

# Basics

Dataset: <https://archive.ics.uci.edu/dataset/186/wine+quality>

Repository: <https://github.com/iamhex7/151A-Wine-Quality.git>

Research Question:

**How do chemical properties differently affect the quality of white and red wines?**

## 0. Data and Modeling Objective

The original data comes in two datasets: one contains 4,898 white-wine observations and another one with 1,599 red-wine observations.

We manually merged them two into a single dataframe with one extra categorical variable called **type** indicating wine type – 0 as red wine, 1 as white wine.

**Response Variable:** **quality** (integer 0–10)

**Key grouping:** **type** (red / white as dummy variable)

**(Potential) Explanatory Variables:** **fixed\_acidity**, **volatile\_acidity**, **citric\_acid**, **residual\_sugar**, **chlorides**, **free\_sulfur\_dioxide**, **total\_sulfur\_dioxide**, **density**, **pH**, **sulphates**, **alcohol**.

## 1. determining if a transform is needed

Plot for each continuous x:

- histogram / density plot
- summary statistics (mean, median, IQR, max/min)

Transform if:

- Spotted strongly right-skewed (long-tailed) pattern → transform:  $\log(x)$  or  $\sqrt{x}$
- If a variable has a value of 0 and cannot use  $\log$ , consider  $\log(x + c)$  ( $c$  is a small constant such as 0.1).

## 2. Basic Main-Effects Model excluding interaction

```
m_main <- lm(quality ~ type + x1 + x2 + ... + x11, data = wine_transformed)
```

### 2.1 Check the residuals

- Residuals vs Fitted: look for non-linearity or heteroscedasticity?
- QQ plot: Is the error roughly close to normal?

### 2.2 Checking collinearity

- Calculate the correlation coefficient matrix for all  $x$
- Calculate the VIF (variance inflation factors) on this model

If some variables are highly correlated:

If both variables are meaningful for the scientific question, they can be retained initially, and simplified later during model selection;

### 2.3 Which Features May Be Removed:

Examine the estimated value and standard error of each main effect

Examine their t-values/p-values

Compare the changes in AIC/BIC before and after removing a certain variable

## 3. Explore & test interaction: type × chemical

Chemically, below are likely strong interactions among features:

free sulfur dioxide & total sulfur dioxide

fixed acidity & pH

alcohol & density

residual sugar & density

citric acid & pH

volatile acidity & pH

### 3.1 Visual Review First, EDA

Are the slopes of the two lines significantly different for red wine and white wine?

For example:

```
ggplot(wine, aes(x = alcohol, y = quality, type = type)) +  
  geom_point(alpha = 0.2) +  
  geom_smooth(method = "lm", se = FALSE)
```

If the regression lines of the two colors are significantly non-parallel, then  $\Rightarrow$  strong candidate: type  $\times$  alcohol interaction.

### 3.2 First, create a "full interaction" model and perform a global test.

```
m_int_full <- lm(quality ~ type * (x1 + x2 + ... + x11), data = wine_transformed)  
type * (...) :
```

All main effects (type + x1 + ... + x11)

Add all type: xj interactions

Then:

Compare using ANOVA incremental F-test: `anova(m_main, m_int_full)`

Compare AIC / BIC: `AIC(m_main, m_int_full) / BIC(m_main, m_int_full)`

## 4. feature selection on the main effects

We have a model:

Some main effects: `type + selected xj`

Some interactions: `type: xj`

### 4.1 General Principles

Main effects corresponding to retained interactions should not be removed.

Variables that do not appear in interactions and have small and unstable coefficients can be considered for removal.

### 4.2 Model Selection Procedure

- AIC/BIC
- Cross-validation

## 5. Model Diagnosis

- Residual vs Fitted: Check for nonlinearity and heteroscedasticity

QQ plot: Check for heavy tails

- Leverage & Cook's distance: Find high leverage/influential points