PREDICTIVE ANALYTICS

SYNDICATE TASK #1 – PREDICTING WINE QUALITIES

SYNDICATE 8

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1. Purpose

The purpose of this report is to predict the wine quality score of red wine based on specific physicochemical properties. The ability to predict wine quality score has several applications. Firstly, it allows winemakers to judge how their wine may turn out in terms of quality score, early in the process. That forecasted score then enables quality improvement interventions and implementation of the proper marketing mix i.e. advertising budget, packaging and pricing. Furthermore, the prediction of the wine quality score also helps to better plan the winemaking process in the upcoming season to optimize the balance between costs and quality score.

2. Methodology

1. Exploratory Data Analysis of wine dataset
    a. Characteristics of each variable
    b. Correlation between variables
2. Multilinear regression with all variables
3. Multilinear stepwise regression with all variables
4. Nonlinear regression
5. Nonlinear stepwise regression
6. Scoring of all models & predictive accuracy

2.1a Characteristics of variables

Each wine has multiple physiochemical variables which affect overall wine quality, and its score. Below is the average value and standard deviation for the different attributes of red wine.

	FA	VA	CA	RS	Ch	FSD	TSD	Density	pH	Sulphates	Alc
Avg	8.32	0.53	0.27	2.54	0.09	15.88	46.47	1.00	3.31	0.66	10.42
St dev σ	1.74	0.18	0.19	1.41	0.05	10.46	32.90	0.00	0.15	0.17	1.07

2.1b Correlation of variables against quality

The below provides a view of which variables are negatively or positively correlated with quality score. It appears ‘Volatile Acidity’ is most negatively correlated whilst ‘Alcohol’ is most positively correlated with the score.

FA	VA	CA	RS	Ch	FSD	TSD	Density	pH	Sulphates	Alc
0.12	-0.39	0.23	0.01	-0.13	-0.05	-0.19	-0.18	-0.06	0.25	0.48

2.2 Multilinear regression with all variables

The multilinear regression with all variables produced an adjusted R-squared of 0.3495, as demonstrated in Appendix 1. There are several variables which the model deems to be statistically insignificant in predicting the quality score, such as ‘Fixed Acidity’, ‘Citric Acid’, ‘Residual Sugar’ and ‘Wine Density’.

Exploring Appendix 2, specifically the fitted values vs actual values, it’s evident that the model tends to overestimate at the low range of the quality score and underestimate at the high range of the quality score.

Apart from that, other residual plots do not seem to indicate any nonlinear relationships between quality score and the explanatory variables.

2.3 Multilinear stepwise regression with all variables

Outlined in Appendix 3, the multilinear stepwise regression slightly improves on the prior model with an adjusted R-squared of 0.3511, highlighting the advantage of utilizing less irrelevant parameters. Despite the improved adjusted R-squared, the multilinear stepwise regression still suffers from the same overestimate and underestimate issues of the quality score.

Similarly, the new set residual plots, as depicted in Appendix 4, do not seem to indicate any nonlinear relationships. However, further analysis is still recommended.

2.4 Nonlinear regression

Outlined in Appendix 5, the nonlinear regression with quadratic and logarithm terms on the seven significant variables (VA, Ch, FSD, TSD, pH, Sulphates, Alc) highlighted by a multilinear stepwise regression improves the adjusted R-squared to 0.3814. But the improvement of adjusted R-squared is not significant, and the issue of overestimating and underestimating remain.

2.5 Nonlinear stepwise regression

Outlined in Appendix 7, the stepwise regression on the nonlinear model improves the adjusted R-squared to 0.3819. The primary concern of systematic over and under estimation still exits, and improvement of R-squared is meagre.

2.6 Scoring of all models & predictive accuracy

All four models have been scored and they perform closely in term of predicting the quality score of wine using existing physiochemical properties. The loss functions metrics in the table below demonstrate their predictive strength relative to each other.

	RMSE	**MAE**	**MAPE**	**MASE**	**# of Parameters**
Linear	0.58593	0.46498	8.66332	0.72938	12
Stepwise	0.58721	0.46462	8.65633	0.72881	8
Nonlinear	0.58349	0.46077	8.61997	0.72278	18
Nonlinear plus stepwise	0.58434	0.46105	8.61332	0.72321	13

3. Analysis

The four models used in predicting wine qualities all scored extremely closely, despite the nonlinear models being more complicated through the use of quadratic and logarithmic terms. In this instance, it is safe to use any of the four reported metrics as there are no extreme values which can affect the RMSE and no values of 0, which would ordinarily affect the MAPE.

The two models which had the best predictive power were the nonlinear ones (without and with stepwise), and in the search for the model which best predicts quality of the wine, either of the two nonlinear models should be selected.

In the nonlinear (without stepwise) model, a prediction deviates on average 0.583 points away from true quality according to RMSE. It varies 0.461 from true quality using the MAE measure. A forecast on average deviates by 8.62% to actual quality scores according to MAPE and the MASE of 0.72 highlights it is worth running a prediction model as it is approximately 28% better than running a naïve prediction.

However, if there were a need to derive causal effects, it would be recommended to use the linear stepwise model as it can explain the majority of what influences the quality score and uses fewer parameters.

To explain how wine quality is affected by the physicochemical properties of wine, the linear stepwise model will be referenced due to the simplicity of explanation. 'Free Sulphur Dioxide', 'Sulphates' and 'Alcohol' all appear to have a positive effect on the score of red wine. 'Volatile Acidity', 'Chlorides', 'Total Sulfur Dioxide' and 'pH' all have a negative effect on the quality of the wine.

These results appear to follow the correlation matrix to a certain extent, except for 'Free Sulphur Dioxide' which has a negative association with quality score in the correlation matrix.

The other physiochemical properties have been excluded from the model, likely due to either being correlated with other variables or being statistically insignificant in predicting the quality of the wine.

4. Limitations

Based on adjusted R-squared, all models could explain less than 40% of wine quality score variation. Furthermore, they tend to overpredict at the low range of observed scores and underestimate at the high range of observed scores. There are several reasons for these issues.

Firstly, all the data available that goes into scoring wine may not be explained purely by physicochemical properties. For example, there are elements of human judgement that goes into choosing a quality score for wine which is not captured in the dataset. There may also be other data points which have not been recorded or unable to be measured but are crucial in determining wine quality.

Secondly, it is possible the regression model is not well suited to predict wine quality from physicochemical properties. The regression models tend to be parametric, which means they follow a smooth pattern. Other non-parametric models, which tends to be more flexible, may do a much better job at predicting quality score from the available variables.

Another limitation is that the analysis and scoring do not place any weighting on over or under predictions. Consequently, winemakers may use different metrics to measure the predictive accuracy of modelling so a user-defined loss function may be more suited in that instance.

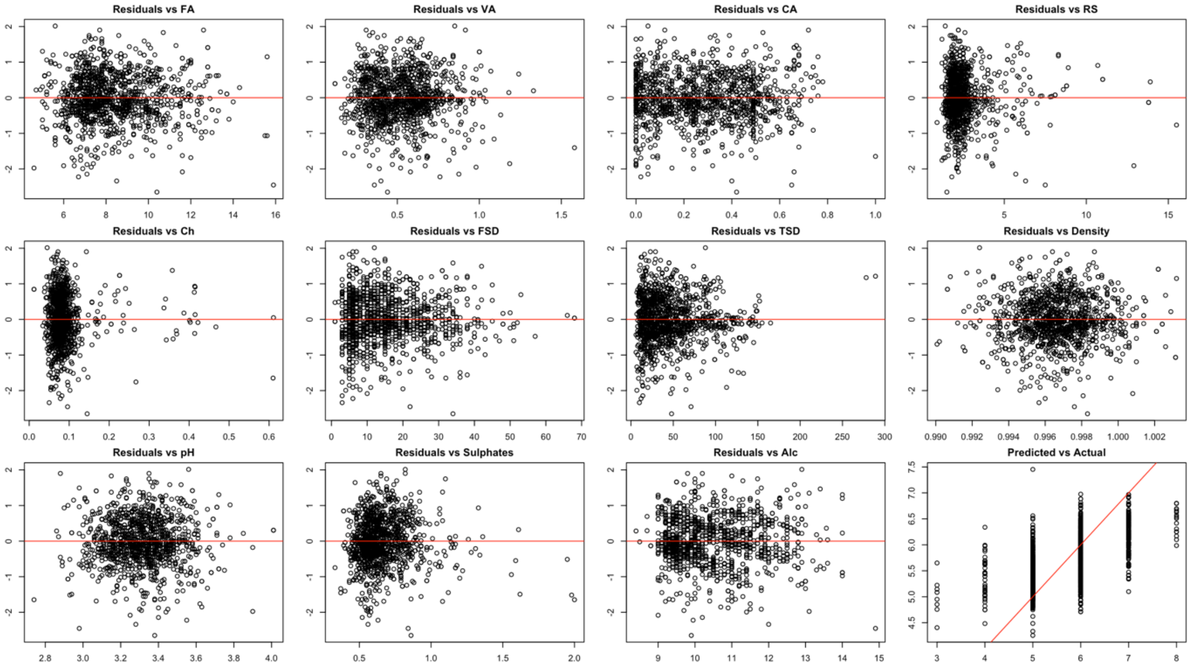
Finally, we acknowledge that each industry will have its own benchmark and a statistical model which generates an adjusted R-squared below 40% and the subsequent loss function results outlined may be considered predictably suitable for the purpose of wine making.

5. Appendix

Appendix 1 – Multilinear Regression Summary

```
Call:
lm(formula = QS ~ ., data = trainData)

Residuals:
     Min       1Q   Median       3Q      Max
-2.65050 -0.38391 -0.04515  0.45702  2.01409

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.490e+01  2.405e+01   0.620  0.53569
FA           1.242e-02  2.998e-02   0.414  0.67877
VA          -1.021e+00  1.398e-01  -7.304 4.91e-13 ***
CA          -1.296e-01  1.687e-01  -0.768  0.44262
RS           6.203e-03  1.749e-02   0.355  0.72284
Ch          -2.059e+00  4.711e-01  -4.371 1.34e-05 ***
FSD          4.145e-03  2.502e-03   1.656  0.09791 .
TSD         -3.561e-03  8.351e-04  -4.264 2.16e-05 ***
Density     -1.024e+01  2.455e+01  -0.417  0.67667
pH          -5.783e-01  2.193e-01  -2.637  0.00846 **
Sulphates    8.651e-01  1.329e-01   6.508 1.09e-10 ***
Alc          2.908e-01  3.040e-02   9.564  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.6634 on 1267 degrees of freedom
Multiple R-squared:  0.3551,    Adjusted R-squared:  0.3495
F-statistic: 63.41 on 11 and 1267 DF,  p-value: < 2.2e-16
```

Appendix 2 – Multilinear Residual Plot

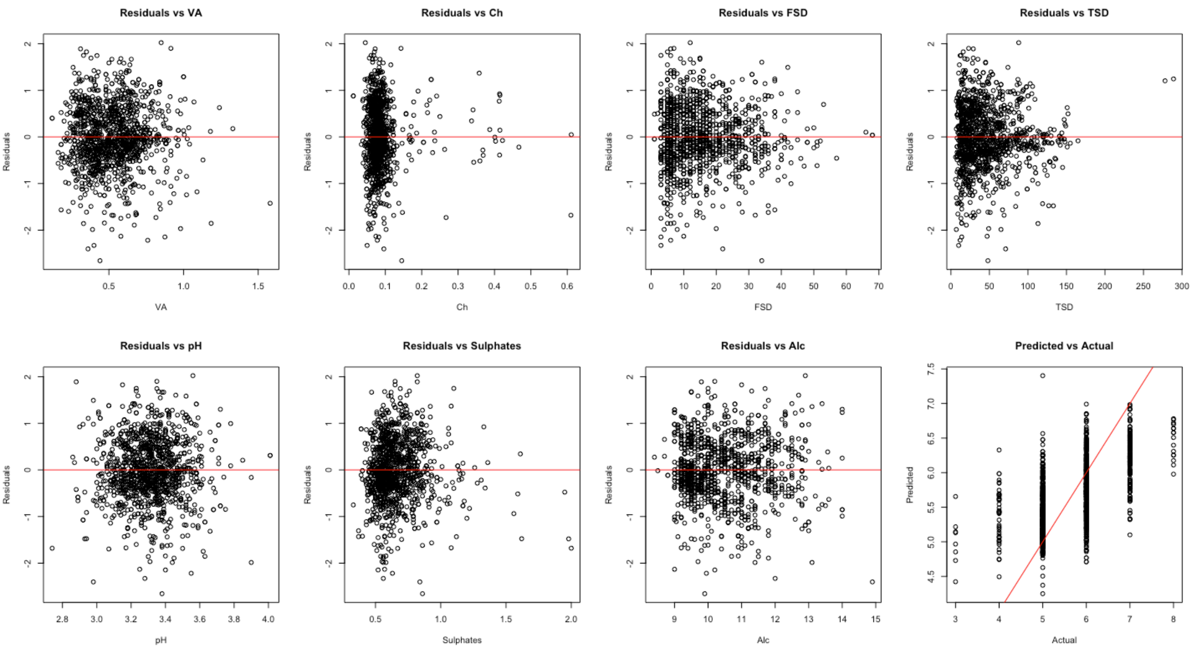


Appendix 3 – Stepwise Multilinear Regression Summary

```
Call:
lm(formula = QS ~ VA + Ch + FSD + TSD + pH + Sulphates + Alc,
    data = trainData)


Residuals:
     Min       1Q   Median       3Q      Max
-2.65513 -0.37980 -0.04544  0.46399  2.02174


Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  4.7312900  0.4552581  10.393  < 2e-16 ***
VA          -0.9654987  0.1151049  -8.388  < 2e-16 ***
Ch          -2.1511320  0.4473199  -4.809 1.70e-06 ***
FSD          0.0045550  0.0024584   1.853   0.0641 .
TSD         -0.0037041  0.0007855  -4.715 2.68e-06 ***
pH          -0.5871845  0.1336715  -4.393 1.21e-05 ***
Sulphates    0.8437438  0.1278251   6.601 5.99e-11 ***
Alc          0.2972283  0.0189738  15.665  < 2e-16 ***
---
```

```
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1


Residual standard error: 0.6626 on 1271 degrees of freedom
Multiple R-squared:  0.3546,   Adjusted R-squared:  0.3511
F-statistic: 99.77 on 7 and 1271 DF,  p-value: < 2.2e-16
```

Appendix 4 - Stepwise Multilinear Regression Residual Plot



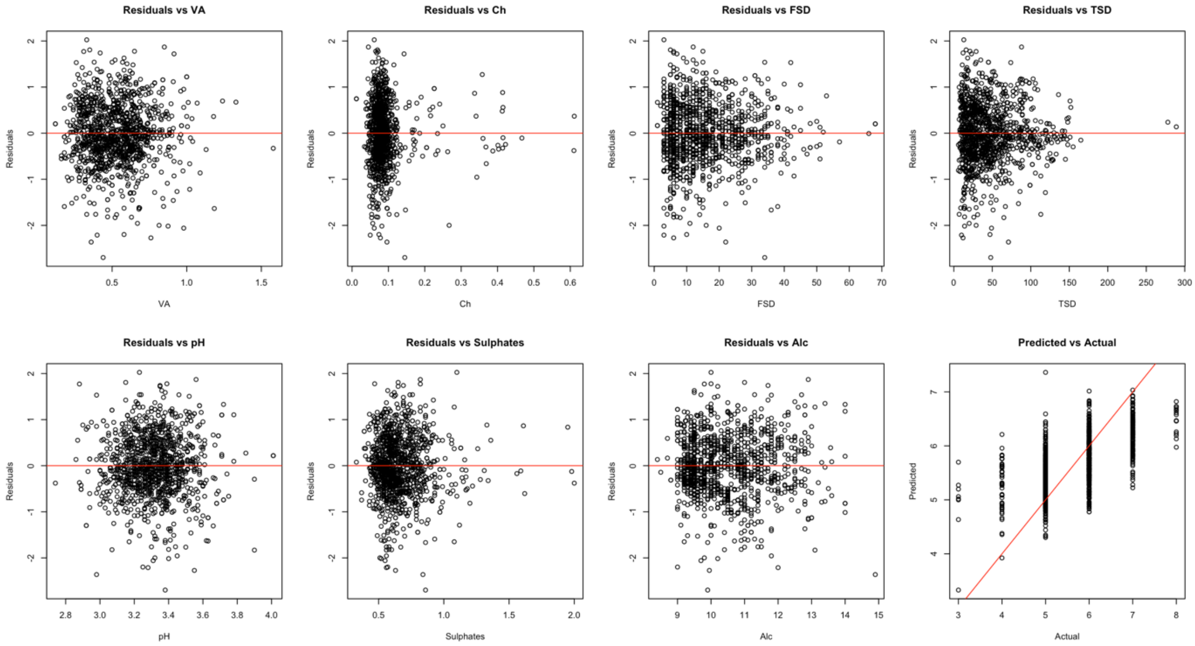
Appendix 5 – Nonlinear Regression Summary

Nonlinear regression with quadratic and logarithm terms added for seven statistically significant predictors identified by the previous stepwise: VA, Ch, FSD, TSD, pH, Sulphates, Alc.

```
Call:
lm(formula = QS ~ VA + I(VA^2) + I(log(VA)) + Ch + I(Ch^2) + 
    I(log(Ch)) + TSD + I(TSD^2) + I(log(TSD)) + FSD + I(FSD^2) + 
    I(log(FSD)) + pH + Sulphates + I(Sulphates^2) + I(log(Sulphates)) + 
    Alc, data = trainData)


Residuals:
     Min       1Q   Median       3Q      Max 
-2.69813 -0.38174 -0.03291  0.43054  2.02515 
```

```
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)        7.372e+00  2.572e+00   2.866 0.004224 **
VA                 2.278e+00  1.967e+00   1.158 0.247177
I(VA^2)           -1.418e+00  8.460e-01  -1.676 0.094036 .
I(log(VA))        -7.178e-01  5.291e-01  -1.357 0.175103
Ch                 7.050e+00  3.620e+00   1.948 0.051662 .
I(Ch^2)           -9.158e+00  4.714e+00  -1.943 0.052239 .
I(log(Ch))        -7.194e-01  2.624e-01  -2.741 0.006210 **
TSD               -1.260e-02  4.270e-03  -2.952 0.003218 **
I(TSD^2)           3.716e-05  1.420e-05   2.616 0.008995 **
I(log(TSD))        1.776e-01  1.315e-01   1.351 0.177011
FSD               -4.246e-03  1.737e-02  -0.245 0.806872
I(FSD^2)           3.004e-05  2.133e-04   0.141 0.888014
I(log(FSD))        1.334e-01  1.455e-01   0.917 0.359365
pH                -7.846e-01  1.348e-01  -5.820 7.45e-09 ***
Sulphates         -6.912e+00  3.181e+00  -2.173 0.029958 *
I(Sulphates^2)     1.071e+00  8.354e-01   1.282 0.199905
I(log(Sulphates))  4.542e+00  1.373e+00   3.308 0.000966 ***
Alc                2.778e-01  1.958e-02  14.184  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.6469 on 1261 degrees of freedom
Multiple R-squared:  0.3896,   Adjusted R-squared:  0.3814
F-statistic: 47.35 on 17 and 1261 DF,  p-value: < 2.2e-16
```

Appendix 6 – Nonlinear Regression Residual Plot



Appendix 7 – Stepwise Nonlinear Regression Summary

```
Call:
lm(formula = QS ~ I(VA^2) + Ch + I(Ch^2) + I(log(Ch)) + TSD + I(TSD^2) +
I(log(TSD)) + I(log(FSD)) + pH + Sulphates + I(log(Sulphates)) + Alc, dat
a = trainData)


Residuals:
     Min       1Q   Median       3Q      Max
-2.74200 -0.38463 -0.03049  0.43293  1.94216


Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)        6.146e+00  1.163e+00   5.283 1.50e-07 ***
I(VA^2)           -6.305e-01  9.359e-02  -6.736 2.46e-11 ***
Ch                 5.977e+00  3.449e+00   1.733  0.08332 .
I(Ch^2)           -7.837e+00  4.530e+00  -1.730  0.08389 .
I(log(Ch))        -6.528e-01  2.498e-01  -2.614  0.00906 **
TSD               -1.316e-02  3.992e-03  -3.298  0.00100 **
I(TSD^2)           3.884e-05  1.382e-05   2.811  0.00502 **
I(log(TSD))        1.925e-01  1.204e-01   1.600  0.10994
```

```
I(log(FSD))         8.972e-02  4.451e-02   2.016  0.04403 *
pH                 -7.719e-01  1.333e-01  -5.791 8.81e-09 ***
Sulphates          -2.895e+00  5.623e-01  -5.149 3.04e-07 ***
I(log(Sulphates))   2.869e+00  4.184e-01   6.857 1.10e-11 ***
Alc                 2.796e-01  1.939e-02  14.420  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.6467 on 1266 degrees of freedom
Multiple R-squared:  0.3877,   Adjusted R-squared:  0.3819
F-statistic: 66.79 on 12 and 1266 DF,  p-value: < 2.2e-16
```