

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 negative 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

```

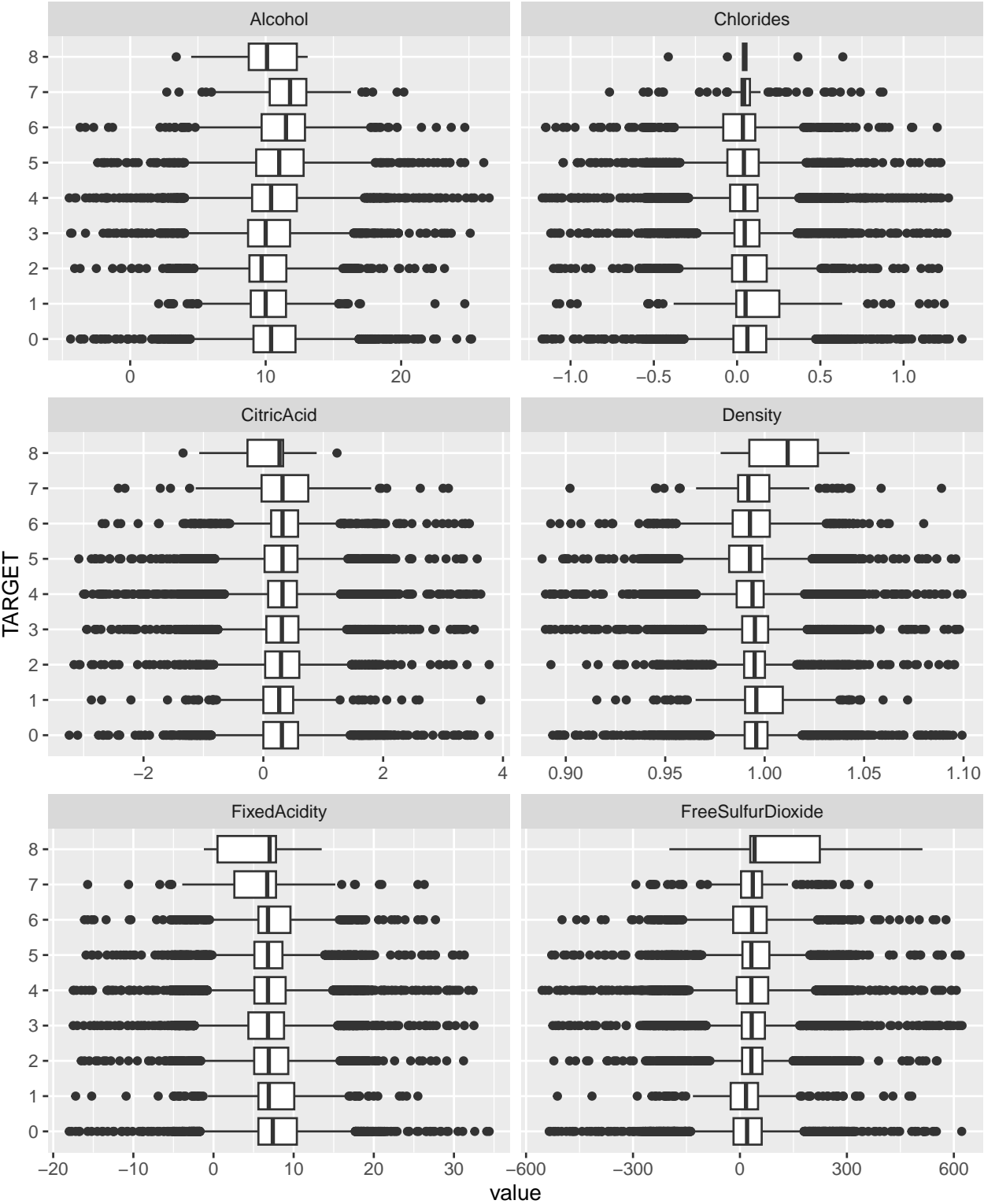
When put in the context of our specific properties of wine they represent, these negative values appear to be erroneous. For example, we expected **Alcohol Content** to have a minimum value of zero instead of a negative value. The same can be said of the other parameters with negative values (Chlorides, 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

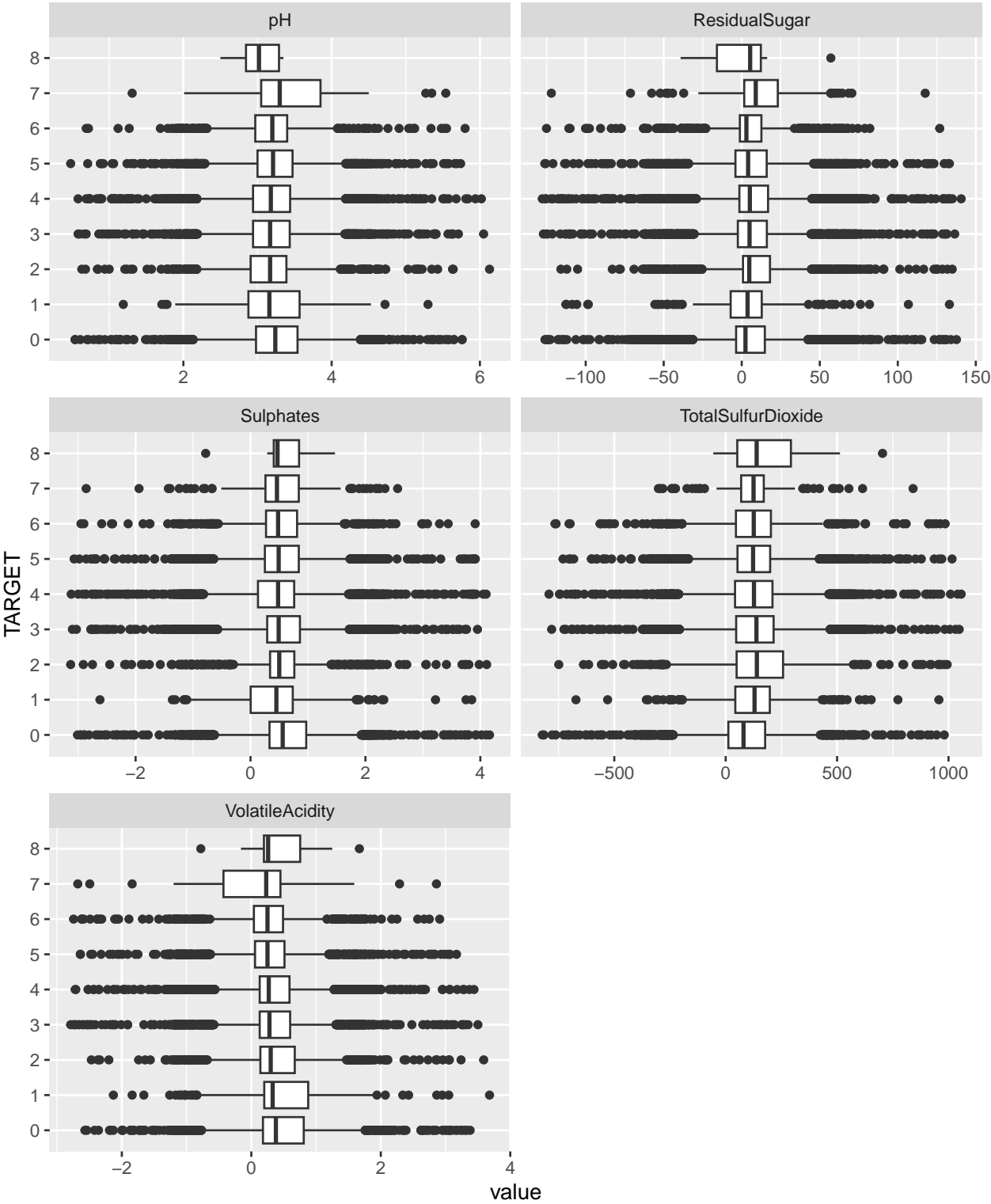
Variable	Q25	Median	Q75	CommonRange	Rows Below Zero
TARGET	2.000	3.000	4.000	0 or higher	0
Alcohol	9.000	10.400	12.400	8% – 15% ABV	118
Chlorides	-0.031	0.046	0.153	0.01 – 0.10 g/L	3197
CitricAcid	0.030	0.310	0.580	0 – 1.0 g/L	2966
Density	0.988	0.994	1.001	0.990 – 1.005 g/cm ³	0
FixedAcidity	5.200	6.900	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

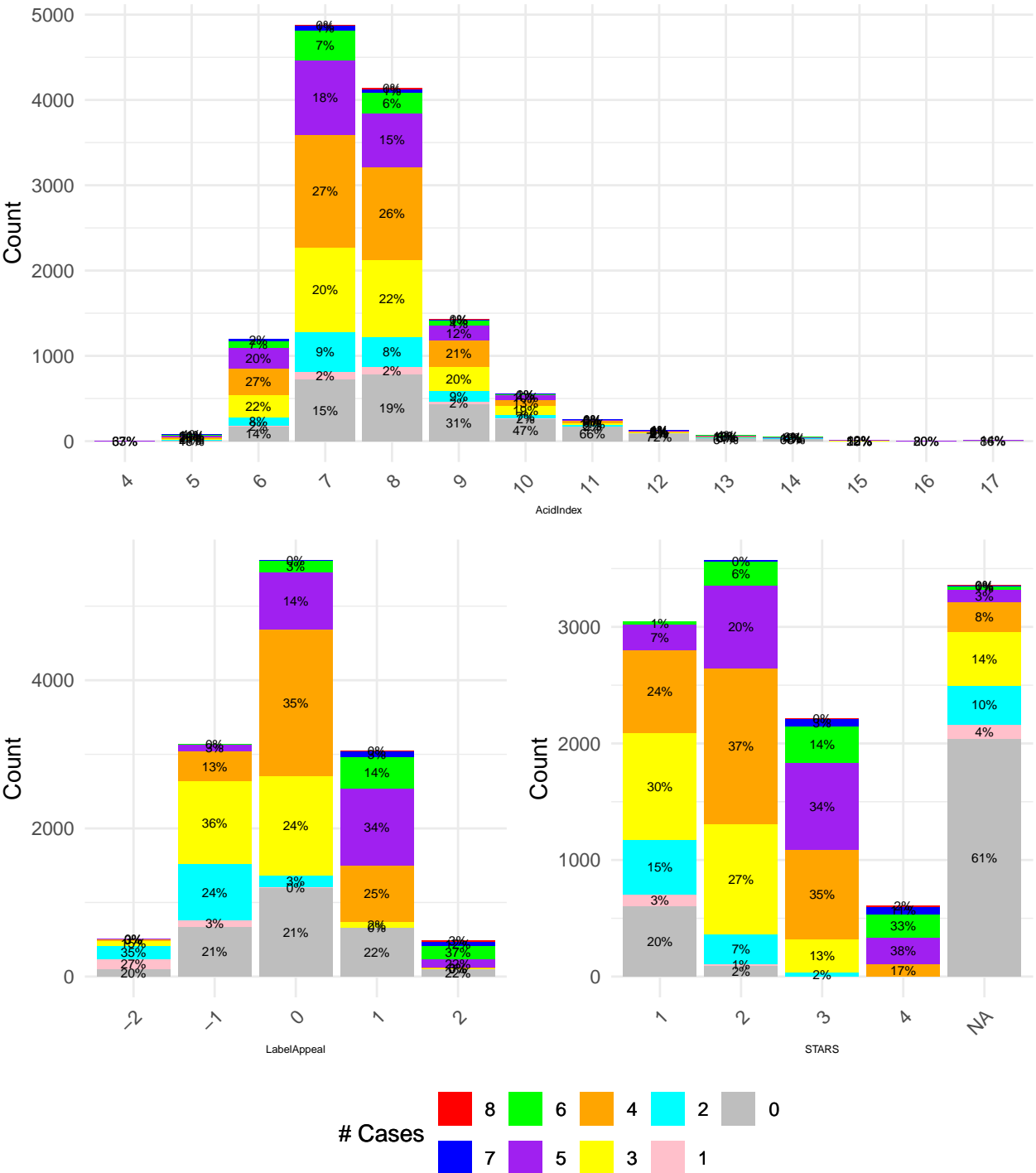


Boxplots of Target vs Param



Examining Categorical Variables

Visualizing the distributions of out 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 suggesting no major e. The STARS rating variable has the most missing values (3359) of any variable; 61% of rows without a STAR rating had zero cases purchased. About half of the total 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
## (0ther): 342
```

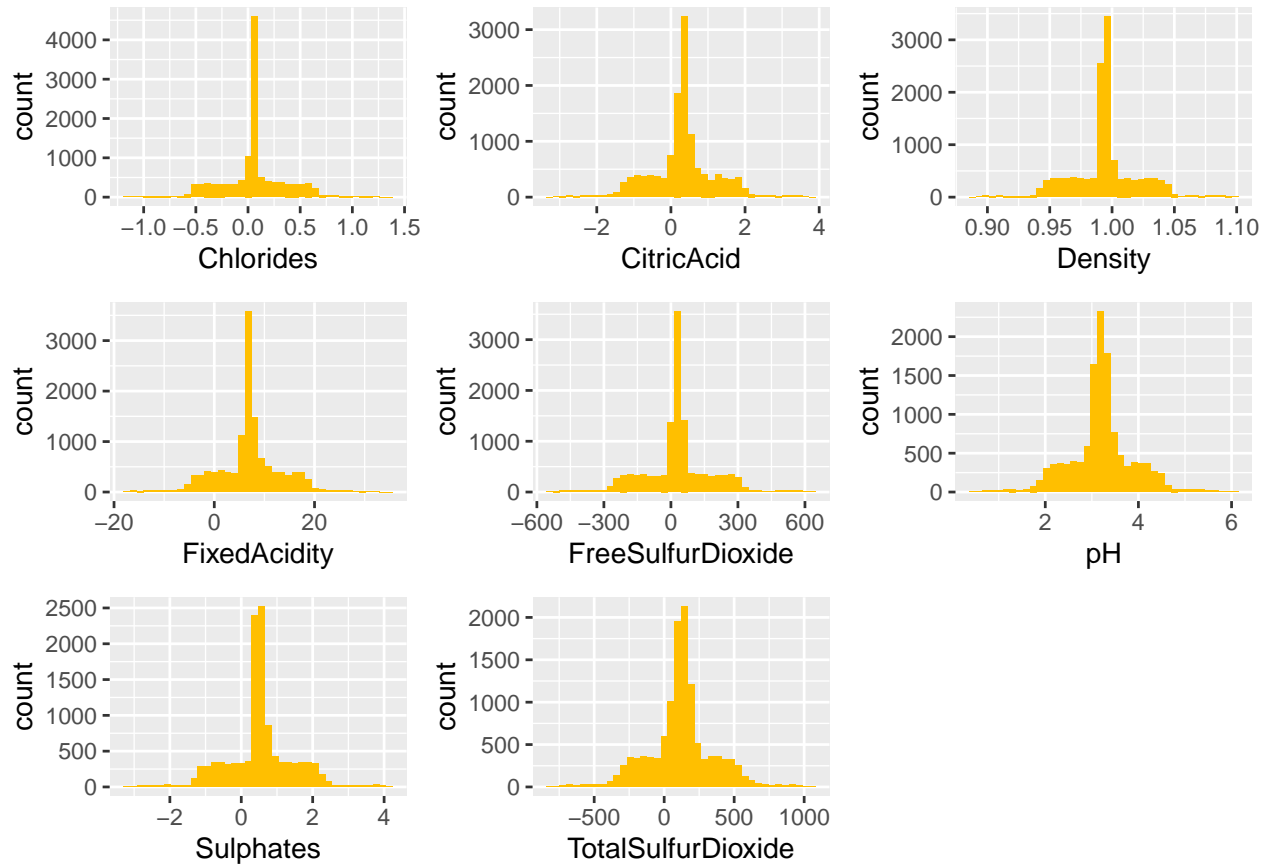
A closer look at LabelAppeal shows relatively few observations had the highest values (-2 or 2). For observations where zero cases were bought (TARGET = 0), label appeal seemed to have very little impact, as there nearly equal number of positive and negative label appeal ratings within their respective categories. However, lower case purchases (1-3) had more lower rankings counts than higher rankings, while higher case purchases (4+) had higher label appeal ratings.



TARGET	-2	-1	0	1	2
0	102	671	1193	660	108
1	136	89	19	0	0
2	177	755	152	7	0
3	74	1118	1347	70	2
4	14	413	1972	765	13
5	1	88	775	1040	110
6	0	2	155	425	183
7	0	0	4	79	59
8	0	0	0	2	15

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. However, as noted earlier, negative values for many of these parameters would be impossible.



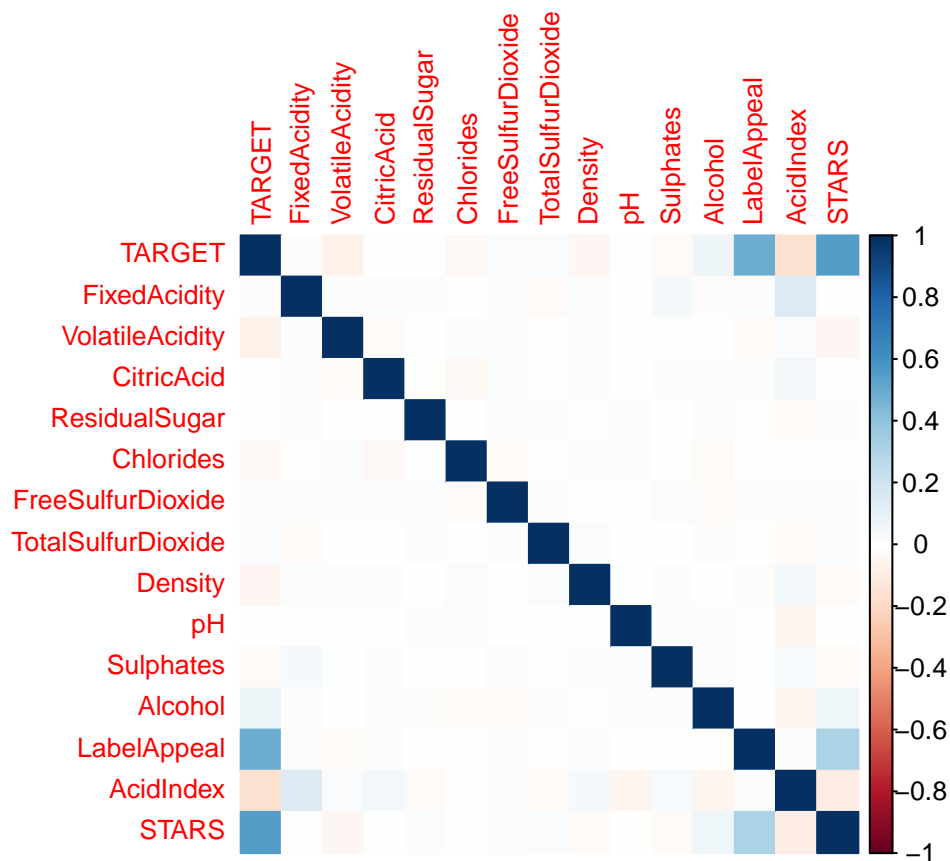
Our skewness test confirms that our numerical variables are nearly symmetrical or almost symmetrical.

Table 3: Skewness

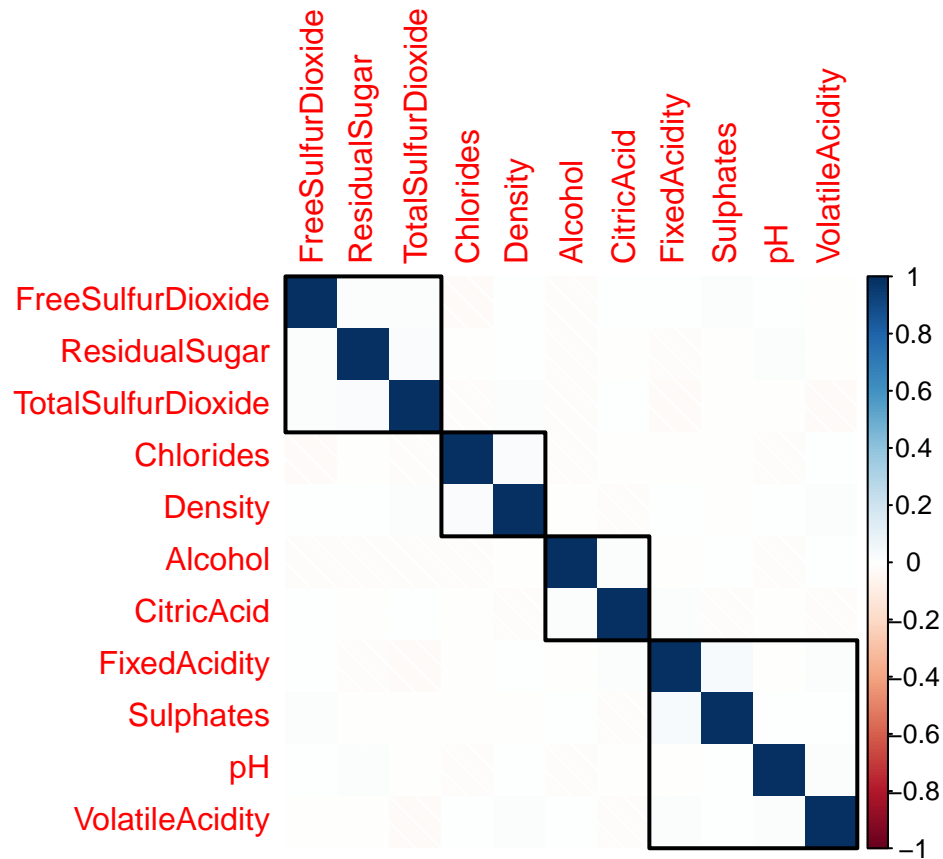
	Variable	Skewness
ResidualSugar	ResidualSugar	-0.0531229
CitricAcid	CitricAcid	-0.0503070
pH	pH	0.0442880
Alcohol	Alcohol	-0.0307158
Chlorides	Chlorides	0.0304272
FixedAcidity	FixedAcidity	-0.0225860
VolatileAcidity	VolatileAcidity	0.0203800
Density	Density	-0.0186938
TotalSulfurDioxide	TotalSulfurDioxide	-0.0071794
FreeSulfurDioxide	FreeSulfurDioxide	0.0063930
Sulphates	Sulphates	0.0059119

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 only the 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.

##		GVI	F	$GVI^{1/(2 \cdot Df)}$
##	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. We won't impute values for STARS since this appears to be an indication that a rating was not given to these observations. When exploring our data, we noticed that 61% of the wines without a STAR rating had zero (0) cases purchased. As such, a NA value may represent useful data for our model. We will convert this variable to -1 for interpretability by our model.

Table 4: 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

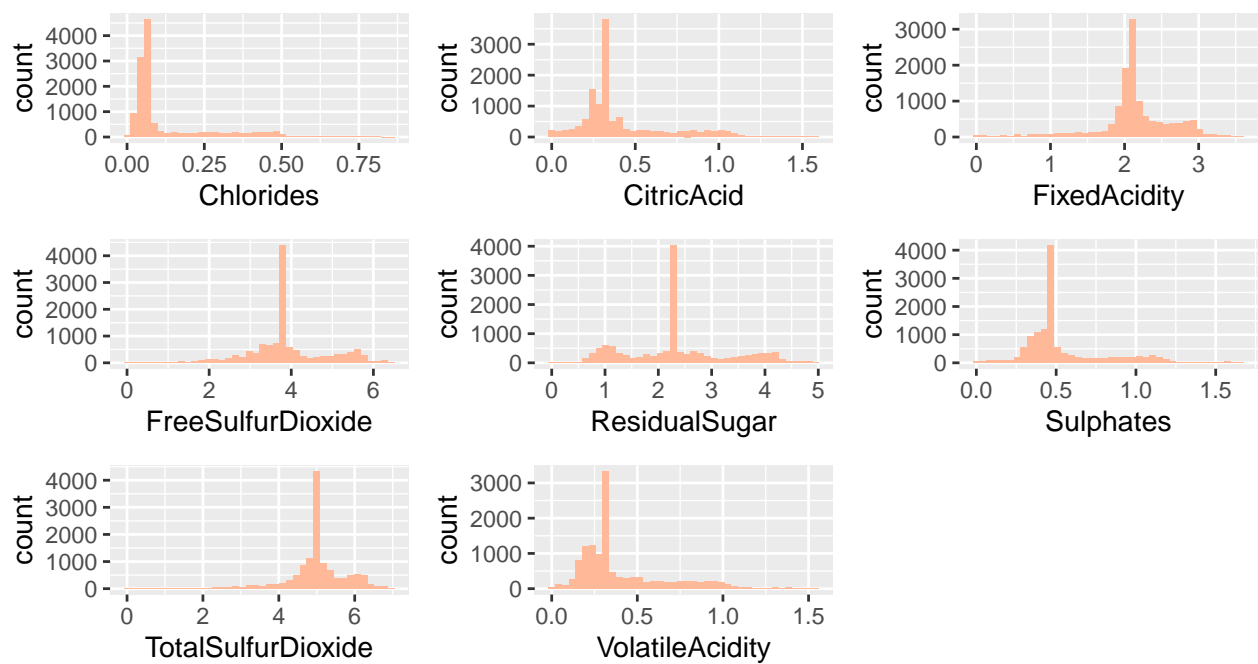
Transformations

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.

Numerical Variables – Before Transformation

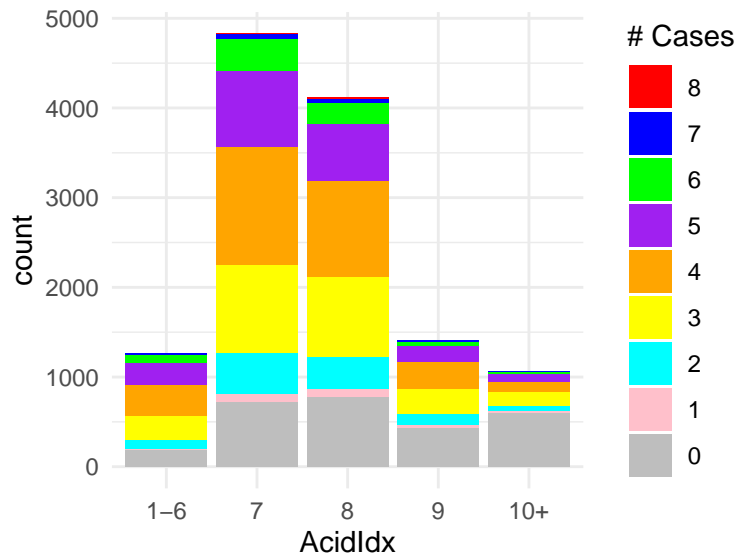


Numerical Variables – Post Transformation



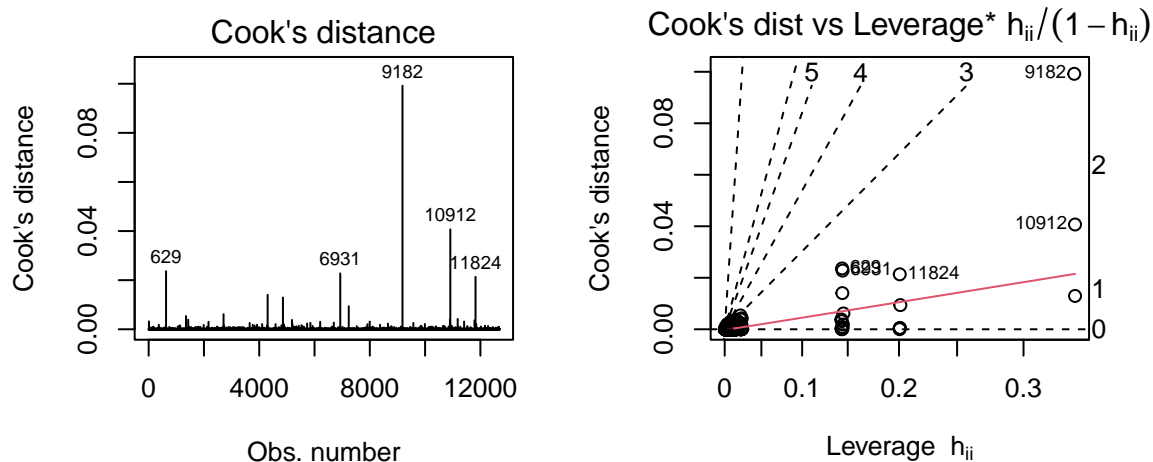
Binned Transformation

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. It will also help free up degrees of freedom in our models.



Possible Outliers

Diagnostic plots show several points with relatively high Cook's Distance values when compared to rest of our data, but Cook's Distance values are fairly low overall and these points may not affect our models much. Prior to transformation, we saw two points with perfect leverage that we flagged for possible removal, but none of the points seem to have strong leverage or influence after transformation.



Model Building
Model Selection