

# Assignment5\_Data621

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## Data Exploration

The training dataset has 12,795 observations across 15 columns and an additional INDEX column. For the purposes of our analysis, we will drop the INDEX column. The parameters STARS, AcidIndex, LabelAppeal appear to be categorical, while the remaining 12 variables, including our TARGET variable, appear numerical. The number of cases purchased (TARGET) ranges from 0-8. Roughly 21.4% (2734) of our observations had a TARGET value of zero.

```
## Rows: 12,795
## Columns: 15
## $ TARGET      <dbl> 3, 3, 5, 3, 4, 0, 0, 4, 3, 6, 0, 4, 3, 7, 4, 0, 0, ~
## $ AcidIndex   <fct> 8, 7, 8, 6, 9, 11, 8, 7, 6, 8, 5, 10, 7, 8, 9, 8, 9~
## $ Alcohol     <dbl> 9.9, NA, 22.0, 6.2, 13.7, 15.4, 10.3, 11.6, 15.0, 1~
## $ Chlorides   <dbl> -0.567, -0.425, 0.037, -0.425, NA, 0.556, 0.060, 0.~
## $ CitricAcid  <dbl> -0.98, -0.81, -0.88, 0.04, -1.26, 0.59, -0.40, 0.34~
## $ Density     <dbl> 0.99280, 1.02792, 0.99518, 0.99640, 0.99457, 0.9994~
## $ FixedAcidity <dbl> 3.2, 4.5, 7.1, 5.7, 8.0, 11.3, 7.7, 6.5, 14.8, 5.5,~
## $ FreeSulfurDioxide <dbl> NA, 15, 214, 22, -167, -37, 287, 523, -213, 62, 551~
## $ LabelAppeal <fct> 0, -1, -1, -1, 0, 0, 0, 1, 0, 0, 1, 0, 1, 2, 0, 0, ~
## $ pH         <dbl> 3.33, 3.38, 3.12, 2.24, 3.12, 3.20, 3.49, 3.20, 4.9~
## $ ResidualSugar <dbl> 54.20, 26.10, 14.80, 18.80, 9.40, 2.20, 21.50, 1.40~
## $ STARS       <fct> 2, 3, 3, 1, 2, NA, NA, 3, NA, 4, 1, 2, 2, 3, NA, NA~
## $ Sulphates   <dbl> -0.59, 0.70, 0.48, 1.83, 1.77, 1.29, 1.21, NA, 0.26~
## $ TotalSulfurDioxide <dbl> 268, -327, 142, 115, 108, 15, 156, 551, NA, 180, 65~
## $ VolatileAcidity <dbl> 1.160, 0.160, 2.640, 0.385, 0.330, 0.320, 0.290, -1~

##
##    0    1    2    3    4    5    6    7    8
## 2734 244 1091 2611 3177 2014  765  142  17
```

## Missing Values

Additionally, eight parameters had missing values ranging from 395 missing values (pH) to 3359 missing values (STARS). Below is the full list of variables with missing values:

##	Alcohol	Chlorides	FreeSulfurDioxide	pH
##	653	638	647	395
##	ResidualSugar	STARS	Sulphates	TotalSulfurDioxide
##	616	3359	1210	682

## Examining Numerical Variables

A review of the summary statistics reveals issues with our data. In particular, nine of the 11 numeric variables show minimum values below zero. Table 1 shows number of missing values.

##	TARGET	Alcohol	Chlorides	CitricAcid
##	Min. :0.000	Min. : -4.70	Min. : -1.1710	Min. : -3.2400
##	1st Qu.:2.000	1st Qu.: 9.00	1st Qu.: -0.0310	1st Qu.: 0.0300
##	Median :3.000	Median :10.40	Median : 0.0460	Median : 0.3100
##	Mean :3.029	Mean :10.49	Mean : 0.0548	Mean : 0.3084
##	3rd Qu.:4.000	3rd Qu.:12.40	3rd Qu.: 0.1530	3rd Qu.: 0.5800
##	Max. :8.000	Max. :26.50	Max. : 1.3510	Max. : 3.8600
##		NA's :653	NA's :638	
##	Density	FixedAcidity	FreeSulfurDioxide	pH
##	Min. :0.8881	Min. : -18.100	Min. : -555.00	Min. :0.480
##	1st Qu.:0.9877	1st Qu.: 5.200	1st Qu.: 0.00	1st Qu.:2.960
##	Median :0.9945	Median : 6.900	Median : 30.00	Median :3.200
##	Mean :0.9942	Mean : 7.076	Mean : 30.85	Mean :3.208
##	3rd Qu.:1.0005	3rd Qu.: 9.500	3rd Qu.: 70.00	3rd Qu.:3.470
##	Max. :1.0992	Max. : 34.400	Max. : 623.00	Max. :6.130
##			NA's :647	NA's :395
##	ResidualSugar	Sulphates	TotalSulfurDioxide	VolatileAcidity
##	Min. : -127.800	Min. : -3.1300	Min. : -823.0	Min. : -2.7900
##	1st Qu.: -2.000	1st Qu.: 0.2800	1st Qu.: 27.0	1st Qu.: 0.1300
##	Median : 3.900	Median : 0.5000	Median : 123.0	Median : 0.2800
##	Mean : 5.419	Mean : 0.5271	Mean : 120.7	Mean : 0.3241
##	3rd Qu.: 15.900	3rd Qu.: 0.8600	3rd Qu.: 208.0	3rd Qu.: 0.6400
##	Max. : 141.150	Max. : 4.2400	Max. :1057.0	Max. : 3.6800
##	NA's :616	NA's :1210	NA's :682	

When put in the context of our specific properties of wine they represent, these negative values appear to be erroneous. For example, we expected **Alcohol Content** to have a minimum value of zero instead of a negative value. The same can be said of the other parameters with negative values (Chlorides, Citric Acid, Fixed Acidity, Free Sulfur Dioxide, Residual Sugar, Sulphates, Total Sulfur Dioxide, and Volatile Acidity). This suggests possible data entry errors or normalization that shifted our actual values to the left.

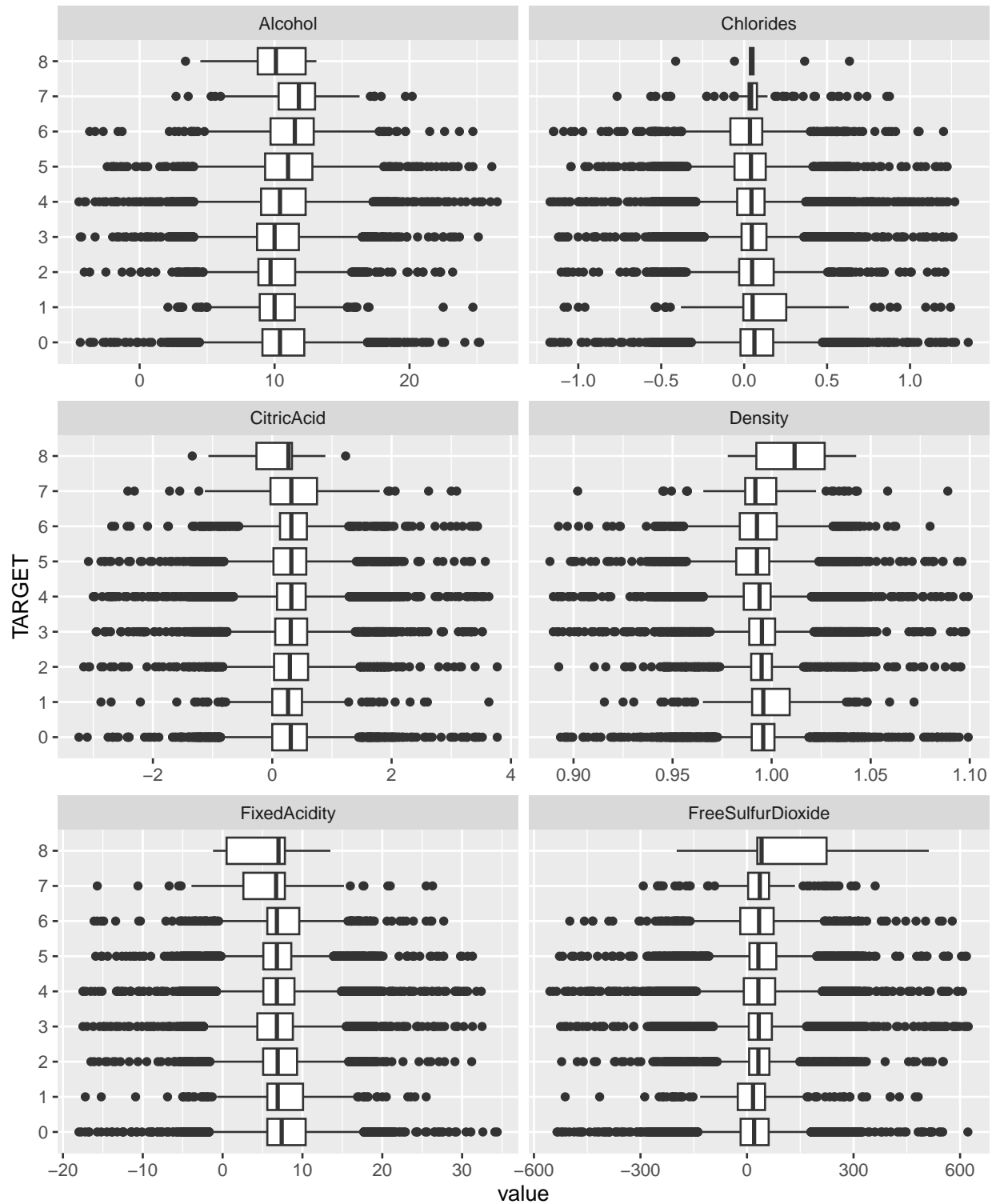
Table 1: Number of negative values

Variable	Q25	Median	Q75	CommonRange	Rows Below Zero
TARGET	2.000	3.000	4.000	0 or higher	0
Alcohol	9.000	10.400	12.400	8% – 15% ABV	118
Chlorides	-0.031	0.046	0.153	0.01 – 0.10 g/L	3197
CitricAcid	0.030	0.310	0.580	0 – 1.0 g/L	2966
Density	0.988	0.994	1.001	0.990 – 1.005 g/cm <sup>3</sup>	0
FixedAcidity	5.200	6.900	9.500	4 – 9 g/L	1621
FreeSulfurDioxide	0.000	30.000	70.000	10 – 70 mg/L	3036
pH	2.960	3.200	3.470	2.9 – 4.0	0
ResidualSugar	-2.000	3.900	15.900	0 – 45 g/L	3136
Sulphates	0.280	0.500	0.860	0.3 – 1.0 g/L	2361
TotalSulfurDioxide	27.000	123.000	208.000	30 – 150 mg/L	2504
VolatileAcidity	0.130	0.280	0.640	0.2 – 0.8 g/L	2827

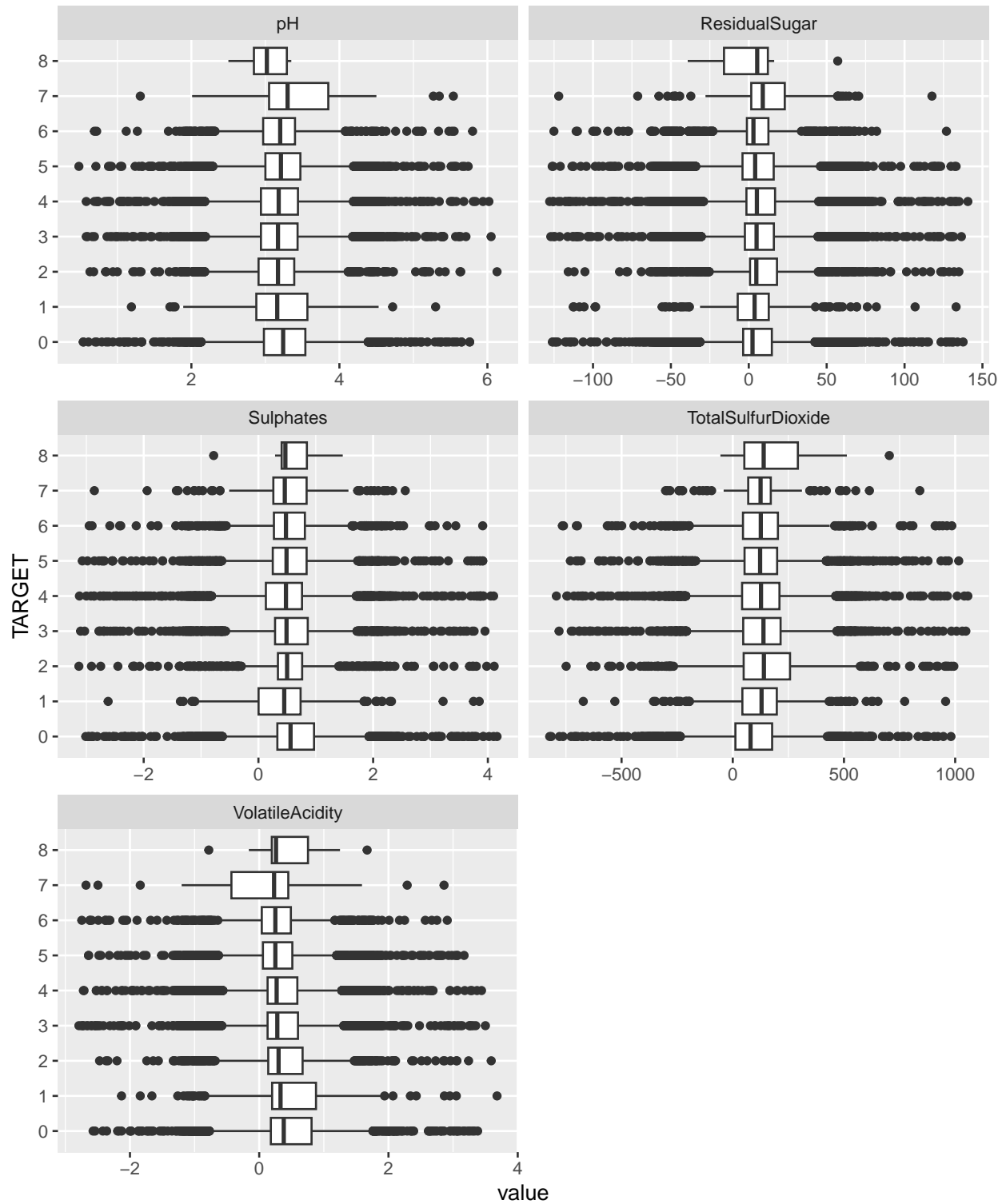
A look at our boxplots shows the IQR's for each parameter are centered around a similar x-axis for each of our case counts. The boxplots confirm the presence of extreme values at lower as well as on the upper

ranges. It should be noted the IQRs for the affected variables are in line with their corresponding typical ranges according to VineEnology.com as shown in Table 1.

Boxplots of Target vs Param



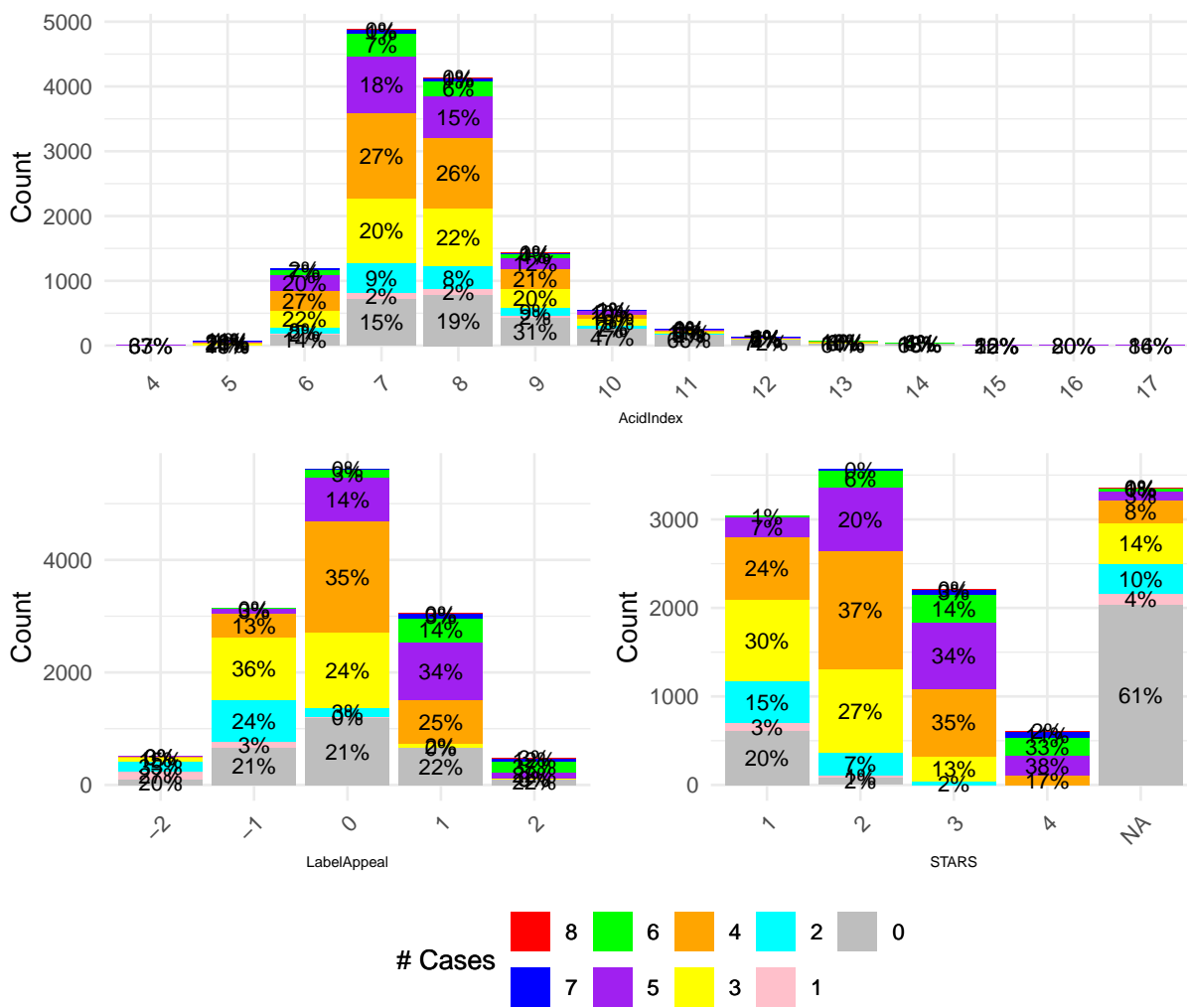
Boxplots of Target vs Param



## Examining Categorical Variables

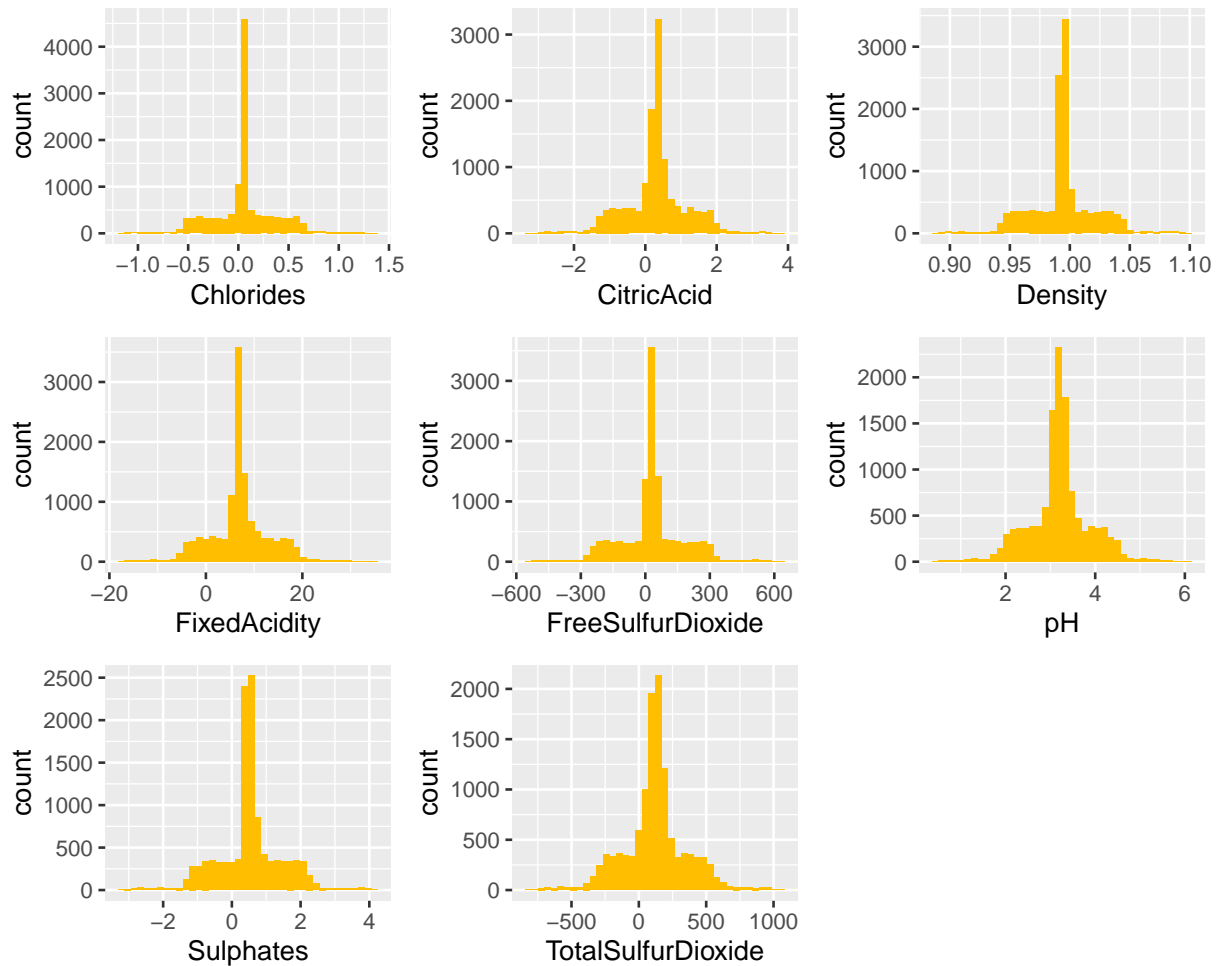
Visualizing the distributions of our categorical variables helps ensure variables are treated as discrete categories, not continuous numbers. Our AcidIndex variable shows that majority of values fall between 6 and 11 with 342 observations collectively making up the remaining values. We may want to bin values for this parameter. LabelAppeal has a normal distribution ranging from -2 to 2 and centered around 0. The our Wine rative variable STARS has the most missing values (3359) of any variable; of missing value, 61% of rows had 0 cases purchased. As would be expected, the majority of observations have a low STARS value (1/2), while few observations have a perfect value of 4.

```
##      AcidIndex      LabelAppeal      STARS
## 7      :4878      -2: 504      1      :3042
## 8      :4142      -1:3136      2      :3570
## 9      :1427      0 :5617      3      :2212
## 6      :1197      1 :3048      4      : 612
## 10     : 551      2 : 490      NA's:3359
## 11     : 258
## (Other): 342
```



## Visualizing Distributions

Next we will visualize the distributions for our numeric variables. Using the histograms, we can quickly spot skewness, check distribution and value ranges, and identify variables with spikes or unusual spread. The histograms show symmetric unimodal distributions strongly peaked with thin tails across our numeric variables.



Our skewness test confirms that our numerical variables are nearly symmetrical or almost symmetrical.

##	Variable	Skewness
## ResidualSugar	ResidualSugar	-0.053122905
## CitricAcid	CitricAcid	-0.050307040
## pH	pH	0.044288014
## Alcohol	Alcohol	-0.030715836
## Chlorides	Chlorides	0.030427175

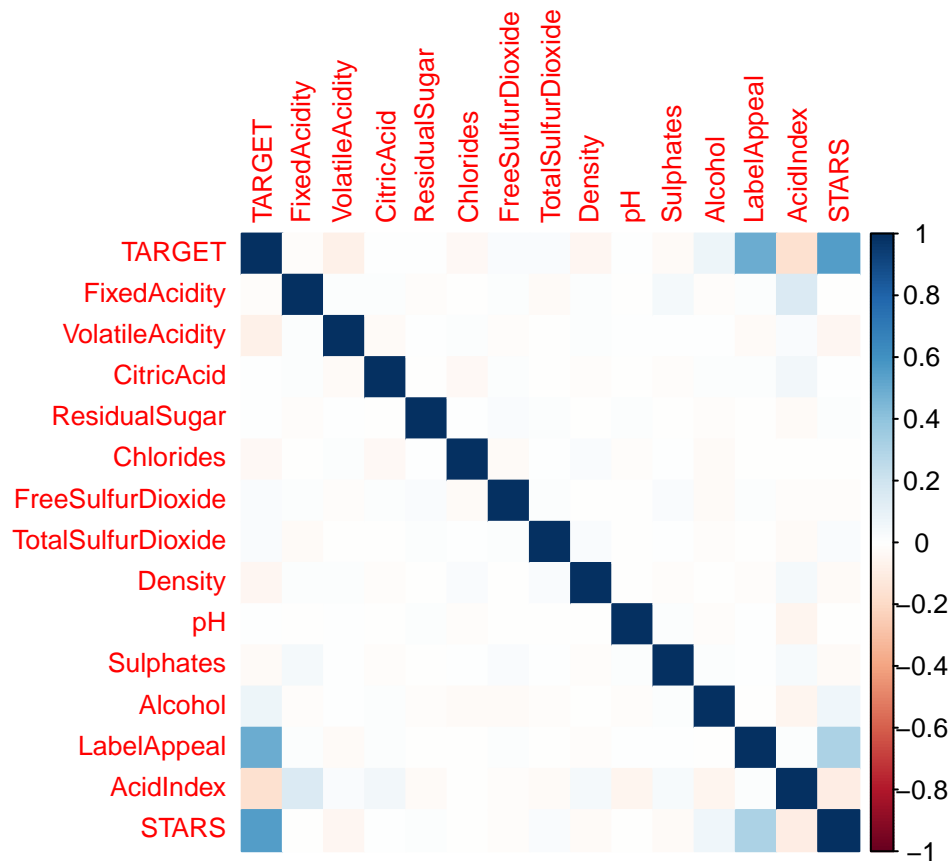
```

## FixedAcidity          FixedAcidity -0.022585961
## VolatileAcidity       VolatileAcidity  0.020379965
## Density               Density -0.018693764
## TotalSulfurDioxide    TotalSulfurDioxide -0.007179351
## FreeSulfurDioxide     FreeSulfurDioxide  0.006393010

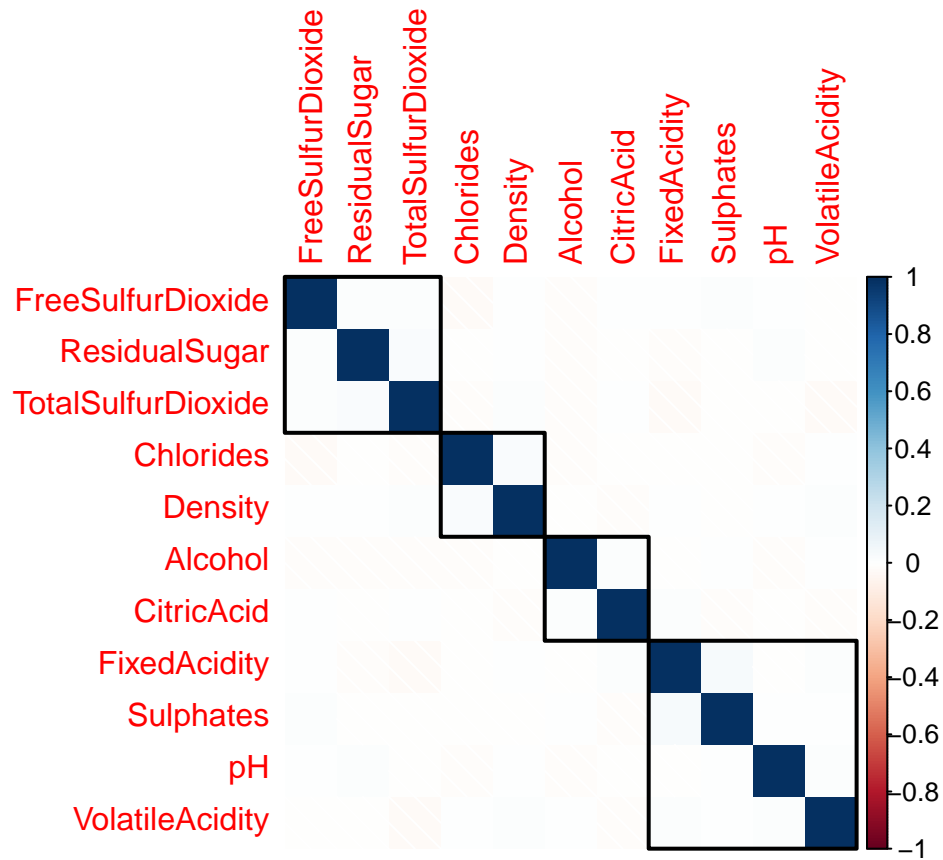
```

## Visualizing Relationships Among Variables

Correlation plots help us understand variable relationships and potential multicollinearity. A correlation plot for all variables shows moderate correlation between our dependent variable TARGET and the variables STARS and LabelAppeal and weak correlation between TARGET and AcidIndex.



STARS, LabelAppeal, and AcidIndex are also three parameters that we identified to be ordinal. The following correlation plot shows the correlation between the remaining numerical parameters. This view also groups the parameters into four clusters that appear to have a relationship with each other.



A Variance Inflation Factor (VIF) test confirms that no major multicollinearity present in between our variables.

##		GVIF	Df	$GVIF^{(1/(2*Df))}$
##	AcidIndex	1.100734	13	1.003698
##	Alcohol	1.013464	1	1.006709
##	Chlorides	1.007238	1	1.003612
##	CitricAcid	1.008134	1	1.004059
##	Density	1.009057	1	1.004518
##	FixedAcidity	1.031541	1	1.015648
##	FreeSulfurDioxide	1.006411	1	1.003200
##	LabelAppeal	1.146432	4	1.017229
##	pH	1.007787	1	1.003886
##	ResidualSugar	1.005833	1	1.002912
##	STARS	1.162161	3	1.025363
##	Sulphates	1.007464	1	1.003725
##	TotalSulfurDioxide	1.007607	1	1.003796
##	VolatileAcidity	1.005933	1	1.002962



## Data Preparation

### Handling Negative Values

In the Data Exploration phase, we discovered that nine out of 11 numerical variables had negative values. While Poisson and Negative Binomial Regression will allow negative predictor values, we know that these values are impossible in the real world. Ignoring these values could lead to biased coefficient estimates that could introduce highly misleading relationships in our models. We will assume that these erroneous values may be the result of data entry or normalization errors and attempt to address them.

As we do not know what transformations may have been applied if normalization occurred, we will need to address the negative values through another method. From our earlier observations, we noted that nearly all of the affected parameters had thousands of affected records, with Chlorides having the most affected rows (3197). This means that nearly 1/4 of our 12,795 may be affected one way or another and we would lose too much data if we were to drop the affected records. We will instead only drop the 118 records with for Alcohol Content as it is a small fraction of the total rows in our dataset. We will then set the remaining negative values to N/A, allowing the values to be imputed if desired. Imputing may introduce some bias into our results, but will retain much of our data; dropping these 118 rows may somewhat help reduce this bias.

### Handling Missing Values

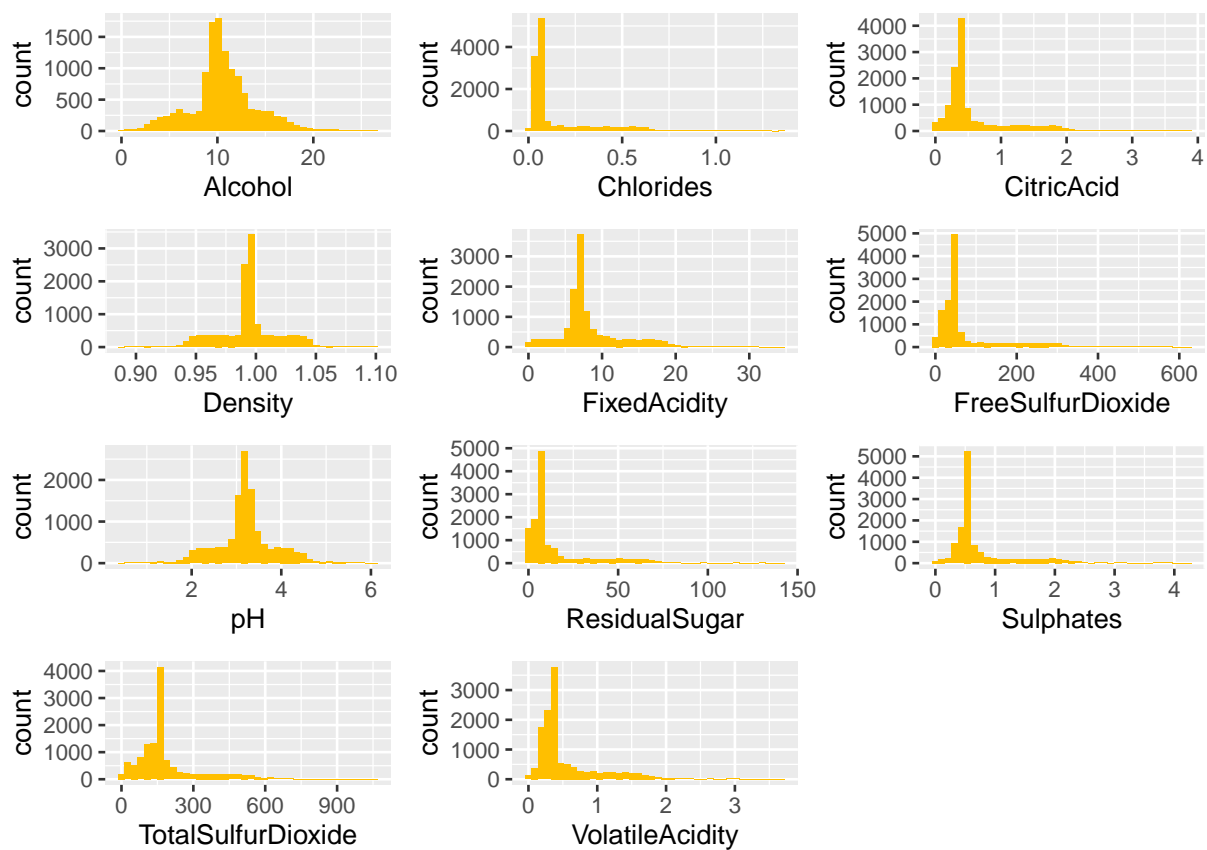
Given that we don't know if our data was previously transformed, we will apply median imputation to our variables with missing data. This method was preferred over multiple imputation or other techniques as it is easier to understand how we have altered the data and simpler to . Additionally, Multiple-imputation may magnify additional bias that may have been introduced if the data was previously transformed.

Table 2: Number of missing values

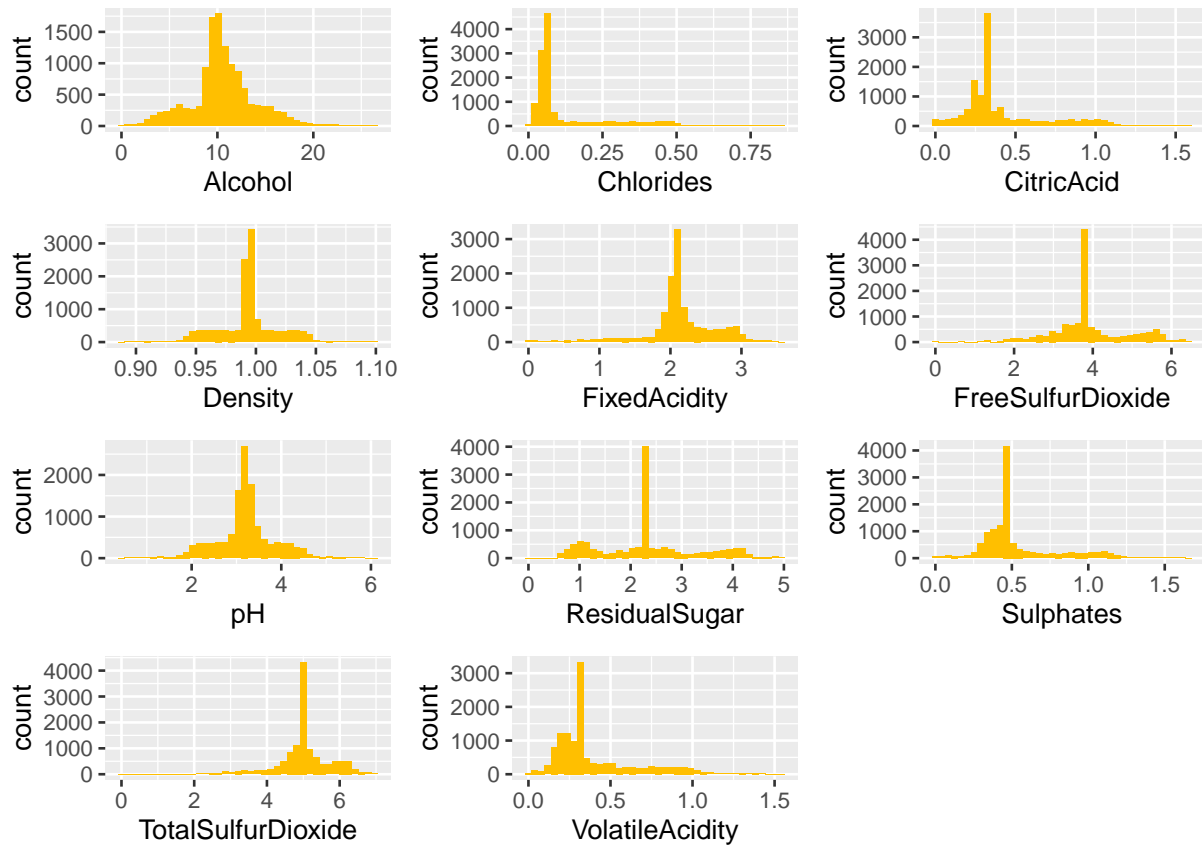
	Original.Missing.Count	New.Missing.Count	After.Imputation
TARGET	0	0	0
AcidIndex	0	0	0
Alcohol	653	653	0
Chlorides	638	3802	0
CitricAcid	0	2933	0
Density	0	0	0
FixedAcidity	0	1608	0
FreeSulfurDioxide	647	3657	0
LabelAppeal	0	0	0
pH	395	392	0
ResidualSugar	616	3714	0
STARS	3359	3329	0
Sulphates	1210	3534	0
TotalSulfurDioxide	682	3151	0
VolatileAcidity	0	2795	0

### Transformations

Dropping our negative values and imputing our missing values introduced skewness into most of the numerical variables. All variables but Alcohol, Density and pH have are right-skewed—though the right tail for FixedAcidity and TotalSulfurDioxide are relatively moderate compared the heavy right tails of the other variables.

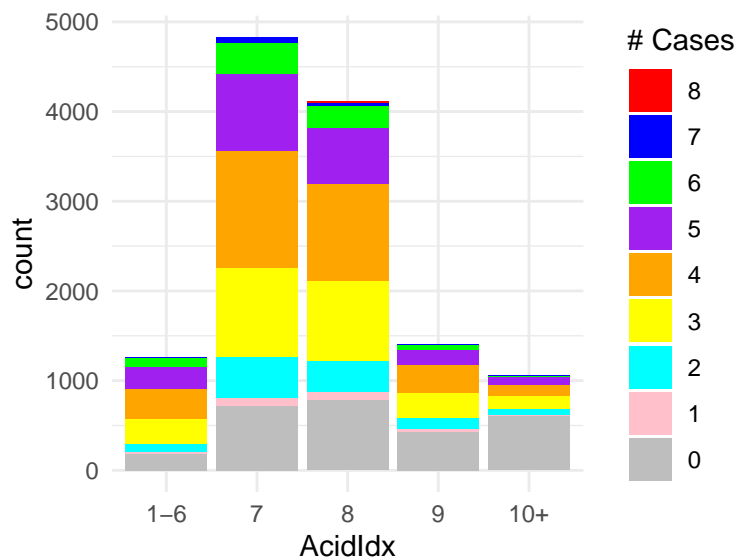


We can apply log transformation to these variables to help address skewness



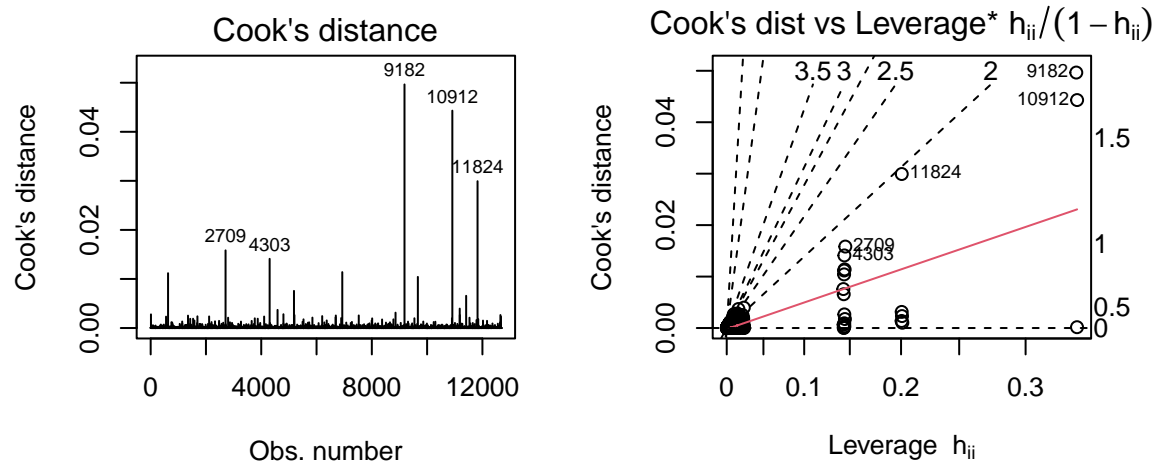
## Binned Transformation

To simplify the effects of AcidIndex, this variable was transformed into categorical bins. This can help reduce the influence of extreme values and better capture non-linear effects in logistic regression.



## Outliers

Diagnostic plots show several points with relatively high Cook's distance values when compared to rest of our data.



## Model Building

## Model Selection