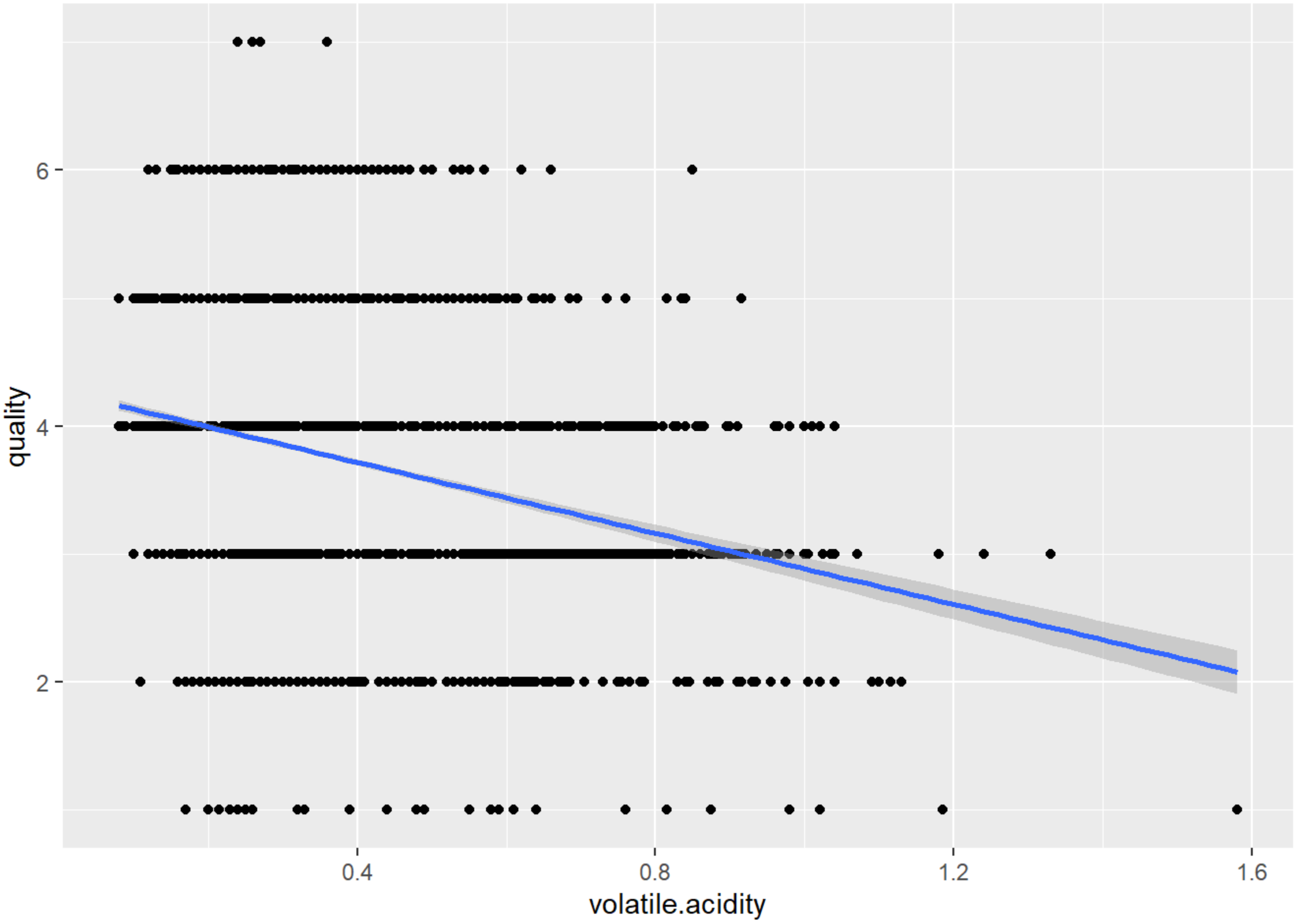
Member	Contribution
Shahzeb Naveed	Plots, Reporting, EDA
Zaryab Javaid	EDA, Data Cleaning
Mohsin Tahir	Regression Modelling

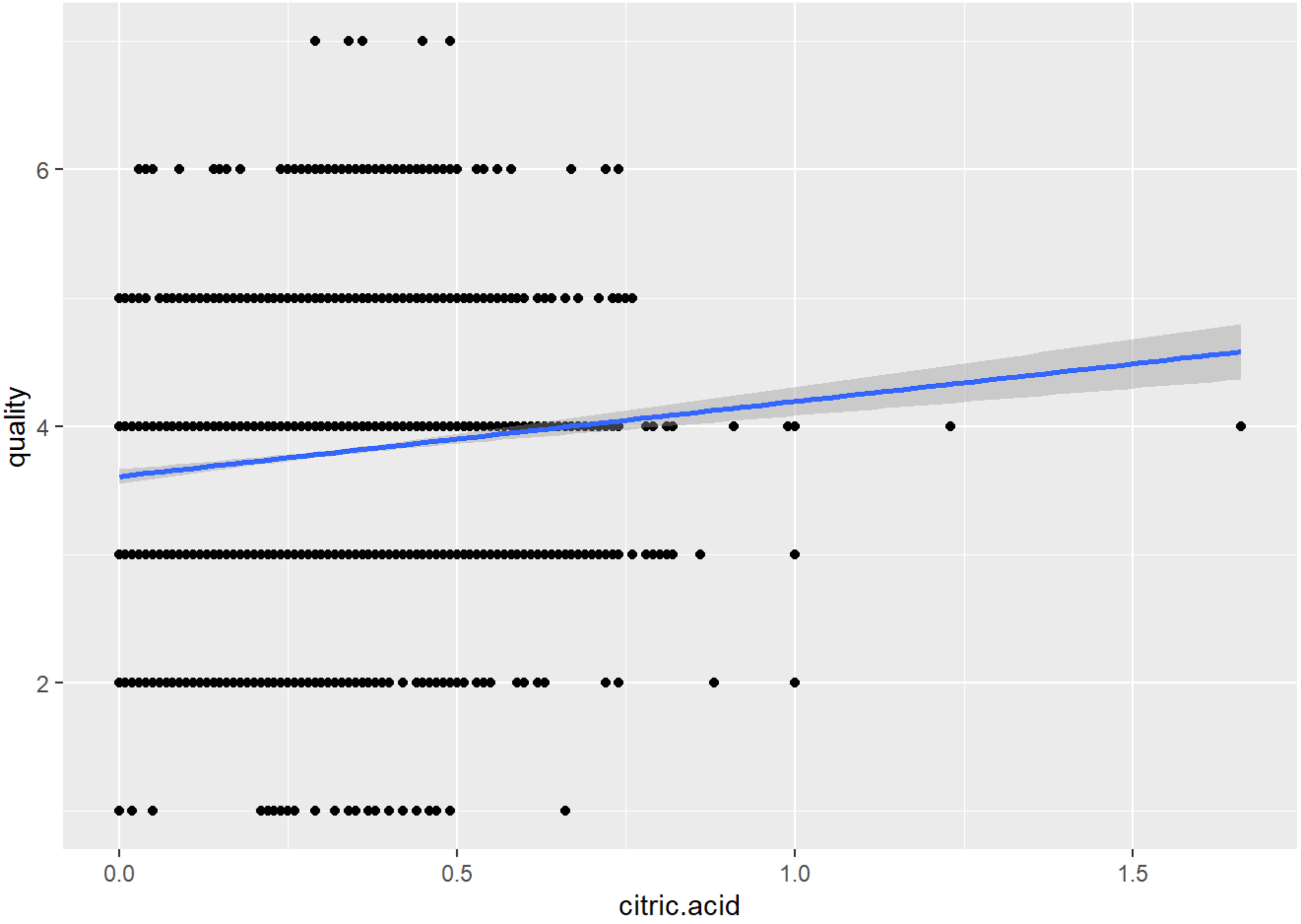
Appendix (i)

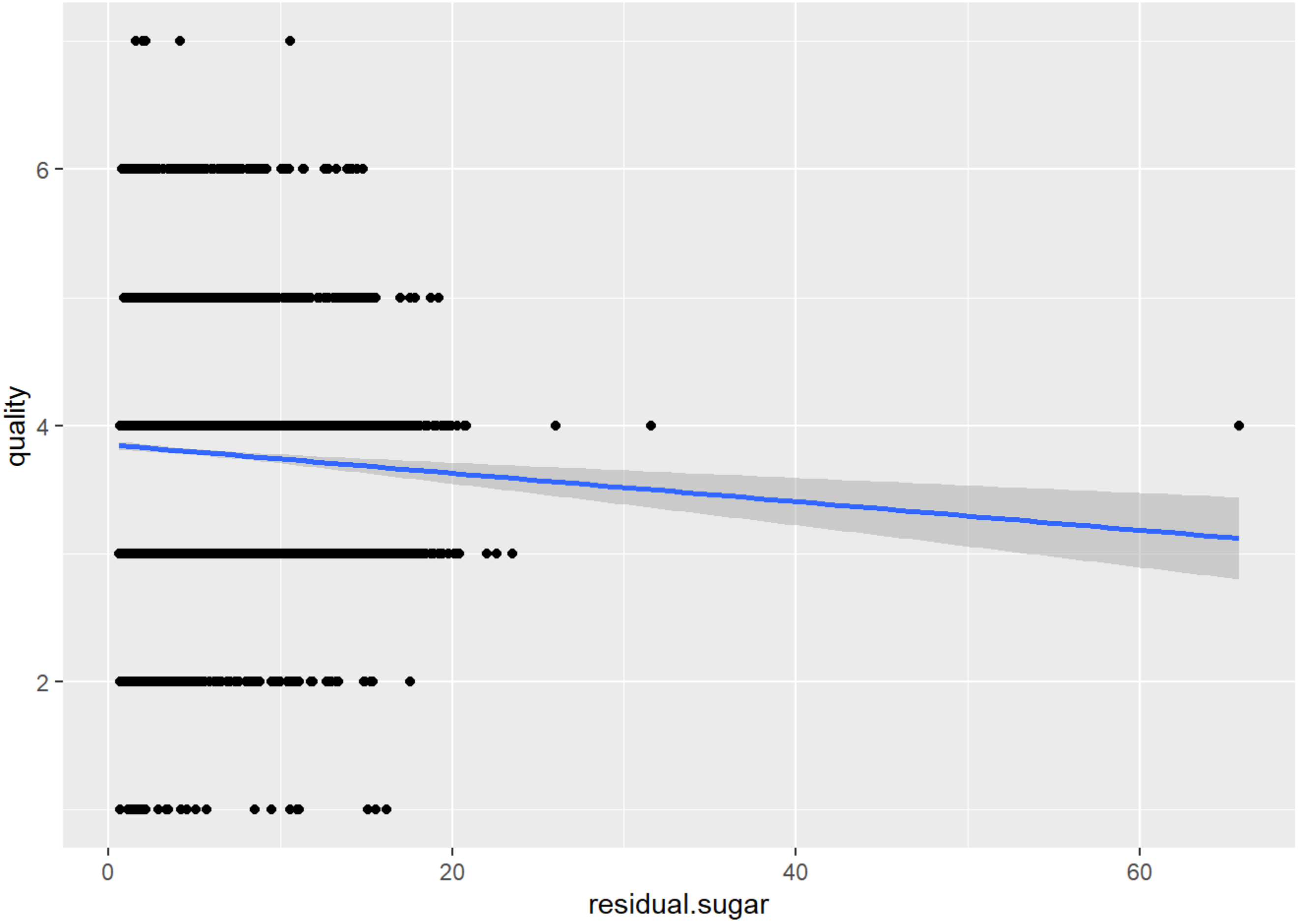

quality
6
4
2
3.0
3.5
4.0
pH

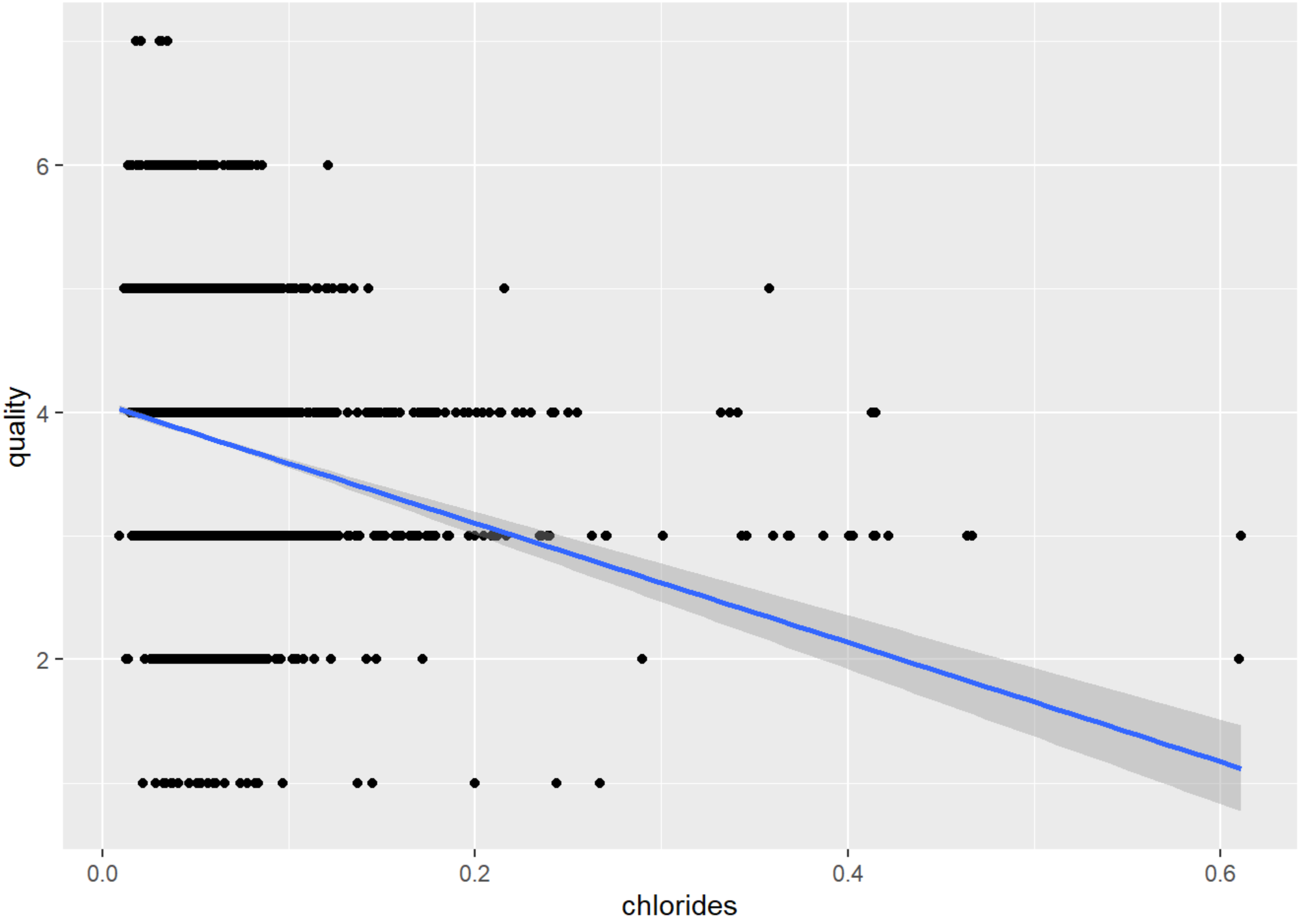

quality
6
4
2
8
10
12
14
alcohol

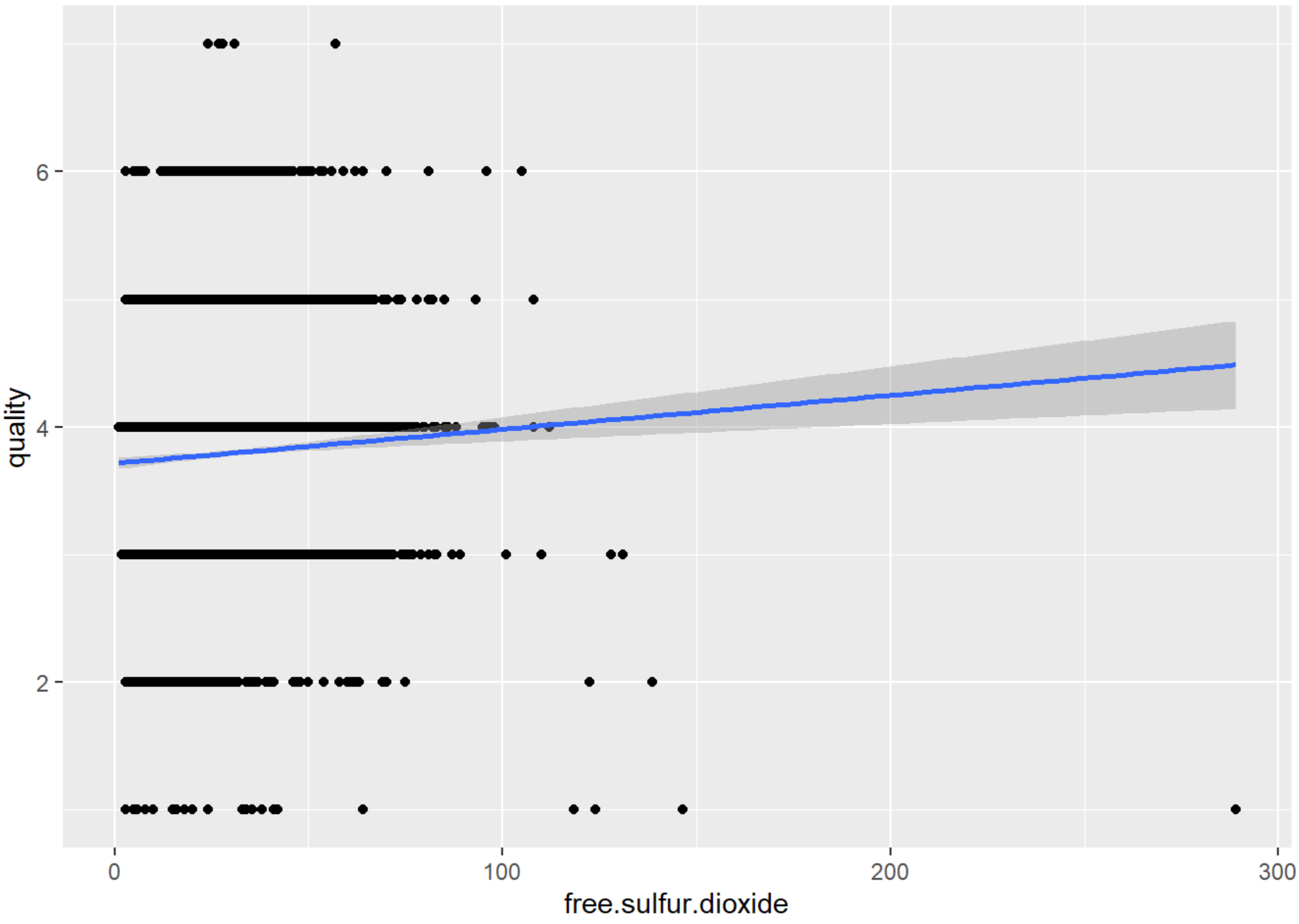

quality
6
4
2
4
8
12
16
fixed.acidity

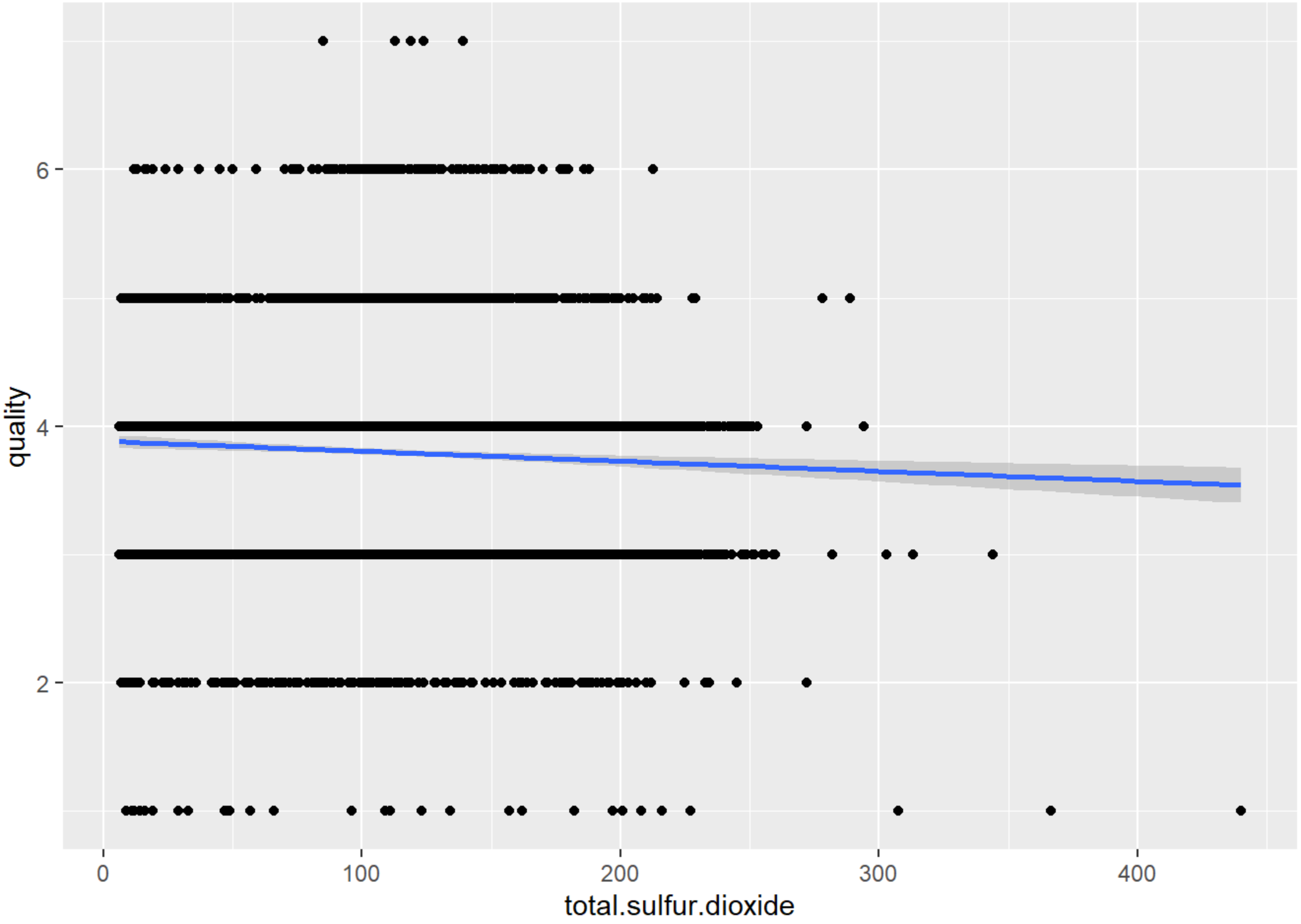

quality
6
4
2
0.4
0.8
1.2
1.6
volatile.acidity

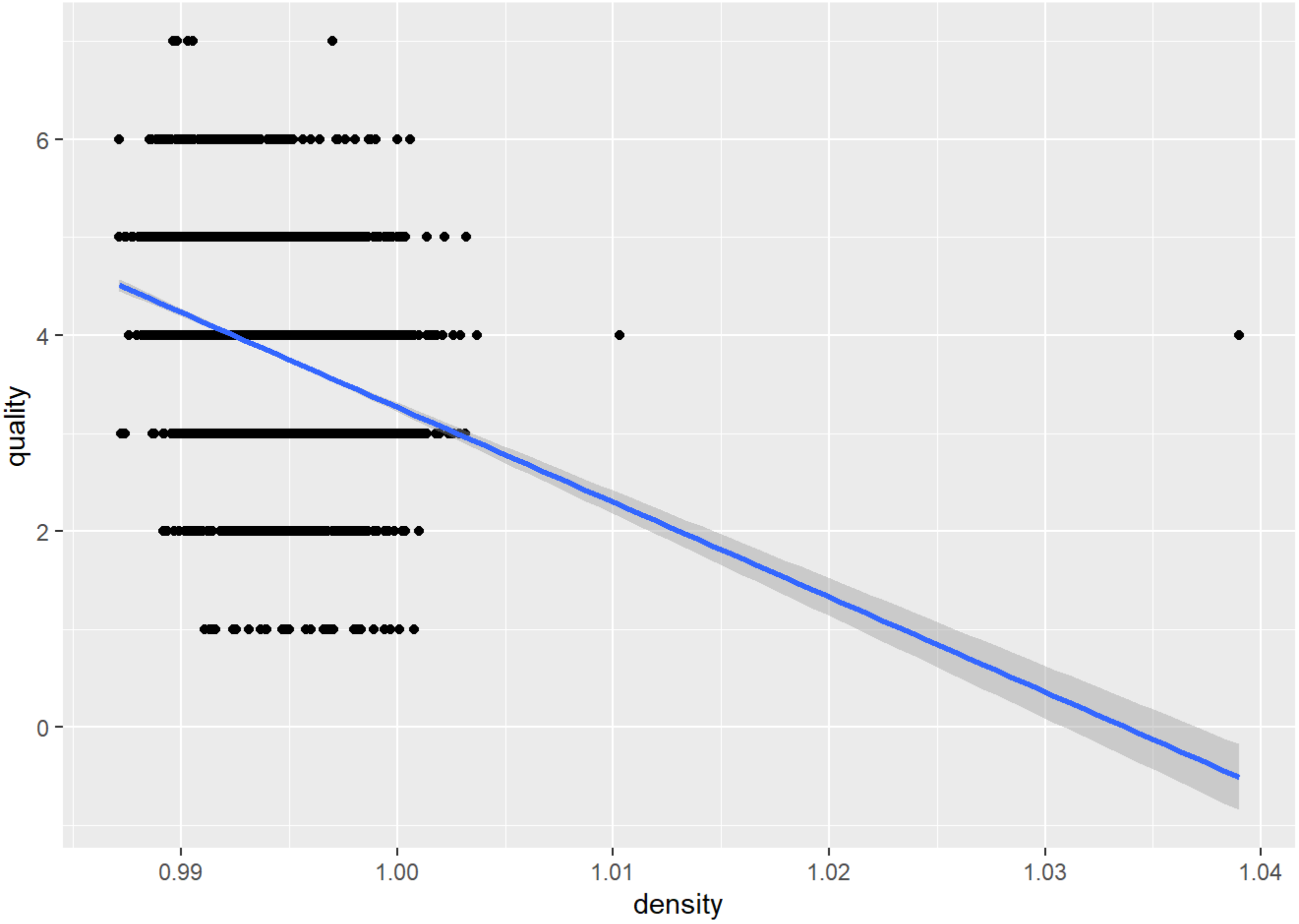

quality
6
4
2
0.0
0.5
1.0
1.5
citric.acid

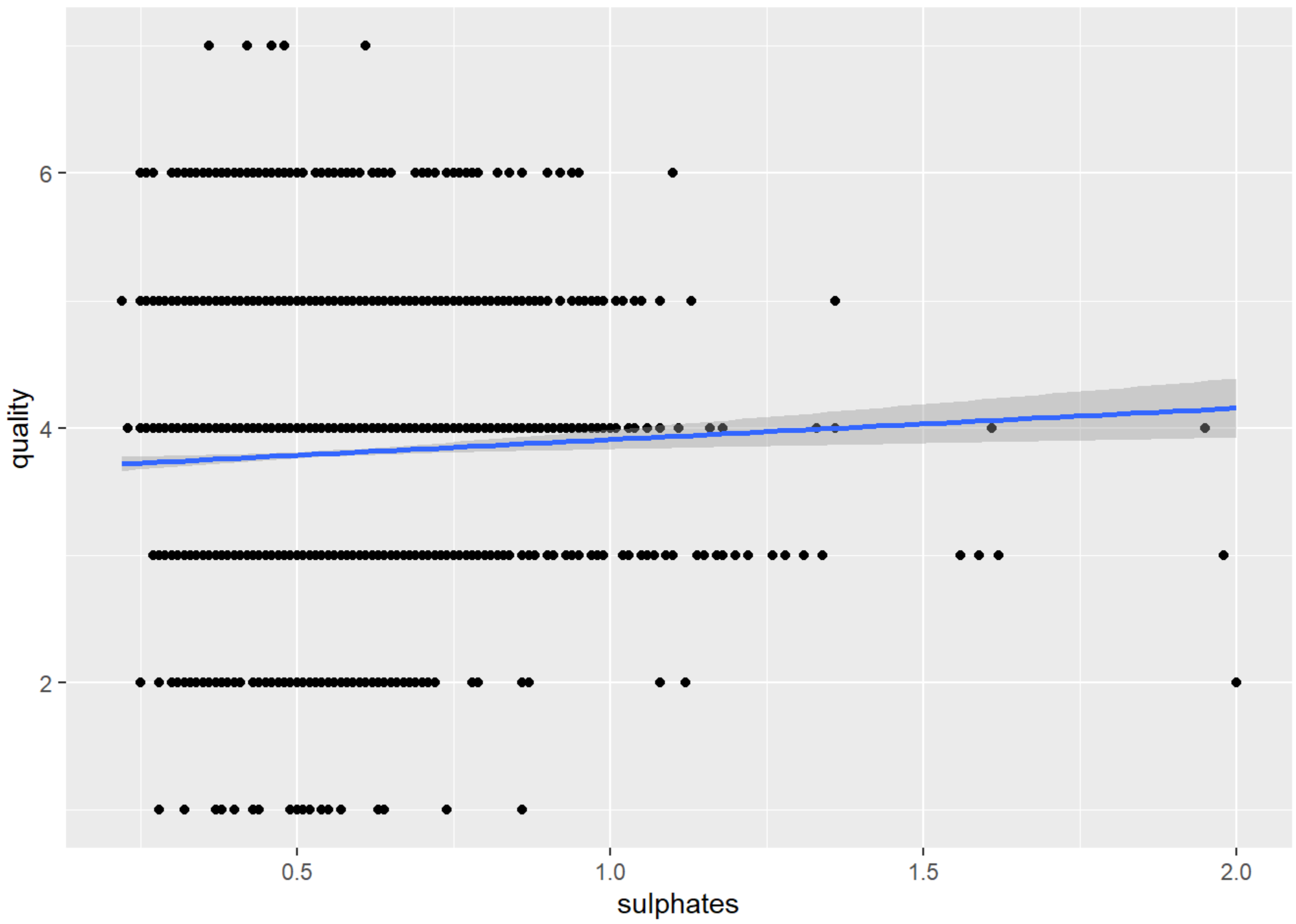

quality
6
4
2
0
20
40
60
residual.sugar


6
4
2
quality
0.0
0.2
0.4
0.6
chlorides


6
4
2
quality
0
100
200
300
free.sulfur.dioxide


quality
6
4
2
0
100
200
300
400
total.sulfur.dioxide


quality
6
4
2
0
0.99
1.00
1.01
1.02
1.03
1.04
density



Appendix (ii)

```
##       fixed.acidity     volatile.acidity       residual.sugar
##            4.483849             2.114120             5.232880
##           chlorides              density  free.sulfur.dioxide
##            1.455882            10.170734             3.598477
## total.sulfur.dioxide                  pH                color
##            6.570343             2.076801             7.231698
##           sulphates              alcohol
##            1.781381             2.577716
```

Appendix (iii)

```
##
## Call:
## glm(formula = quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     chlorides + density + free.sulfur.dioxide + total.sulfur.dioxide +
##     pH + color + sulphates + alcohol, family = binomial(), data = final)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -3.8361   0.0505   0.0707   0.0987   0.8752
##
## Coefficients:
##                        Estimate Std. Error z value Pr(>|z|)
## (Intercept)          -64.564099 196.414364  -0.329 0.742372
## fixed.acidity         -0.807737   0.218956  -3.689 0.000225 ***
## volatile.acidity      -5.319662   0.957892  -5.554  2.8e-08 ***
## residual.sugar        -0.032271   0.093590  -0.345 0.730237
## chlorides            -12.013227   3.742827  -3.210 0.001329 **
## density               88.301371 199.369972   0.443 0.657837
## free.sulfur.dioxide   -0.036657   0.010816  -3.389 0.000701 ***
## total.sulfur.dioxide   0.008427   0.006846   1.231 0.218290
## pH                    -4.446619   1.582166  -2.810 0.004947 **
## color                  2.865665   1.093708   2.620 0.008789 **
## sulphates              3.374793   1.959029   1.723 0.084945 .
## alcohol                0.299832   0.296180   1.012 0.311380
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 370.51  on 5319  degrees of freedom
## Residual deviance: 304.15  on 5308  degrees of freedom
## AIC: 328.15
##
## Number of Fisher Scoring iterations: 9
```

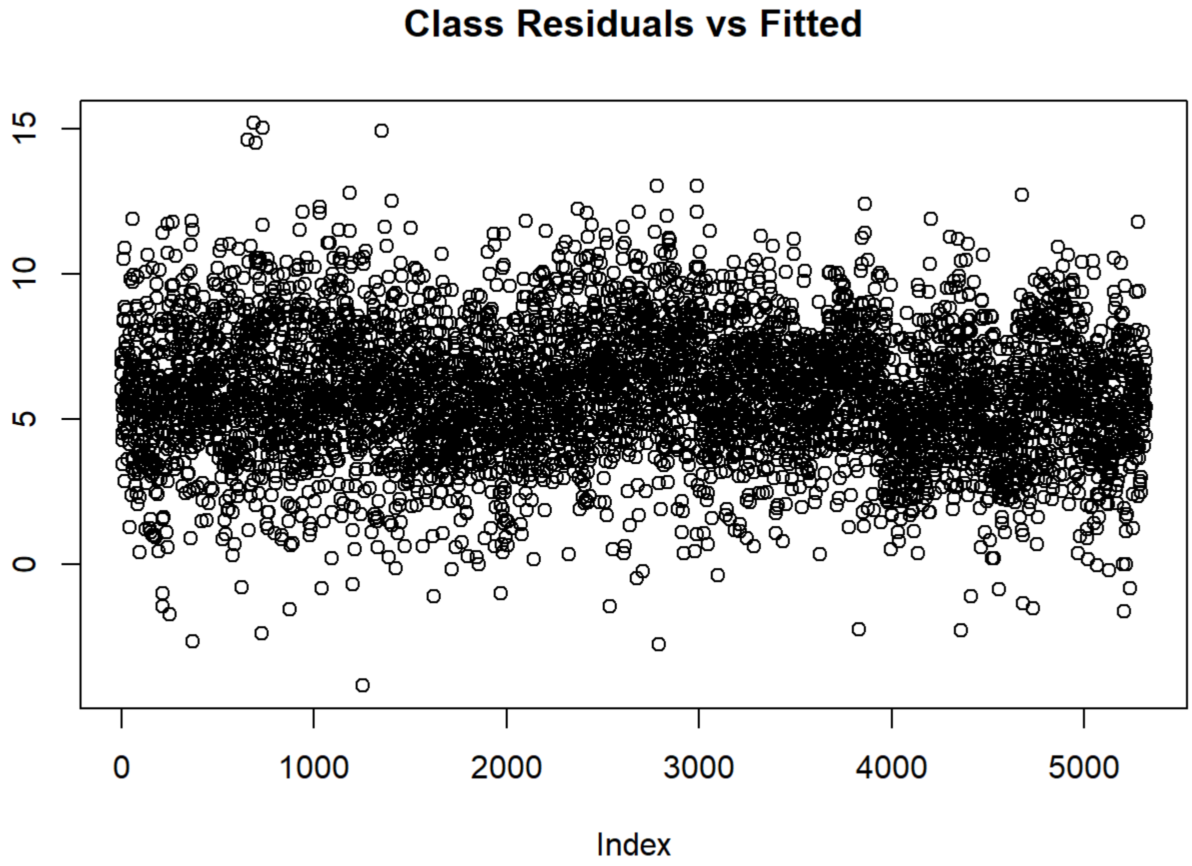
Appendix (iv)

```
## Start:  AIC=11719.3
## quality ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar +
##     chlorides + total.sulfur.dioxide + sulphates + alcohol
##
##                        Df   AIC
## - citric.acid           1 11717
## - fixed.acidity         1 11718
## <none>                    11719
## - chlorides             1 11724
## - total.sulfur.dioxide  1 11736
## - residual.sugar        1 11758
## - sulphates             1 11815
## - volatile.acidity      1 12027
## - alcohol               1 12790
##
## Step:  AIC=11717.31
## quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     chlorides + total.sulfur.dioxide + sulphates + alcohol
##
##                        Df   AIC
## - fixed.acidity         1 11716
## <none>                    11717
## - chlorides             1 11723
## - total.sulfur.dioxide  1 11735
## - residual.sugar        1 11756
## - sulphates             1 11813
## - volatile.acidity      1 12095
## - alcohol               1 12807
##
## Step:  AIC=11716.53
## quality ~ volatile.acidity + residual.sugar + chlorides + total.sulfur.dioxide +
##     sulphates + alcohol
##
##                        Df   AIC
## <none>                    11716
## - chlorides             1 11722
## - total.sulfur.dioxide  1 11733
## - residual.sugar        1 11755
## - sulphates             1 11812
## - volatile.acidity      1 12096
## - alcohol               1 12830
```

Appendix (V)

```
##                              Value   Std. Error    t value       p value
## volatile.acidity     -3.680594811 0.1920680588 -19.162972  7.544023e-82
## residual.sugar        0.043944326 0.0069212601   6.349180  2.164657e-10
## chlorides            -2.500683839 0.8868676528  -2.819681  4.807142e-03
## total.sulfur.dioxide -0.002620399 0.0006062559  -4.322266  1.544347e-05
## sulphates             1.963793250 0.2012843657   9.756313  1.733431e-22
## alcohol               0.905261810 0.0285225223  31.738491 4.577244e-221
## 3|4                   3.192979759 0.4001568320   7.979321  1.471406e-15
## 4|5                   5.348236534 0.3619094681  14.777830  2.036220e-49
## 5|6                   8.378000222 0.3628078594  23.092113 5.556908e-118
## 6|7                  11.002758103 0.3796697579  28.979812 1.182151e-184
## 7|8                  13.345507455 0.3960133694  33.699639 5.851558e-249
## 8|9                  16.841969138 0.5930228029  28.400205 2.010367e-177
```

Appendix (vi)


Class Residuals vs Fitted
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