

STAT 462 Final Project

Regression Analysis for Wine Data

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Abstract

Introduction

Exploratory Data Analysis

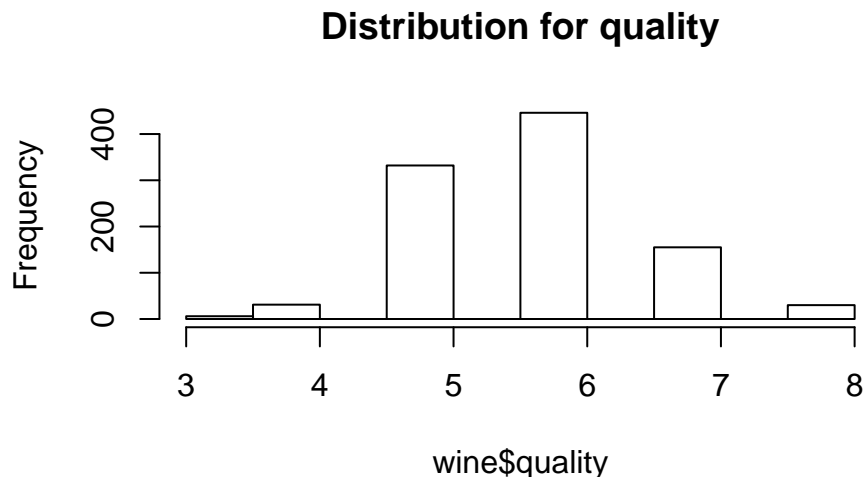
| The two datasets are related to red and white variants of the Portuguese “Vinho Verde” wine. We obtained the dataset from: <http://archive.ics.uci.edu/ml/datasets/Wine+Quality> . The website also provided the following references.

1. Paulo Cortez, University of Minho, Guimar?es, Portugal, <http://www3.dsi.uminho.pt/pcortez> 2. A. Cerdeira, F. Almeida, T. Matos and J. Reis, Viticulture Commission of the Vinho Verde Region(CVRVV), Porto, Portugal,2009. | We randomly select 1000 samples of the dataset. It contains the following variables (units are not given in the dataset description):

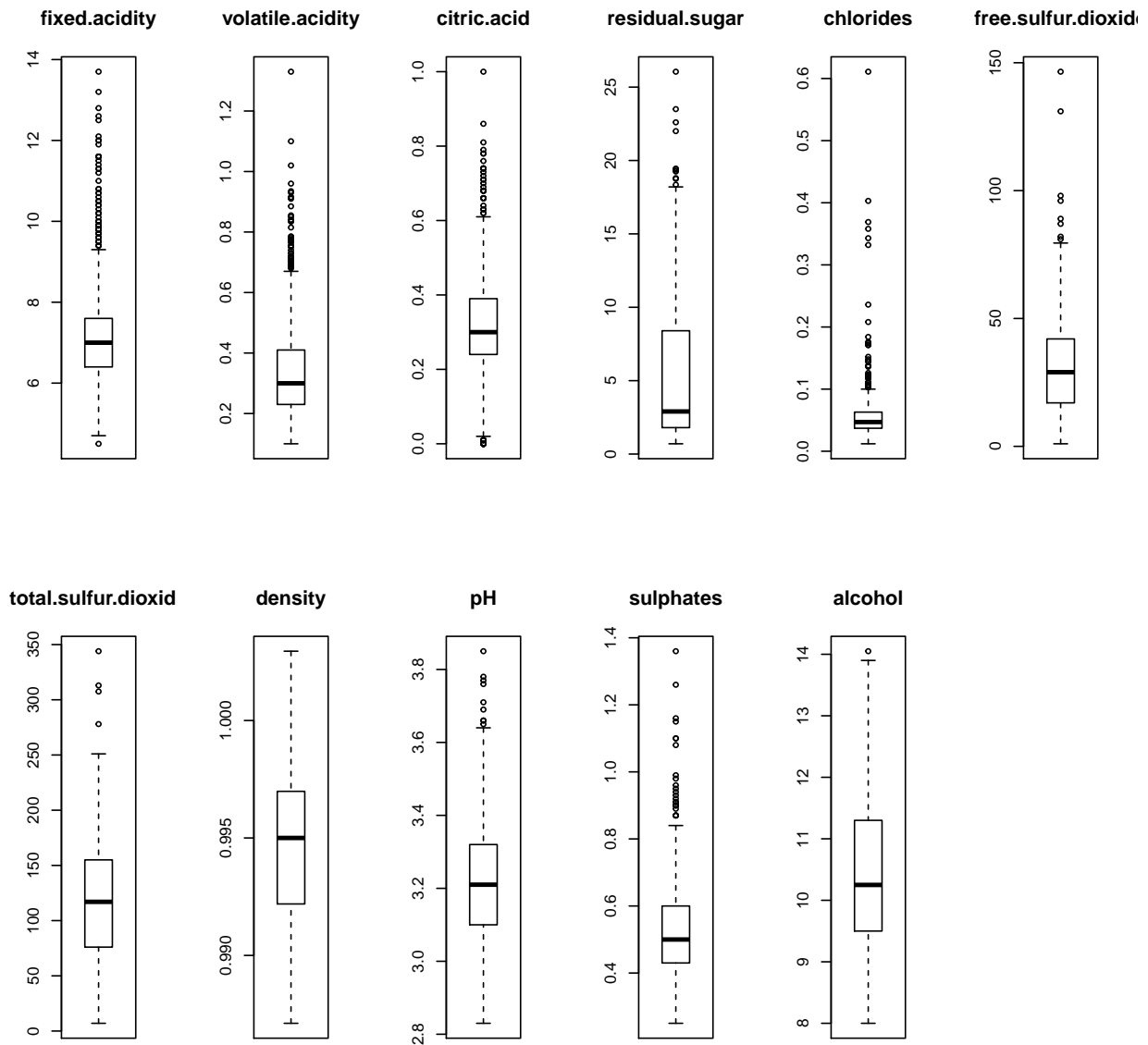
- fixed acidity (grams/liter)
- volatile acidity (grams/liter)
- citric acid (grams/liter)
- residual sugar (grams/liter)
- chlorides (grams/liter)
- free sulfur dioxide (milligrams/liter)
- total sulfur dioxide (milligrams/liter)
- density (grams/cubic centimeter)
- pH: acidity (below 7) or alkalinity (over 7)
- sulphates:potassium sulfate (grams/liter)
- alcohol:percentage alcohol (% volume) *t type: type of wine (red/white)
- Output variable (based on sensory data): quality (score between 0 and 10)

In this report, we are interested in what impact the different quality of red wine and white wine. We build two different models, treating quality as continuous variable and categorical variable regardingly. Here are some simple summary output of this dataset:

Consider quality as a response, these is the distribution for quality.



These are the boxplot for all continuous variables. Density is the only variable does not have outliers and roughly symmetric (due to the random sample; few outliers exist when considering the whole dataset). Extreme outliers can be noticed within the chlorides variables. Most variables are skewed to the right with the outliers on the larger side.



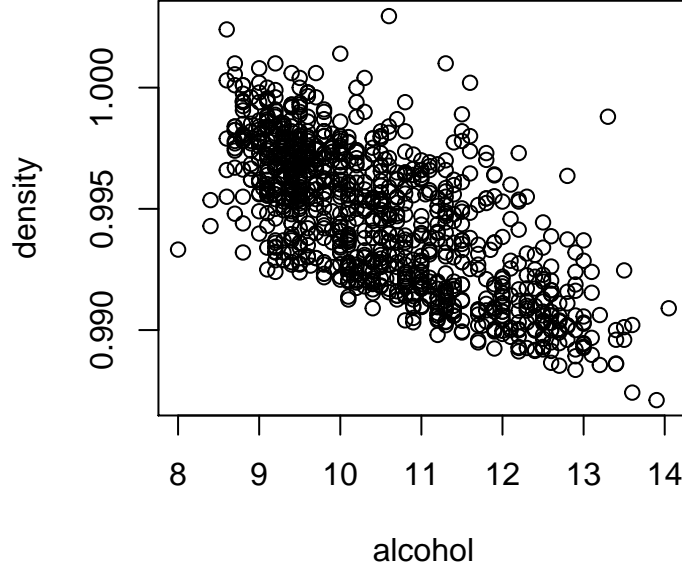
| According to the boxplots above, there are some extreme outliers have high chlorides. Since the dataset is really big, looking at the pairwise scatterplots will be relatively hard to identify outliers, we calculate the leverage of the potential predictors. Still considering the quality as response, we calculate the leverage of the potential model.

There are the points with leverage greater then the threshold $3 \cdot p/n$:

```
## 145 153 204 220 224 269 279 298 321 388 402 597 608 655 658 669 696 699
## 145 153 204 220 224 269 279 298 321 388 402 597 608 655 658 669 696 699
## 745 800 856 881 902 932 989
## 745 800 856 881 902 932 989
```

Method

1. Check Collinearity and Re-Scaling X's



From the VIF table we can see density has VIF of 25.061323 which mean severe collinearity (the plot shows the linear relationship between density and alcoho). So we have to remove this predictor, and this is the new VIF result.

	vif1		vif2
fixed.acidity	5.04	fixed.acidity	2.23
volatile.acidity	2.12	volatile.acidity	2.09
citric.acid	1.59	citric.acid	1.59
residual.sugar	10.70	residual.sugar	1.52
chlorides	1.63	chlorides	1.63
free.sulfur.dioxide	2.38	free.sulfur.dioxide	2.37
total.sulfur.dioxide	3.97	total.sulfur.dioxide	3.89
density	25.06	pH	1.71
pH	2.73	sulphates	1.50
sulphates	1.61	alcohol	1.41
alcohol	6.61	type	4.89
type	7.63		

(a) VIF Full Predictor

(b) VIF Remove Density

Table 1: VIF table

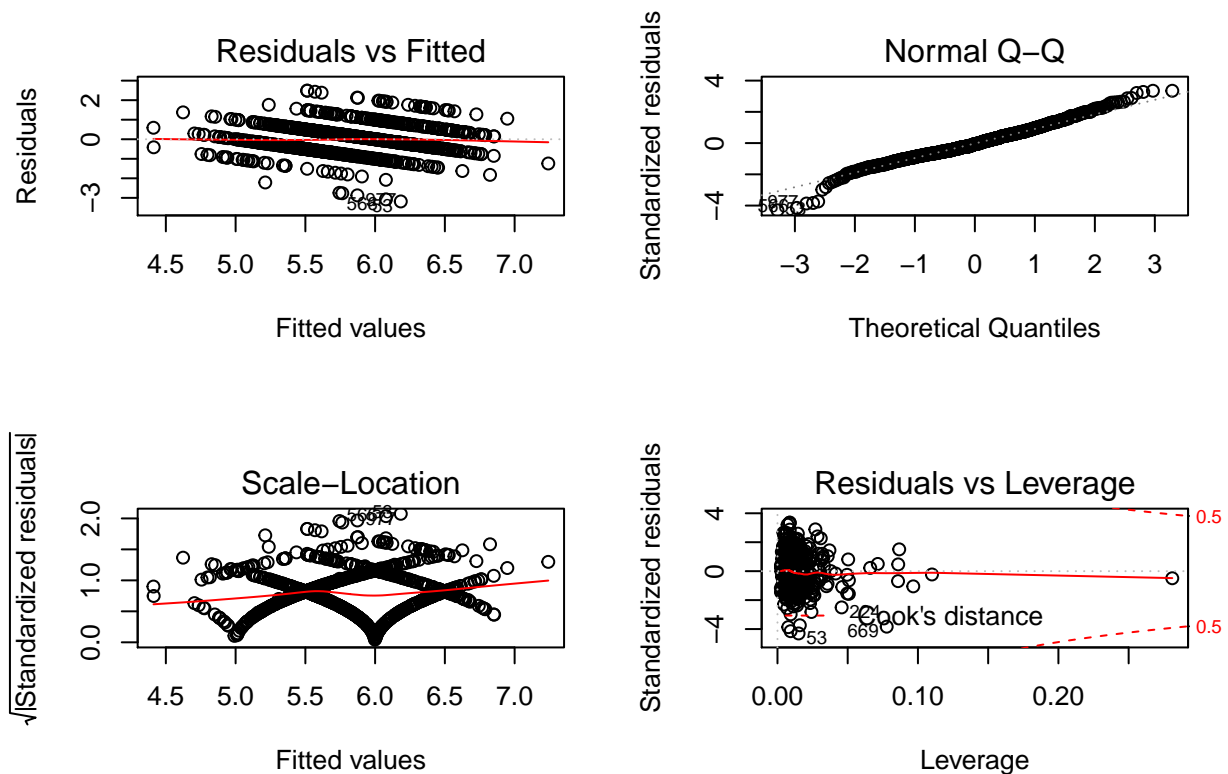
Looking at the new VIF result, no predictor variabel has VIF greater than 4. Thus the collinearity problem is eliminated. We also look in to the scale of X's. Since the original full linear model shows there is about 100 times difference between two β , we decided to scale the X's using the method "scale". In the following analysis, all continuous predictors are scaled.

2. Regression Model treating Quality as continuous Variable and Model Selection

2.1 Full model

First we create dummy variable for type variable, for which type red is 1, and type white is 0. Then we build a full model using quality as response variable. Here shows the full model summary and diagnostic plot

```
##
## Call:
## lm(formula = wine$quality ~ scaled.wine$fixed.acidity + scaled.wine$volatile.acidity +
##     scaled.wine$citric.acid + scaled.wine$residual.sugar + scaled.wine$chlorides +
##     scaled.wine$free.sulfur.dioxide + scaled.wine$total.sulfur.dioxide +
##     scaled.wine$pH + scaled.wine$sulphates + scaled.wine$alcohol +
##     dummy)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.1840 -0.4840 -0.0502  0.4462  2.4867
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      5.734427   0.037795 151.726 < 2e-16 ***
## scaled.wine$fixed.acidity -0.037839   0.035257  -1.073  0.28343
## scaled.wine$volatile.acidity -0.248168   0.034091 -7.280 6.83e-13 ***
## scaled.wine$citric.acid    0.001008   0.029788   0.034  0.97300
## scaled.wine$residual.sugar  0.090266   0.029114   3.100  0.00199 **
## scaled.wine$chlorides     -0.059595   0.030083  -1.981  0.04787 *
## scaled.wine$free.sulfur.dioxide  0.051370   0.036322   1.414  0.15759
## scaled.wine$total.sulfur.dioxide -0.020356   0.046515  -0.438  0.66176
## scaled.wine$pH           -0.010799   0.030804  -0.351  0.72598
## scaled.wine$sulphates      0.140478   0.028867   4.866 1.32e-06 ***
## scaled.wine$alcohol        0.383226   0.028002  13.686 < 2e-16 ***
## dummy                  0.282193   0.121560   2.321  0.02047 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7456 on 988 degrees of freedom
## Multiple R-squared:  0.264, Adjusted R-squared:  0.2558
## F-statistic: 32.21 on 11 and 988 DF, p-value: < 2.2e-16
```



| The residuals vs fitted looks like this because quality is a categorical variable with 6 levels. However, since it has so many level, we treat it as a continuous variable. Hence, the residuals vs fitted plot breaks into 6 lines. According to the Q-Q plot, the residuals follows a normal distribution. According to the residuals vs leverage plot, there is no influential point because there is no leverage exceed 0.5.

2.2 Select model

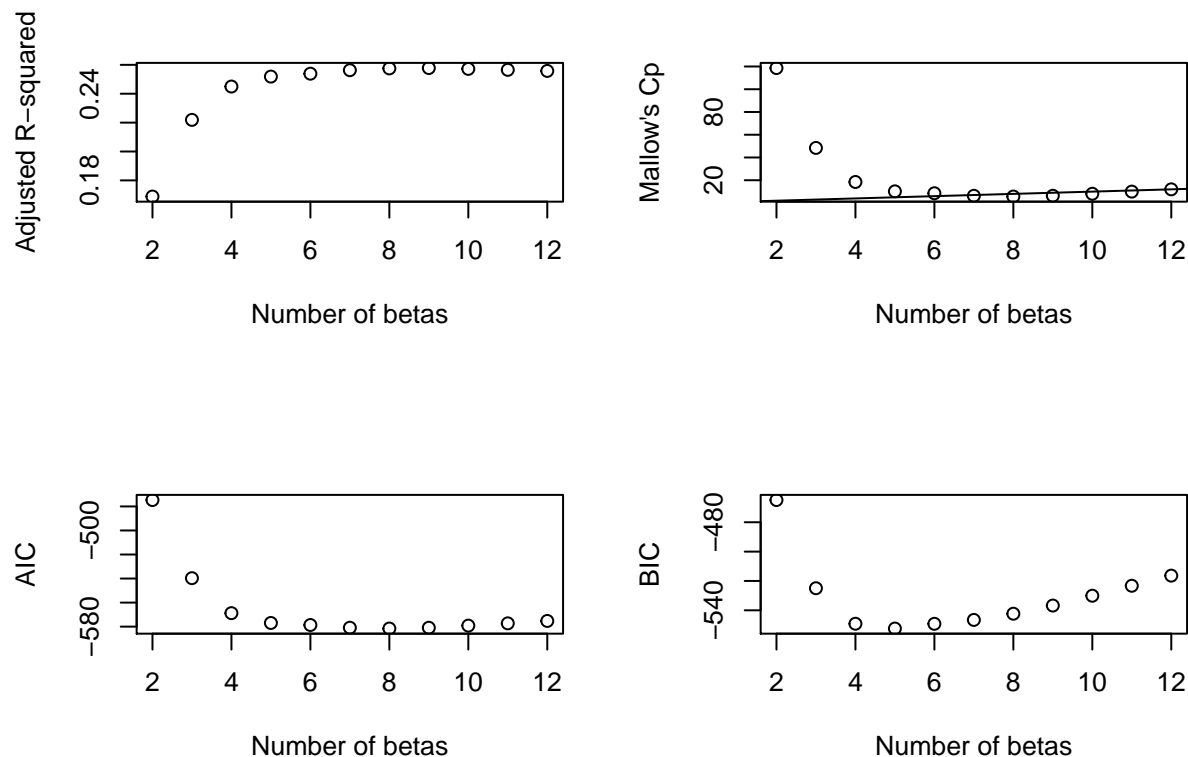
Using backward selection

```
##
## Call:
## lm(formula = wine$quality ~ +scaled.wine$volatile.acidity + scaled.wine$residual.sugar +
##     scaled.wine$chlorides + scaled.wine$sulphates + scaled.wine$alcohol +
##     dummy)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.2383 -0.4721 -0.0555  0.4603  2.4962
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      5.75054    0.03209  179.213  < 2e-16 ***
## scaled.wine$volatile.acidity -0.25059    0.03130   -8.006 3.29e-15 ***
## scaled.wine$residual.sugar    0.09719    0.02755    3.527 0.000439 ***
## scaled.wine$chlorides      -0.05980    0.02906   -2.058 0.039858 *
## scaled.wine$sulphates      0.13880    0.02829    4.907 1.08e-06 ***
## scaled.wine$alcohol        0.38286    0.02654   14.424 < 2e-16 ***
## dummy              0.21590    0.08961    2.409 0.016161 *
```

```
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7453 on 993 degrees of freedom
## Multiple R-squared:  0.2608, Adjusted R-squared:  0.2563
## F-statistic: 58.38 on 6 and 993 DF,  p-value: < 2.2e-16
```

We end up with 6 predictors. The reduced model includes volatile.acidity, residual.sugar, chlorides, sulphates, alcohol and dummy variables.

using R_{adj}^2 to select model:



Max adjusted R^2 with 8 predictors. The model include fixed.acidity, volatile.acidity, residual.sugar, chlorides, free.sulfur.dioxide, sulphates, alcohol and dummy variables.

Using C_p : when $p=7$, with 6 predictors. The model include volatile.acidity, residual.sugar, chlorides, sulphates, alcohol and dummy variables.

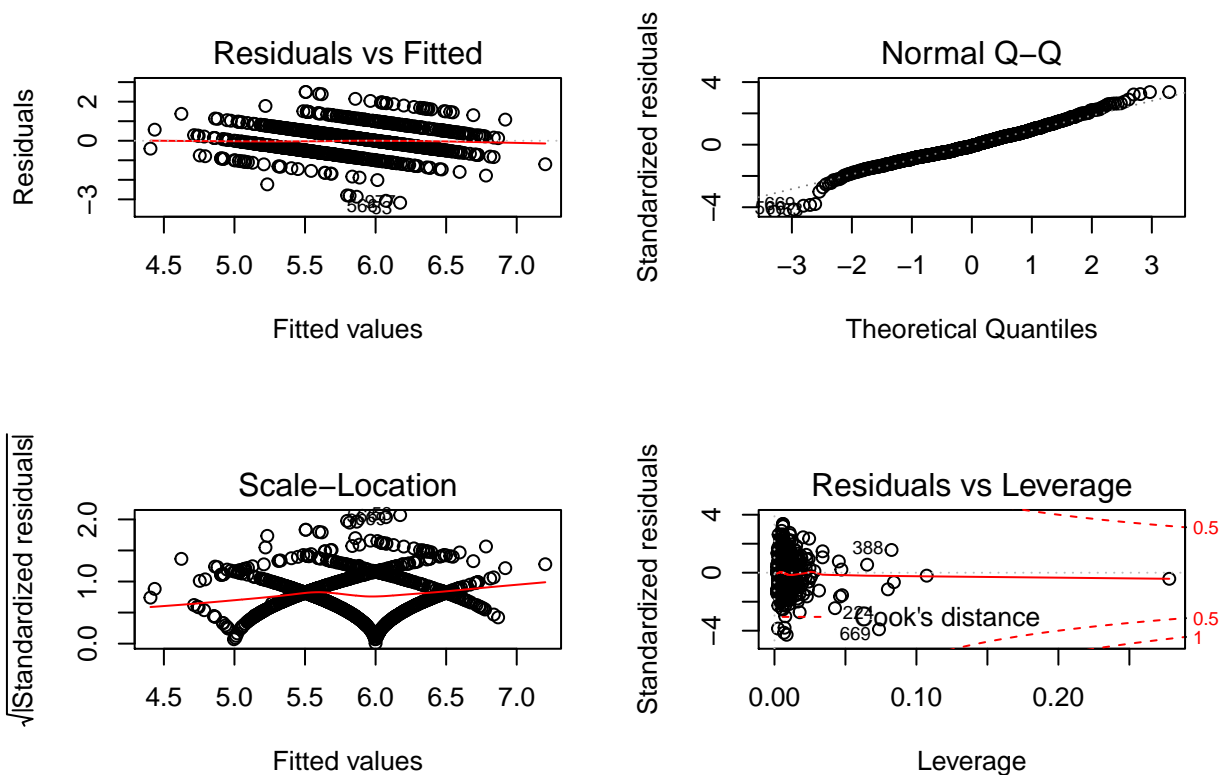
Using AIC: when $p=8$, with 7 predictors. The model includes volatile.acidity, residual.sugar, chlorides, free.sulfur.dioxide, sulphates, alcohol and dummy variables.

Using BIC: when $p=5$, 4 predictors. The model includes volatile.acidity, residual.sugar, sulphates, alcohol and dummy variables.

In conclusion, we should use the model with 7 predictors because it has relatively big R_{adj}^2 , low C_p , low aic and low bic. The final models includes volatile.acidity, residual.sugar, chlorides, free.sulfur.dioxide, sulphates, alcohol and dummy variables.

```
##
## Call:
```

```
## lm(formula = wine$quality ~ scaled.wine$volatile.acidity + scaled.wine$residual.sugar +
##      scaled.wine$chlorides + scaled.wine$free.sulfur.dioxide +
##      scaled.wine$sulphates + scaled.wine$alcohol + dummy)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.1741 -0.4819 -0.0591  0.4581  2.4950
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      5.74086    0.03260  176.075 < 2e-16 ***
## scaled.wine$volatile.acidity -0.24599    0.03140  -7.834 1.21e-14 ***
## scaled.wine$residual.sugar    0.08712    0.02821   3.088 0.00207 **
## scaled.wine$chlorides      -0.05860    0.02904  -2.018 0.04388 *
## scaled.wine$free.sulfur.dioxide 0.04658    0.02855   1.632 0.10304
## scaled.wine$sulphates       0.13643    0.02830   4.820 1.66e-06 ***
## scaled.wine$alcohol         0.38821    0.02672  14.527 < 2e-16 ***
## dummy                0.25572    0.09280   2.756 0.00597 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7447 on 992 degrees of freedom
## Multiple R-squared:  0.2627, Adjusted R-squared:  0.2575
## F-statistic: 50.5 on 7 and 992 DF, p-value: < 2.2e-16
```



According to the summary output, the final model is

$$y = 5.741 - 0.246X_{\text{volatile.acidity}} + 0.087X_{\text{residual.sugar}} - 0.059X_{\text{chlorides}} + 0.047X_{\text{free.sulfur.dioxide}} +$$

$$0.136X_{sulphates} + 0.388X_{alcohol} + 0.256d_{type}$$

However, R^2 for this model is 0.2627 which means this model only represent 26.27% of the quality response. Hence, we need to use other method to find a better model.

3. Logistic Model treating Quality as Categorical Variable and Model Selection

3.1 Prepare Response Variable for Logistic Regression

To successfully perform the logistic regression analysis, we divide the quality variable into two groups, quality 3-5 is marked as low quality, which is assigned as value 0; quality 6-8 is marked as high quality, which is assigned as value 1. Using the function glm with family parameter of binomial. We get a full model of logistic regression.

```
##      Min. 1st Qu.  Median      Mean 3rd Qu.      Max.
##      3.000   5.000   6.000   5.803   6.000   8.000

##
## Call:
## glm(formula = quality_logi ~ scaled.wine, family = binomial(link = "logit"))
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
## -2.6833  -0.9472   0.4378   0.8311   2.3008
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)      0.53081    0.12564   4.225 2.39e-05 ***
## scaled.winefixed.acidity -0.14286    0.11137  -1.283  0.1996
## scaled.winevolatile.acidity -0.67837    0.11555 -5.871 4.34e-09 ***
## scaled.winecitric.acid -0.01938    0.09110  -0.213  0.8315
## scaled.wineresidual.sugar  0.20489    0.09044   2.266  0.0235 *
## scaled.winechlorides -0.17178    0.08962  -1.917  0.0553 .
## scaled.winefree.sulfur.dioxide 0.19536    0.11748   1.663  0.0963 .
## scaled.winetotal.sulfur.dioxide -0.09020    0.14920  -0.605  0.5455
## scaled.winepH -0.07578    0.09865  -0.768  0.4424
## scaled.winesulphates  0.41448    0.10106   4.101 4.11e-05 ***
## scaled.winealcohol  1.12115    0.10797  10.384 < 2e-16 ***
## scaled.winedummy    0.81345    0.40885   1.990  0.0466 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##      Null deviance: 1316.8  on 999  degrees of freedom
## Residual deviance: 1058.1  on 988  degrees of freedom
## AIC: 1082.1
##
## Number of Fisher Scoring iterations: 4
```

3.2 Model Selection

Observing the full logsitc regression summary, there are some variable not significantly contribute to the model. Using the function bestglm from the package “bestglm”, the best logistic model is selected according to AIC. Then a presudo R^2 is calculated using deviance and null deviance from the model summary. The result is 0.1948436. This is a relatively low R^2 , regardless this is not a “true” R^2

```
## Morgan-Tatar search since family is non-gaussian.
```

```
## AIC
## BICq equivalent for q in (0.867623212288942, 0.93125399684379)
## Best Model:
##           Estimate Std. Error  z value    Pr(>|z|)
## (Intercept)    0.5480113 0.10806465  5.071143 3.954328e-07
## volatile.acidity -0.6622902 0.10716867 -6.179886 6.414783e-10
## residual.sugar   0.1942633 0.08810508  2.204904 2.746080e-02
## chlorides       -0.1620564 0.08707090 -1.861201 6.271583e-02
## free.sulfur.dioxide 0.1666271 0.09174542  1.816189 6.934133e-02
## sulphates       0.3828727 0.09775920  3.916487 8.984855e-05
## alcohol        1.1291147 0.10358885 10.899963 1.153037e-27
## dummy          0.7121395 0.30641529  2.324099 2.012019e-02
```

4. Ordinal Logistic Regression

4.1 Even though logistic regression explain the relationship between significant predictors and quality as two level categorical variable, it does not fully explain the true nature of quality as a 6 level categorical variable. Thus, an ordinal logistic regression model is build to fully take consideration of 6 levels of quality.

Using the function polr from package MASS, treating quality as an ordered factor (with ordered level: 3<4<5<6<7<8), the full ordinal logistic model is constructed. Later, the p-value for each individual t-test is performed. Using backward selection, only variable volatile.acidity, residual.sugar, sulphates, and alcohol are left at $\alpha=0.05$. The best model summary is shown below (a new page called “ordinal” is used, since the clm function has a better output than polr function):

```
## Warning in library(package, lib.loc = lib.loc, character.only = TRUE,
## logical.return = TRUE, : there is no package called 'Hmisc'

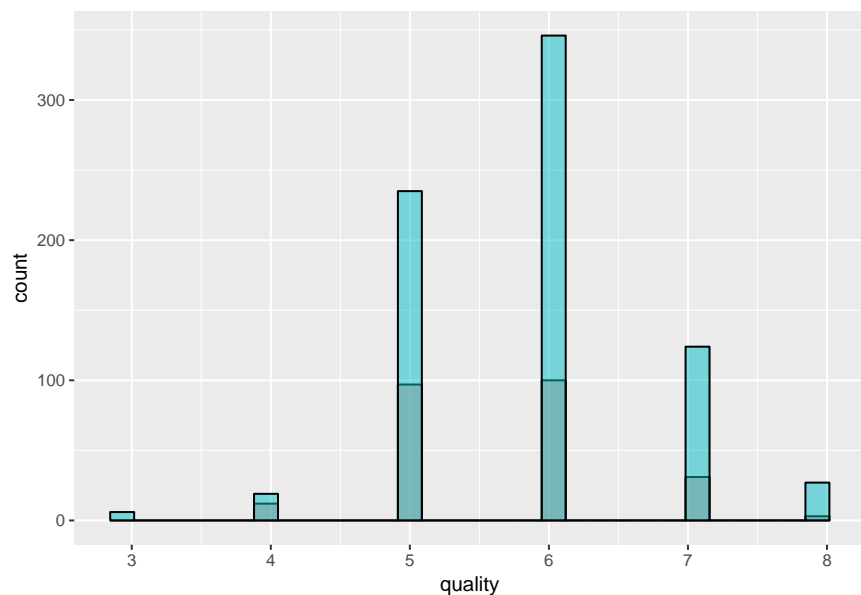
## formula:
## quality_order ~ volatile.acidity + residual.sugar + sulphates + alcohol
##
## link threshold nobs logLik  AIC      niter max.grad cond.H
## logit flexible 1000 -1100.95 2219.90 7(0) 2.01e-09 1.1e+05
##
## Coefficients:
##           Estimate Std. Error z value Pr(>|z|)
## volatile.acidity -3.41919    0.41900  -8.160 3.34e-16 ***
## residual.sugar   0.04725    0.01427   3.312 0.000925 ***
## sulphates       2.68418    0.46102   5.822 5.80e-09 ***
## alcohol         0.87910    0.06174  14.240 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Threshold coefficients:
##           Estimate Std. Error z value
## 3|4    3.9381    0.8266  4.764
## 4|5    5.8492    0.7390  7.915
## 5|6    9.0082    0.7454 12.084
## 6|7   11.5812    0.7888 14.683
## 7|8   13.7805    0.8247 16.709
```

4.2 ANOVA Analysis for Variable Type

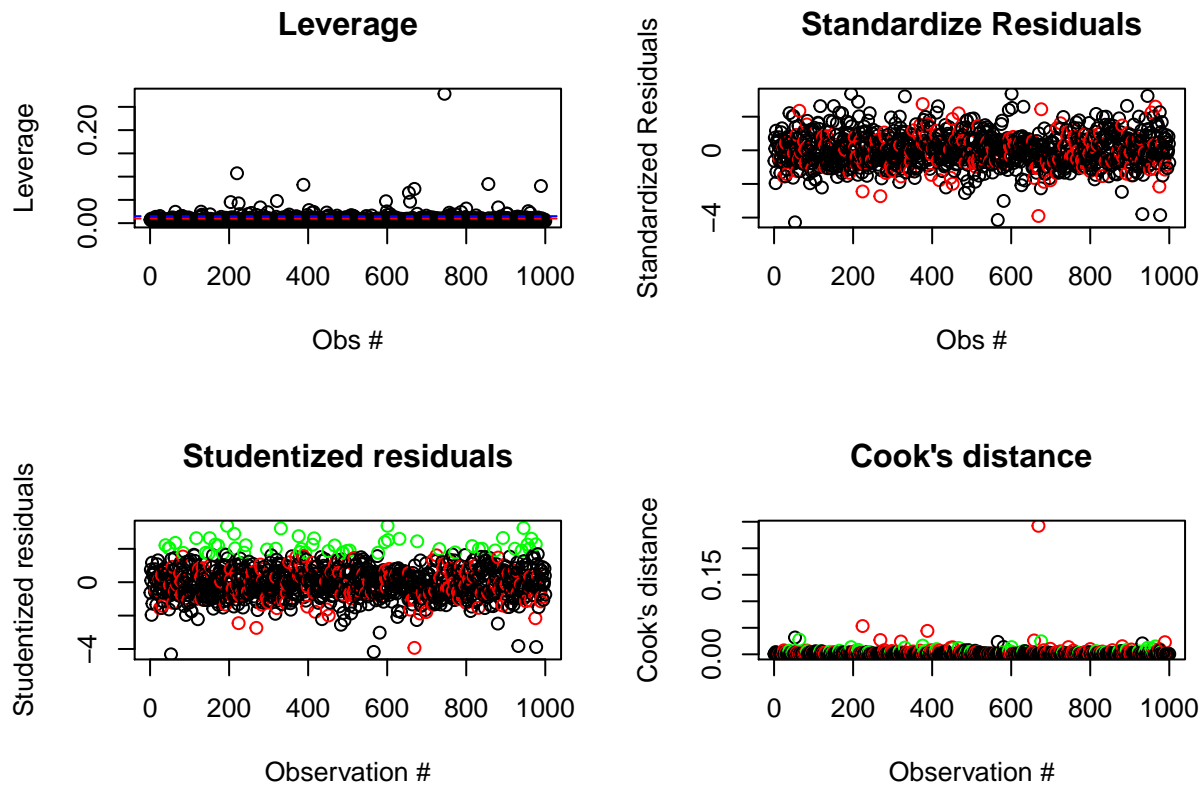
During the model selection for ordinal logsitic selection, the dummy variable type caught our attention. It is the last variable to be removed from the backward selection with p-value of 0.0579 which is slightly above 0.05. Will this categorical variable of wine type actually impact the wine quality. A seperated anova analysis

is performed along with a histogram overlaying the distribution of quality for red wine and white wine. The NOVA table shows that the quality is significantly different from red wine and white wine.

```
##           Df Sum Sq Mean Sq F value    Pr(>F)
## type         1      7.1    7.096    9.582 0.00202 **
## Residuals   998   739.1    0.741
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



5. Check Potential Outlier



| According to these plots, there are a lot of observations that have very high leverage (red points in leverage plot are observations with leverage greater than threshold $2p/n$) which is most likely due to the fact that a logistic model would better represent them

Result

Conclusion

Team Member Contribution

Reference