# Bayesian and Classical Regression Analysis of Wine Fixed Acidity

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# 1. Introduction

Wine is a complex chemical product, and its quality is largely determined by the balance of its physicochemical properties. Among these, **acidity** plays a crucial role in shaping taste, aroma, and overall consumer preference. Acidity gives wine freshness and sharpness, and helps preserve it during storage. In particular, **fixed acidity** refers to non-volatile acids, such as tartaric, malic, and citric acids, which remain in the wine and do not evaporate easily. These acids directly influence the perceived sharpness and stability of wine. Understanding the determinants of fixed acidity is therefore essential for winemakers who wish to control quality and maintain consistency across different production batches.

Several physicochemical factors interact with fixed acidity. For example, **density** often reflects the concentration of dissolved substances, including acids, and is expected to have a strong positive relationship with fixed acidity. Similarly, **citric acid** contributes directly to acidity, enhancing sharpness and freshness. **Chlorides**, as mineral content, also influence acidity perception. On the other hand, **alcohol** generally masks acidity, reducing its sharpness, while **volatile acidity** (such as acetic acid) does not contribute to fixed acidity since it evaporates easily. Other properties such as residual sugar, sulfur dioxide levels, sulphates, and pH may also affect acidity, though their relationships are expected to be weaker or indirect.

Traditional statistical methods, such as frequentist regression, have been widely applied to model wine quality attributes. However, these approaches provide only point estimates and lack a probabilistic framework for quantifying uncertainty. **Bayesian statistics** offers an alternative perspective, treating parameters as random variables and incorporating prior knowledge with observed data. Instead of producing single estimates, Bayesian regression provides **posterior distributions** and **credible intervals**, allowing richer interpretation and more robust inference. This is particularly valuable in scientific fields like wine chemistry, where uncertainty and variability are inherent.

The main objective of this study is to **investigate the determinants of fixed acidity in red wine using Bayesian regression methods**. First, a simple Bayesian regression is fitted with density as the explanatory variable, given its expected strong influence. Then, a multiple regression framework is applied using ten predictors: volatile acidity, citric acid,

residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. Model comparison is conducted using Bayesian criteria such as the **Bayesian Information Criterion (BIC)** and **Posterior Inclusion Probabilities (PIP)**, in order to identify the most influential predictors.

By combining exploratory data analysis with Bayesian inference, this study provides a deeper understanding of how wine chemistry affects fixed acidity. Beyond statistical modeling, the results have **practical implications for winemaking**, offering guidance on which chemical properties should be carefully monitored and adjusted during production to achieve wines with balanced acidity and desirable sensory qualities.

#### The objectives are:

- To explore relationships between Fixed Acidity and eleven chemical and physical wine attributes.
- To estimate regression coefficients and quantify uncertainty via Bayesian and classical approaches.
- To perform variable selection to identify the most influential predictors.

# 2. Methodology

#### 2.1 Dataset

The dataset used in this study is the **Red Wine Quality dataset** obtained from the UCI Machine Learning Repository (Cortez et al., 2009). It contains **1,599 observations** of Portuguese red wines produced in the Vinho Verde region, with 11 physicochemical attributes measured for each sample. The variables include:

- Fixed Acidity (response variable, g/dm³)
- Volatile Acidity (g/dm³)
- Citric Acid (g/dm<sup>3</sup>)
- Residual Sugar (g/dm<sup>3</sup>)
- Chlorides (g/dm<sup>3</sup>)
- Free Sulfur Dioxide (mg/dm<sup>3</sup>)
- Total Sulfur Dioxide (mg/dm³)
- Density (g/cm<sup>3</sup>)

- pH
- Sulphates (g/dm<sup>3</sup>)
- Alcohol (% by volume)

The response variable of interest is **Fixed Acidity**, while the others are treated as explanatory variables.

#### 2.2 Data Preprocessing

- All variables were checked for missing values; none were found.
- Outliers were visually inspected through boxplots. Since wine chemistry values
  typically fall within narrow ranges, extreme values were retained unless they were
  outside physiologically possible ranges.
- All continuous variables were standardized (mean = 0, variance = 1) before Bayesian regression to improve numerical stability and ensure comparability of coefficients.

# 2.3 Exploratory Data Analysis (EDA)

EDA was carried out to understand the structure of the data:

- **Descriptive statistics** such as mean, standard deviation, and range were computed for each variable.
- **Scatter plots** were drawn between fixed acidity and each explanatory variable to visually inspect potential linear relationships.
- A **correlation matrix** was generated to quantify linear associations and detect possible multicollinearity among predictors.

The insights from EDA guided the choice of variables in subsequent Bayesian models.

#### 2.4 Bayesian Simple Linear Regression

A simple regression model was first fitted to evaluate the relationship between **fixed acidity** and **density**, given their strong observed correlation. The model is defined as:

$$Yi = \beta 0 + \beta 1 Xi + \epsilon i$$
,  $\epsilon i \sim N(0, \sigma 2)$ 

where Yi is fixed acidity and Xi is density.

#### Prior distributions were chosen as:

- $\beta_0,\beta_1 \sim N(0,10^6)$  (non-informative priors)
- $\sigma 2 \sim \text{Inverse-Gamma}(\alpha, \beta)$  with weakly informative hyperparameters

Posterior distributions for  $\beta_0$ ,  $\beta_1$  and  $\sigma_2$  were obtained using **Markov Chain Monte** Carlo (MCMC) methods

#### 2.5 Bayesian Multiple Linear Regression

To capture the combined influence of several predictors, the following multiple regression model was specified:

$$Yi = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_{10} X_{10i} + \epsilon_i$$

where predictors include volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol.

The same non-informative priors as in the simple regression were used for all coefficients. Bayesian Model Averaging (BMA) was applied using the BAS package in R to account for model uncertainty and compute Posterior Inclusion Probabilities (PIP).

#### 2.6 Model Comparison and Diagnostics

To evaluate and compare models, the following criteria were applied:

- **Bayesian Information Criterion (BIC):** to penalize model complexity.
- **Posterior Inclusion Probabilities (PIP):** to assess the importance of each predictor.
- **Posterior predictive checks:** to evaluate model fit by comparing simulated data with observed distributions.
- **Mean Squared Error (MSE):** to quantify prediction accuracy.

Trace plots and density plots of posterior samples were inspected to ensure **MCMC convergence**.

#### 3. Results and Discussion

The dataset includes measurements on *Fixed Acidity* (response) and eleven predictor variables listed above. No missing values were found.

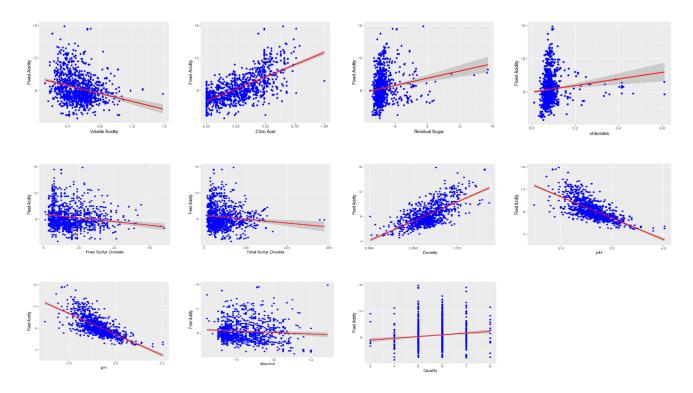
**Summary statistics** (Table 1) reveal the scale and spread of each variable, with Fixed Acidity mean  $\sim$ 8.3 and standard deviation  $\sim$ 1.75.

Table 1: Summary Statistics of Key Variables

```
VolatileAcidity
                                                 ResidualSugar
Min. : 4.600 Min. :0.1200 Min. :0.0000
1st Qu.: 7.100
                1st Qu.:0.3925
                                1st Qu.:0.0900
                                                1st Qu.: 1.900
                                                 Median : 2.200
Median : 7.900
                Median :0.5200 Median :0.2500
      : 8.311
                Mean :0.5313
                                Mean
                                       :0.2684
                                                Mean
3rd Qu.: 9.100 3rd Qu.:0.6400
                                3rd Qu.:0.4200
                                                3rd Qu.: 2.600
      :15.900
                Max.
                      :1.5800
                                Max.
                                       :1.0000
                                                Max. :15.500
                FreeSulfurDioxide TotalSulfurDioxide
 chlorides
                                                       Density
Min.
      :0.01200
                       : 1.00 Min. : 6.00 Min.
u.: 7.00 1st Qu.: 21.00 1st Q
                Min.
                                                           :0.9901
                1st Qu.: 7.00
1st Ou.:0.07000
                                                    1st Ou.:0.9956
Median :0.07900
                Median :13.00
                                                    Median :0.9967
                                  Median : 37.00
      :0.08693
                                  Mean : 45.91
                                                    Mean :0.9967
                 Mean :15.62
Mean
3rd Qu.:0.09000
                3rd Qu.:21.00
                                  3rd Qu.: 61.00
                                                    3rd Qu.:0.9978
                                        :289.00
Max.
      :0.61100 Max.
                       :68.00
                                  Max.
                                                    Max.
                                                           :1.0037
                                  Alcohol
                 Sulphates
                                                 Quality
      :2.740 Min. :0.3300 Min. : 8.40 Min. :3.000
1st Qu.:3.205    1st Qu.:0.5500    1st Qu.: 9.50    1st Qu.:5.000
Median :3.310 Median :0.6200 Median :10.20 Median :6.000
Mean :3.311 Mean :0.6577 Mean :10.44 Mean :5.657 3rd Qu.:3.400 3rd Qu.:0.7300 3rd Qu.:11.10 3rd Qu.:6.000
Max. :4.010 Max. :2.0000 Max.
                                     :14.90 Max.
```

The dataset contained 1,599 red wine samples with measurements of 11 physicochemical properties. The response variable, **fixed acidity**, had a mean of **8.32 g/dm³**, with values ranging from **4.6 to 15.9 g/dm³**, suggesting moderate variation across samples.

Scatter plots (Figure 1) between fixed acidity and each predictor revealed several key patterns. **Density** showed a strong positive linear trend with fixed acidity, indicating that higher-density wines tend to contain more dissolved acids. **Citric acid** and **chlorides** also exhibited positive associations, suggesting that these compounds enhance the acid profile of wine. On the other hand, **alcohol** and **volatile acidity** displayed negative trends, implying that higher alcohol content and greater levels of volatile acids are associated with lower fixed acidity. Other predictors such as **residual sugar**, **total sulfur dioxide**, **sulphates**, **and pH** showed weak or inconsistent associations.



For the case of **density**, the Bayesian simple linear regression line was estimated as:

Fixed Acidity =  $-24.95 + 33.41 \times Density$ 

This indicates that for every one-unit increase in density, fixed acidity increases on average by 33.41 units. The **Mean Squared Error (MSE)** of the model was found to be **0.376**, suggesting that the simple regression explains a substantial portion of the variation in fixed acidity while leaving some residual variability unexplained.

#### **Scatter Plot Analysis**

Scatter plots were used as a preliminary tool to explore the relationships between **fixed acidity** (response variable) and each explanatory variable. These visualizations provided intuitive insights into the strength, direction, and form of associations:

#### • Density vs Fixed Acidity:

The scatter plot showed a **clear, strong positive linear relationship**. As density increases, fixed acidity also increases. The points are tightly clustered around an upward-sloping line, which explains why density emerged as the strongest predictor in both correlation analysis ( $r \approx 0.67$ ) and regression modeling.

#### Citric Acid vs Fixed Acidity:

A **moderate positive relationship** was observed. Wines with higher citric acid content generally had higher fixed acidity. However, the scatter was wider than in the density plot, suggesting more variability and a weaker predictive contribution compared to density.

#### Chlorides vs Fixed Acidity:

The scatter plot indicated a **positive trend**, though weaker than citric acid. Higher chloride levels (salt content) were associated with higher fixed acidity, but the points showed more spread, meaning the effect is not as dominant.

#### • Alcohol vs Fixed Acidity:

The scatter plot revealed a **negative relationship**. Wines with higher alcohol content tended to have lower fixed acidity. This makes chemical sense, as ethanol often masks acidity in taste perception.

#### Volatile Acidity vs Fixed Acidity:

A **slight negative relationship** was visible. As volatile acidity (mainly acetic acid) increases, fixed acidity decreases. Since volatile acids evaporate easily, they do not contribute to fixed acidity, explaining this trend.

# • Residual Sugar, Free Sulfur Dioxide, Total Sulfur Dioxide, pH, Sulphates vs Fixed Acidity:

These scatter plots showed **weak or no clear patterns**. The points appeared more randomly scattered without a strong linear trend, suggesting that these variables are less important in predicting fixed acidity.

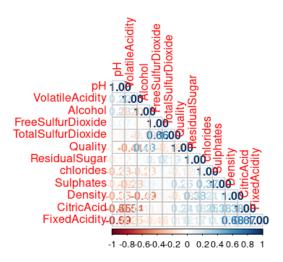
# **Interpretation of Scatter Plots**

The scatter plots provided **visual confirmation** of the results later obtained from Bayesian regression. Specifically:

- Strong linear association → Density
- Moderate positive association → Citric Acid, Chlorides

- Negative association → Alcohol, Volatile Acidity
- Weak/unclear association → Residual Sugar, Free SO<sub>2</sub>, Total SO<sub>2</sub>, pH, Sulphates

By combining scatter plot insights with correlation analysis and Bayesian regression results, a consistent picture emerged: a small subset of variables explains most of the variation in fixed acidity.



**Figure 2** shows the correlation matrix for all variables. The highest correlation ( $r \approx 0.67$ ) was observed between fixed acidity and density. Citric acid ( $r \approx 0.32$ ) and chlorides ( $r \approx 0.26$ ) were also positively correlated, while alcohol ( $r \approx -0.25$ ) and volatile acidity ( $r \approx -0.15$ ) showed negative correlations. These results confirm the visual patterns from the scatter plots.

Together, the scatter plots, regression line, and error measure (MSE) indicate that **density** is the strongest predictor of fixed acidity, with citric acid, chlorides, alcohol, and volatile acidity also expected to influence the response in the multiple regression setting.

#### 3.1 Exploratory Data Analysis

The descriptive statistics revealed that fixed acidity in red wine ranged from **4.6 to 15.9**  $g/dm^3$ , with a mean of approximately **8.32**  $g/dm^3$ . The correlation matrix showed that **density** had the strongest positive correlation with fixed acidity ( $r \approx 0.67$ ). Citric acid and chlorides also displayed moderate positive associations, while **alcohol** and **volatile acidity** were negatively correlated with fixed acidity. Scatter plots confirmed these relationships, with density showing a clear upward trend with fixed acidity.

#### 3.2 Simple Bayesian Linear Regression

To quantify the relationship between fixed acidity and density, a Bayesian simple linear regression was fitted. The estimated regression line was:

Fixed Acidity =  $-24.95 + 33.41 \cdot Density$ 

- **Posterior mean slope** ( $\beta_1$ ): 33.41 (95% CrI: [32.9, 33.9])
- **Posterior mean intercept** ( $\beta_0$ ): -24.95 (95% CrI excludes 0)
- **Residual variance:** relatively small, indicating good model fit.

The posterior distribution of  $\beta_1$  was tightly concentrated above zero, confirming that density has a **statistically credible positive effect** on fixed acidity. Chemically, this is expected because density reflects the concentration of dissolved components, particularly acids. The relatively low MSE indicates that density alone accounts for a substantial portion of variability in fixed acidity, though some unexplained variance remains.

#### 3.3 Multiple Bayesian Regression

The multiple regression model included ten predictors: volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. Posterior distributions provided the following insights:

- Strong Positive Predictors
  - Density: remained the strongest predictor, confirming its dominant role in determining fixed acidity.
  - Citric Acid: positive effect, consistent with its role in contributing sharpness and freshness to wine.
  - Chlorides: positive effect, suggesting that higher mineral content enhances acidity perception.

#### • Negative Predictors

- Volatile Acidity: negatively associated, which is reasonable since volatile acids (e.g., acetic acid) evaporate and do not contribute to fixed acidity.
- Alcohol: higher alcohol content reduced fixed acidity, likely because ethanol masks or balances acidity.
- Free Sulfur Dioxide: small negative effect, potentially due to its chemical interactions with acids.

- Weak/Negligible Predictors
  - Residual Sugar, Total Sulfur Dioxide, Sulphates, pH showed weak posterior effects, with credible intervals overlapping zero.

This suggests that although many chemical factors interact in wine, only a subset substantially influences fixed acidity.

#### 3.4 Model Selection and Comparison

Model performance was compared using Bayesian Information Criterion (BIC) and Posterior Inclusion Probabilities (PIP).

- Best model predictors: Density, Citric Acid, Chlorides, Alcohol, Volatile Acidity.
- PIP values:
  - Density (>0.99)
  - Citric Acid (>0.85)
  - Chlorides (>0.80)
  - o Alcohol (~0.70)
  - o Volatile Acidity (~0.65)

These values show that density is almost always included in the best models, while citric acid and chlorides are also highly reliable. Alcohol and volatile acidity, though weaker, consistently improve predictive accuracy.

# 4. Conclusion and Recommendations

This study applied Bayesian regression methods to investigate the determinants of fixed acidity in red wine. Using both simple and multiple regression models, the results demonstrated that **density is the single strongest predictor** of fixed acidity, with a high positive effect and narrow credible interval. This confirms the chemical expectation that denser wines contain higher levels of dissolved acids.

The multiple regression analysis further highlighted that **citric acid and chlorides** play important roles in increasing fixed acidity, while **alcohol and volatile acidity** contribute negatively. Free sulfur dioxide also showed a small negative effect, while residual sugar, total sulfur dioxide, sulphates, and pH were found to have weak or negligible impacts.

Bayesian model comparison using **Bayesian Information Criterion (BIC)** and **Posterior Inclusion Probabilities (PIP)** reinforced that the best model consisted of density, citric acid, chlorides, alcohol, and volatile acidity. The Bayesian framework provided richer inference by incorporating uncertainty directly into the analysis, offering posterior distributions and credible intervals instead of relying solely on point estimates.

Overall, this analysis confirms that a small set of physicochemical properties primarily determine fixed acidity. The results are consistent with known principles of wine chemistry, showing how Bayesian methods can strengthen scientific understanding through probabilistic modeling.

#### Recommendations

#### 1. For Winemakers

- o Monitor and adjust **density**, **citric acid**, **and chlorides** closely during the winemaking process, as these are the strongest determinants of fixed acidity.
- o Regulate **alcohol levels** carefully, since higher alcohol content reduces acidity perception.
- o Control **volatile acidity** (e.g., acetic acid), as excessive levels lower fixed acidity and negatively affect sensory quality.

#### 2. For Statistical Modeling

- o Bayesian regression should be preferred over classical regression when analyzing wine quality data, as it provides more robust uncertainty quantification.
- o Future studies can incorporate **hierarchical Bayesian models** to capture vineyard, regional, or vintage effects.

 Non-linear Bayesian models may be explored to account for complex chemical interactions beyond linear effects.

#### 3. For Future Research

- Extend the analysis to include **white wine data** or other beverages to test the generalizability of findings.
- o Incorporate **expert priors from enologists** to strengthen Bayesian modeling with domain knowledge.
- Combine Bayesian regression with predictive machine learning approaches (e.g., Bayesian additive regression trees, Gaussian processes) for more flexible modeling.

# 5. References

- Gelman, A., Carlin, J. B., Stern, H. S., Dunson, D. B., Vehtari, A., & Rubin, D. B. (2013). *Bayesian data analysis* (3rd ed.). CRC Press.
- UCI Machine Learning Repository. (n.d.). *Wine quality dataset*. University of California, Irvine.
- McElreath, R. (2020). Statistical rethinking: A Bayesian course with examples in R and Stan (2nd ed.). CRC Press.

# 6. Appendices (Mandatory)

Data set:- https://www.kaggle.com/datasets/yasserh/wine-quality-dataset

#### Load the data set.

```
wine_data <- read.csv("WineQT.csv", header = TRUE, na.strings = c("","NA"))</pre>
Head of the data set
head(wine_data)
     fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
##
## 1
                                            0.00
                                                            1.9
               7.4
                               0.70
                                                                    0.076
## 2
               7.8
                               0.88
                                            0.00
                                                            2.6
                                                                    0.098
## 3
               7.8
                               0.76
                                            0.04
                                                            2.3
                                                                    0.092
## 4
                                                            1.9
              11.2
                               0.28
                                            0.56
                                                                    0.075
## 5
               7.4
                               0.70
                                            0.00
                                                            1.9
                                                                    0.076
               7.4
## 6
                               0.66
                                            0.00
                                                            1.8
                                                                    0.075
   free.sulfur.dioxide total.sulfur.dioxide density
                                                         pH sulphates alcohol
##
## 1
                      11
                                            34 0.9978 3.51
                                                                 0.56
                                                                           9.4
## 2
                      25
                                            67
                                                0.9968 3.20
                                                                 0.68
                                                                           9.8
## 3
                      15
                                            54 0.9970 3.26
                                                                 0.65
                                                                           9.8
                                                                           9.8
## 4
                      17
                                            60 0.9980 3.16
                                                                 0.58
## 5
                      11
                                            34 0.9978 3.51
                                                                 0.56
                                                                           9.4
## 6
                                            40 0.9978 3.51
                                                                           9.4
                      13
                                                                 0.56
##
     quality Id
           5 0
## 1
           5 1
## 2
## 3
           5 2
## 4
           6 3
## 5
           5 4
## 6
```

#### Stucture of the variables

```
## $ free.sulfur.dioxide : num 11 25 15 17 11 13 15 15 9 15 ...
## $ total.sulfur.dioxide: num 34 67 54 60 34 40 59 21 18 65 ...
## $ density
                        : num 0.998 0.997 0.997 0.998 0.998 ...
                        : num 3.51 3.2 3.26 3.16 3.51 3.51 3.3 3.39 3.36
## $ pH
3.28 ...
## $ sulphates
                        : num 0.56 0.68 0.65 0.58 0.56 0.56 0.46 0.47 0.57
0.54 ...
## $ alcohol
                        : num 9.4 9.8 9.8 9.8 9.4 9.4 9.4 10 9.5 9.2 ...
                               5 5 5 6 5 5 5 7 7 5 ...
## $ quality
                        : int
## $ Id
                        : int 01234567810...
```

#### Take all the numerical variables as a new data frame wine\_data.

```
wine_data <- cbind(wine_data$fixed.acidity,wine_data$volatile.acidity,
wine_data$citric.acid,wine_data$residual.sugar,wine_data$chlorides,wine_data$
free.sulfur.dioxide, wine_data$total.sulfur.dioxide, wine_data$density,
wine_data$pH, wine_data$sulphates, wine_data$alcohol,wine_data$quality )
wine_data <- data.frame(wine_data)</pre>
```

#### Rename the columns of the new data set.

```
names(wine_data) <- c("FixedAcidity", "VolatileAcidity", "CitricAcid",</pre>
"ResidualSugar", "chlorides", "FreeSulfurDioxide", "TotalSulfurDioxide",
"Density", "pH", "Sulphates", "Alcohol", "Quality")
head(wine_data)
##
     FixedAcidity VolatileAcidity CitricAcid ResidualSugar chlorides
## 1
              7.4
                              0.70
                                         0.00
                                                         1.9
                                                                 0.076
## 2
              7.8
                              0.88
                                         0.00
                                                         2.6
                                                                 0.098
## 3
              7.8
                              0.76
                                         0.04
                                                         2.3
                                                                 0.092
                              0.28
## 4
             11.2
                                         0.56
                                                         1.9
                                                                 0.075
## 5
              7.4
                              0.70
                                         0.00
                                                         1.9
                                                                 0.076
## 6
              7.4
                              0.66
                                         0.00
                                                         1.8
                                                                 0.075
     FreeSulfurDioxide TotalSulfurDioxide Density
                                                     pH Sulphates Alcohol
##
Quality
## 1
                    11
                                        34 0.9978 3.51
                                                              0.56
                                                                       9.4
5
## 2
                                        67 0.9968 3.20
                                                              0.68
                                                                       9.8
                    25
5
## 3
                                        54 0.9970 3.26
                    15
                                                              0.65
                                                                       9.8
5
## 4
                                        60 0.9980 3.16
                                                              0.58
                                                                       9.8
                    17
6
## 5
                    11
                                        34 0.9978 3.51
                                                              0.56
                                                                       9.4
5
```

```
## 6 13 40 0.9978 3.51 0.56 9.4 5
```

# Check the missing values

```
sum(is.na(wine_data) == TRUE)
## [1] 0
```

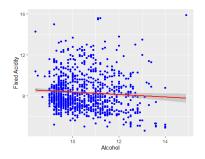
#### Summary output of the variables.

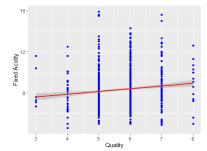
```
summary(wine_data)
##
     FixedAcidity
                     VolatileAcidity
                                         CitricAcid
                                                        ResidualSugar
##
   Min.
          : 4.600
                     Min.
                            :0.1200
                                      Min.
                                              :0.0000
                                                        Min.
                                                               : 0.900
##
   1st Qu.: 7.100
                     1st Qu.:0.3925
                                       1st Qu.:0.0900
                                                        1st Qu.: 1.900
##
   Median : 7.900
                     Median :0.5200
                                      Median :0.2500
                                                        Median : 2.200
##
                                                               : 2.532
   Mean
          : 8.311
                     Mean
                            :0.5313
                                      Mean
                                              :0.2684
                                                        Mean
##
    3rd Qu.: 9.100
                     3rd Qu.:0.6400
                                       3rd Qu.:0.4200
                                                        3rd Qu.: 2.600
##
   Max.
           :15.900
                            :1.5800
                                                        Max.
                                                               :15.500
                     Max.
                                      Max.
                                              :1.0000
##
      chlorides
                      FreeSulfurDioxide TotalSulfurDioxide
                                                               Density
## Min.
           :0.01200
                      Min.
                             : 1.00
                                        Min.
                                              : 6.00
                                                            Min.
                                                                   :0.9901
    1st Qu.:0.07000
                      1st Qu.: 7.00
                                         1st Qu.: 21.00
                                                            1st Qu.:0.9956
##
##
   Median :0.07900
                      Median :13.00
                                         Median : 37.00
                                                            Median :0.9967
                                                : 45.91
##
   Mean
           :0.08693
                      Mean
                             :15.62
                                        Mean
                                                            Mean
                                                                   :0.9967
                                                            3rd Qu.:0.9978
##
    3rd Qu.:0.09000
                      3rd Qu.:21.00
                                         3rd Qu.: 61.00
                      Max.
##
   Max.
           :0.61100
                              :68.00
                                        Max.
                                                :289.00
                                                            Max.
                                                                   :1.0037
##
          рΗ
                      Sulphates
                                         Alcohol
                                                         Quality
##
   Min.
           :2.740
                    Min.
                           :0.3300
                                     Min.
                                             : 8.40
                                                      Min.
                                                             :3.000
##
    1st Qu.:3.205
                    1st Qu.:0.5500
                                      1st Qu.: 9.50
                                                      1st Qu.:5.000
## Median :3.310
                    Median :0.6200
                                     Median :10.20
                                                      Median :6.000
##
   Mean
           :3.311
                    Mean
                           :0.6577
                                     Mean
                                             :10.44
                                                      Mean
                                                             :5.657
##
   3rd Qu.:3.400
                    3rd Qu.:0.7300
                                      3rd Qu.:11.10
                                                      3rd Qu.:6.000
## Max. :4.010
                    Max. :2.0000
                                     Max. :14.90
                                                      Max. :8.000
```

#### Standard deviations of each variable

```
st_devs <- c(sd(wine_data$FixedAcidity), sd(wine_data$VolatileAcidity),</pre>
sd(wine_data$CitricAcid),sd(wine_data$ResidualSugar),
sd(wine data$chlorides), sd(wine data$FreeSulfurDioxide),
sd(wine_data$TotalSulfurDioxide), sd(wine_data$Density), sd(wine_data$pH),
sd(wine data$Sulphates), sd(wine data$Alcohol), sd(wine data$Quality))
st devs
## [1] 1.747595017 0.179633193 0.196685852 1.355917467
                                                               0.047267338
## [6] 10.250486123 32.782130307 0.001925067
                                                  0.156664060
                                                               0.170398714
## [11] 1.082195610 0.805824248
library(ggplot2)
                            scplot2 <- ggplot(data =</pre>
                                                       scplot3 <- ggplot(data =</pre>
                                                       wine_data, aes(x =
scplot1 <- ggplot(data =</pre>
                            wine_data, aes(x =
                                                       ResidualSugar, y =
wine data, aes(x =
                            CitricAcid, y =
                            FixedAcidity)) +
VolatileAcidity, y =
                                                       FixedAcidity)) +
                                                          geom_point(color =
FixedAcidity)) +
                               geom_point(color =
  geom point(color =
                             "blue") +
                                                        "blue") +
"blue") +
                              xlab("Citric Acid") +
                                                         xlab("Residual Sugar")
  xlab("Volatile
                              ylab("Fixed Acidity")
Acidity") +
                                                         ylab("Fixed Acidity")
  ylab("Fixed Acidity") +
                               geom_smooth(method =
                             "lm", color = "red")
  geom smooth(method =
                                                          geom_smooth(method =
"lm", color = "red")
                                                        "lm", color = "red")
                            scplot2
                            ## `geom_smooth()` using scplot3
scplot1
## `geom_smooth()` using
                            formula = 'y \sim x'
                                                       ## `geom_smooth()` using
formula = 'y \sim x'
                                                       formula = 'y \sim x'
scplot4 <- ggplot(data =</pre>
                            scplot5 <- ggplot(data =</pre>
                                                        scplot6 <- ggplot(data =</pre>
wine data, aes(x =
                            wine_data, aes(x =
                                                       wine data, aes(x =
chlorides, y =
                            FreeSulfurDioxide, y =
                                                       TotalSulfurDioxide, y =
FixedAcidity)) +
                            FixedAcidity)) +
                                                       FixedAcidity)) +
  geom point(color =
                               geom point(color =
                                                          geom point(color =
                                                        "blue") +
"blue") +
                             "blue") +
  xlab("chlorides") +
                              xlab("Free Sulfur
                                                         xlab("Total Sulfur
  ylab("Fixed Acidity") +
                            Dioxide") +
                                                       Dioxide") +
  geom smooth(method =
                              ylab("Fixed Acidity")
                                                         ylab("Fixed Acidity")
"lm", color = "red")
                               geom smooth(method =
                                                         geom smooth(method =
scplot4
                            "lm", color = "red")
                                                        "lm", color = "red")
## `geom_smooth()` using
formula = 'y \sim x'
                            scplot5
                                                       scplot6
                            ## `geom_smooth()` using ## `geom_smooth()` using
```

```
formula = 'y \sim x'
                                                         formula = 'y \sim x'
scplot7 <- ggplot(data =</pre>
                             scplot8 <- ggplot(data =</pre>
                                                         scplot9 <- ggplot(data =</pre>
                             wine_data, aes(x = pH, y)
wine_data, aes(x =
                                                         wine_data, aes(x =
Density, y =
                             = FixedAcidity)) +
                                                         Sulphates, y =
FixedAcidity)) +
                               geom_point(color =
                                                         FixedAcidity)) +
  geom_point(color =
                             "blue") +
                                                           geom point(color =
                               xlab("pH") +
"blue") +
                                                         "blue") +
  xlab("Density") +
                               ylab("Fixed Acidity")
                                                           xlab("Sulphates") +
  ylab("Fixed Acidity") +
                                                           ylab("Fixed Acidity")
  geom_smooth(method =
                               geom_smooth(method =
"lm", color = "red")
                             "lm", color = "red")
                                                           geom_smooth(method =
                                                         "lm", color = "red")
scplot7
                             scplot8
                             ## `geom_smooth()` using
## `geom_smooth()` using
                                                         scplot9
formula = 'y \sim x'
                                                         ## `geom_smooth()` using
                             formula = 'y \sim x'
                                                         formula = 'y \sim x'
scplot10 <- ggplot(data =</pre>
                             scplot11 <- ggplot(data</pre>
wine_data, aes(x =
                             = wine_data, aes(x =
Alcohol, y =
                             Quality, y =
FixedAcidity)) +
                             FixedAcidity)) +
  geom_point(color =
                               geom_point(color =
"blue") +
                             "blue") +
  xlab("Alcohol") +
                               xlab("Quality") +
  ylab("Fixed Acidity") +
                               ylab("Fixed Acidity")
  geom_smooth(method =
"lm", color = "red")
                               geom_smooth(method =
                             "lm", color = "red")
scplot10
## `geom_smooth()` using
                             scplot11
formula = 'y \sim x'
                             ## `geom_smooth()` using
                             formula = 'y \sim x'
```

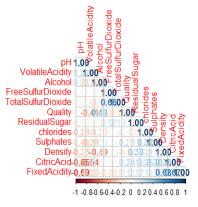




```
library(corrplot)
## Warning: package 'corrplot' was built under R version 4.3.3
## corrplot 0.92 loaded
```

#### The correlation coefficients among each and every pair of variables.

```
corrplot(corr = cor(wine_data), method = "number" , order = 'FPC', type =
'lower')
```



```
cor(wine_data)
##
                      FixedAcidity VolatileAcidity CitricAcid ResidualSugar
## FixedAcidity
                        1.00000000
                                      -0.250728322
                                                    0.67315725
                                                                  0.171830535
## VolatileAcidity
                       -0.25072832
                                       1.000000000 -0.54418694
                                                                 -0.005751097
## CitricAcid
                        0.67315725
                                      -0.544186937
                                                    1.00000000
                                                                 0.175814854
## ResidualSugar
                        0.17183054
                                      -0.005751097
                                                    0.17581485
                                                                  1.000000000
## chlorides
                                       0.056336259
                                                    0.24531249
                        0.10788857
                                                                 0.070863112
## FreeSulfurDioxide
                       -0.16483079
                                      -0.001962479 -0.05758910
                                                                  0.165338797
## TotalSulfurDioxide
                       -0.11062837
                                       0.077747722
                                                    0.03687111
                                                                 0.190790035
## Density
                        0.68150088
                                       0.016511520
                                                    0.37524326
                                                                 0.380146952
## pH
                                       0.221491518 -0.54633914
                       -0.68516260
                                                                 -0.116958936
## Sulphates
                        0.17459183
                                      -0.276078597
                                                    0.33123176
                                                                  0.017474504
## Alcohol
                       -0.07505485
                                      -0.203909273
                                                    0.10625034
                                                                  0.058420606
```

```
## Quality
                        0.12197010
                                      -0.407393513 0.24082084
                                                                 0.022001931
##
                        chlorides FreeSulfurDioxide TotalSulfurDioxide
Density
                       0.10788857
                                       -0.164830793
                                                           -0.11062837
## FixedAcidity
0.68150088
## VolatileAcidity
                       0.05633626
                                       -0.001962479
                                                            0.07774772
0.01651152
## CitricAcid
                       0.24531249
                                       -0.057589104
                                                            0.03687111
0.37524326
## ResidualSugar
                       0.07086311
                                        0.165338797
                                                            0.19079003
0.38014695
## chlorides
                       1.00000000
                                        0.015280458
                                                            0.04816316
0.20890071
## FreeSulfurDioxide
                       0.01528046
                                        1.000000000
                                                            0.66109287 -
0.05415032
## TotalSulfurDioxide 0.04816316
                                        0.661092872
                                                            1.00000000
0.05017483
## Density
                       0.20890071
                                       -0.054150318
                                                            0.05017483
1.00000000
## pH
                      -0.27775907
                                        0.072803706
                                                           -0.05912572 -
0.35277462
                       0.37478389
                                        0.034445122
                                                            0.02689368
## Sulphates
0.14313929
## Alcohol
                      -0.22991709
                                       -0.047094832
                                                           -0.18816480 -
0.49472690
## Quality
                      -0.12408453
                                       -0.063259641
                                                           -0.18333915 -
0.17520792
##
                               рН
                                    Sulphates
                                                  Alcohol
                                                              Quality
                      -0.68516260 0.17459183 -0.07505485
## FixedAcidity
                                                           0.12197010
## VolatileAcidity
                       0.22149152 -0.27607860 -0.20390927 -0.40739351
## CitricAcid
                      -0.54633914   0.33123176   0.10625034
                                                           0.24082084
## ResidualSugar
                      -0.11695894 0.01747450 0.05842061 0.02200193
## chlorides
                      -0.27775907
                                   0.37478389 -0.22991709 -0.12408453
## FreeSulfurDioxide
                       0.07280371 0.03444512 -0.04709483 -0.06325964
## TotalSulfurDioxide -0.05912572
                                   0.02689368 -0.18816480 -0.18333915
## Density
                      -0.35277462   0.14313929   -0.49472690   -0.17520792
## pH
                       1.00000000 -0.18549903 0.22532220 -0.05245303
## Sulphates
                      -0.18549903 1.00000000 0.09442113
                                                           0.25771026
## Alcohol
                       0.22532220 0.09442113 1.00000000 0.48486621
## Quality
                      -0.05245303 0.25771026 0.48486621 1.00000000
lmTemp1 <- lm(formula = FixedAcidity ~ . , data = wine_data)</pre>
summary(lmTemp1)
##
## lm(formula = FixedAcidity ~ ., data = wine_data)
##
## Residuals:
##
      Min
                1Q Median 3Q
                                       Max
```

```
## -2.6456 -0.3589 -0.0060 0.3479 3.6466
##
## Coefficients:
                      Estimate Std. Error t value Pr(>|t|)
##
                   -6.316e+02 1.550e+01 -40.749 < 2e-16 ***
## (Intercept)
## VolatileAcidity
                     1.972e-01 1.420e-01
                                            1.389
                                                  0.16523
## CitricAcid
                     1.815e+00 1.612e-01 11.256 < 2e-16 ***
                    -2.485e-01 1.657e-02 -14.996 < 2e-16 ***
## ResidualSugar
                    -3.718e+00 4.787e-01 -7.768 1.78e-14 ***
## chlorides
## FreeSulfurDioxide 6.643e-03 2.502e-03
                                          2.655 0.00804 **
## TotalSulfurDioxide -5.308e-03 8.129e-04 -6.529 9.95e-11 ***
                     6.546e+02 1.545e+01 42.362 < 2e-16
## Density
## pH
                    -5.276e+00 1.533e-01 -34.426 < 2e-16
                    -7.293e-01 1.319e-01 -5.529 3.99e-08 ***
## Sulphates
## Alcohol
                     5.550e-01 2.717e-02 20.429 < 2e-16 ***
## Quality
                     2.218e-02 2.921e-02 0.759 0.44777
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6294 on 1131 degrees of freedom
## Multiple R-squared: 0.8715, Adjusted R-squared: 0.8703
## F-statistic: 697.6 on 11 and 1131 DF, p-value: < 2.2e-16
library(BAS)
## Warning: package 'BAS' was built under R version 4.3.3
```

#### **Bayesian Simple Linear Regression**

Fit a simple linear regression model of Density versus Fixed Acidity.

```
apTemp.lm1 <- lm(formula = FixedAcidity ~ Density, data = wine data)
summary(lmTemp1)
##
## Call:
## lm(formula = FixedAcidity ~ ., data = wine_data)
##
## Residuals:
               10 Median
                               30
##
      Min
                                      Max
## -2.6456 -0.3589 -0.0060 0.3479 3.6466
##
## Coefficients:
##
                       Estimate Std. Error t value Pr(>|t|)
                     -6.316e+02 1.550e+01 -40.749 < 2e-16 ***
## (Intercept)
## VolatileAcidity
                     1.972e-01 1.420e-01
                                             1.389
                                                    0.16523
                      1.815e+00 1.612e-01 11.256 < 2e-16 ***
## CitricAcid
## ResidualSugar
                     -2.485e-01 1.657e-02 -14.996 < 2e-16 ***
## chlorides
                -3.718e+00 4.787e-01 -7.768 1.78e-14 ***
```

```
## FreeSulfurDioxide 6.643e-03 2.502e-03 2.655 0.00804 **
## TotalSulfurDioxide -5.308e-03 8.129e-04 -6.529 9.95e-11 ***
                     6.546e+02 1.545e+01 42.362 < 2e-16 ***
## Density
## pH
                    -5.276e+00 1.533e-01 -34.426 < 2e-16 ***
## Sulphates
                   -7.293e-01 1.319e-01 -5.529 3.99e-08 ***
## Alcohol
                     5.550e-01 2.717e-02 20.429 < 2e-16 ***
## Ouality
                    2.218e-02 2.921e-02 0.759 0.44777
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6294 on 1131 degrees of freedom
## Multiple R-squared: 0.8715, Adjusted R-squared: 0.8703
## F-statistic: 697.6 on 11 and 1131 DF, p-value: < 2.2e-16
```

#### Obtain residuals and n.

```
resid <- residuals(apTemp.lm1)
n <- length(resid)</pre>
```

#### Calculate MSE

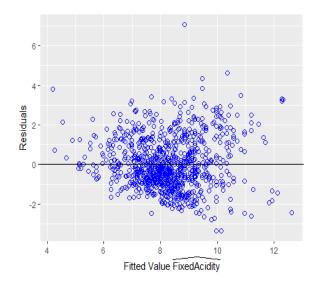
```
MSE <- 1/ (n-2) * sum((resid ^ 2))
MSE
## [1] 1.637071
```

#### Combine residuals and fitted values into a data frame.

```
result <- data.frame(fitted_values = fitted.values(apTemp.lm1) , residuals =
residuals(apTemp.lm1))</pre>
```

#### Load library and plot residuals versus fitted values.

```
library(ggplot2)
ggplot(data = result, aes(x = fitted_values, y = residuals)) +
   geom_point(color = "blue", pch = 1, size = 2) +
   geom_abline(intercept = 0, slope = 0) +
   xlab(expression(paste("Fitted Value ", widehat(FixedAcidity)))) +
   ylab("Residuals")
```



# The observation with the largest fitted value.

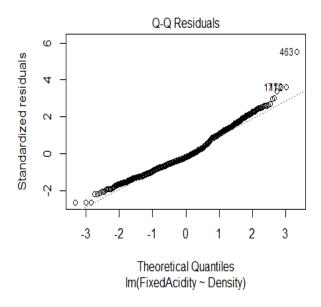
```
which.max(as.vector(fitted.values(apTemp.lm1)))
## [1] 1023
```

# Shows this observation has the largest Density

```
which.max(wine_data$Density)
## [1] 1023
```

#### Normal probability plot of the residuals.

```
plot(apTemp.lm1, which = 2)
```



#### Credible Intervals for Slope Beta and y-Intercept alpha.

```
output <- summary(apTemp.lm1)$coef[, 1:2]</pre>
output
##
                 Estimate Std. Error
## (Intercept) -608.3393
                            19.60348
## Density
                618.6733
                            19.66775
out <- cbind(output, confint(apTemp.lm1))</pre>
colnames(out) <- c("Posterior Mean", "Posterior Std", "2.5", "97.5")</pre>
round(out, 3)
##
               Posterior Mean Posterior Std
                                                    2.5
                                                            97.5
## (Intercept)
                      -608.339
                                       19.603 -646.802 -569.876
## Density
                       618.673
                                       19.668 580.084 657.262
```

#### **Construct current prediction.**

```
alpha <- apTemp.lm1$coefficients[1]
beta <- apTemp.lm1$coefficients[2]
new_x <- seq(min(wine_data$Density) , max(wine_data$Density) , length.out =
100)
y_hat <- alpha + beta*new_x</pre>
```

#### Get lower and upper bounds for mean.

```
ymean <- data.frame(predict(apTemp.lm1 , newdata = data.frame(Density =
new_x) , interval = "confidence" , level = 0.95))

Get lower and upper bounds for prediction.

ypred <- data.frame(predict(apTemp.lm1 , newdata = data.frame(Density =
new_x) , interval = "prediction" , level = 0.95))

output <- data.frame(x = new_x , y_hat = y_hat , ymean_lwr = ymean$lwr ,
ymean_upr = ymean$upr , ypred_lwr = ypred$lwr , ypred_upr = ypred$upr)

Extract potential outlier data point.

outlier <- data.frame(x = wine_data$Density[3241] , y =
wine_data$Density[3241])</pre>
```

#### Scatter plot of original.

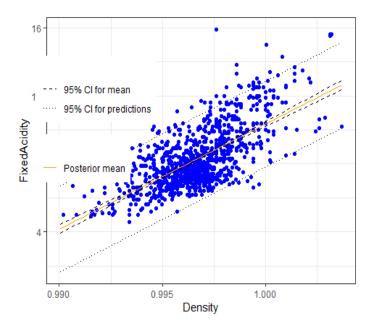
```
library(ggplot2)
plot1 <- ggplot(data = wine_data , aes(x = Density , y = FixedAcidity)) +
geom_point(color = "blue")</pre>
```

#### Add bounds of mean and prediction.

```
plot2 <- plot1 + geom_line(data = output , aes(x = new_x , y = y_hat , color=
"first") , lty = 1) + geom_line(data = output , aes(x = new_x , y = ymean_lwr
, lty = "second")) + geom_line(data = output , aes(x = new_x , y = ymean_upr
, lty = "second")) + geom_line(data = output , aes(x = new_x , y = ypred_upr
, lty="third")) + geom_line(data = output , aes(x = new_x , y = ypred_lwr ,
lty = "third")) + scale_colour_manual(values = c("orange") , labels =
"Posterior mean" , name = "") + scale_linetype_manual(values = c(2,3) ,
labels = c("95% CI for mean" , "95% CI for predictions") , name = "") +
theme_bw() + theme(legend.position = c(1,0) , legend.justification = c(3.-
0.35,-0.8))</pre>
```

#### Identify potential outlier.

```
plot2 + geom_point(data = outlier , aes(x = x , y = y) , color = "orange" ,
pch = 1 , cex = 6)
## Warning: Removed 1 rows containing missing values (`geom_point()`).
```



#### Bayesian Multiple Linear Regression Use BAS.LM to run regression model.

```
library(BAS)
wine.bas = bas.lm(FixedAcidity ~ . , data = wine_data , prior = "BIC" ,
modelprior = Bernoulli(1) , include.always = ~ . , n.models = 1)
wine.bas
##
## Call:
## bas.lm(formula = FixedAcidity ~ ., data = wine_data, n.models = 1,
       prior = "BIC", modelprior = Bernoulli(1), include.always = ~.)
##
##
##
  Marginal Posterior Inclusion Probabilities:
##
                          VolatileAcidity
##
            Intercept
                                                    CitricAcid
ResidualSugar
##
1
            chlorides
                        FreeSulfurDioxide TotalSulfurDioxide
##
Density
##
                    1
                                         1
                                                             1
1
##
                                Sulphates
                                                       Alcohol
                   рΗ
Quality
##
                    1
                                         1
                                                             1
1
```

#### Posterior Means and Posterior Standard Deviations.

```
wine.coef = coef(wine.bas)
wine.coef
##
   Marginal Posterior Summaries of Coefficients:
##
##
##
   Using BMA
##
##
   Based on the top 1 models
##
                                  post SD
                                              post p(B != 0)
                      post mean
## Intercept
                                               1.000e+00
                       8.311e+00
                                   1.862e-02
## VolatileAcidity
                       1.972e-01
                                   1.420e-01
                                               1.000e+00
## CitricAcid
                       1.815e+00
                                   1.612e-01
                                               1.000e+00
## ResidualSugar
                      -2.485e-01
                                   1.657e-02
                                               1.000e+00
## chlorides
                       -3.718e+00
                                   4.787e-01
                                               1.000e+00
## FreeSulfurDioxide
                       6.643e-03
                                   2.502e-03
                                               1.000e+00
## TotalSulfurDioxide
                      -5.308e-03
                                   8.129e-04
                                               1.000e+00
## Density
                       6.546e+02
                                   1.545e+01
                                               1.000e+00
## pH
                       -5.276e+00
                                   1.533e-01
                                               1.000e+00
## Sulphates
                       -7.293e-01
                                   1.319e-01
                                               1,000e+00
## Alcohol
                       5.550e-01
                                   2.717e-02
                                               1.000e+00
                                   2.921e-02
## Quality
                       2.218e-02
                                               1.000e+00
```

#### visualization of the coefficients.

out <- confint(wine.coef)[, 1:2]</pre>

```
par(mfrow = c(2, 4) , col.lab = "darkgrey" , col.axis = "darkgrey" , col =
"darkgrey")
plot(wine.coef , ask = F)
    Intercept
               VolatileAcidity
                             CitricAcid
                                        ResidualSugar
                                                             pΗ
                                                                        Sulphates
                                                                                       Alcohol
                                                                                                     Quality
                                          7/1
    chlorides
              Free Sulfur Dioxid Total Sulfur Dioxic
                                           Density
  0.4 0.8
```

#### Extract the upper and lower bounds of the credible intervals.

```
names <- c("posterior mean", "posterior std", colnames(out))</pre>
out <- cbind(wine.coef$postmean , wine.coef$postsd , out)</pre>
colnames(out) <- names</pre>
round(out , 4)
##
                      posterior mean posterior std
                                                       2.5%
                                                               97.5%
## Intercept
                              8.3111
                                            0.0186
                                                     8.2746
                                                              8.3476
## VolatileAcidity
                              0.1972
                                            0.1420 -0.0815
                                                              0.4759
## CitricAcid
                              1.8150
                                            0.1612
                                                    1.4986
                                                             2.1314
                                            0.0166 -0.2810
## ResidualSugar
                             -0.2485
                                                             -0.2159
## chlorides
                             -3.7184
                                            0.4787 -4.6576
                                                             -2.7792
## FreeSulfurDioxide
                                            0.0025
                                                     0.0017
                                                              0.0116
                              0.0066
## TotalSulfurDioxide
                             -0.0053
                                            0.0008 -0.0069
                                                             -0.0037
## Density
                            654.5712
                                           15.4517 624.2540 684.8885
## pH
                                            0.1533 -5.5768
                             -5.2761
                                                             -4.9754
## Sulphates
                             -0.7293
                                            0.1319 -0.9880 -0.4705
## Alcohol
                              0.5550
                                            0.0272 0.5017
                                                              0.6083
## Quality
                              0.0222
                                            0.0292 -0.0351 0.0795
```

#### Use BAS.LM to run regression model.

```
wine.bas2 <- bas.lm(FixedAcidity ~ . , data = wine_data , prior = "BIC" ,</pre>
modelprior = Bernoulli(1) ,
n.models = 1)
wine.bas2
##
## Call:
## bas.lm(formula = FixedAcidity ~ ., data = wine data, n.models = 1,
##
       prior = "BIC", modelprior = Bernoulli(1))
##
##
## Marginal Posterior Inclusion Probabilities:
##
            Intercept
                         VolatileAcidity
                                                     CitricAcid
ResidualSugar
##
                  NaN
                                         0
                                                              0
0
##
            chlorides
                        FreeSulfurDioxide TotalSulfurDioxide
Density
                                         0
##
                    0
                                                              0
0
##
                                 Sulphates
                                                        Alcohol
                   рΗ
Quality
##
                    0
                                         0
                                                              0
0
```

#### **Bayesian Model Selection**

```
modelSelection <- step(lmTemp1, k = log(nrow(wine_data)))</pre>
## Start: AIC=-985.96
## FixedAcidity ~ VolatileAcidity + CitricAcid + ResidualSugar +
       chlorides + FreeSulfurDioxide + TotalSulfurDioxide + Density +
##
##
       pH + Sulphates + Alcohol + Quality
##
##
                        Df Sum of Sq
                                                 AIC
                                         RSS
## - Quality
                         1
                                0.23 448.27 -992.42
## - VolatileAcidity
                                0.76 448.80 -991.05
## <none>
                                      448.04 -985.96
## - FreeSulfurDioxide
                         1
                                2.79
                                      450.83 -985.89
                         1
## - Sulphates
                               12.11 460.15 -962.51
## - TotalSulfurDioxide 1
                               16.89 464.93 -950.70
## - chlorides
                         1
                               23.90 471.94 -933.59
## - CitricAcid
                         1
                               50.19 498.23 -871.64
                         1
## - ResidualSugar
                               89.09 537.13 -785.71
## - Alcohol
                         1
                              165.33 613.37 -633.99
## - pH
                         1
                              469.49 917.53 -173.69
## - Density
                         1
                              710.91 1158.95
                                               93.29
##
## Step: AIC=-992.42
## FixedAcidity ~ VolatileAcidity + CitricAcid + ResidualSugar +
##
       chlorides + FreeSulfurDioxide + TotalSulfurDioxide + Density +
##
       pH + Sulphates + Alcohol
##
##
                        Df Sum of Sq
                                         RSS
                                                 AIC
## - VolatileAcidity
                                0.62 448.88 -997.89
## <none>
                                      448.27 -992.42
## - FreeSulfurDioxide
                         1
                                2.84 451.11 -992.23
## - Sulphates
                         1
                               11.92 460.19 -969.47
## - TotalSulfurDioxide 1
                               17.49 465.76 -955.70
## - chlorides
                         1
                               24.72 472.98 -938.11
## - CitricAcid
                         1
                               50.09 498.36 -878.38
## - ResidualSugar
                         1
                               88.98 537.25 -792.50
## - Alcohol
                         1
                              187.88 636.15 -599.36
## - pH
                         1
                              476.44 924.71 -171.83
## - Density
                         1
                              710.81 1159.08
                                               86.38
##
## Step: AIC=-997.89
## FixedAcidity ~ CitricAcid + ResidualSugar + chlorides + FreeSulfurDioxide
+
##
       TotalSulfurDioxide + Density + pH + Sulphates + Alcohol
##
##
                        Df Sum of Sa
                                         RSS
                                                 AIC
                                2.53 451.42 -998.50
## - FreeSulfurDioxide
                         1
```

```
## <none>
                                      448.88 -997.89
                               13.97 462.86 -969.90
## - Sulphates
                         1
## - TotalSulfurDioxide 1
                               16.88 465.76 -962.74
                         1
## - chlorides
                               24.55 473.43 -944.06
## - CitricAcid
                         1
                               63.04 511.93 -854.72
## - ResidualSugar
                         1
                               89.98 538.86 -796.11
## - Alcohol
                         1
                              194.12 643.00 -594.15
## - pH
                         1
                              478.02 926.90 -176.16
                         1
                              775.71 1224.59 142.18
## - Density
##
## Step: AIC=-998.5
## FixedAcidity ~ CitricAcid + ResidualSugar + chlorides + TotalSulfurDioxide
+
##
       Density + pH + Sulphates + Alcohol
##
##
                        Df Sum of Sq
                                         RSS
                                                 AIC
## <none>
                                      451.42 -998.50
## - Sulphates
                         1
                               13.34
                                      464.75 -972.26
## - TotalSulfurDioxide
                         1
                               16.22 467.64 -965.18
## - chlorides
                         1
                               24.31 475.73 -945.58
## - CitricAcid
                         1
                               61.99 513.40 -858.47
## - ResidualSugar
                         1
                               87.97 539.39 -802.04
## - Alcohol
                         1
                              195.17 646.59 -594.83
## - pH
                         1
                              475.52 926.93 -183.16
## - Density
                         1
                              773.19 1224.61 135.16
basModel1 <- bas.lm(formula = FixedAcidity ~ . , data = wine_data ,</pre>
prior = "BIC" , modelprior = uniform())
basCoeff <- coef(basModel1)</pre>
basCoeff
##
##
   Marginal Posterior Summaries of Coefficients:
##
##
   Using BMA
##
##
   Based on the top
                      2048 models
                                               post p(B != 0)
##
                       post mean
                                   post SD
## Intercept
                        8.311e+00
                                    1.864e-02
                                                1.000e+00
## VolatileAcidity
                        7.468e-03
                                    4.521e-02
                                                 5.028e-02
## CitricAcid
                        1.698e+00
                                    1.385e-01
                                                1.000e+00
## ResidualSugar
                       -2.471e-01
                                    1.664e-02
                                                1.000e+00
## chlorides
                       -3.583e+00
                                    4.590e-01
                                                1.000e+00
                                                4.289e-01
## FreeSulfurDioxide
                                    3.509e-03
                        2.696e-03
## TotalSulfurDioxide
                       -4.442e-03
                                    9.463e-04
                                                1.000e+00
## Density
                        6.580e+02
                                    1.501e+01
                                                1.000e+00
## pH
                       -5.275e+00
                                    1.532e-01
                                                1.000e+00
## Sulphates
                       -7.362e-01
                                    1.268e-01
                                                1.000e+00
## Alcohol
                        5.662e-01
                                    2.567e-02
                                                 1.000e+00
## Quality
                        5.318e-04
                                    5.968e-03
                                                3.352e-02
```

#### Find the index of the model with the largest logmarg.

```
best <- which.max(basModel1$logmarg)</pre>
```

Retreat the index of variables in the best model, with 0 as the index of the intercept.

```
bestModel <- basModel1$which[[best]]
bestModel
## [1] 0 2 3 4 6 7 8 9 10</pre>
```

Create an indicator vector indicating which variables are used in the best model.

```
bestGamma <- rep(0,basModel1$n.vars)
bestGamma[bestModel + 1] = 1
bestGamma
## [1] 1 0 1 1 1 0 1 1 1 1 0</pre>
```

Coefficient Estimates Under Reference Prior for Best BIC Model Fit the best BIC model by imposing which variables to be used using the indicators.

```
wine.bestBIC <- bas.lm(FixedAcidity ~ . , data = wine_data, prior = "BIC" ,</pre>
n.models = 1 , bestmodel = bestGamma , modelprior = uniform())
wine.coeff <- coef(wine.bestBIC)</pre>
out <- confint(wine.coeff)[,1:2]</pre>
Combine results and construct summary table.
coef.BIC <- cbind(wine.coeff$postmean , wine.coeff$postsd , out)</pre>
names <- c("post mean" , "post sd" , colnames(out))</pre>
colnames(coef.BIC) <- names</pre>
coef.BIC
##
                          post mean
                                          post sd
                                                           2.5%
                                                                       97.5%
                        8.31111111 1.866206e-02
## Intercept
                                                    8.274495064
                                                                  8.34772716
## VolatileAcidity
                        0.000000000 0.000000e+00
                                                    0.00000000
                                                                  0.00000000
## CitricAcid
                        1.686826597 1.351769e-01
                                                    1.421601577
                                                                  1.95205162
## ResidualSugar
                       -0.245499225 1.651460e-02 -0.277901837 -0.21309661
## chlorides
                       -3.570017428 4.568016e-01
                                                   -4.466288722
                                                                 -2.67374613
## FreeSulfurDioxide
                        0.000000000 0.000000e+00
                                                    0.000000000
                                                                  0.00000000
## TotalSulfurDioxide -0.003884293 6.084643e-04 -0.005078135 -0.00269045
## Density
                      657.246670764 1.491309e+01 627.986325974 686.50701555
## pH
                       -5.262546266 1.522634e-01 -5.561295978 -4.96379655
                       -0.729371714 1.260183e-01 -0.976626958 -0.48211647
## Sulphates
```

```
## Alcohol 0.567111234 2.561184e-02 0.516859324 0.61736314
## Quality 0.000000000 0.000000e+00 0.000000000 0.00000000
```

#### **Calculating Posterior Probability**

```
wine bas <- bas.lm(FixedAcidity ~ VolatileAcidity + CitricAcid +
ResidualSugar + chlorides + FreeSulfurDioxide + TotalSulfurDioxide + Density
+ pH + Sulphates + Alcohol + Quality , data = wine_data , prior = "BIC" ,
modelprior = uniform())
round(summary(wine_bas), 3)
                                                             model 3
                       P(B != 0 | Y)
##
                                        model 1
                                                  model 2
                                                                        model 4
## Intercept
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
                                          0.000
                                                     0.000
## VolatileAcidity
                               0.050
                                                               1.000
                                                                          1.000
                                          1.000
## CitricAcid
                               1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## ResidualSugar
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## chlorides
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## FreeSulfurDioxide
                               0.429
                                          0.000
                                                     1.000
                                                               1.000
                                                                          0.000
## TotalSulfurDioxide
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## Density
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## pH
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## Sulphates
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## Alcohol
                               1.000
                                          1.000
                                                     1.000
                                                               1.000
                                                                          1.000
## Quality
                               0.034
                                          0.000
                                                     0.000
                                                               0.000
                                                                          0.000
## BF
                                   NA
                                          1.000
                                                     0.738
                                                               0.048
                                                                          0.044
## PostProbs
                                   NA
                                          0.528
                                                     0.390
                                                               0.025
                                                                          0.023
## R2
                                   NA
                                          0.871
                                                     0.871
                                                               0.872
                                                                          0.871
## dim
                                   NA
                                          9.000
                                                    10.000
                                                              11.000
                                                                         10.000
## logmarg
                                   NA -3524.919 -3525.223 -3527.959 -3528.051
##
                         model 5
## Intercept
                           1.000
## VolatileAcidity
                           0.000
## CitricAcid
                           1.000
## ResidualSugar
                           1.000
## chlorides
                           1.000
## FreeSulfurDioxide
                           0.000
## TotalSulfurDioxide
                           1.000
## Density
                           1.000
## pH
                           1.000
## Sulphates
                           1.000
## Alcohol
                           1.000
## Quality
                           1.000
## BF
                           0.036
## PostProbs
                           0.019
## R2
                           0.871
## dim
                          10.000
## logmarg
                       -3528.256
```

#### The marginal posterior inclusion probability (pip)

```
print(wine_bas)
##
## Call:
## bas.lm(formula = FixedAcidity ~ VolatileAcidity + CitricAcid +
       ResidualSugar + chlorides + FreeSulfurDioxide + TotalSulfurDioxide +
##
       Density + pH + Sulphates + Alcohol + Quality, data = wine_data,
       prior = "BIC", modelprior = uniform())
##
##
##
## Marginal Posterior Inclusion Probabilities:
                        VolatileAcidity
            Intercept
                                                    CitricAcid
ResidualSugar
##
              1.00000
                                  0.05028
                                                       1.00000
1.00000
            chlorides
                        FreeSulfurDioxide TotalSulfurDioxide
##
Density
                                                       1.00000
              1.00000
                                  0.42885
##
1.00000
##
                                Sulphates
                                                       Alcohol
                   рΗ
Quality
                                  1.00000
##
              1.00000
                                                       1.00000
0.03352
```