DATA 621 Homework 5

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Summary

The goal of the project is to test approaches for evaluating the data set containing various wine characteristics and to predict the number of cases ordered. This report includes comparison of linear, poisson, negative binomial regression models (including zero-inflated negative binomial model).

There are some questions about real-world validity of evaluation data since there are a lot of negative values for variables that should not have them. Earlier in the analysis, an attempt was made to use the absolute value for modeling, but that did not improve models and generally does not fit the distribution of variables.

Data Exploration

The data set includes 12,795 observations with 14 variables (excluding the target variable).

Summary of Variables

The data set includes 14 independent variables:

- `AcidIndex`: Proprietary method of testing total acidity of wine by using a weighted average.
- `Alcohol`: Alcohol content of wine.
- `Chlorides`: Chloride content of wine.
- `CitricAcid`: Citric acid content of wine.
- `Density`: Density of wine.
- `FixedAcidity`: Fixed Acidity of wine.
- `FreeSulfurDioxide`: Sulfur dioxide content of wine.
- `LabelAppeal`: Marketing score indicating the appeal of label design for consumers.
- `ResidualSugar`: Residual sugar of wine.
- `STARS`: Wine rating by a team of experts. Ranges from 1 (Poor) to 4 (Excellent) stars.
- `Sulphates`: Sulfate content of wine.
- `TotalSulfurDioxide`: Total sulfur dDioxide of wine.
- `VolatileAcidity`: Volatile acid content of wine.
- `pH`: pH of wine

Dependent variable is `TARGET` representing number of cases of wine purchased.

The table below shows summary of all variables.

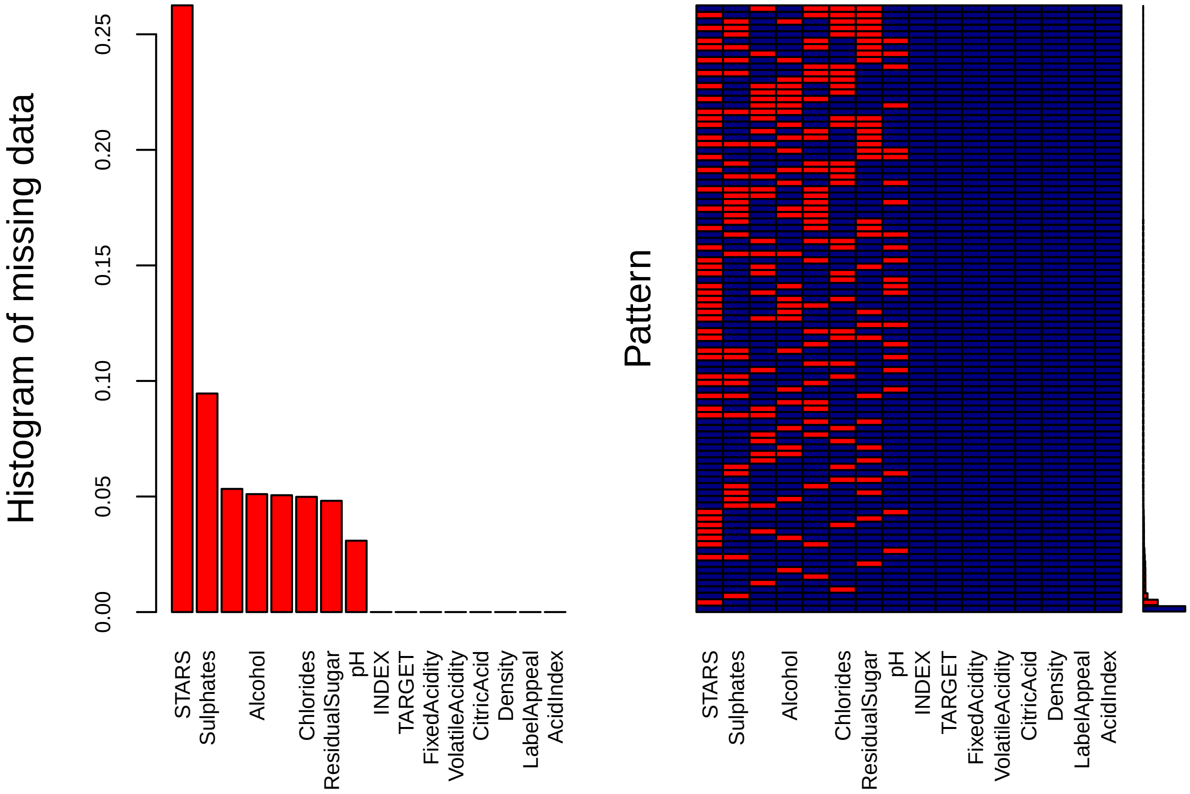
Variable	Class	Min	Median	Mean	SD	Max
FixedAcidity	numeric	-18.1	6.9	7.076	6.318	34.4
VolatileAcidity	numeric	-2.79	0.28	0.3241	0.784	3.68
CitricAcid	numeric	-3.24	0.31	0.3084	0.8621	3.86
ResidualSugar	numeric	-127.8	3.9	5.419	33.75	141.2
Chlorides	numeric	-1.171	0.046	0.05482	0.3185	1.351
FreeSulfurDioxide	numeric	-555	30	30.85	148.7	623
TotalSulfurDioxide	numeric	-823	123	120.7	231.9	1057
Density	numeric	0.8881	0.9945	0.9942	0.02654	1.099
pH	numeric	0.48	3.2	3.208	0.6797	6.13
Sulphates	numeric	-3.13	0.5	0.5271	0.9321	4.24
Alcohol	numeric	-4.7	10.4	10.49	3.728	26.5
LabelAppeal	integer	-2	0	-0.009066	0.8911	2
AcidIndex	integer	4	8	7.773	1.324	17
STARS	integer	1	2	2.042	0.9025	4

Variable	Num of NAs	Num of Zeros	Num of Neg Values
FixedAcidity	0	39	1621
VolatileAcidity	0	18	2827
CitricAcid	0	115	2966
ResidualSugar	616	6	3136
Chlorides	638	5	3197
FreeSulfurDioxide	647	11	3036
TotalSulfurDioxide	682	7	2504
Density	0	0	0
pH	395	0	0
Sulphates	1210	22	2361
Alcohol	653	2	118
LabelAppeal	0	5617	3640
AcidIndex	0	0	0
STARS	3359	0	0

All but three independent variables are continous. Variables `LabelAppeal`, `AcidIndex` and `STARS` are categorical, but represented by numeric values in logical order. The distances between categories/values can be considered equal (i.e. the difference between `-2` and `-1` for `LabelAppeal` is the same as the difference between 0 and 1). As such these variables can be used in modeling as numeric variables.

Missing Values

Majority variables have negative values. Eight variables have some `NA` values. The plot and table below show how the missing values are spread out within the data set. About quarter of observations are missing a `STARS` value. The rest of variables contain missing values for at most 9.5% of observations.

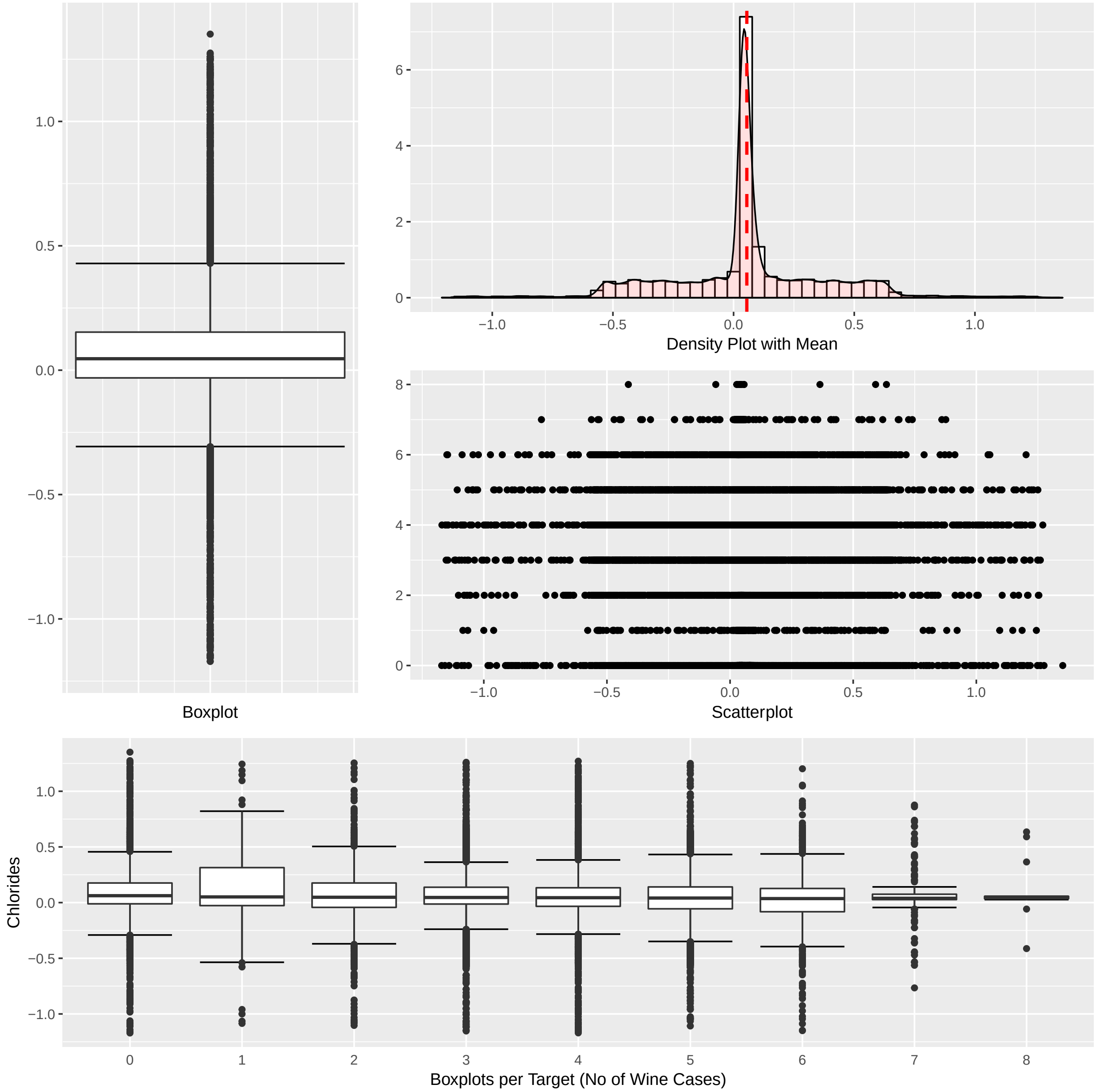


```
##
##  Variables sorted by number of missings:
##            Variable      Count
##               STARS 0.26252442
##           Sulphates 0.09456819
##  TotalSulfurDioxide 0.05330207
##             Alcohol 0.05103556
##   FreeSulfurDioxide 0.05056663
##           Chlorides 0.04986323
##       ResidualSugar 0.04814381
##                  pH 0.03087143
##               INDEX 0.00000000
##              TARGET 0.00000000
##        FixedAcidity 0.00000000
##     VolatileAcidity 0.00000000
##          CitricAcid 0.00000000
##             Density 0.00000000
##         LabelAppeal 0.00000000
##           AcidIndex 0.00000000
```

Exploratory Plots

All dependent variables were inspected using boxplots, density plots and scatterplots. Distribution is similar for all variables - unimodal and symmetrical. Boxplots are also very similar across all possible outcomes with the exception of the last category - 8 cases purchased. This is due to the fact that the data set contains very few observations with this outcome.

Plots below illustrate results for `Chlorides`. Other variables produced similar plots.



Correlation Matrix

Correlation matrix below shows that there is very little correlation between variables. All can contribute in the modeling.

	TARGET	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	Chlorides	FreeSO2	TotalSO2	Density	pH	Sulphates	Alcohol	LabelAppeal	AcidIndex	STARS
TARGET	1	-0.05	-0.09	0.01	0.02	-0.04	0.04	0.05	-0.04	-0.01	-0.04	0.06	0.36	-0.25	0.56
FixedAcidity	-0.05	1	0.01	0.01	-0.02	0	0	-0.02	0.01	-0.01	0.03	-0.01	0	0.18	-0.01
VolatileAcidity	-0.09	0.01	1	-0.02	-0.01	0	-0.01	-0.02	0.01	0.01	0	0	-0.02	0.04	-0.03
CitricAcid	0.01	0.01	-0.02	1	-0.01	-0.01	0.01	0.01	-0.01	-0.01	-0.01	0.02	0.01	0.07	0
ResidualSugar	0.02	-0.02	-0.01	-0.01	1	-0.01	0.02	0.02	0	0.01	-0.01	-0.02	0	-0.01	0.02
Chlorides	-0.04	0	0	-0.01	-0.01	1	-0.02	-0.01	0.02	-0.02	0	-0.02	0.01	0.03	0
FreeSO2	0.04	0	-0.01	0.01	0.02	-0.02	1	0.01	0	0.01	0.01	-0.02	0.01	-0.04	-0.01
TotalSO2	0.05	-0.02	-0.02	0.01	0.02	-0.01	0.01	1	0.01	0	-0.01	-0.02	-0.01	-0.05	0.01
Density	-0.04	0.01	0.01	-0.01	0	0.02	0	0.01	1	0.01	-0.01	-0.01	-0.01	0.04	-0.02
pH	-0.01	-0.01	0.01	-0.01	0.01	-0.02	0.01	0	0.01	1	0.01	-0.01	0	-0.06	0
Sulphates	-0.04	0.03	0	-0.01	-0.01	0	0.01	-0.01	-0.01	0.01	1	0	0	0.03	-0.01
Alcohol	0.06	-0.01	0	0.02	-0.02	-0.02	-0.02	-0.02	-0.01	-0.01	0	1	0	-0.04	0.07
LabelAppeal	0.36	0	-0.02	0.01	0	0.01	0.01	-0.01	-0.01	0	0	0	1	0.02	0.33
AcidIndex	-0.25	0.18	0.04	0.07	-0.01	0.03	-0.04	-0.05	0.04	-0.06	0.03	-0.04	0.02	1	-0.09
STARS	0.56	-0.01	-0.03	0	0.02	0	-0.01	0.01	-0.02	0	-0.01	0.07	0.33	-0.09	1

Dependent Variable

The dependent variable `TARGET` ranges from 0 (no cases purchased) to 8 cases of wine purchased. The most common outcome is 4 cases at 25% of all observations followed closely with no purchase (0 cases) at 21%. Not counting the 0 outcome, it seems that the variable has unimodal, symmetrical distribution resembling normal distibution centered around 4.

Outcome	No of Observations	Percent of Total
0	2734	0.21
1	244	0.02
2	1091	0.09
3	2611	0.2
4	3177	0.25
5	2014	0.16
6	765	0.06
7	142	0.01
8	17	0

Data Preparation

This data set requires very few transformations as most of the variables appear to be good for analysis as they exist. Two main areas to consider are missing and negative values.

Missing Values

The `STARS` variables contains 3,359 missing values. It represents experts' rating. A missing value - weither it is an intentionally omitted rating or not - may have a meaning for modeling - number of cases purchased for wines without rating is influenced by the fact that there is no rating. **For this analysis missing values for `STARS` have been replaced with 0.**

Two other categorical variables - `LabelAppeal` and `AcidIndex` - do not have any missing values.

Other variables with missing values are good candidates for imputation. Imputation has been done using the `mice` R package and its method `norm`.

Negative Values

`Alcohol` variable has a few negative values - only 118 observations. Negative values for this variable are not possible since 0 would be a non-alcoholic beverage. **The variable has been transformed by taking absolute value of all observations.**

For other variables there is significantly more observations with negative values. Based on some research it seems unlikely that most variables allow for negative values; however, because the distributions for all variables are symmetrical it does not appear that the negative values are data entry or measurement errors. Perhaps, the data was manipulated/shifted or variables were measured using non-standard units. For this analysis, **negative values for all variables except `STARS` remained unchanged.**

Training/Testing Split

Data set has been split into a training (75% of observations) and testing (25% of observations) sets. Splitting has been accomplished using the `caTools` R package based on the `TARGET` variable to make sure that each set has a proportional number of various target classes.

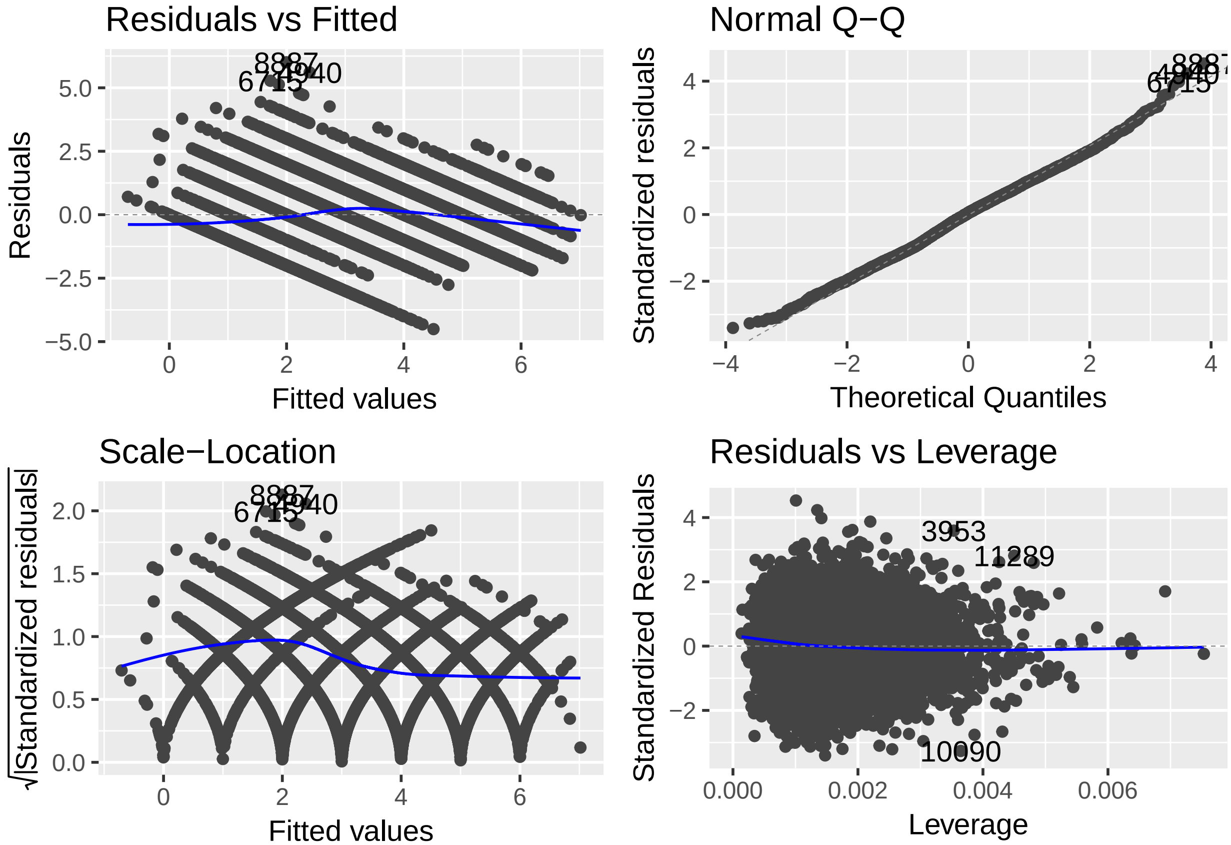
Modeling: Linear

Two main linear models developed were developed and analyzed. The first one included all available variables. It resulted in R^2 of 0.5268, RMSE of 1.3184 and accuracy in predicting the outcomes in the testing set of 0.2853. The second model used stepwise process in both directions to optimize the model (using the `stepAIC` function). It resulted in R^2 of 0.5266, RMSE of 1.3193 and accuracy of 0.2847. It appears that the full model performed very slightly better than the stepwise model.

Below is the summary of the full model.

```
##
## Call:
## lm(formula = TARGET ~ . - INDEX, data = wineTRAIN)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -4.5069 -0.9507  0.0674  0.9089  6.0046
##
## Coefficients:
##                      Estimate  Std. Error t value            Pr(>|t|)
## (Intercept)         3.67369630  0.51997673   7.065     0.00000000000172
## FixedAcidity        0.00017354  0.00218877   0.079             0.936806
## VolatileAcidity    -0.09128121  0.01732010  -5.270     0.00000013920351
## CitricAcid          0.02277522  0.01575707   1.445             0.148379
## ResidualSugar       0.00019360  0.00040400   0.479             0.631792
## Chlorides          -0.11475363  0.04279211  -2.682             0.007338
## FreeSulfurDioxide   0.00032030  0.00009067   3.532             0.000414
## TotalSulfurDioxide  0.00010772  0.00005848   1.842             0.065493
## Density            -0.60095976  0.51208962  -1.174             0.240607
## pH                 -0.02452450  0.01993802  -1.230             0.218713
## Sulphates          -0.03980772  0.01455681  -2.735             0.006256
## Alcohol             0.01340460  0.00376286   3.562             0.000369
## LabelAppeal         0.41927617  0.01575148  26.618 < 0.0000000000000002
## AcidIndex          -0.20162864  0.01068154 -18.876 < 0.0000000000000002
## STARS               0.98317365  0.01199592  81.959 < 0.0000000000000002
##
## (Intercept)        ***
## FixedAcidity
## VolatileAcidity    ***
## CitricAcid
## ResidualSugar
## Chlorides          **
## FreeSulfurDioxide  ***
## TotalSulfurDioxide .
## Density
## pH
## Sulphates          **
## Alcohol            ***
## LabelAppeal        ***
## AcidIndex          ***
## STARS              ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.326 on 9580 degrees of freedom
## Multiple R-squared:  0.5268, Adjusted R-squared:  0.5261
## F-statistic: 761.7 on 14 and 9580 DF,  p-value: < 0.00000000000000022
```

Looking at the diagnostic plots we can see that the model performs reasonably well. Some of the plots are not very suitable for this data set because the dependent variable is a count variable.



The accuracy is fairly low at 28.53%; however, if we examine full confusion matrix below we can see that the model mostly errors only by 1 or 2 cases which may be reasonable enough for a business application. The bigger problem is difficulty in predicting no purchase. There may be significant cost associated with this error.

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1   2   3   4   5   6   7   8
##          0  24   2   1   3   0   0   0   0   0
##          1 313  29  68  80  22   7   0   0   0
##          2 256  26 115 178 109  28  10   2   0
##          3  86   3  74 236 223  71   9   0   0
##          4   5   1  14 129 301 197  42   3   0
##          5   0   0   1  27 128 155  76  14   1
##          6   0   0   0   0  11  45  51  15   1
##          7   0   0   0   0   0   1   3   2   2
##          8   0   0   0   0   0   0   0   0   0
##
## Overall Statistics
##
##                Accuracy : 0.2853
##                 95% CI : (0.2697, 0.3013)
##     No Information Rate : 0.2481
##     P-Value [Acc > NIR] : 0.0000008841
##
##                   Kappa : 0.1642
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 0 Class: 1 Class: 2 Class: 3 Class: 4 Class: 5
## Sensitivity          0.035088 0.475410  0.42125  0.36141  0.37909  0.30754
## Specificity          0.997615 0.843899  0.79194  0.81704  0.83749  0.90838
## Pos Pred Value       0.800000 0.055877  0.15884  0.33618  0.43497  0.38557
## Neg Pred Value       0.791798 0.988064  0.93619  0.83307  0.80343  0.87527
## Prevalence           0.213750 0.019062  0.08531  0.20406  0.24813  0.15750
## Detection Rate       0.007500 0.009062  0.03594  0.07375  0.09406  0.04844
## Detection Prevalence 0.009375 0.162188  0.22625  0.21937  0.21625  0.12562
## Balanced Accuracy    0.516351 0.659655  0.60659  0.58922  0.60829  0.60796
##                      Class: 6 Class: 7 Class: 8
## Sensitivity           0.26702 0.055556  0.00000
## Specificity           0.97607 0.998104  1.00000
## Pos Pred Value        0.41463 0.250000      NaN
## Neg Pred Value        0.95450 0.989348  0.99875
## Prevalence            0.05969 0.011250  0.00125
## Detection Rate        0.01594 0.000625  0.00000
## Detection Prevalence  0.03844 0.002500  0.00000
## Balanced Accuracy     0.62154 0.526830  0.50000
```

Modeling: Poisson

The linear model seemed to perform good with all variables. So for the poisson regression similar strategy was applied - a model with all variables and a model optimized by the stepwise method. There was no considerable imrovement using the stepwise method, so for comparison reasons below is the summary for the full model. RMSE for this model is 1.39855, slightly worse than for the linear model.

```
##
## Call:
## glm(formula = TARGET ~ . - INDEX, family = poisson, data = wineTRAIN)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.9561  -0.7237   0.0709   0.5750   3.2336
##
## Coefficients:
##                       Estimate  Std. Error z value            Pr(>|z|)
## (Intercept)         1.41611137  0.22551127   6.280        0.00000000034
## FixedAcidity       -0.00028475  0.00095364  -0.299             0.765252
## VolatileAcidity    -0.03184819  0.00753753  -4.225        0.00002386398
## CitricAcid          0.00849643  0.00682495   1.245             0.213166
## ResidualSugar       0.00001864  0.00017560   0.106             0.915463
## Chlorides          -0.03927542  0.01860154  -2.111             0.034737
## FreeSulfurDioxide   0.00013161  0.00003924   3.354             0.000797
## TotalSulfurDioxide  0.00004204  0.00002562   1.641             0.100768
## Density            -0.21687294  0.22128775  -0.980             0.327062
## pH                 -0.01221488  0.00864782  -1.412             0.157808
## Sulphates          -0.01570441  0.00633604  -2.479             0.013191
## Alcohol             0.00331670  0.00164184   2.020             0.043371
## LabelAppeal         0.12981840  0.00699730  18.553 < 0.0000000000000002
## AcidIndex          -0.08412083  0.00525625 -16.004 < 0.0000000000000002
## STARS               0.31327867  0.00518717  60.395 < 0.0000000000000002
##
## (Intercept)        ***
## FixedAcidity
## VolatileAcidity    ***
## CitricAcid
## ResidualSugar
## Chlorides          *
## FreeSulfurDioxide  ***
## TotalSulfurDioxide
## Density
## pH
## Sulphates          *
## Alcohol            *
## LabelAppeal        ***
## AcidIndex          ***
## STARS              ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for poisson family taken to be 1)
##
##     Null deviance: 17142  on 9594  degrees of freedom
## Residual deviance: 11060  on 9580  degrees of freedom
## AIC: 35045
##
## Number of Fisher Scoring iterations: 5
```

Confusion matrix below comparing predicted values to the test data shows that the model does not predict *no purchase* outcome (count is 0). Additionally, it often predicts fewer cases than the test data indicates. Accuracy is lower than for the linear model.

```
## Accuracy
## 0.233125
```

```
##           Reference
## Prediction   0   1   2   3   4   5   6   7   8   9  10
##         0    0   0   0   0   0   0   0   0   0   0   0
##         1  204  19  35  39   6   4   0   0   0   0   0
##         2  421  38 166 282 178  45  12   2   0   0   0
##         3   58   4  64 231 305 118  12   1   0   0   0
##         4    1   0   6  75 186 155  36   2   0   0   0
##         5    0   0   2  24  94 103  53  11   1   0   0
##         6    0   0   0   2  18  53  32   6   0   0   0
##         7    0   0   0   0   5  19  28   9   1   0   0
##         8    0   0   0   0   2   6  17   4   0   0   0
##         9    0   0   0   0   0   1   0   1   2   0   0
##         10   0   0   0   0   0   0   1   0   0   0   0
```

Modeling: Negative Binomial

Using the MASS R package, negative binomial model was created using all variables. This model turned out to be nearly identical to the poisson model. Because of this details are not included in this report. Code used to create and analyze the model is available in the Appendix B.

Both models exhibited over-dispersion.

Modeling: Zero-Inflated Negative Binomial

Poisson and negative binomial models do not account for the 0 outcome. So a zero-inflated negative binomial model was attempted using the pscl R package. RMSE for this model is 1.2727, the best one out of all models.

```
## 
## Call:
## zeroinfl(formula = TARGET ~ . - INDEX, data = wineTRAIN, dist = "negbin")
## 
## Pearson residuals:
##       Min        1Q    Median        3Q       Max 
## -2.105481 -0.406840 -0.007311  0.370580  5.885059 
## 
## Count model coefficients (negbin with log link):
##                       Estimate  Std. Error z value             Pr(>|z|)
## (Intercept)          1.38749237  0.23290861   5.957        0.00000000257
## FixedAcidity         0.00032298  0.00098200   0.329              0.74223
## VolatileAcidity     -0.01187606  0.00778309  -1.526              0.12704
## CitricAcid           0.00276410  0.00700564   0.395              0.69317
## ResidualSugar       -0.00010593  0.00018122  -0.585              0.55887
## Chlorides           -0.02437025  0.01911366  -1.275              0.20230
## FreeSulfurDioxide    0.00001724  0.00003963   0.435              0.66350
## TotalSulfurDioxide -0.00003882  0.00002549  -1.523              0.12771
## Density             -0.23328109  0.22802503  -1.023              0.30628
## pH                   0.00388454  0.00891545   0.436              0.66305
## Sulphates           -0.00109531  0.00652144  -0.168              0.86662
## Alcohol              0.00718892  0.00167871   4.282        0.00001848844
## LabelAppeal          0.23205485  0.00727633  31.892 < 0.0000000000000002
## AcidIndex           -0.01776608  0.00566333  -3.137              0.00171
## STARS                0.10279921  0.00596377  17.237 < 0.0000000000000002
## Log(theta)          17.28537035  3.53384182   4.891        0.00000100130
## 
## (Intercept)        ***
## FixedAcidity       
## VolatileAcidity    
## CitricAcid         
## ResidualSugar      
## Chlorides          
## FreeSulfurDioxide  
## TotalSulfurDioxide 
## Density            
## pH                 
## Sulphates          
## Alcohol            ***
## LabelAppeal        ***
## AcidIndex          **
## STARS              ***
## Log(theta)         ***
##
## Zero-inflation model coefficients (binomial with logit link):
##                      Estimate Std. Error z value             Pr(>|z|)
## (Intercept)        -4.4655671  1.5648983  -2.854             0.004323 **
## FixedAcidity       -0.0002386  0.0064138  -0.037             0.970328
## VolatileAcidity     0.1521474  0.0500156   3.042             0.002350 **
## CitricAcid         -0.0168663  0.0463038  -0.364             0.715669
## ResidualSugar      -0.0014057  0.0011789  -1.192             0.233085
## Chlorides          -0.0439587  0.1239199  -0.355             0.722789
## FreeSulfurDioxide  -0.0009263  0.0002715  -3.412             0.000645 ***
## TotalSulfurDioxide -0.0007884  0.0001692  -4.659           0.00000318 ***
## Density             0.6619423  1.5366213   0.431             0.666630
## pH                  0.1873466  0.0580398   3.228             0.001247 **
## Sulphates           0.1280083  0.0425673   3.007             0.002637 **
## Alcohol             0.0233231  0.0110155   2.117             0.034236 *
## LabelAppeal         0.7547693  0.0495578  15.230 < 0.0000000000000002 ***
## AcidIndex           0.4345200  0.0300666  14.452 < 0.0000000000000002 ***
## STARS              -2.3833377  0.0698006 -34.145 < 0.0000000000000002 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Theta = 32132236.8215
## Number of iterations in BFGS optimization: 60
## Log-likelihood: -1.53e+04 on 31 Df
```

This model has the accuracy of 35.78%, again the best one out of all models. It predicts 0 outcomes (not ideally, but perhaps it can be improved with more research).

```
##  Accuracy
## 0.3578125
```

```
##           Reference
## Prediction   0   1   2   3   4   5   6   7   8
##          0 107   1   0   6   4   3   1   1   0
##          1 323  15  34  76  39  16   5   1   0
##          2 138  36 125 118  39  11   4   0   0
##          3 103   9 107 308 246  64   4   0   0
##          4  13   0   7 140 373 200  33   3   0
##          5   0   0   0   5  81 164  75  11   0
##          6   0   0   0   0  12  36  45  12   0
##          7   0   0   0   0   0  10  20   8   4
##          8   0   0   0   0   0   0   4   0   0
```

Model Comparison

Considering log-likelihood of all models, it is clear that zero-inflated negative binomial model is the best option. More research in that direction will probably be beneficial.

	Log-Likelihood	DF
Linear	-16316	16
Poisson	-17507	15
NB	-17507	16
ZINB	-15303	31

Using full models in all methods allows comparison of coefficients. For the most part coefficients are similar in sign and in magnitude. There are a couple of small coefficients that change signs between NB and ZINB models.

	Linear	Poisson	NB	ZINB (Count)
(Intercept)	3.674	1.416	1.416	1.387
FixedAcidity	0.000174	-0.000285	-0.000285	0.000323
VolatileAcidity	-0.09128	-0.03185	-0.03185	-0.01188
CitricAcid	0.02278	0.008496	0.008497	0.002764
ResidualSugar	0.000194	0.000019	0.000019	-0.000106
Chlorides	-0.1148	-0.03927	-0.03928	-0.02437
FreeSulfurDioxide	0.00032	0.000132	0.000132	0.000017
TotalSulfurDioxide	0.000108	0.000042	0.000042	-0.000039
Density	-0.601	-0.2169	-0.2169	-0.2333
pH	-0.02453	-0.01222	-0.01222	0.003885
Sulphates	-0.03981	-0.0157	-0.01571	-0.001095
Alcohol	0.01341	0.003317	0.003317	0.007189
LabelAppeal	0.4193	0.1298	0.1298	0.2321
AcidIndex	-0.2016	-0.08412	-0.08412	-0.01777
STARS	0.9832	0.3133	0.3133	0.1028

APPENDIX A: Evaluation Data Set

Please note that this appendix includes first 100 observations from the evaluation set.

Index	Predicted Value	Predicted Outcome
3	1.894	2
9	3.826	4
10	2.513	3
18	2.492	2
21	0.7126	1
30	5.695	6
31	3.595	4
37	1.343	1
39	0.2309	0
47	1.468	1
60	2.693	3
62	0.2158	0
63	3.539	4
64	1.329	1
68	1.176	1
75	2.761	3
76	2.517	3
83	0.0539	0
87	3.674	4
92	5.435	5
98	2.317	2
106	1.682	2
107	0.473	0
113	2.537	3
120	3.448	3
123	5.88	6
125	2.838	3
126	5.872	6
128	4.508	5
129	2.449	2
131	4.213	4
135	0.9485	1
141	4.205	4
147	3.249	3
148	1.312	1
151	3.745	4
156	3.179	3
157	3.38	3
174	1.655	2
186	0.5061	1
193	2.592	3
195	0.9228	1
212	0.6654	1
213	0.6855	1
217	2.986	3
223	3.834	4
226	3.158	3
228	4.544	5
230	4.127	4

Index	Predicted Value	Predicted Outcome
241	2.628	3
243	3.746	4
249	1.071	1
281	4.079	4
288	0.277	0
294	1.913	2
295	1.963	2
300	5.567	6
302	4.323	4
303	1.856	2
308	1.706	2
319	4.84	5
320	0.9056	1
324	2.964	3
331	2.665	3
343	2.961	3
347	2.422	2
348	3.685	4
350	4.667	5
357	1.443	1
358	3.605	4
360	4.18	4
366	3.558	4
367	2.621	3
368	4.894	5
376	2.318	2
380	3.275	3
388	0.5946	1
396	4.575	5
398	4.527	5
403	3.921	4
410	2.043	2
412	0.6185	1
420	2.501	3
434	2.495	2
440	3.049	3
450	3.489	3
453	2.763	3
464	4.602	5
465	4.51	5
466	4.76	5
473	2.475	2
476	1.708	2
478	1.517	2
479	3.189	3
493	2.733	3
497	3.061	3
503	3.663	4
504	3.592	4
505	2.192	2
507	0.2199	0

APPENDIX B: R Script

```
# Required libraries
library(ggplot2)    # plotting
library(dplyr)      # data manipulation
library(gridExtra)  # display
library(knitr)      # display
library(kableExtra) # display
library(mice)       # imputation
library(caTools)    # train-test split
library(MASS)       # boxcox
library(Metrics)    # rmse
library(caret)      # confusion matrix
library(VIM)        # plotting NAs
library(ggfortify)  # plotting lm diagnostic
library(car)        # VIF
library(pscl)       # zero-inflated model

# Import data
wine <- read.csv(url(paste0("https://raw.githubusercontent.com/",
                           "ilyakats/CUNY-DATA621/master/hw5/",
                           "wine-training-data.csv")),
                 na.strings=c("","NA"))
colnames(wine)[1] <- "INDEX"

# Basic statistic
nrow(wine); ncol(wine)
summary(wine)

# Summary table
sumtbl = data.frame(Variable = character(),
                    Class = character(),
                    Min = integer(),
                    Median = integer(),
                    Mean = double(),
                    SD = double(),
                    Max = integer(),
                    Num_NAs = integer(),
                    Num_Zeros = integer(),
                    Num_Neg = integer())
for (i in c(3:16)) {
  sumtbl <- rbind(sumtbl, data.frame(Variable = colnames(wine)[i],
                                     Class = class(wine[,i]),
                                     Min = min(wine[,i], na.rm=TRUE),
                                     Median = median(wine[,i], na.rm=TRUE),
                                     Mean = mean(wine[,i], na.rm=TRUE),
                                     SD = sd(wine[,i], na.rm=TRUE),
                                     Max = max(wine[,i], na.rm=TRUE),
                                     Num_NAs = sum(is.na(wine[,i])),
                                     Num_Zeros = length(which(wine[,i]==0)),
                                     Num_Neg = sum(wine[,i]<0 & !is.na(wine[,i]))))
}
colnames(sumtbl) <- c("Variable", "Class", "Min", "Median", "Mean", "SD", "Max",
                      "Num of NAs", "Num of Zeros", "Num of Neg Values")
sumtbl

# Categorical variables
table(wine$LabelAppeal)
table(wine$AcidIndex)
table(wine$STARS)

# Exploratory plots
v <- "FixedAcidity"
v <- "VolatileAcidity"
v <- "CitricAcid"
v <- "ResidualSugar"
v <- "Chlorides"
v <- "FreeSulfurDioxide"
v <- "TotalSulfurDioxide"
v <- "Density"
v <- "pH"
v <- "Sulphates"
v <- "Alcohol"
v <- "LabelAppeal"
v <- "AcidIndex"
v <- "STARS"
pd <- as.data.frame(cbind(wine[, v], wine$TARGET)); colnames(pd) <- c("X", "Y")
bp <- ggplot(pd, aes(x = 1, y = X)) + stat_boxplot(geom ='errorbar') +
  geom_boxplot() +
  xlab("Boxplot") + ylab("") + theme(axis.text.x=element_blank(),
                                     axis.ticks.x=element_blank())
hp <- ggplot(pd, aes(x = X)) + geom_histogram(aes(y=..density..),
                                              colour="black", fill="white") +
  geom_density(alpha=.2, fill="#FF6666") + ylab("") +
  xlab("Density Plot with Mean") +
  geom_vline(aes(xintercept=mean(X, na.rm=TRUE)),
             color="red", linetype="dashed", size=1)
sp <- ggplot(pd, aes(x=X, y=Y)) + geom_point() + xlab("Scatterplot")
grid.arrange(bp, hp, sp, layout_matrix=rbind(c(1,2,2),c(1,3,3)))

ggplot(wine, aes(x = as.factor(TARGET), y = Chlorides)) +
  stat_boxplot(geom ='errorbar') + geom_boxplot() +
  xlab("Boxplots per No of Wine Cases") + ylab("pH") +
  theme(axis.ticks.x=element_blank())

# Correlation matrix
cm <- cor(wine[,2:16], use="pairwise.complete.obs")
cm <- round(cm, 2)
cmout <- as.data.frame(cm) %>% mutate_all(function(x) {
  cell_spec(x, "html", color = ifelse(x>0.5 | x<(-0.5),"blue","black"))
})
rownames(cmout) <- colnames(cmout)
cmout %>%
  kable("html", escape = F, align = "c", row.names = TRUE) %>%
  kable_styling("striped", full_width = F)
```

```r
# IMPUTATION / TRANSFORMATION
wineOriginal <- wine # Backup of original data

wine$STARS[is.na(wine$STARS)] <- 0 # Missing STARS are 0 score
# Missing values - table
md.pattern(wine)
# Missing values - plot
aggr_plot <- aggr(wine, col=c('navyblue','red'),
                  numbers=FALSE, sortVars=TRUE, labels=names(wine),
                  cex.axis=.7, gap=3,
                  ylab=c("Histogram of missing data","Pattern"))
# Imputation
wineImputed <- mice(wine, m=5, maxit=20, meth='norm', seed=500)
summary(wineImputed)
wine <- complete(wineImputed)
summary(wine)

# Proportion of target variable
table(wine$TARGET)
table(wine$TARGET)/sum(table(wine$TARGET))

wine$Alcohol <- abs(wine$Alcohol)

# Split into train and validation sets
set.seed(88)
split <- sample.split(wine$TARGET, SplitRatio = 0.75)
wineTRAIN <- subset(wine, split == TRUE)
wineTEST <- subset(wine, split == FALSE)
table(wineTRAIN$TARGET)/sum(table(wineTRAIN$TARGET))

# LINEAR MODEL

# All variables
lmModel <- lm(TARGET ~ .-INDEX,data = wineTRAIN)
summary(lmModel)
# stepAIC
lmModel <- stepAIC(lmModel, trace=FALSE, direction='both')
summary(lmModel)
# Model returned by step AIC
lmModel <- lm(TARGET ~ VolatileAcidity + CitricAcid +
                Chlorides + FreeSulfurDioxide +
                TotalSulfurDioxide + Sulphates + Alcohol +
                LabelAppeal + AcidIndex + STARS,
              data = wineTRAIN)
summary(lmModel)
# Manual variations
lmModel <- lm(TARGET ~ VolatileAcidity + Chlorides +
                FreeSulfurDioxide +
                TotalSulfurDioxide + Sulphates + Alcohol +
                LabelAppeal + AcidIndex + STARS,
              data = wineTRAIN)
summary(lmModel)
lmModel <- lm(TARGET ~ VolatileAcidity + Chlorides +
                FreeSulfurDioxide +
                TotalSulfurDioxide + Alcohol +
                LabelAppeal + AcidIndex + STARS,
              data = wineTRAIN)
summary(lmModel)

# Calculate RMSE
pred <- predict(lmModel, newdata=wineTEST)
rmse(wineTEST$TARGET, pred)

# Confusion matrix
predRound <- as.factor(round(pred,0))
table(predRound)
levels(predRound) <- levels(as.factor(wineTEST$TARGET))
confusionMatrix(predRound, as.factor(wineTEST$TARGET))

autoplot(lmModel)

# Model plots
plot(lmModel$residuals, ylab="Residuals")
abline(h=0)

plot(lmModel$fitted.values, lmModel$residuals,
     xlab="Fitted Values", ylab="Residuals")
abline(h=0)

qqnorm(lmModel$residuals)
qqline(lmModel$residuals)

# POISSON and NB REGRESSION MODEL

# Poisson 1
glmModel <- glm (TARGET ~ .-INDEX, data = wineTRAIN, family = poisson)
summary(glmModel)
pred <- predict(glmModel, newdata=wineTEST, type='response')
rmse(wineTEST$TARGET, pred)
predRound <- as.factor(round(pred,0))
testData <- as.factor(wineTEST$TARGET)
levels(predRound) <- c("1", "2", "3", "4", "5", "6", "7", "8", "9", "10", "0")
levels(testData) <- c("0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "10")
confusionMatrix(predRound, testData)

# Poisson 2
glmModel2 <- stepAIC(glmModel, trace=FALSE, direction='both')
summary(glmModel2)
pred <- predict(glmModel2, newdata=wineTEST, type='response')
rmse(wineTEST$TARGET, pred)
predRound <- as.factor(round(pred,0))
testData <- as.factor(wineTEST$TARGET)
levels(predRound) <- c("1", "2", "3", "4", "5", "6", "7", "8", "9", "10", "0")
levels(testData) <- c("0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "10")
confusionMatrix(predRound, testData)
```

```
# Poisson 3
glmModel3 <- glm(TARGET ~ VolatileAcidity + Chlorides + FreeSulfurDioxide +
                 Sulphates + Alcohol + LabelAppeal +
                 AcidIndex + STARS, family = poisson, data = wineTRAIN)
summary(glmModel3)
pred <- predict(glmModel3, newdata=wineTEST, type='response')
rmse(wineTEST$TARGET, pred)
predRound <- as.factor(round(pred,0))
testData <- as.factor(wineTEST$TARGET)
levels(predRound) <- c("1", "2", "3", "4", "5", "6", "7", "8", "9", "10", "0")
levels(testData) <- c("0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "10")
confusionMatrix(predRound, testData)

# NB
nbModel <- glm.nb(TARGET ~ .-INDEX, data = wineTRAIN)
summary(nbModel)
pred <- predict(nbModel, newdata=wineTEST, type='response')
rmse(wineTEST$TARGET, pred)
predRound <- as.factor(round(pred,0))
testData <- as.factor(wineTEST$TARGET)
levels(predRound) <- c("1", "2", "3", "4", "5", "6", "7", "8", "9", "10", "0")
levels(testData) <- c("0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "10")
confusionMatrix(predRound, testData)

# Zero Inflated
zrModel <- zeroinfl(TARGET ~ .-INDEX, data = wineTRAIN, dist = "negbin")
summary(zrModel)
pred <- predict(zrModel, newdata=wineTEST, type='response')
rmse(wineTEST$TARGET, pred)
predRound <- as.factor(round(pred,0))
testData <- as.factor(wineTEST$TARGET)
confusionMatrix(predRound, testData)

# Deviance residuals
anova(glmModel, test="Chisq")
anova(glmModel2, test="Chisq")
anova(glmModel3, test="Chisq")
anova(nbModel, test="Chisq")
anova(zrModel, test="Chisq")

# VIF
vif(glmModel)
vif(nbModel)
vif(zrModel)

# Coefficients
coef <- as.data.frame(lmModel$coefficients)
coef <- cbind(coef, as.data.frame(glmModel$coefficients))
coef <- cbind(coef, as.data.frame(nbModel$coefficients))
coef <- cbind(coef, as.data.frame(zrModel$coefficients))

# Prediction
eval <- read.csv(url(paste0("https://raw.githubusercontent.com/",
                            "ilyakats/CUNY-DATA621/master/hw5/",
                            "wine-evaluation-data.csv")),
                 na.strings=c("","NA"))
colnames(eval)[1] <- "INDEX"

sumtbl = data.frame(Variable = character(),
                    Class = character(),
                    Min = integer(),
                    Median = integer(),
                    Mean = double(),
                    SD = double(),
                    Max = integer(),
                    Num_NAs = integer(),
                    Num_Zeros = integer(),
                    Num_Neg = integer())
for (i in c(3:16)) {
  sumtbl <- rbind(sumtbl, data.frame(Variable = colnames(eval)[i],
                                     Class = class(eval[,i]),
                                     Min = min(eval[,i], na.rm=TRUE),
                                     Median = median(eval[,i], na.rm=TRUE),
                                     Mean = mean(eval[,i], na.rm=TRUE),
                                     SD = sd(eval[,i], na.rm=TRUE),
                                     Max = max(eval[,i], na.rm=TRUE),
                                     Num_NAs = sum(is.na(eval[,i])),
                                     Num_Zeros = length(which(eval[,i]==0)),
                                     Num_Neg = sum(eval[,i]<0 & !is.na(eval[,i]))))
}
colnames(sumtbl) <- c("Variable", "Class", "Min", "Median", "Mean", "SD", "Max",
                      "Num of NAs", "Num of Zeros", "Num of Neg Values")
sumtbl

eval$STARS[is.na(eval$STARS)] <- 0
eval$Alcohol <- abs(eval$Alcohol)

evalImputed <- mice(eval, m=5, maxit=10, meth='norm', seed=500)
eval <- complete(evalImputed)

pred <- predict(zrModel, newdata=eval, type="response")
results <- eval[, c("INDEX")]
results <- cbind(results, prob=round(pred,4))
results <- cbind(results, predict=round(pred,0))
colnames(results) <- c("Index", "Predicted Value", "Predicted Outcome")
pander(head(results, 100))
```