Group 18

Red Wine Quality

Inferential Analysis

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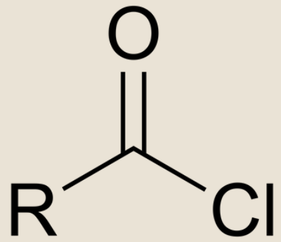
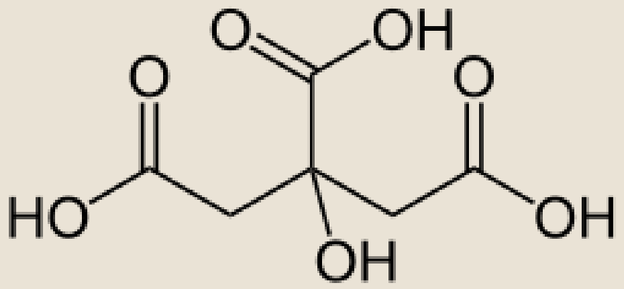
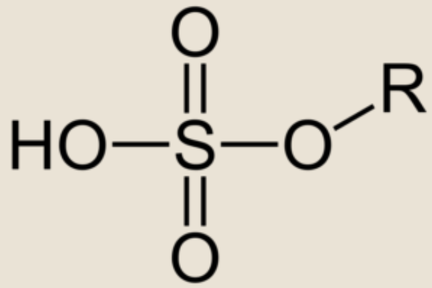
Goal of our analysis

Investigating how physiochemical properties affect the quality of the Portuguese "Vinho Verde" red wine.

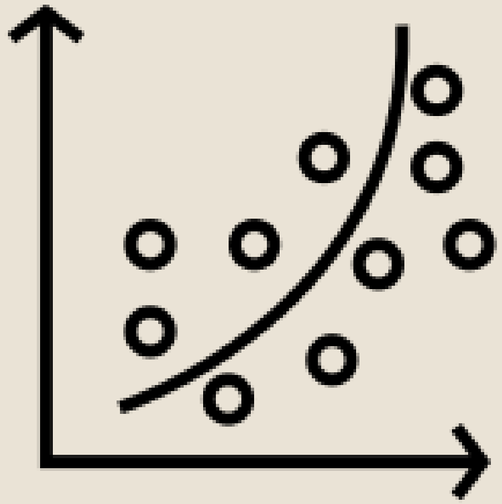






Models:

- Ordered multinomial model
- Binomial model



Conclusions:

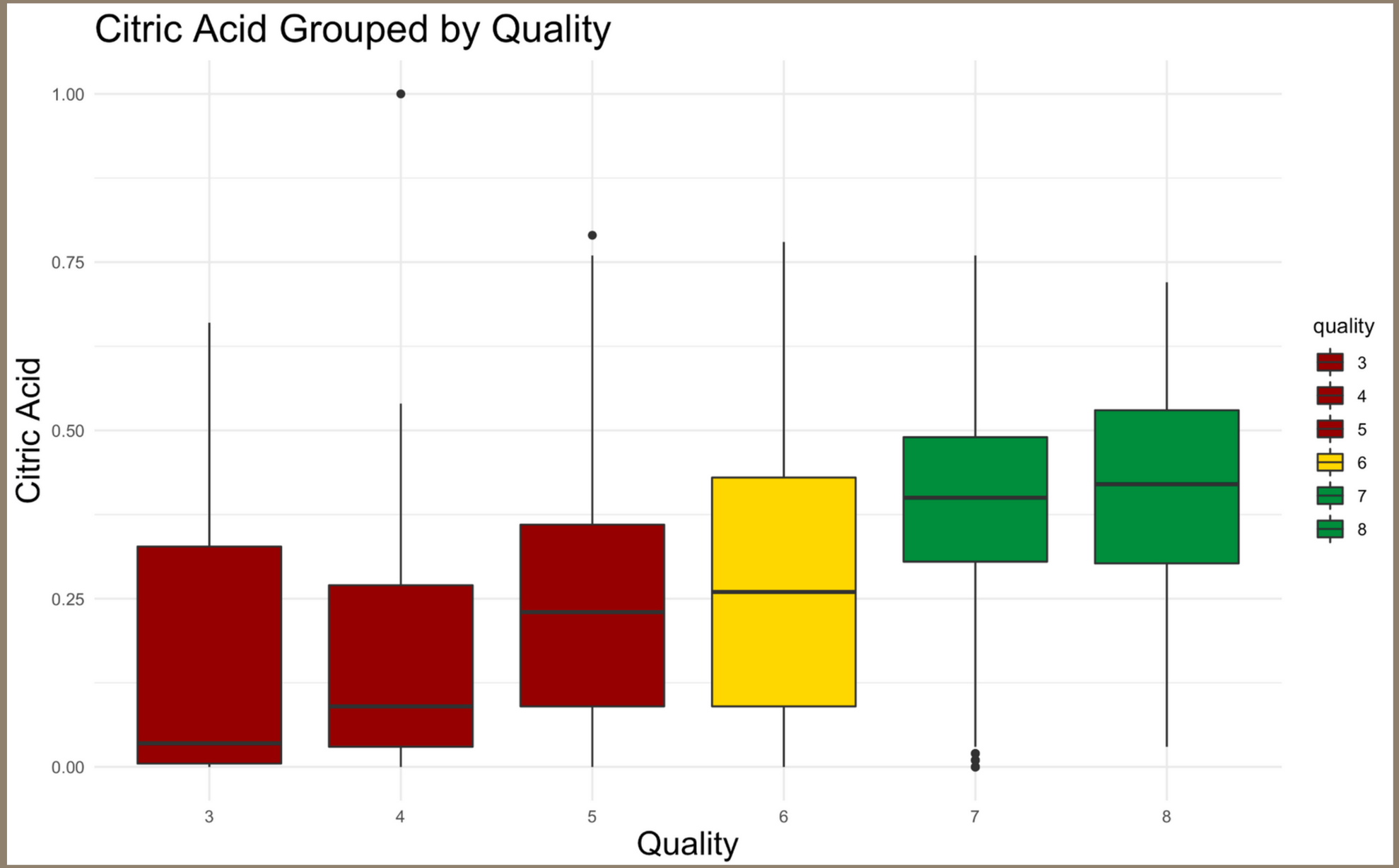
The two models lead us to very similar results

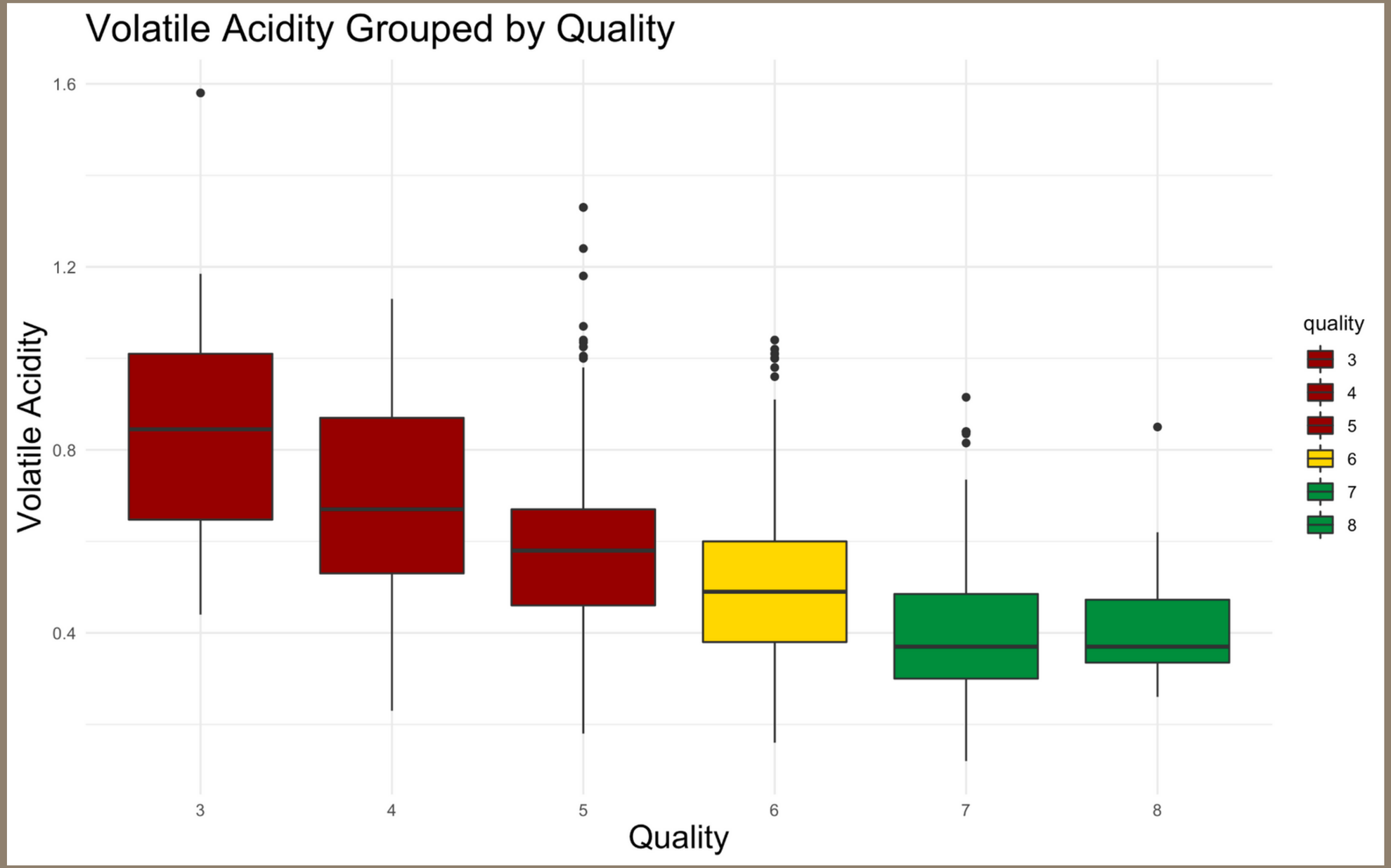
Dataset

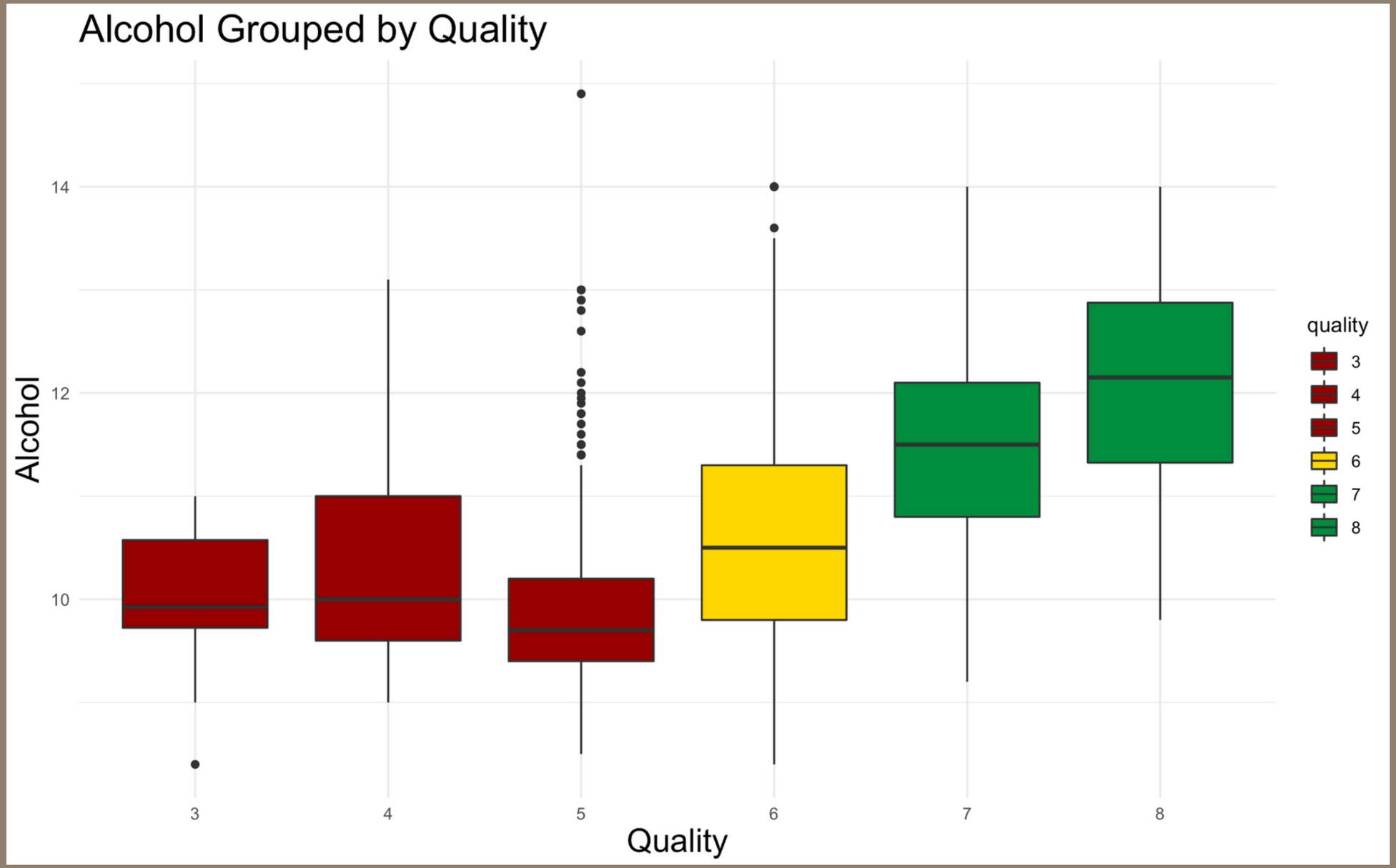
11 numerical variables
1 categorical response

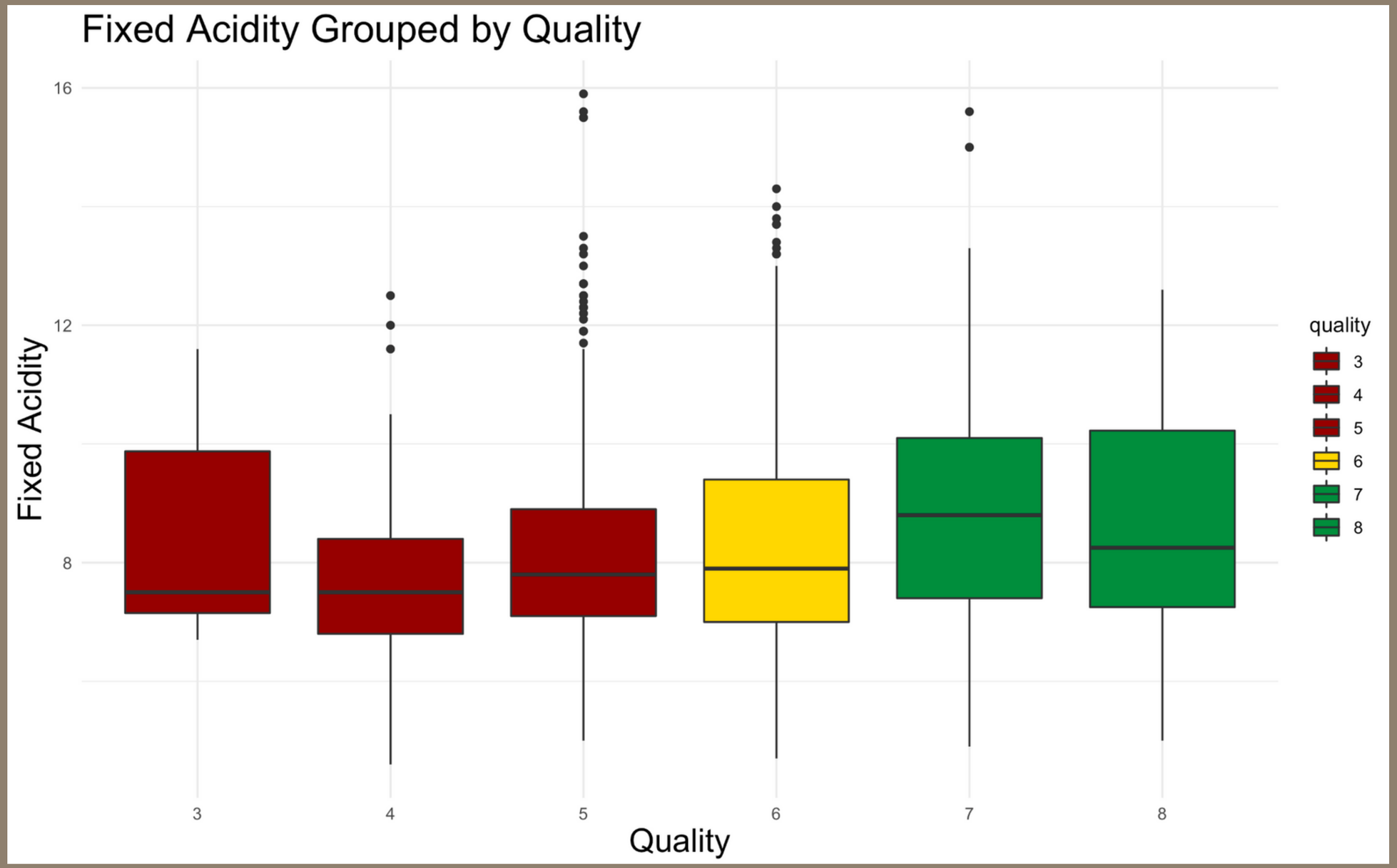
- **Quality**: quality on a sale from 3 to 8
- **Fixed acidity**: most of the acids in wine
- **Volatile acidity**: the amount of acetic acid, which in high quantities can lead to an unpleasant vinegar taste
- **Citric acid**: found in small quantities, it adds freshness and flavour to wine
- **Residual sugar**: sugars remaining after fermentation stops

- **Chlorides**: the amount of salt in wine
- **Free sulfur dioxide**: prevents microbial growth and fermentation of wine
- **Total sulfur dioxide**: sum of free and bound sulfur dioxide, in high concentrations it becomes evident in taste and nose
- **Density**: close to density of water
- **pH**: how acid the wine is. Most wines are between 3 and 4
- **Sulphates**: added to wine because it's an antimicrobilal and antioxidant
- **Alcohol**: amount of alcohol in the wine

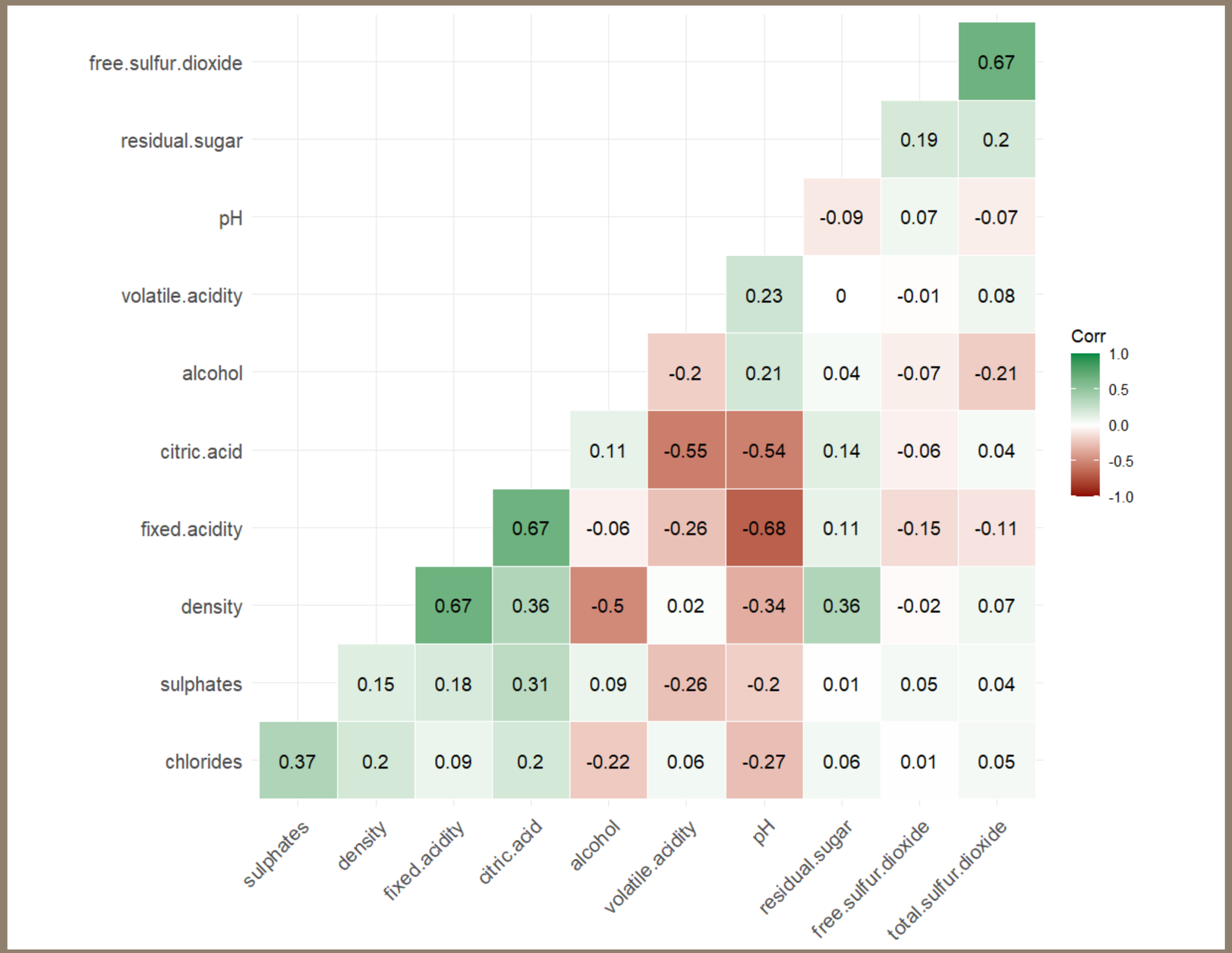

Citric Acid Grouped by Quality
Citric Acid
1.00
0.75
0.50
0.25
0.00
3
4
5
6
7
8
Quality
quality
3
4
5
6
7
8


Volatile Acidity Grouped by Quality
Volatile Acidity
1.6
1.2
0.8
0.4
3
4
5
6
7
8
Quality
quality
3
4
5
6
7
8


Alcohol Grouped by Quality
Alcohol
14
12
10
3
4
5
6
7
8
Quality
quality
3
4
5
6
7
8

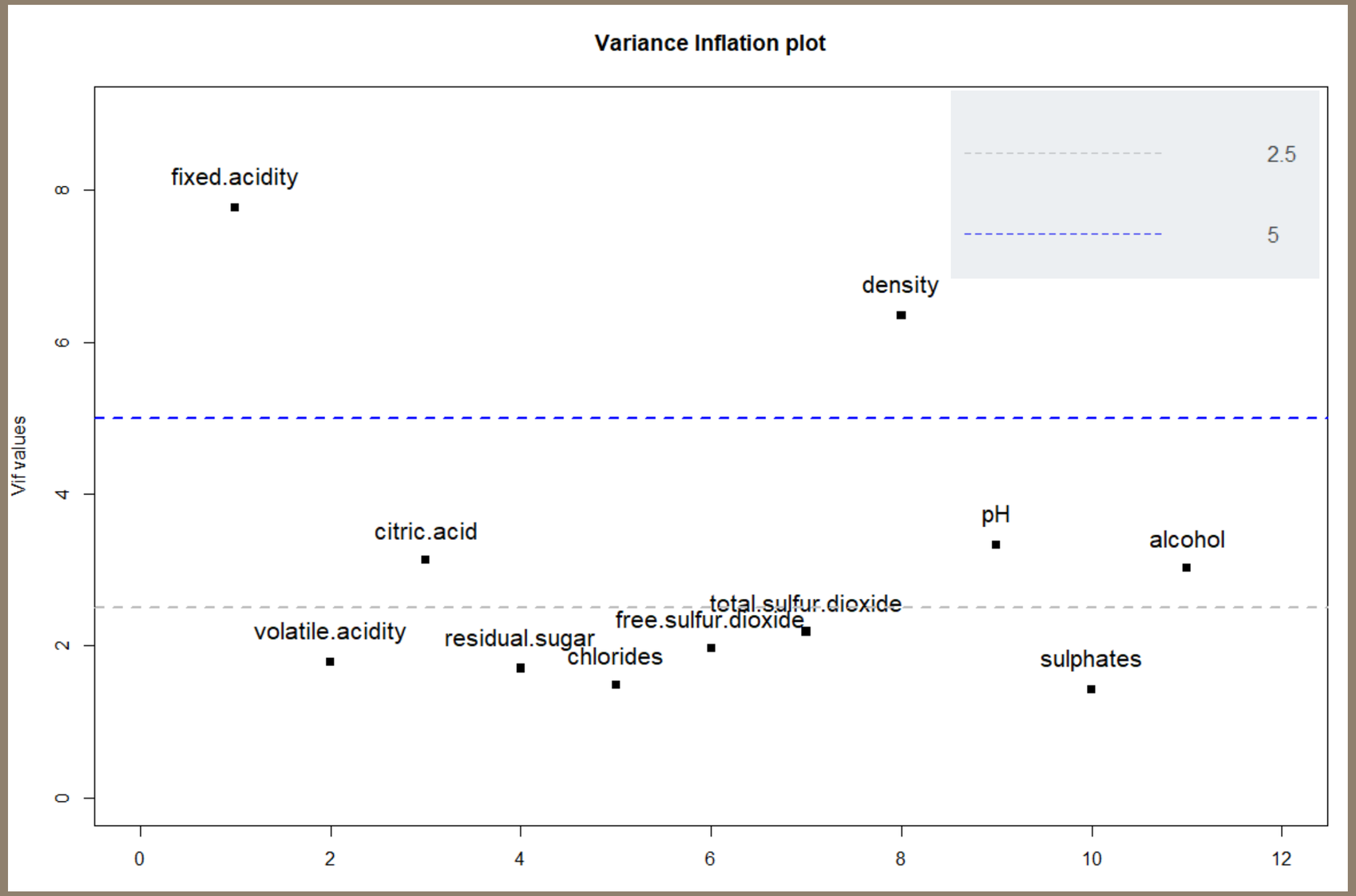

Fixed Acidity Grouped by Quality
16
12
8
Fixed Acidity
3
4
5
6
7
8
Quality
quality
3
4
5
6
7
8

Correlation matrix with initial variables



VIF

Fixed acidity and density above the VIF=5 conventional threshold



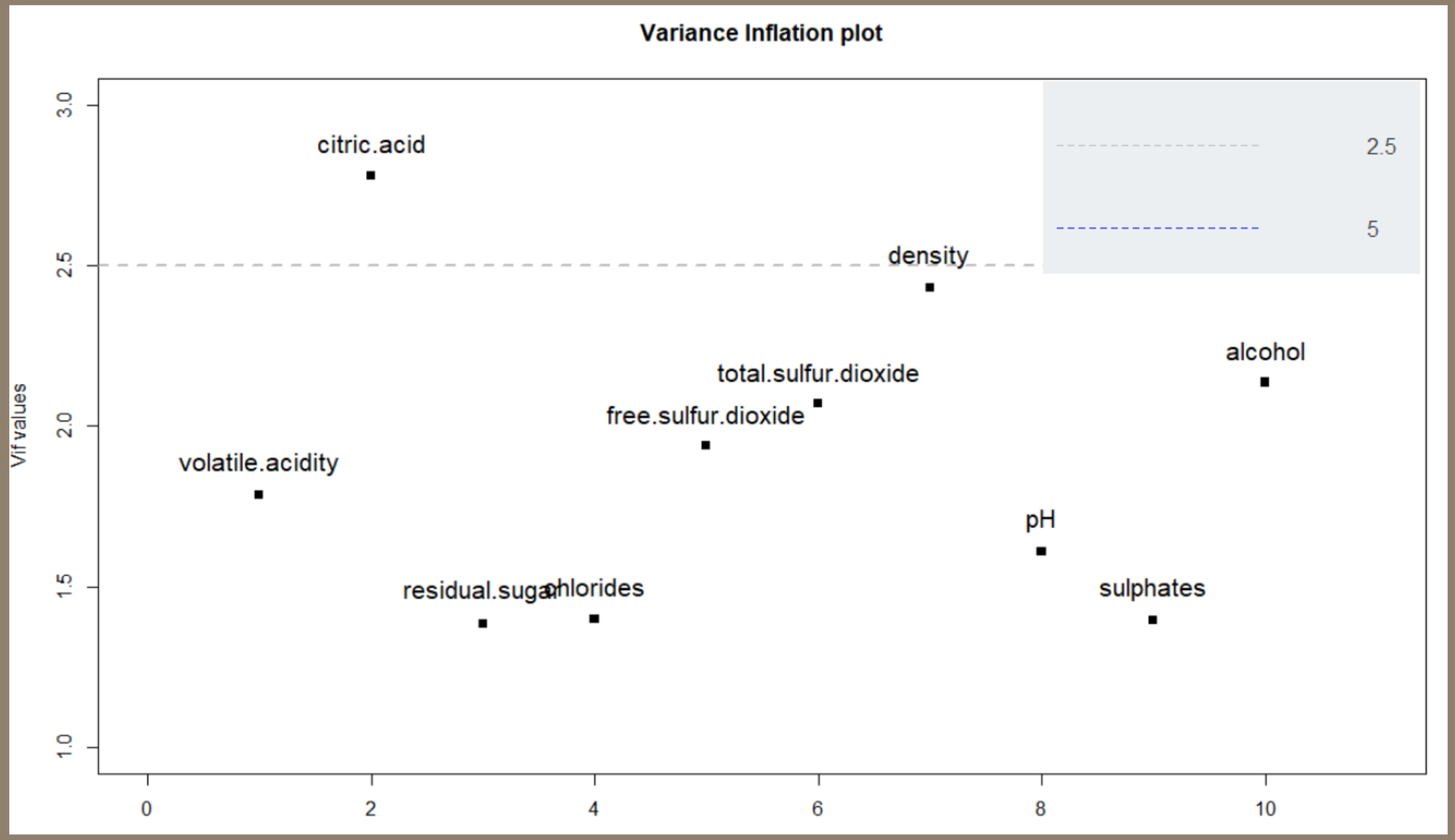
Variable selection

Fixed Acidity vs All other variables: R-squared 0.8713

Total sulfur dioxide - free sulfur dioxide ⟶ Bound sulfur dioxide

VIF

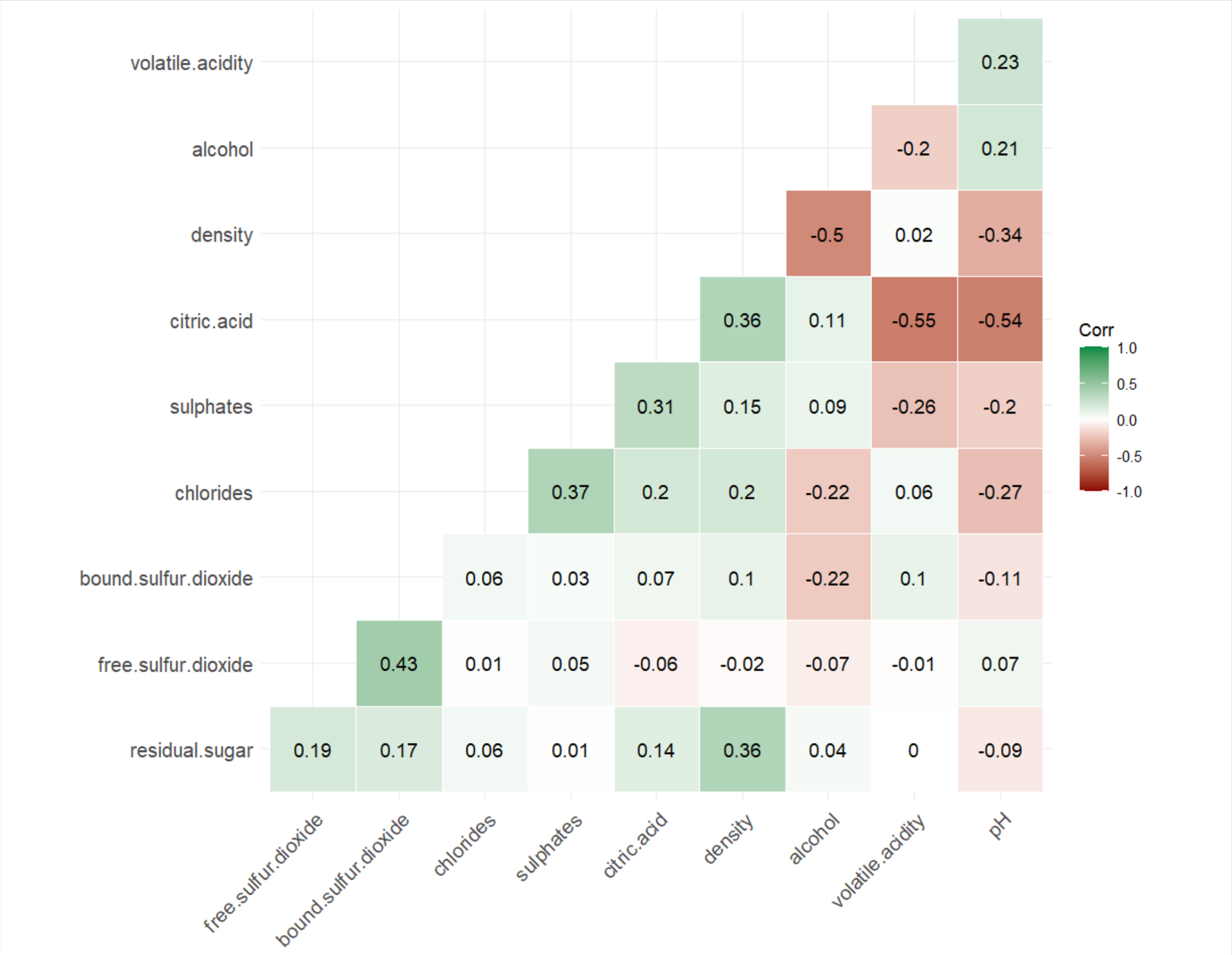
No problems anymore with any variable



Variable selection

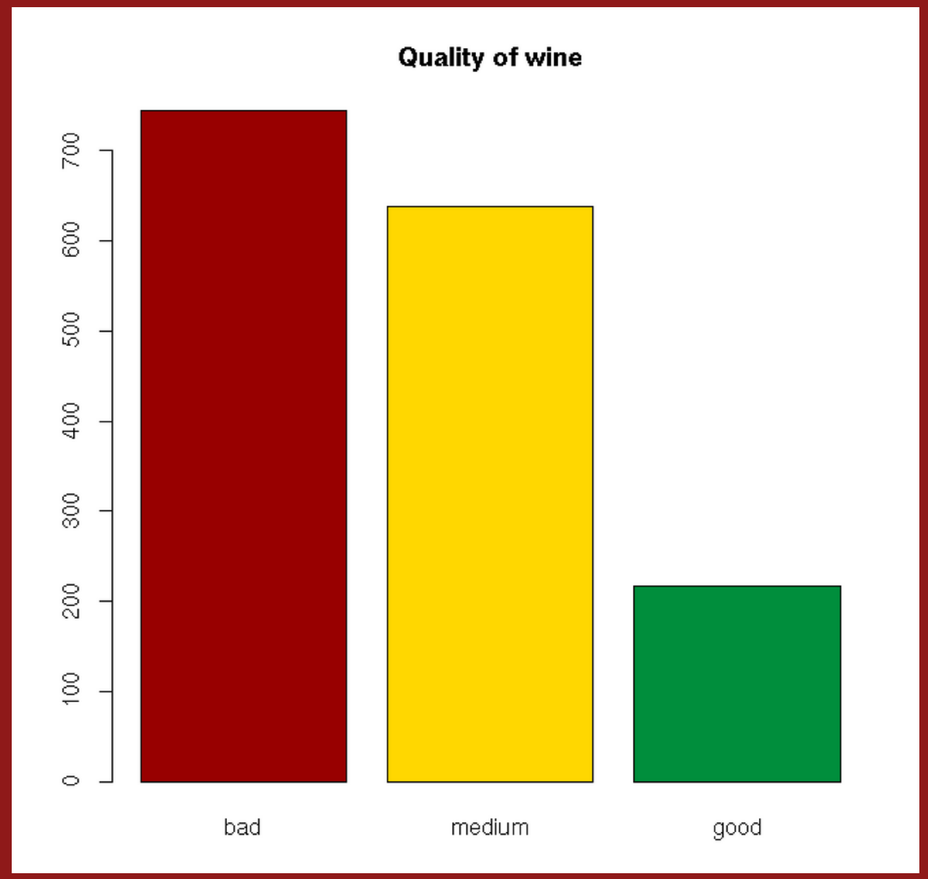
Fixed Acidity vs All other variables: R-squared 0.8713

Total sulfur dioxide - free sulfur dioxide ⟶ Bound sulfur dioxide



Correlation matrix with initial variables

Ordered Multinomial Model



Grades 3, 4 and 5 → bad

Grade 6 → medium

Grades 7 and 8 → good

Mathematical aspects

$$\gamma_{ij} = P(Y_i \leq j)$$

Cumulative probabilities

$$g(\gamma_{ij}) = \theta_j - \beta^T x_i$$

General form of the link function

$$\log\left(\frac{\gamma_{ij}}{1-\gamma_{ij}}\right)$$

Log-odds function

Final model

$$logit(P(\text{bad})) = 5.17 - 2.80x_1 - 5.91x_2 - 1.04x_3 + 3.01x_4 + 0.90x_5 - 0.02x_6$$

$$logit(P(\text{medium or bad})) = 8.06 - 2.80x_1 - 5.91x_2 - 1.04x_3 + 3.01x_4 + 0.90x_5 - 0.02x_6$$

Coefficients:

		Value	Std. Error	t value	p value
x_1	volatile.acidity	-2.80816	0.34939	-8.037	9.189600e-16
x_2	chlorides	-5.91108	1.37260	-4.306	1.658703e-05
x_3	pH	-1.04281	0.38016	-2.743	6.087140e-03
x_4	sulphates	3.01230	0.36389	8.278	1.252269e-16
x_5	alcohol	0.90718	0.05916	15.333	4.584314e-53
x_6	bound.sulfur.dioxide	-0.01761	0.00241	-7.308	2.716690e-13

Intercepts:

		Value	Std. Error	t value	p value
θ_1	bad|medium	5.1728	1.3022	3.9724	7.113811e-05
θ_2	medium|good	8.0583	1.3144	6.1309	8.736129e-10

Residual Deviance: 2457.885
AIC: 2473.885

Model Selection

Criterion-based test:

- AIC
- BIC

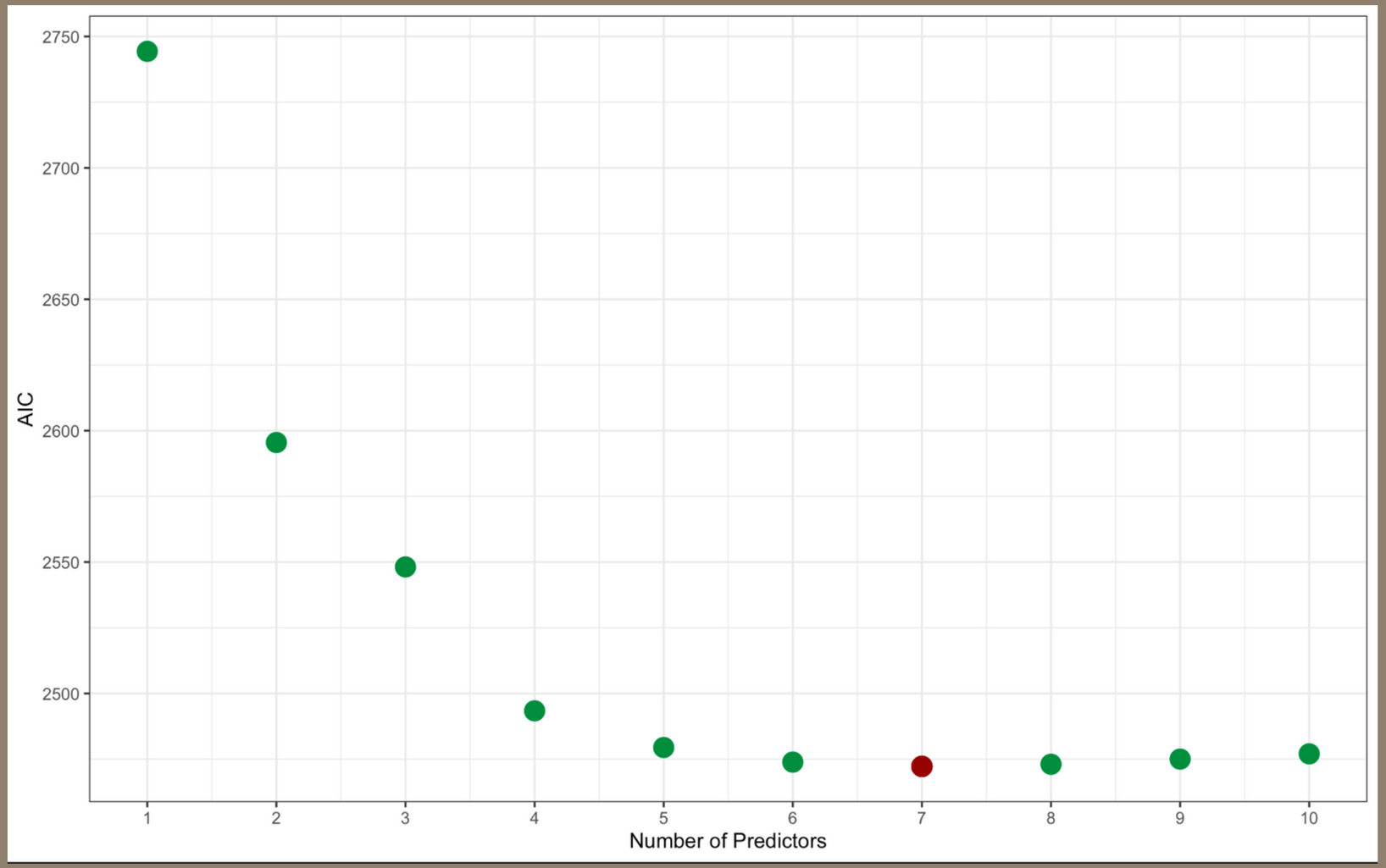
Testing-based procedures:

- Single term deletion with "Chi Square" test

Comparison with the full model:

ANOVA with X^2 test

AIC



7 predictors

- volatile acidity
- chlorides
- pH
- sulphates
- alcohol
- bound sulphur dioxide
- residual sugar

Alternative model

with 7 variables

Coefficients:

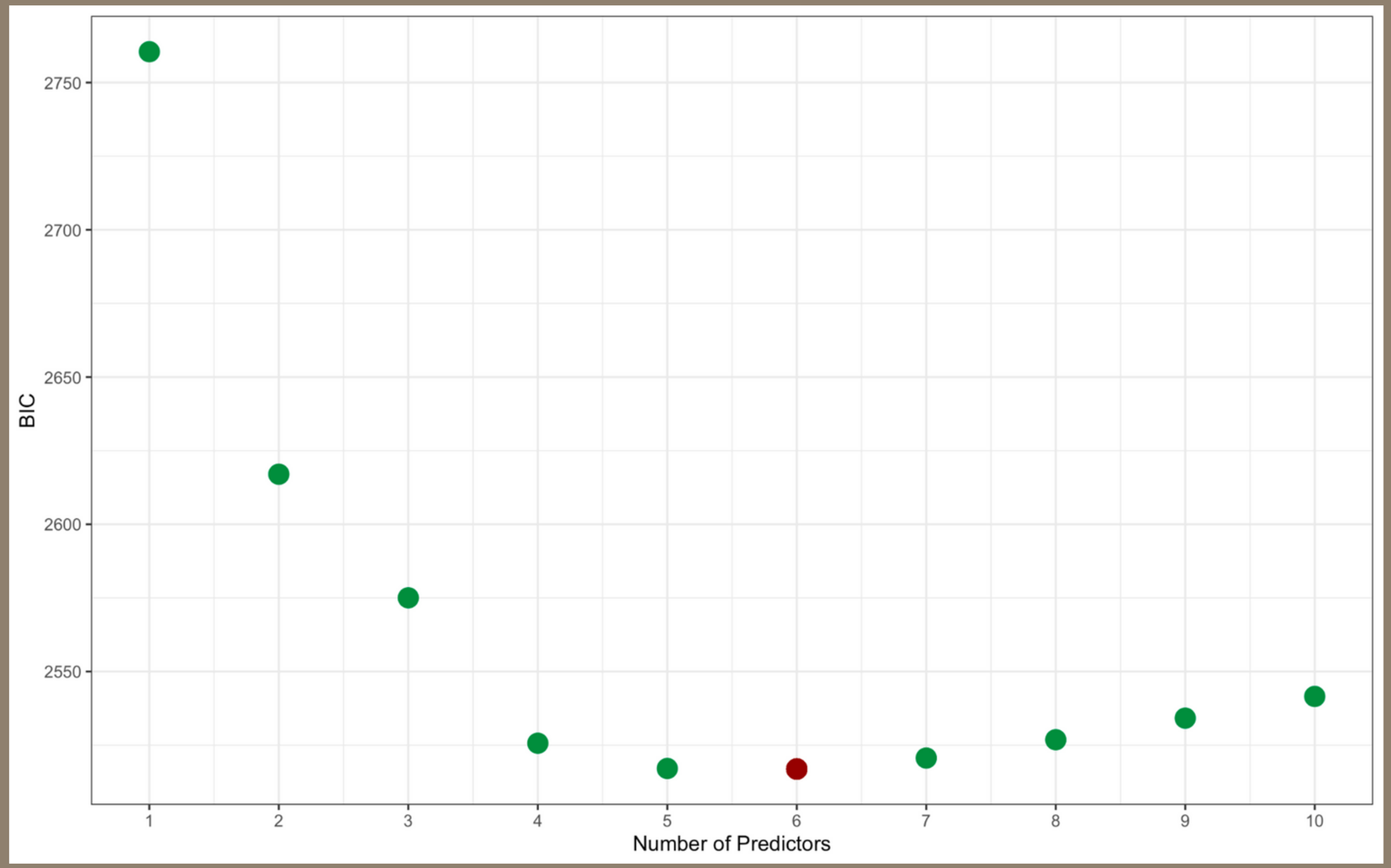
		Value	Std. Error	t value	p value
x_1	volatile.acidity	-2.81720	0.350156	-8.046	0.000
x_2	chlorides	-6.09406	1.387370	-4.393	0.000
x_3	pH	-0.99637	0.381419	-2.612	0.009
x_4	sulphates	3.05175	0.364630	8.369	0.000
x_5	alcohol	0.89775	0.059351	15.126	0.000
x_6	bound.sulfur.dioxide	-0.01851	0.002471	-7.492	0.000
x_7	residual.sugar	0.07500	0.038838	1.931	0.053

Intercepts:

		Value	Std. Error	t value	p value
θ_1	bad|medium	5.3962	1.3093	4.1215	0.000
θ_2	medium|good	8.2849	1.3216	6.2687	0.000

Residual Deviance: 2454.24
AIC: 2472.24

BIC



6 predictors

- volatile acidity
- chlorides
- pH
- sulphates
- alcohol
- bound sulphur dioxide

Stepwise elimination

Based on "Chi square" test

```
Single term deletions

Model:
quality ~ volatile.acidity + chlorides + pH + sulphates + alcohol +
    bound.sulfur.dioxide + residual.sugar
                      Df    AIC     LRT  Pr(>Chi)
<none>                     2472.2
volatile.acidity       1 2539.0  68.757 < 2.2e-16 ***
chlorides              1 2491.3  21.084 4.396e-06 ***
pH                     1 2477.1   6.846  0.008884 **
sulphates              1 2544.4  74.127 < 2.2e-16 ***
alcohol                1 2727.9 257.660 < 2.2e-16 ***
bound.sulfur.dioxide   1 2534.0  63.797 1.379e-15 ***
residual.sugar         1 2473.9   3.645  0.056229 .
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

The test suggests using a model with 6 variables

Statistical tests

"Chi square" test of LR

	Resid. df	Resid. Dev	Test	Df	LR stat.	Pr(Chi)
Final model	1591	2457.885				
Total model	1587	2453.016	1 vs 2	4	4.869737	0.3009263

H0: the parameters we removed are all equal to 0

We can remove these variables:

- Citric acid
- Free sulphur dioxide
- Density
- Residual sugar

Model diagnostic

Proportional odds assumption:

Test for	X2	df	probability
Omnibus	7.36	6	0.29
volatile.acidity	0.51	1	0.47
chlorides	1.36	1	0.24
pH	2.88	1	0.09
sulphates	1.08	1	0.3
alcohol	1.29	1	0.26
bound.sulfur.dioxide	0.05	1	0.82

H0: Parallel Regression Assumption holds

Brant test

$$\begin{cases} \mathrm{H}_0 : \ \beta_k = \beta \\ \mathrm{H}_1 : \ \beta_k = \phi_k \beta \end{cases}$$

$$logit\left(\gamma_1(x)\right) - logit\left(\gamma_2(x)\right) = \theta_1 - \theta_2$$

Model diagnostic

Test for goodness of fit: Hosmer-Lemeslow test

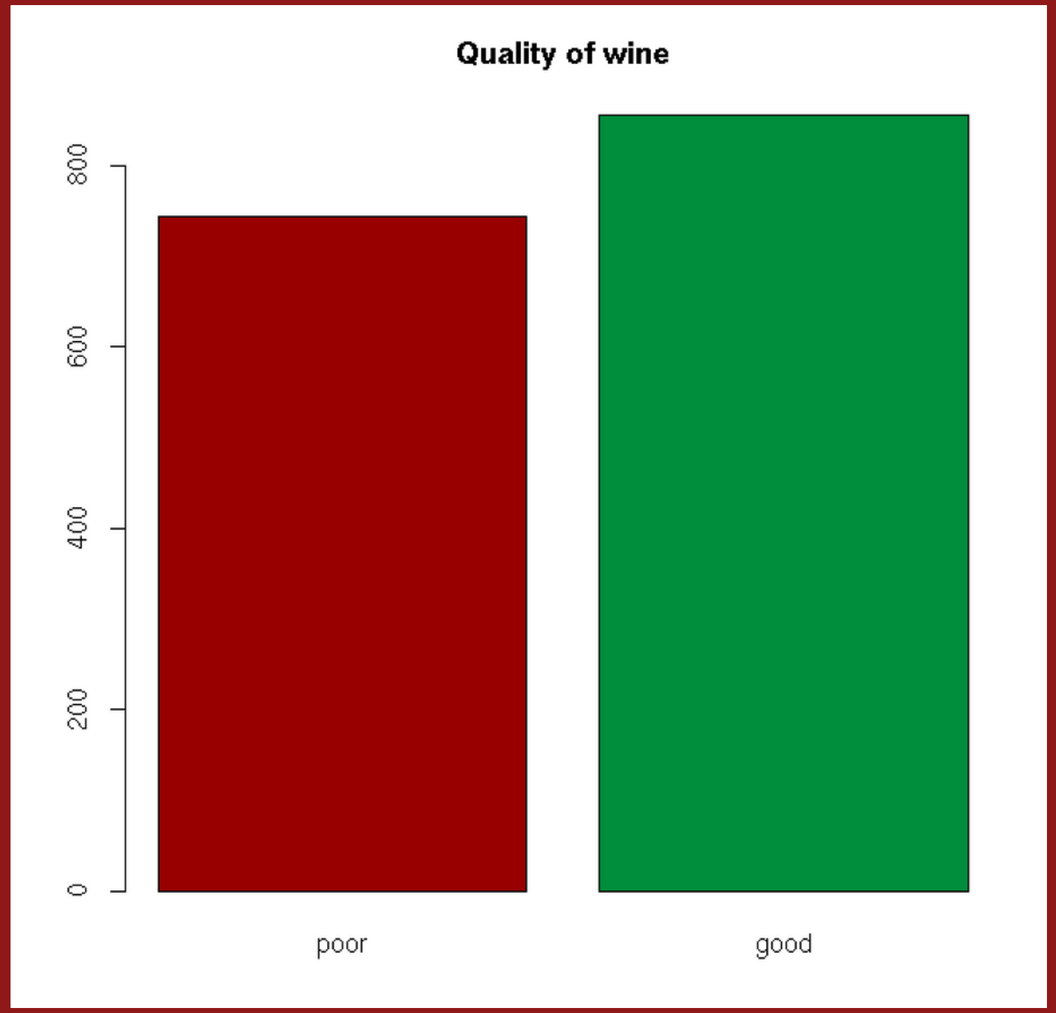
```
        Hosmer and Lemeshow test (ordinal model)

data:  data2$quality, fitted(poltt)
X-squared = 24.835, df = 17, p-value = 0.09847
```

$$\begin{cases} \boldsymbol{H_0: Model\ suits\ the\ data} \\ \boldsymbol{H_1: Model\ doesn't\ suit\ the\ data} \end{cases}$$

$$X^2_{LS} = \sum_{j=1}^{J} \frac{(y_j - m_j\hat{p}_j)^2}{m_j\hat{p}_j(1-\hat{p}_j)}$$

Binomial Model



Grades 3, 4, and 5 → bad
Grades 6, 7, and 8 → good

With the division we chose, both categories are well represented

Mathematical aspects

$$Y_i \sim Bin(n_i, p_i)$$

Binomial Distribution

$$P(Y_i = y_i) = \binom{n_i}{y_i} p_i^{y_i}(1 - p_i)^{n_i - p_i}$$

$$\eta = log(\frac{p}{1-p}) = \beta_0 + \beta_1 x_1 + .. + \beta_q x_q$$

Logit Link Model

$$p = g^{-1}(\eta) = \frac{e^\eta}{e^\eta + 1}$$

Inverse of Logit

Final Model

$$\eta_i = -8.10 - 2.91x_1 - 4.45x_2 + 0.86x_3 + 2.71x_4 - 0.02x_5$$

```
   Coefficients:
                          Estimate Std. Error z value Pr(>|z|)
   (Intercept)            -8.09506    0.80702 -10.031  < 2e-16 ***
x1 volatile.acidity       -2.91314    0.37034  -7.866 3.66e-15 ***
x2 chlorides              -4.45501    1.43196  -3.111  0.00186 **
x3 alcohol                 0.86127    0.07078  12.168  < 2e-16 ***
x4 sulphates               2.71473    0.42875   6.332 2.43e-10 ***
x5 bound.sulfur.dioxide   -0.01639    0.00244  -6.718 1.84e-11 ***
   ---

       Null deviance: 2209.0  on 1598  degrees of freedom
   Residual deviance: 1665.7  on 1593  degrees of freedom
```

Model Selection

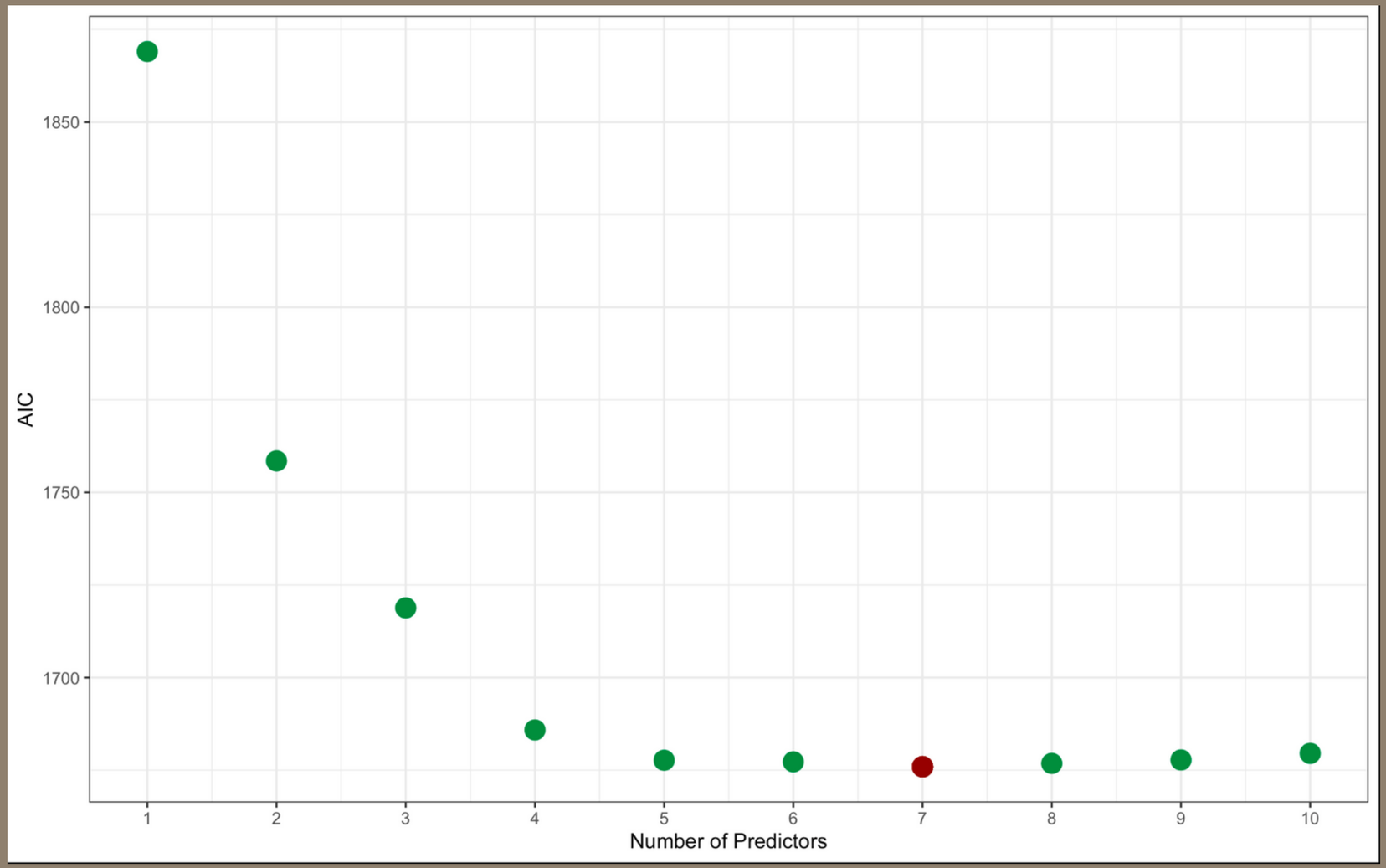
Criterion-based test:

- AIC
- BIC

Testing-based procedures:

- Backward elimination

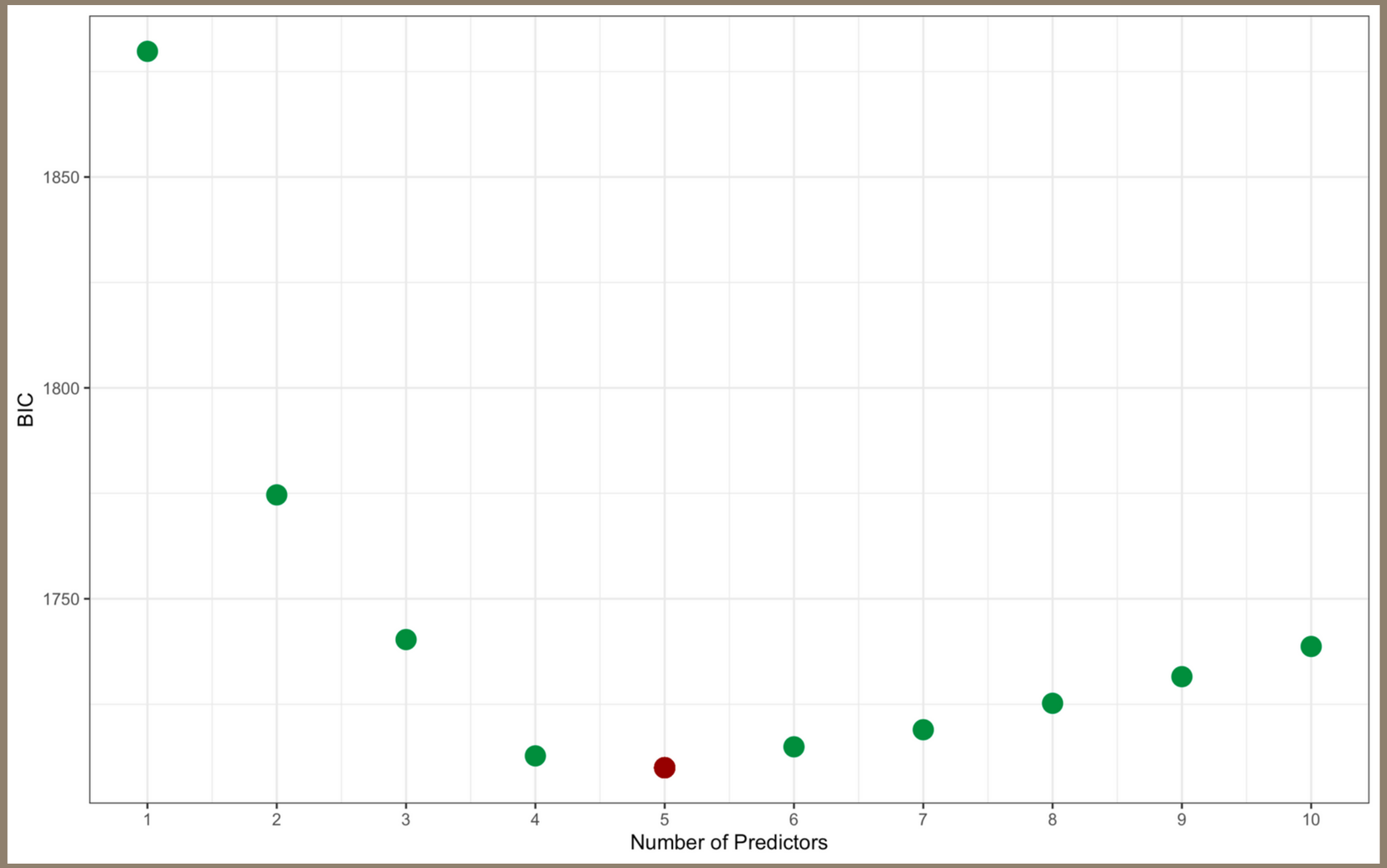
AIC



7 predictors

- volatile acidity
- chlorides
- sulphates
- alcohol
- bound sulphur dioxide
- citric acid
- pH

BIC



5 predictors

- volatile acidity
- chlorides
- sulphates
- alcohol
- bound sulphur dioxide

Model Selection

Criterion-based test:

- AIC
- BIC

Testing-based procedures:

- Backward elimination

To compare the models:

- ANOVA with χ^2 test

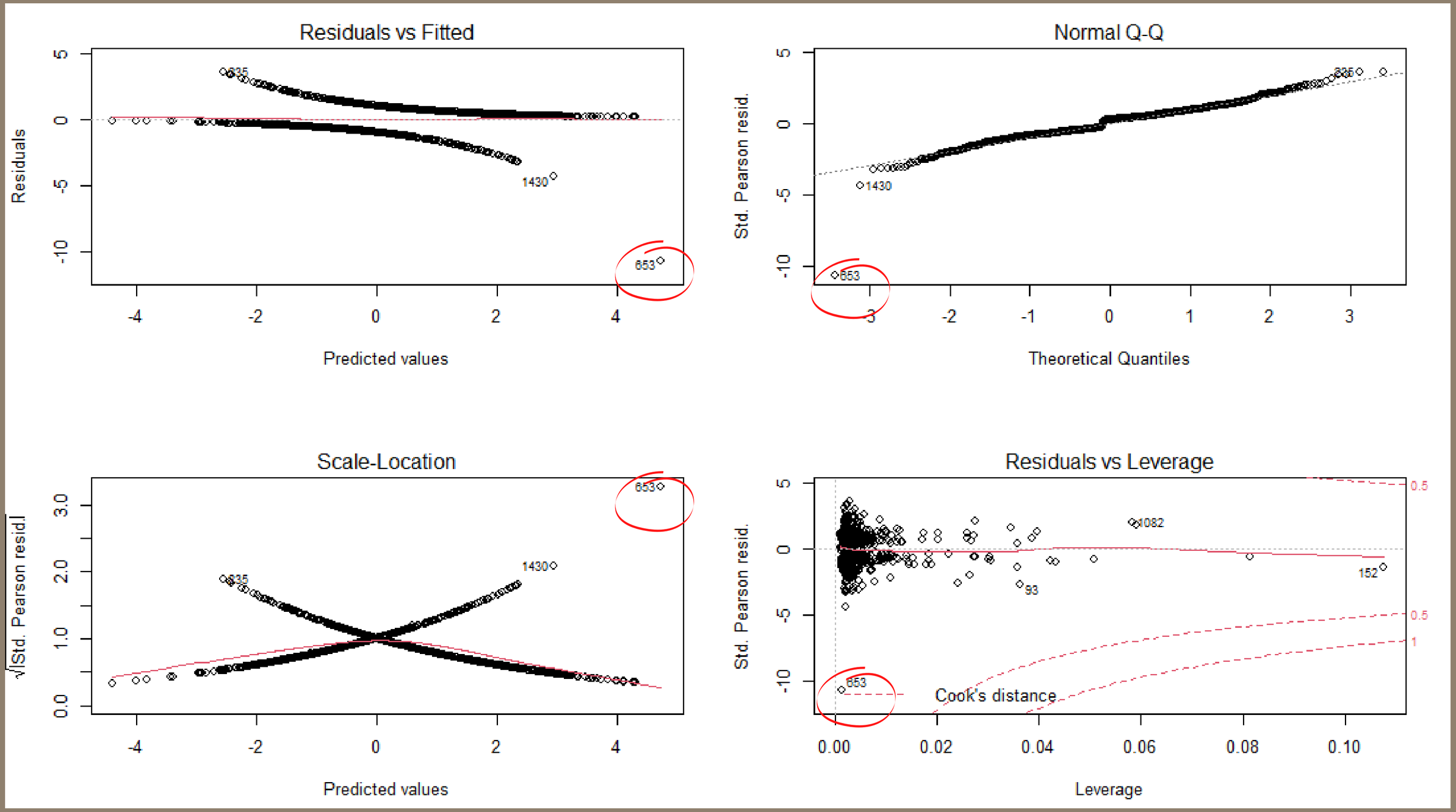
p-value: 0.1487

Goodness of fit:

- Hosmer-Lemeshow test

p-value: 0.7571

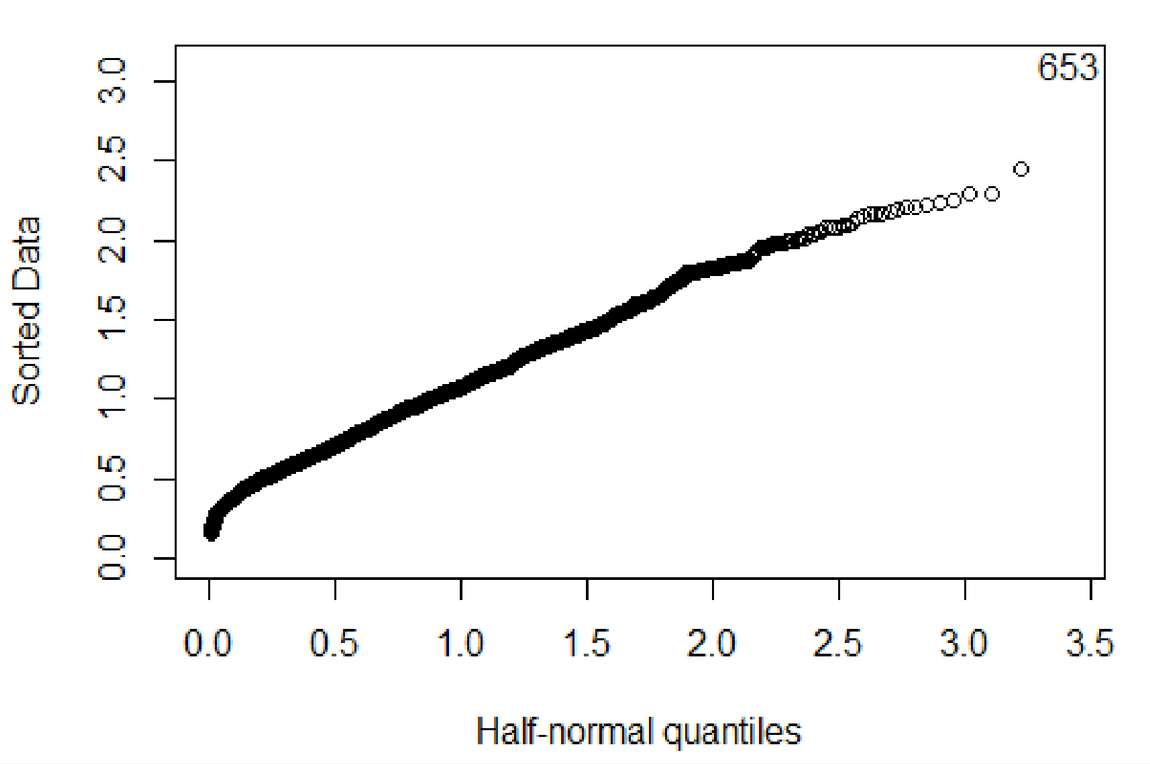
$$\begin{cases} H_0: Model\ suits\ the\ data \\ H_1: Model\ doesn't\ suit\ the\ data \end{cases}$$


Residuals vs Fitted
Residuals
Predicted values
635
1430
653
Normal Q-Q
Std. Pearson resid.
Theoretical Quantiles
635
1430
653
Scale-Location
√|Std. Pearson resid.|
Predicted values
653
1430
635
Residuals vs Leverage
Std. Pearson resid.
Leverage
Cook's distance
1082
152
93
653
0.5
0.5
1

Model Diagnostic

Checking for outliers

Studentized residuals in halfnorm plot:



Test:

$$|t_i| > t_{\alpha/(2*n)}(n-p-1)$$

$$t_{\alpha/(2*n)}(n-p-1) = 4.17604$$

$$\begin{cases} H_0 : i\text{-th observation is not an outlier} \\ H_1 : i\text{-th observation is an outlier} \end{cases}$$

Model Diagnostic

Checking for influential observations

- Cook's distance
- dfbeta function observation n° 755

summary estimates with 755

```
Coefficients:
                    Estimate Pr(>|z|)
(Intercept)         -8.09506  < 2e-16 ***
volatile.acidity    -2.91314 3.66e-15 ***
chlorides           -4.45501  0.00186 **
alcohol              0.86127  < 2e-16 ***
sulphates            2.71473 2.43e-10 ***
bound.sulfur.dioxide -0.01639 1.84e-11 ***
```

summary estimates without 755

```
Coefficients:
                    Estimate Pr(>|z|)
(Intercept)         -8.07995  < 2e-16 ***
volatile.acidity    -2.90497 4.47e-15 ***
chlorides           -4.84960 0.000959 ***
alcohol              0.86143  < 2e-16 ***
sulphates            2.72851 2.11e-10 ***
bound.sulfur.dioxide -0.01632 2.23e-11 ***
```

To Sum Up:

- Data visualisation
- Data manipulation
- Model selection
- Model diagnostic

CONCLUSIONS

BINOMIAL MODEL:

	Estimate
(Intercept)	-8.09506
volatile.acidity	-2.91314
chlorides	-4.45501
alcohol	0.86127
sulphates	2.71473
bound.sulfur.dioxide	-0.01639

MULTINOMIAL MODEL:

Coefficients:

	Value
volatile.acidity	-2.80816
chlorides	-5.91108
pH	-1.04281
sulphates	3.01230
alcohol	0.90718
bound.sulfur.dioxide	-0.01761

Intercepts:

	Value	Std. Error
bad|medium	5.1728	1.3022
medium|good	8.0583	1.3144

Conclusions

Initial goal: finding how physiochemical properties affect the quality of the Portuguese "Vinho Verde"

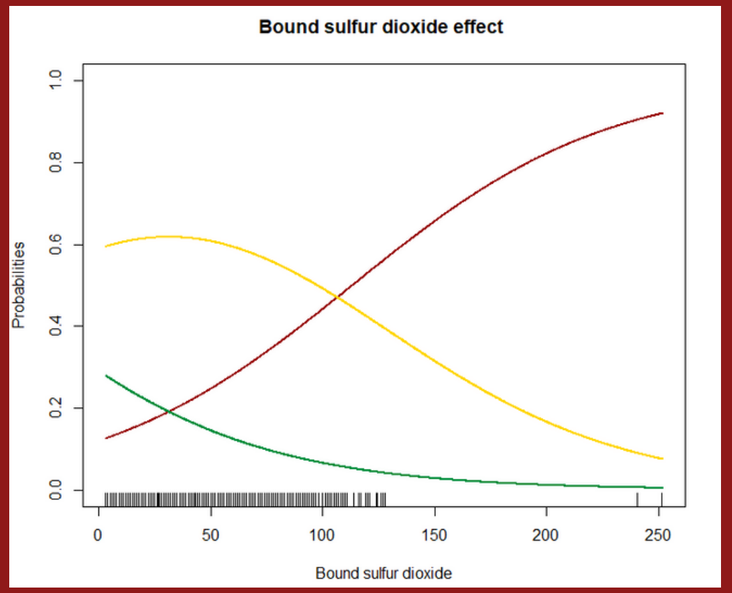
The two different approaches that we used lead us to similar models

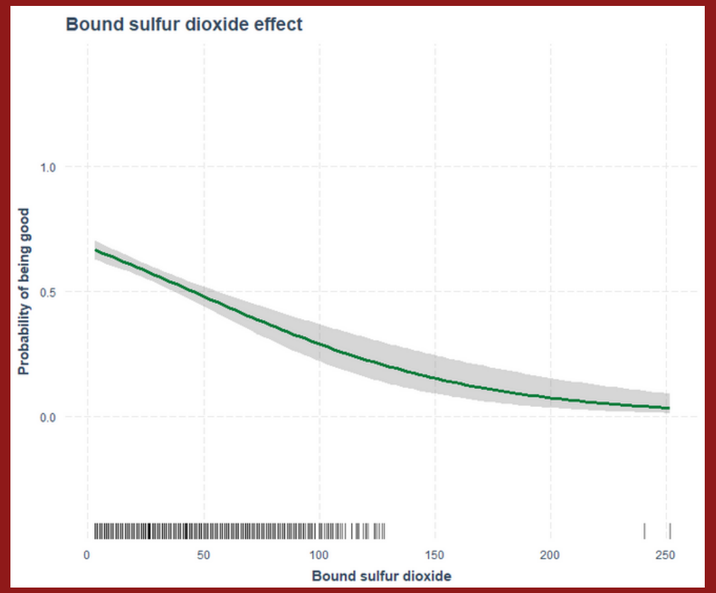
- Same 5 variables significant in the 2 models
- The only different variable is pH
- The effects of the common variables have the same sign

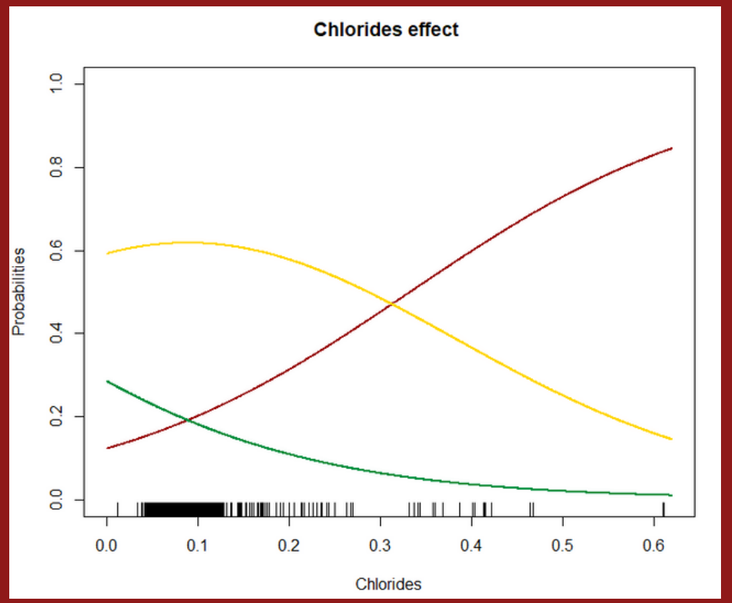
Multinomial

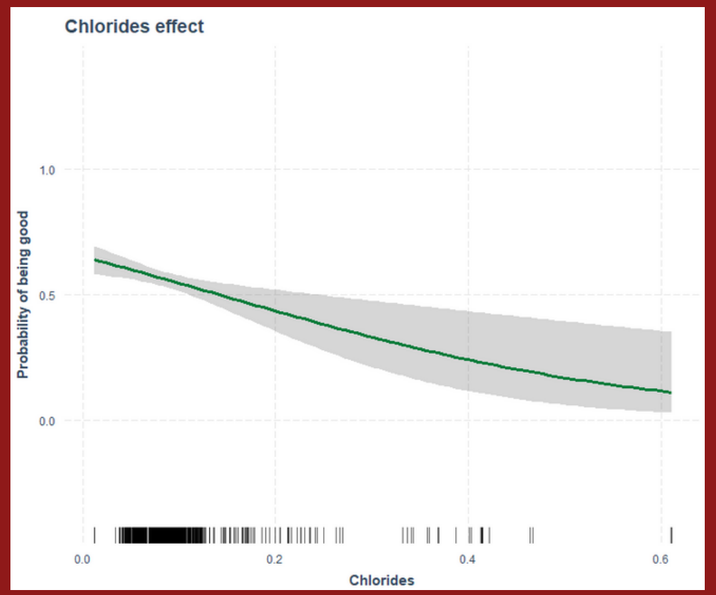
Binomial

bad
medium
good





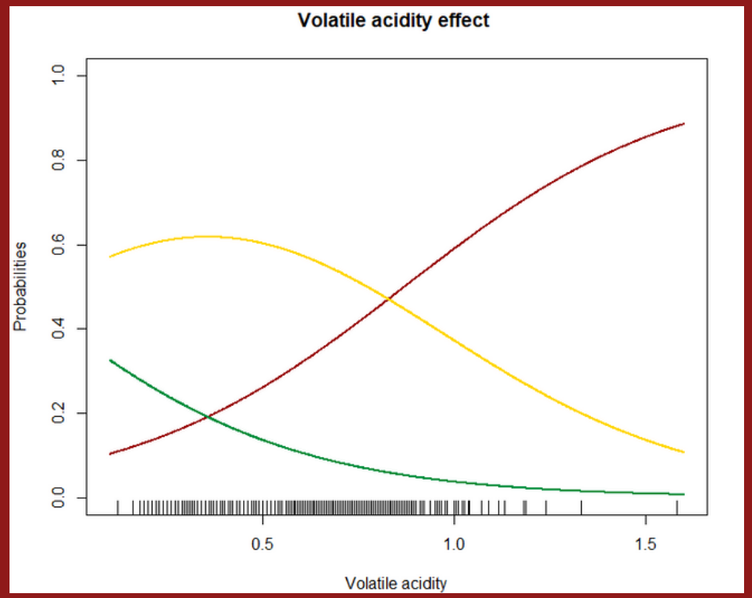


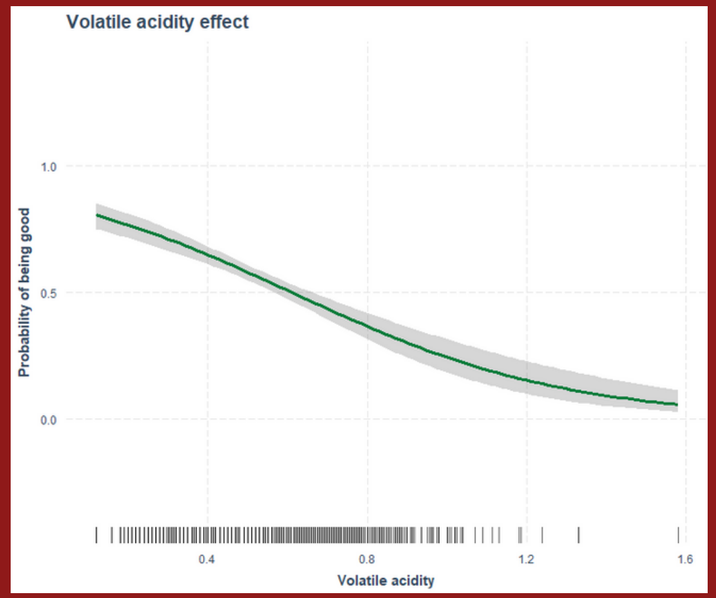


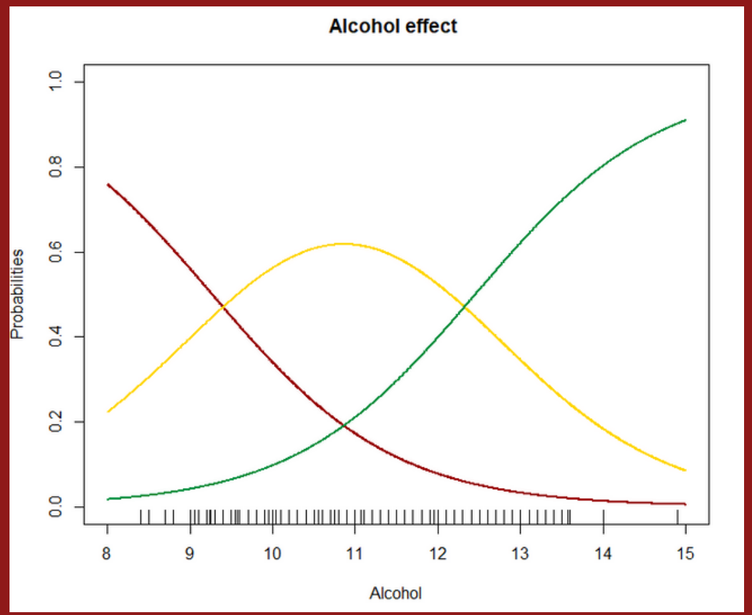
Multinomial

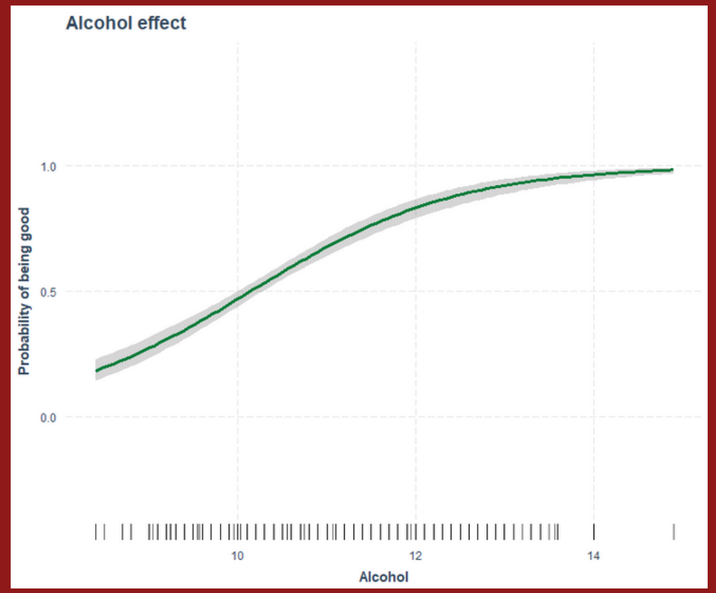
Binomial

bad
medium
good









Multinomial

Binomial

bad
medium
good