# Prediction of Wine Quality: Comparing Machine Learning Models in R Programming

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Abstract: The consideration of wine quality before consumption or use is not a new decision scheme across ages, fields, and people. Gone were the days when quality of wine solely depended on taste or other physical checks. In this age of data science and machine learning, we can make decisions on the best wine quality with reference to different features/variables. This work was done with in predicting the dependent variable while using existing models to analyze the independent variables. This work utilizes the R programming language for this prediction, while comparing different machine learning models like Linear regression, Neural network, Naive Bayes Classification, Linear Discriminant Analysis (LDA), Classification and Regression Trees (CART), k-Nearest Neighbors (kNN), Support Vector Machines (SVM) with a linear kernel, and Random Forest (RF). The provided data was divided into the testing and training portions with parts for validation. It was achieved that Random Forest has a better model for this prediction when cross crossvalidated in 10-folds. The accuracy was then used to select the optimal model. Hence, alcohol is the feature variable that contributes more to wine quality while volatile acidity and chloride contribute the least to the quality of wine. This would assist breweries in determining the right additions and subtraction when wine quality is in question.

*Keywords*: Random Forest, R programming, Machine learning models, Wine quality, Algorithms, RF

# I. INTRODUCTION

ndustries, especially the chemical industries have evolved Lover the years in determining values and analyzing data. Vast collaborations are vast permeating the research atmosphere. Wine is regarded as the commonest beverage across cultures and fields in the global sphere, and its values are weighed by different features in different societies [1]. Determining the quality of wine is always of great interest to both researchers and consumers. Wine quality are generally determined by two basic tests; which are the sensory tests and the physicochemical tests. Considering the fact that physicochemical test is a laboratory test, with no human expertise required and sensory test requires human expertise; researchers come into a difficult terrain in determining the quality of wine [2] [3]. Complex data analysis as wine quality assessment feature therefore requires a better approach for full understanding. Racing through the lane of history,

determining wine quality is expensive and time consuming [1].

This century doesn't only allow for collaboration among seemingly contrasting fields, but gives a push for a paradigm shift in technological advancements and tool utilization [4]. Data scientists, computer scientists, chemical engineers, material engineers and others can seamlessly work together for better research in determining the quality of wine today. Utilizing object-oriented programming like python has been of great benefits in the industry [5]. R programming is not only instructive in the academic world, but produces advance results for optimal predictions in the industrial sphere as well. Hence, R is also used for the machine learning prediction and that has been established in this research with the consideration of different algorithms and easy to use packages in CRAN.

# II. GENERAL OVERVIEW

Machine learning predictions have become easier through the advent of different algorithms and ML models. With much on supervised and unsupervised learning, researchers can now make right predictions through the right and available tools. Engineers and scientists need the right tools in decision making, proper data interpretation and statistical analysis. R among other programming tools is highly effective in data analytics and machine learning. In the fields, much of the machine learning works have been on the door of Python programming and the available packages. Interestingly however, R provides another strong reinforcement in machine learning and statistics. Statistical data is getting the proper attention through these tools, and statisticians are computer scientists to achieve feats.

The data for this work was provided by Kaggle, as uploaded on 15th January, 2022 [6]. R programming tools were utilized to achieve the correct prediction of the quality of wine. Knowing the right package to install in R for data analysis is very pivotal to the success of any research work with it. R programmers have a bunch of similar packages that perform similar operations. Choice, desire and flexibility are few of the factors that inform the use of a package. Linear regression, Neural network, Naive Bayes Classification, Linear Discriminant Analysis (LDA), Classification and Regression Trees (CART), k-Nearest Neighbors (kNN), Support Vector Machines (SVM) with a linear kernel, and Random Forest (RF) were considered for this project as provided by the R packages in use. Different data visualization scheme was also done.

### **III. LITERATURE REVIEW**

With advent of machine learning models in the recent years, determining wine quality have gone through different analysis and modelling [21]. Some previous works of Moreno et. al was to categorize 54 samples of a particular wine using the popular probabilistic neural network [18]. Authors Yu et al. also worked on something related. 147 bottles of rice wine were analyzed and estimated using spectral measurements [19]. Three different Chilean wine was classified by Beltran et al. [20] using basically three machine leaning models; SVM, linear discriminate analysis and neural network.

Wine has been initially analyzed through the use of electric nose [7]. Different wines could also be classified through the use of taste sensor as applied to neural networks [8]. Larkin used stacked generalization to predict wine preferences. There have also been previous application applications of machine wine prediction, recommendation learning in and classification [10][11][12]. Despite all these works, R as a statistical and machine learning tool has often been neglected in the previous works [13]. According to Hackenberger's research in 2020, there was a general believe that R is unfriendly, but probably the best tool. R is not just open source but easily accessible. It was stated that the power of R is closely based on the availability of packages with functions, algorithms, and flexibility [14]. A major comparison initially done compared R, Python and SAS, and found R efficient but often neglected [15]. R has always been on the frontline for teaching purposes. It seems industries over the years are glued to other tools and would not explore the beauties of R [16]. Hence, bringing the machine learning ability of R is part of the focus of this work.

### **IV. THE DATASET**

This dataset gearing towards the prediction of wine quality is related to red variants of the Portuguese "Vinho Verde" wine [6]. According to a report in 2021, USA consumers have grown to love this type of Portuguese wine, and almost becoming a household name [17]. It basically describes the various chemicals present in wine and their possible effects on the quality

This dataset as obtained from Kaggle has 13 columns and divided into three subsections:

- a) The input variables by physicochemical tests:
  - 1. Fixed acidity: This is the non-volatile acid in the wine

- 2. Volatile acidity: This the amount of acetic acid in the wine
- 3. Citric acid: This adds flavor to a wine
- 4. Residual sugar: This is the amount of sugar in the wine
- 5. Chlorides: This is the amount of salt in the wine
- 6. Free sulfur dioxide: This is in wine to prevent microbial growth/oxidation.
- 7. Total sulfur dioxide: This is total presence of sulfur dioxide in the wine
- 8. Density: The density of the substance
- 9. PH: This is the measure of acidity and basicity of the wine- from 0-14
- 10. Sulphates: Added to wine to aid the supply of sulfur dioxide
- 11. Alcohol: Percentage of alcohol in the wine
- b) Output variable by sensory data:
  - 12. Quality: Quality of the wine score between 0 and 10
- *c)* The wine ID:

13. Id: The label on the wine

I. The Dataset at a Glance

This data has a dimension of 1143 x 13. As displayed in Figures 1, 2, 3, and 4, the summary of what the dataset entails could be seen. The datatypes, measures of central tendencies and other features are displayed.

	fixed.acidity	volatile.acidity	citric.ac:	id resid	ual.sug	ar chlo	rides
1	7.4	0.70	0.00		1.9	0.076	
2	7.8	0.88	0.00		2.6	0.098	
3	7.8	0.76	0.04		2.3	0.092	
4	11.2	0.28	0.56		1.9	0.075	
5	7.4	0.70	0.00		1.9	0.076	
	free.sulfur.di	oxide total.sulfu	r.dioxide d	density	pH su	lphates	alcohol
1	11	1	34	0.9978	3.51	0.56	9.4
2	25	(	57	0.9968	3.20	0.68	9.8
3	15	5	54	0.9970	3.26	0.65	9.8
4	17	(	50	0.9980	3.16	0.58	9.8
5	11	1	34	0.9978	3.51	0.56	9.4
	quality Id						
1	5 0						
2	5 1						
3	5 2						
4	6 3						
5	5 4						

Figure 1: The first five lines of the dataset

	fixed.ac	iditv	volati	le.acidity	citric.	acid resid	ual.suga	r chlor	ides
1139		6.3		0.510	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	.13	2.3	~~~	076
1140		6.8		0.620	0	.08	1.9	0.	068
1141		6.2		0.600	0	.08	2.0	0.	090
1142		5.9		0.550	0	.10	2.2	0.	062
1143		5.9		0.645	0	.12	2.0	0.	075
	free.sul	fur.di	ioxide	total.sulfu	ur.dioxi	de density	pH su	lphates	alcohol
1139			29		40	0.99574	3.42	0.75	11.0
1140			28		38	0.99651	3.42	0.82	9.5
1141			32		44	0.99490	3.45	0.58	10.5
1142			39		51	0.99512	3.52	0.76	11.2
1143			32		44	0.99547	3.57	0.71	10.2
	quality	Id							
1139	6	1592							
1140	6	1593							
1141	5	1594							
1142	6	1595							
1143	5	1597							

Figure 2: The last five lines of the dataset

The Summary of the data

##			/ citric.acid	
##		Min. :0.1200		Min. : 0.900
##	1st Qu.: 7.100	1st Qu.:0.3925	1st Qu.:0.0900	1st Qu.: 1.900
##	Median : 7.900	Median :0.5200	Median :0.2500	Median : 2.200
##	Mean : 8.311	Mean :0.5313	Mean :0.2684	Mean : 2.532
##	3rd Qu.: 9.100		3rd Qu.:0.4200	
##	Max. :15.900		Max. :1.0000	
##				.dioxide density
##			Min. : 6.	
##				
	1st Qu.:0.0/000	1st Qu.: 7.00	1st Qu.: 21.	00 1st Qu.:0.9956
##				00 Median :0.9967
##				91 Mean :0.9967
##				00 3rd Qu.:0.9978
##	Max. :0.61100	Max. :68.00	Max. :289.	00 Max. :1.0037
##	pH	sulphates	alcohol	quality
##	Min. :2.740	Min. :0.3300	Min. : 8.40 M	in. :3.000
##	1st Ou.:3.205	1st Ou.:0.5500	1st Qu.: 9.50 1	st Ou.:5.000
##			Median :10.20 M	
##		Mean :0.6577		lean :5.657
##		3rd Qu.:0.7300		rd Qu.:6.000
##	Max. :4.010			ax. :8.000
##	Id			
##	Min. : 0			
##	1st Qu.: 411			
##	Median : 794			
##	Mean : 805			
##	3rd Ou.:1210			
##	Max. :1597			

Figure 3: The Summary of the dataset

### V. DATA PRE-PROCESSING

Id is just a label of the wine and was removed. Hence, it will not be needed as an input variable. The dataset is clean with no NA or voided spaces.

##	fixed.acidity	volatile.acidity	citric.acid	
##	"numeric"	"numeric"	"numeric"	
##	residual.sugar	chlorides	free.sulfur.dioxide	
##	"numeric"	"numeric"	"numeric"	
##	total.sulfur.dioxide	density	pН	
##	"numeric"	"numeric"	"numeric"	
##	sulphates	alcohol	quality	
##	"numeric"	"numeric"	"integer"	

Figure 4: Data types of all the input variables

### I. Working with the data

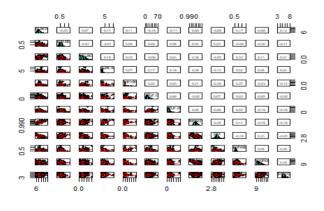


Figure 5: Plot to compare linear relationship

After cleaning the data, it was established a zero linear relationship between quality and other covariants as seen in Figure 5. This indicates that a simple linear regression might not work as an approach. Whenever a linear relationship isn't established between an output and featured inputs, linear models are not fully trusted.

## VI. BUILDING A MODEL WITH EXISTING AND SUGGESTED ALGORITHMS

It should be noted that several R packages were utilized for this project aside the normal base functions. These packages contain several in-built functions and algorithms that makes machine learning easy. With just few lines of commands, the dataset was partitioned into the training and testing sets, and cross-validation were done through the proper use of these R packages. These packages include:

- neuralnet for neural networks: This is used to train neural networks using backpropagation, test it and make predictions through existing/supplied data.
- naivebayes for naïve Bayes classification: This is an easy-to-use classification technique that uses the Bayes' Theorem. It works with independence assumptions of independence while predicting.
- ggplot2: This is basically for data representation and visualization. It contains lots of features used to visualize our data in this work.
- lattice: This is also for data visualization. A very powerful tool to visualize data before categorization.
- Caret: This is an indispensable package in R for this project. It is used for training data and encapsulates several machine learning models and algorithm already prepared (It has a great training tool with over 200 models that could be used by simple syntax). This includes the RF model that is suggested in this work.
- dplyr: This is for data manipulation (in tidyverse package)
- psych: This is an important tool for multivariate analysis.

All these tools and packages were effectively utilized for this work because the models have built into some of them.

49.43	freq percentage	
44		
00		
0.0		
12.12	Shapiro-Wilk normality test	
49.49		
	data: wineDrop\$quality	
48.48	W = 0.8547, p-value < 2.2e-16	
	(Intercept) fixed.acidity volatile.acidity	
88	(intercept) Tixed.acidity volatile.acidity 20.293497160 0.012741945 -1.095591018	
	citric.acid residual.sugar chlorides	
	-0.075781469 0.005005595 -2.295359928	
44.44	free.sulfur.dioxide total.sulfur.dioxide density	
48.48	0.004124116 -0.003054712 -15.595314032	
44.44	pH sulphates alcohol	
***	-0.541336255 0.987771558 0.269242123	
	Call:	
	lm(formula = quality ~ ., data = trainingset)	
49.49		
48.48	Residuals:	
48.48	Min 1Q Median 3Q Max	
	-2.41383 -0.36463 -0.04622 0.43338 2.00655	
49.43		
00	Coefficients: Estimate Std. Error t value Pr(> t )	
	(Intercept) 2.029e+01 2.627e+01 0.772 0.440011	
	fixed acidity 1,274e-02 3,228e-02 0,395 0,693151	
	volatile.acidity -1.096e+00 1.469e-01 -7.457 1.90e-13 ***	
	citric.acid -7.578e-02 1.804e-01 -0.420 0.674551	
	residual.sugar 5.006e-03 2.003e-02 0.250 0.802667	
	chlorides -2.295e+00 5.355e-01 -4.286 1.99e-05 ***	
	free.sulfur.dioxide 4.124e-03 2.683e-03 1.537 0.124532	
	total.sulfur.dioxide -3.055e-03 8.657e-04 -3.529 0.000437 ***	
	density -1.560e+01 2.681e+01 -0.582 0.560876 pH -5.412e-01 2.3090-01 -2.304 0.021404 *	
	pH -5.413e-01 2.349e-01 -2.304 0.021404 * sulphates 9.878e-01 1.473e-01 6.708 3.27e-11 ***	
	alcohol 2,692e-01 3,324e-02 8,099 1,57e-15 ***	
	Signif, codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1	
49.43		
	Residual standard error: 0.6344 on 1017 degrees of freedom	
	Multiple R-squared: 0.3834, Adjusted R-squared: 0.3767	
***	F-statistic: 57.49 on 11 and 1017 DF, p-value: < 2.2e-16	
49.42	Min, 1st Qu. Median Mean 3rd Qu. Max.	
11.12	4,708 5,342 5,640 5,674 6,028 6,751	

Figure 6: Classifying the Quality variable and creating a partition for data training and testing

From Figure 6, the output variable(quality) is only represented on the scale of 3,4,5,6,7,8. Majority of the data fell between 5 and 6. This is an unbalanced data. The data was partitioned into two. 20% was selected of the data for validation and the remaining 80% of data for training and testing the models.

It is clear that it failed the normal test. The algorithms were run using a-10-fold cross validation approach. This splits the dataset into ten different parts with nine for training and one for testing.

# VII. VISUALIZING THE OUTPUT DATA AND INPUT DATA



Figure 7: Histogram of the Quality of wine

I. Multivariate plots

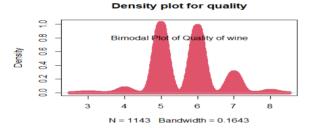


Figure 8: Density plot of quality

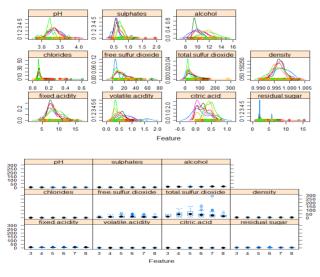
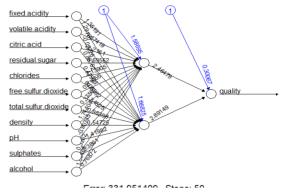


Figure 9 and 10: Feature plots of the dataset

# II. Neural Network

Using logistic neural network on the training dataset, we have the result as seen in figure 11 below. The predictions of the wine quality as determined by the features in the network.







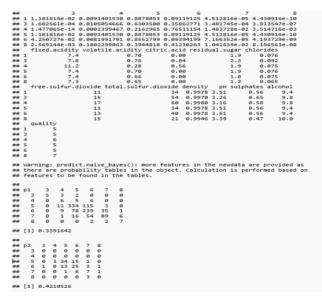
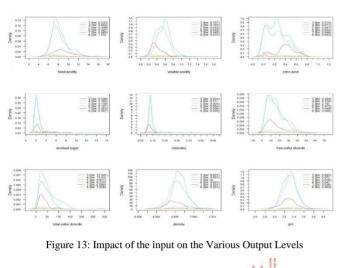


Figure 12: Naïve Bayes classification results

From above, the errors in classification are about 34% and 42%- This isn't good. Naïve Bayes classification couldn't produce the best classification because of this range of error.

### IV. Other models

From these results, it could be seen that alcohol, sulphates, fixed acidity and citric acid have the greatest impact on the quality of wine.



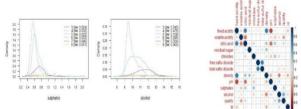


Figure 14: Impact of the inputs and their relationship with outputs

## Linear Discriminant Analysis
##
## 1030 samples
## 11 predictor
## 6 classes: '3', '4', '5', '6', '7', '8'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 927, 926, 927, 926, 927, 929, ...
## Summary of sample sizes: 927, 926, 927, 926, 927, 929, ...
##
Accuracy Kappa
## 0.5971743 0.3517683
## 0.5971743 ## CART ## ## 1030 samples ## 11 predicto ## 6 classes: ## 11 predictor 6 classes: '3', '4', '5', '6', '7', '8' No pre-processing Resampling: Cross-Validated (10 fold) Summary of sample sizes: 927, 926, 927, 926, 927, 929, ... Resampling results across tuning parameters: ## ## ## ## ## ## cp Accuracy Kappa 0.02013423 0.5475948 0.2438928 0.02265101 0.5514783 0.2465860 0.23657718 0.5318994 0.2016864 ## ## ## Accuracy was used to select the optimal model using the largest value. The final value used for the model was cp = 0.02265101. ## k-Nearest Neighbors ## ##
## 1030 samples
## 11 predictor
## 6 classes: '3', '4', '5', '6', '7', '8'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 927, 926, 927, 92 No pre-processing Resampling: Cross-Validated (10 fold) Summary of sample sizes: 927, 926, 927, 926, 927, 929, ... Resampling results across tuning parameters: ## ## ## ## k Accuracy Kappa 5 0.4855390 0.1673174 7 0.5068631 0.1896854 9 0.5096714 0.1914213 ## Accuracy was used to select the optimal model using the largest value. ## The final value used for the model was k = 9. ## Support Vector Machines with Radial Basis Function Kernel

## 1030 samples ## 11 predicts 11 predictor

Figure 15: Cross-validation results

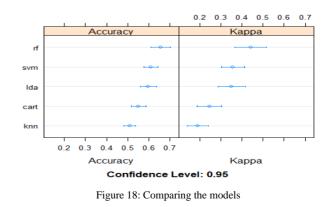
## ##	6 classes: '3', '4', '5', '6', '7', '8'
	No pre-processing
	Resampling: Cross-Validated (10 fold)
	Summary of sample sizes: 927, 926, 927, 926, 927, 929,
##	Resampling results across tuning parameters:
##	C Accuracy Kappa
##	0.25 0.5913012 0.3050919
## ##	0.50 0.6028875 0.3391112
##	1.00 0.6107495 0.3579503
##	Tuning parameter 'sigma' was held constant at a value of 0.09940508
	Accuracy was used to select the optimal model using the largest value.
##	The final values used for the model were sigma = $0.09940508$ and C = 1.
	Random Forest
##	1020 complex
##	1030 samples 11 predictor
##	6 classes: '3', '4', '5', '6', '7', '8'
##	No
	No pre-processing Resampling: Cross-Validated (10 fold)
	Summary of sample sizes: 927, 926, 927, 926, 927, 929,
	Resampling results across tuning parameters:
## ##	mtry Accuracy Kappa
##	2 0.6571082 0.4421066
##	6 0.6492928 0.4319499
## ##	11 0.6434863 0.4229817
	Accuracy was used to select the optimal model using the largest value.
	The final value used for the model was mtry = 2.
##	
##	Call:
	<pre>summary.resamples(object = results)</pre>
##	Models: lda, cart, knn, svm, rf
	Number of resamples: 10
##	
## ##	Accuracy Min. 1st Qu. Median Mean 3rd Qu. Max. NA's
	Ida 0.5096154 0.5686847 0.5922330 0.5971743 0.6393064 0.6732673 0
	cart 0.4851485 0.5048077 0.5679612 0.5514783 0.5834682 0.6213592 0
	knn 0.4368932 0.4879808 0.5168969 0.5096714 0.5406274 0.5533981 0
	svm 0.5384615 0.5926896 0.6019417 0.6107495 0.6502932 0.6826923 0 rf 0.5841584 0.5980209 0.6568298 0.6571082 0.6939180 0.7572816 0
##	11 0.3641364 0.3360203 0.0368236 0.0371662 0.0333186 0.7372610 0
	Kappa
##	Min. 1st Qu. Median Mean 3rd Qu. Max. NA's 1da 0.20048236 0.2982057 0.3533139 0.3517683 0.4233487 0.4707844 0
	cart 0.12144530 0.1860865 0.2669623 0.2465860 0.2924220 0.3809524 0
	knn 0.07751699 0.1535515 0.1996619 0.1914213 0.2508068 0.2654264 0
	Figure 16: Cross-validation results of other models

## svm 0.24346076 0.3255471 0.3409335 0.3579503 0.4240990 0.4764302 a ## rf 0.31624758 0.3495987 0.4393483 0.4421066 0.5004141 0.6031746 ۵

Figure 17: Ten-fold Cross-validation of SVM and RF

## V. Ten-fold Cross-validation

Linear Discriminant Analysis (LDA), Classification and Regression Trees (CART), k-Nearest Neighbors (kNN), Support Vector Machines (SVM) with a linear kernel, and Random Forest (RF) were considered as seen above, considering the accuracy level, Random Forest is said to be the best. Comparing these models, the confidence level is 95%. Random Forest is a form classification model, and it generates its output based on classified inputs. The training sets in this work was selected and classified to predict the feature that could enhance better quality of wine.



##	# Confusion Matrix and Statistics							
##								
##	Reference							
##	Prediction 3 4	56	78					
##	3 5 0	0 0	0 0					
##	4 0 31	0 0	0 0					
##	5 0 0 4	34 0	0 0					
##	600	0 416	0 0					
##	7 0 0	0 01	29 0					
##	8 0 0	0 0	0 15					
##								
##	Overall Statistics							
##								
##	Accur	acy : 1						
##	95%	CI : (0	.9964,	1)				
##	No Information Rate : 0.4214							
##	P-Value [Acc > N	IR] : <	2.2e-16					
##								
##	Ka	ppa : 1						
##								
##	Mcnemar's Test P-Va	lue : NA						
##								
	Statistics by Class:							
##								
##				: 4 Class: 5				
	Sensitivity	1.00000		000 1.0000				
	Specificity	1.00000		000 1.0000				
	Pos Pred Value	1.00000		000 1.0000				
	Neg Pred Value	1.00000		000 1.0000				
	Prevalence	0.00485		301 0.4214				
	Detection Rate	0.00485		301 0.4214				
	Detection Prevalence			301 0.4214				
##	Balanced Accuracy	1.00000	0 1.0	000 1.0000	1.0000	1.0000	1.00000	

#### Figure 19: Overall statistics

### VIII. CONCLUSION

The best classification model for this analysis is the Random Forest over the ten-fold classification. Based on the results, the accuracy of the wine quality prediction scores greatly hinges on alcohol level above others. Aside, this accuracy would significantly improve by not only increasing the amount of alcohol level but also the fixed acidity, citric acid, and sulfates. The amount of volatile acidity and chlorides should also be decreased because they contribute the least to the quality of the wine.

The main challenge with this work is that our data was unbalanced. The major values of quality of the wine data were between just the scores 5 and 6. This poses a difficulty in analyzing the plots due to overplotting. The machine learning models themselves could be enhanced for accuracy by using a larger dataset with a greater even distributions of wine quality scores. It's also discovered that R has easy to use model in the caret and psych package that researchers are encouraged to use in future works.

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