STAT 6340 Statistical Machine Learning

Mini Project 2

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February 25, 2021

1 Answers

Question 1.a We explored the correlations of our variables, both predictors and response on Figure 1. Visualizing the correlation matrix we can see that predictors Oakiness and Clarity have a very low correlation with Quality. We infer that these variables are not much relevant to predict Quality and are the most likely to be removed from future models. On the other hand predictors Aroma, Flavor and Region has a high correlation with Quality, making them good candidates for our models.
Another point to notice is that variable Body presents some correlation with Quality, although, it is not as high as other predictors, therefore we require further analysis to determine its relevance for the response variable. Finally, predictors Aroma, Body, Flavor and Region are highly correlated. This can cause overfitting issues, since the data would be over explained, so with further analysis one or some of this predictors might be dropped since they can be explained by other predictors.

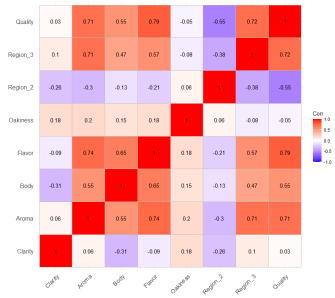

Figure 1: Correlation Matrix

Figure 2: Scatter Plots

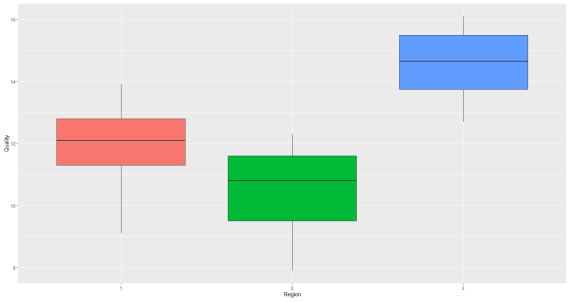

Figure 3: Quality by Region

We present the scatterplot of our variables on Figure 2. As expected from the correlation matrix we can notice that the predictors Aroma, Body and Flavor exhibit a positive linear relation with Quality. On Figure 3 we present the Quality boxplots by Region. Pay attention to the clear distribution of Quality by Region (high on 3, medium on 1, low on 2). This fact evidences the importance of this predictor for determining the Quality of a wine.

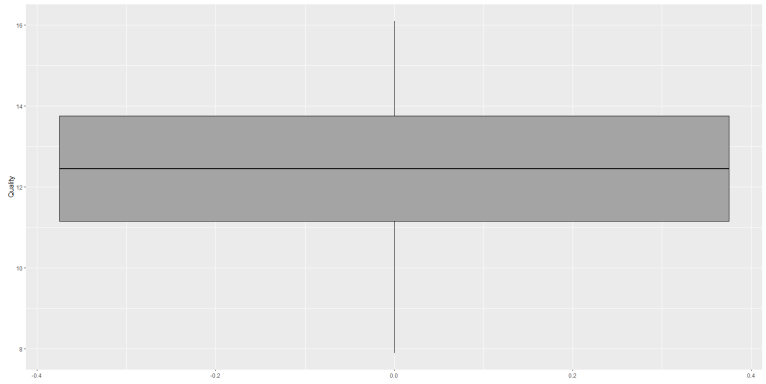

Figure 4: Quality Boxplot

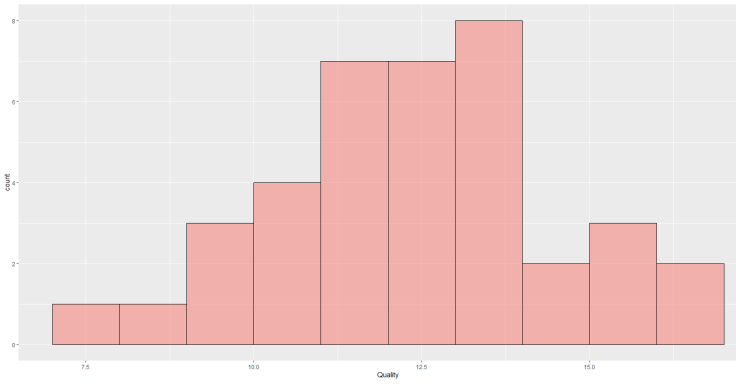

Figure 5: Quality Histogram

Question 1.b We explore the variable Quality using boxplots to identify possible outliers (Figure 4). We did not detect any outlier. We also explore the underlying distribution of Quality using histograms (Figure 5). We can appreciate that data distribution looks approximately normal. At this moment we consider that transformation is not required and we will check model assumptions once we build an appropriate model.

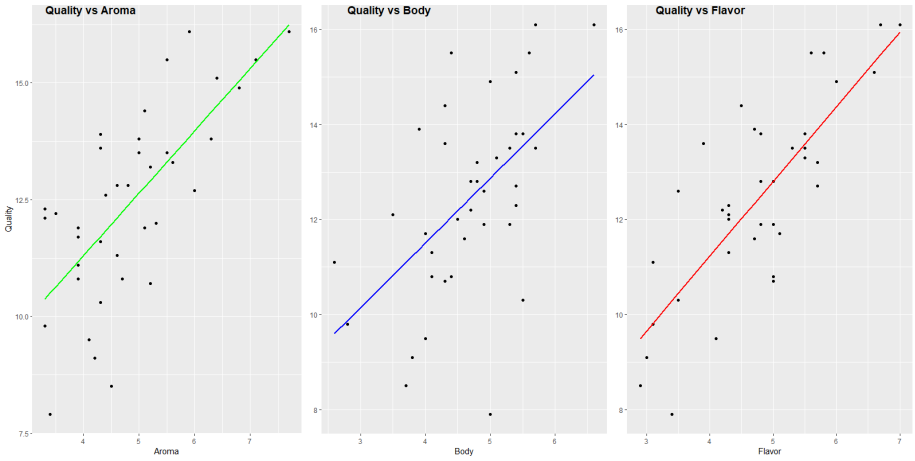

Figure 6: Quality vs Continuous Predictors

Question 1.c We fitted a simple linear regression model for every predictor (Tables 1 to 6). Taking a look to the p-values of every model we can affirm that there is a statistically significant association between the predictor and the response variable on all models except for the models with predictors Clarity (p-value = 0.865) and Oakiness (p-value = 0.779). This is consistent with our previous exploration. We can see on Figure 6 how there is a clear linear relation for predictors Flavor, Aroma and Body. Also we discussed on question 1.a how Region is relevant to predict Quality (Figure 3).

Table 1:

	Estimate	Pr(>|t|)
(Intercept)	12.0034	3.89e-5
Clarity	0.4692	0.865

Table 2:

	Estimate	Pr(>|t|)
(Intercept)	5.9583	4.51e-6
Aroma	1.3365	6.87e-7

Table 3:

	Estimate	Pr(>|t|)
(Intercept)	6.0580	0.0007
Body	1.3618	0.0004

Table 4:

	Estimate	Pr(>|t|)
(Intercept)	4.9414	1.57e-5
Flavor	1.5719	3.68e-9

Table 5:

	Estimate	Pr(>|t|)
(Intercept)	12.9916	1.4e-7
Oakiness	-0.1304	0.779

Table 6:

	Estimate	Pr(>|t|)
(Intercept)	11.9765	2e-16
Region2	-1.5320	0.00757
Region3	2.6069	7.01e-6

Question 1.d From the summary of the full model we can reject the null hypothesis for the Flavor and Region predictors, meaning that this predictors are relevant in order to predict Quality.

Table 7: Full Model

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	7.8144	1.9694	3.97	0.0004
Clarity	0.0171	1.4563	0.01	0.9907
Aroma	0.0890	0.2525	0.35	0.7269
Body	0.0797	0.2677	0.30	0.7681
Flavor	1.1172	0.2403	4.65	6.25e-5
Oakiness	-0.3464	0.2330	-1.49	0.1475
Region2	-1.5129	0.3923	-3.86	0.0006
Region3	0.9726	0.5102	1.91	0.0662

Table 8: Resulting Model

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	7.0943	0.7912	8.97	1.76e-10
Flavor	1.1155	0.1738	6.42	2.49e-07
Region2	-1.5335	0.3688	-4.16	0.0002
Region3	1.2234	0.4003	3.06	0.0043

Question 1.e To start building our model, we will proceed to drop one variable at a time from the full model until all predictors remaining are relevant for our response variable. Starting from the highest p-value predictor and rechecking the test hypothesis results for every new model. After this process we ended up with the model Quality ~Flavor + Region (Table 8) where all variables are . The anova test(Table 9) between the full model and the current model confirms our findings. With a p-value of 0.6528, we fail to reject the null hypothesis, this is all extra predictors are 0.
Now we will proceed to explore interactions between these two predictors. We will compare the model Quality ~Flavor + Region with the model Quality ~Fla-

Table 9: Anova with Full Model

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	34	27.21				
2	30	25.14	4	2.07	0.62	0.6528

Table 10: Anova vs Interactions

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	34	27.21				
2	32	25.43	2	1.78	1.12	0.3378

vor + Region + Flavor:Region. By carrying out an anova test we obtained a p-value of 0.3378, meaning that we fail to reject the null hypothesis, this is all additional predictors are 0. Therefore the interactions between Flavor and Region are not meaningful for our model.

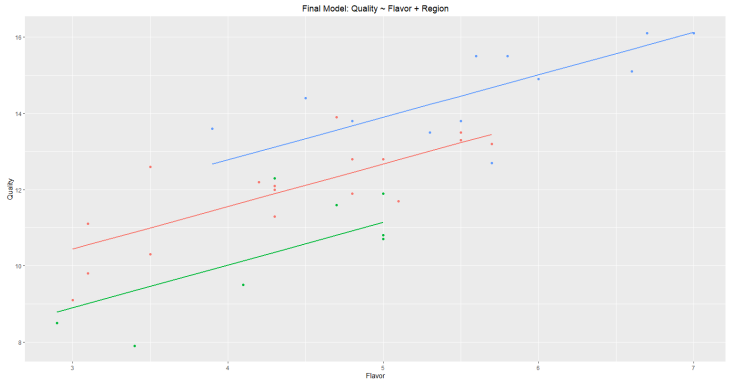

Figure 7: Final Model

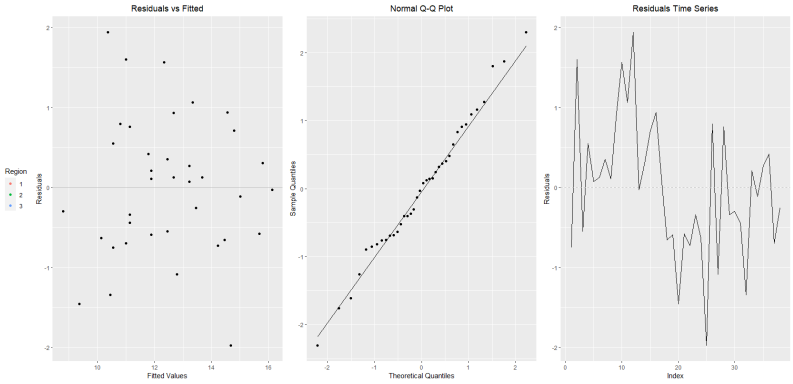

Figure 8: Model Assumptions

We can appreciate the three resulting regression lines of our model for each region on Figure 7. Clearly our model captures the linear trend on each region. Also we present several diagnostics plots on Figure 8 in order to check for model assumptions.
We can see in the Residuals vs Fitted plot how the points are scattered around zero and there is no a clear pattern, verifying that our errors have an approximate zero mean and constant variance. For the Q-Q Plot, observe how for an exception of a few points the errors are close to be normally distributed. Finally checking on the Residuals Time Series, there is not a clear dependence of the residuals, verifying the independence assumption.

Question 1.f Final model:
Quality = 7.0943 + 1.1155(Flavor) -1.53351$\mathbb{1}_{(Region2)}$ + 1.22341$\mathbb{1}_{(Region3)}$

Where $\mathbb{1}$ is an indicator function. We can interpret our model as follows: Approximately every level change in Flavor will directly change the Quality by one level. Region 1 wine has base quality of 7, Region 3 offers an additional level (quality base around 8) and Region 2 a decrease of 1.5 (quality base approximately of 5.5).

Question 1.g Our prediction of Quality for a wine from Region 1 with a mean Flavor is: 12.41371.
We obtained a 95% confidence interval of [11.95152, 12.8759], this is that given an average Flavor wine and assuming it is from Region 1, 95% of intervals of this form will contain the true value of the wine Quality.
Also we obtained a 95% prediction interval of [10.53775, 14.28967], meaning that we can be 95% confident that the Quality of an average Flavor wine from Region 1 will lie in this range.

Question 2.a On Figure 9 we present several plots to explore how the GMAT and GPA can help to predict the group of an applicant. We can observe in the graph of GMAT vs GPA, how the GPA predictor can clearly separate the

three groups. Moreover in the GPA boxplot we have a clear distribution of the GPA by group, evidence of how much this predictor contributes to identify the correct group. For the GMAT boxplot there is some confusion for applicants of group 2 and 3, but a clear distinction for applicants of group 1, meaning that GMAT also helps us characterizes the possible group of an applicant.

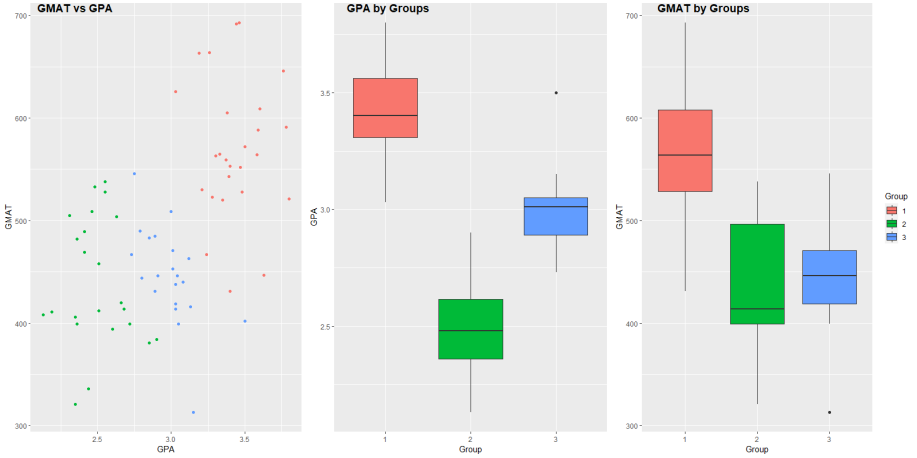

Figure 9:

Question 2.b We present the confusion matrix for training and testing sets on Tables 11 and 16 obtained from the LDA. The misclassification error rate for training set is around 8.5% while is 20% for testing set. We superimpose the decision boundary over the training data on Figure 10. We can notice how group 1 can be confused with group 2 and group 2 with group 3. The misclassification not only happens close to the decision boundary

Table 11: LDA Training

		Actual		
		1	2	3
	1	24	0	1
	2	0	21	1
Predicted	3	2	2	19

Class Error Rate: 0.08571

Table 12: LDA Testing

		Actual		
		1	2	3
	1	2	0	0
	2	0	5	0
Predicted	3	3	0	5

Class Error Rate: 0.2

Table 13: QDA Training

		Actual		
		1	2	3
	1	26	0	1
	2	0	22	0
Predicted	3	0	1	20

Class Error Rate: 0.02857

Table 14: QDA Testing

		Actual		
		1	2	3
	1	4	0	0
	2	0	5	0
Predicted	3	1	0	5

Class Error Rate: 0.06667

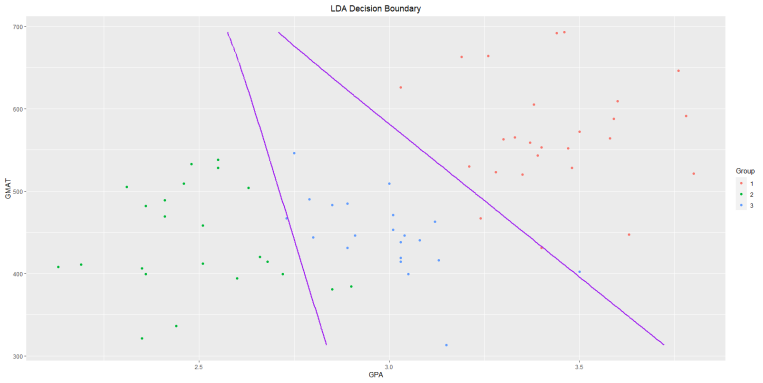

Figure 10: LDA Decision Boundary

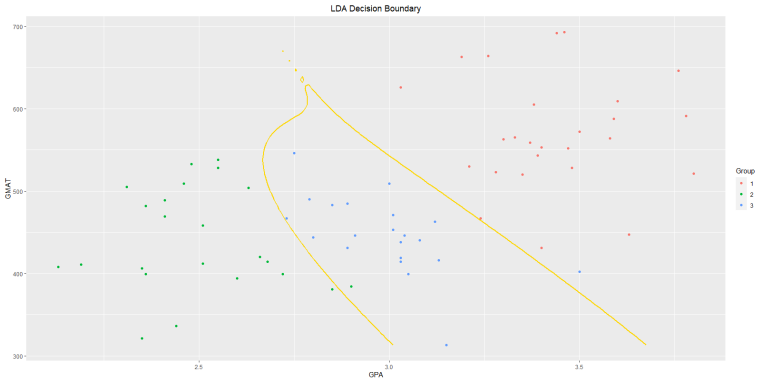

Figure 11: QDA Decision Boundary

Question 2.c We present the confusion matrix for training and testing sets on Tables 13 and 14 obtained from the QDA. The misclassification error rate for training set is around 2.8% and 6.7% for testing set. We superimpose the

decision boundary over the training data on Figure 11. We can see how QDA manage to correctly classify the challenging observations that LDA missed. The QDA decision boundary is less sensible that LDA's decision

Question 2.d We recommend QDA over LDA as the classifier for our data. We observe QDA manage to correctly classify the challenging observations that LDA missed. Also QDA offered us a less sensible decision boundary than LDA.

Question 3.a The data is unbalanced having 1316 observations labelled as 0(non diabetic) and 684 as 1(diabetic). This fact can cause that classification algorithms may have a high accuracy but a low sensitivity (setting 1 as the positive response). We explored several boxplots to investigate how our predictors affect the classes (Figure 12, Figure 13). Predictors Glucose and Age separates the two classes in some degree (Figure 14)

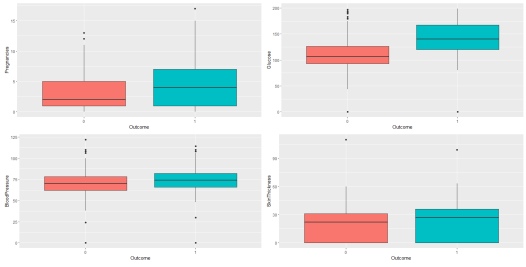

Figure 12: Pregnancies, Glucose, BP, SkinThickness

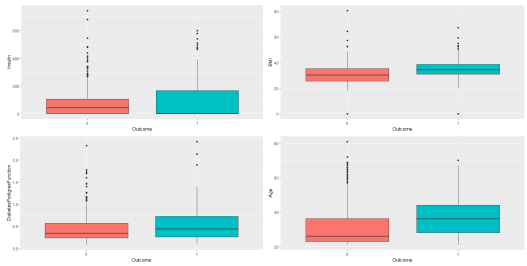

Figure 13: Insulin, BMI, DPF, Age

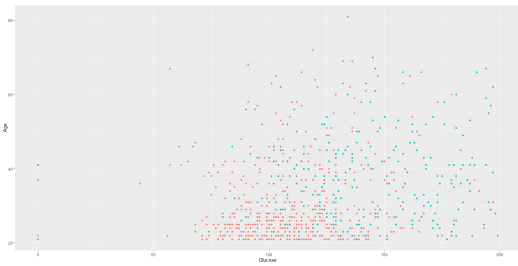

Figure 14: Age vs Glucose

Question 3.b and Question 3.c
Perform an LDA of the data. Compute the confusion matrix, sensitivity, speci city, and overall misclassi
cation rate based on 0.5 cutoff for the posterior probability. Plot the ROC curve. What do you observe

Table 15: LDA Classifier

		Actual 0	Actual 1
Predicted	0	1174	298
	1	142	386

Table 16: QDA Classifier

		Actual 0	Actual 1
Predicted	0	1135	290
	1	181	394

Table 17:

	Error.Rate	Sensitivity	Specificity
LDA	0.22	0.5643275	0.8920973
QDA	0.2355	0.5760234	0.8624620

Question 3.d
From our previous analysis we recommend the use of the LDA classifier. We want to improve our Sensitivity without sacrifying as much Specificity and overall accuracy. So we decided to find a cutoff of the best trade-off between Sensitivity and Specificity using Youden's J statistic, this is the cutoff that offers the maximum value for J = sensitivity + specificity - 1.

2 Code