STAT6020_PredictiveAnalytics_Assignment2 Prepared by Tim Virga

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We are interested in developing a tool that can classify wines into one of the three types based on the other variables provided.

Linear and Quadratic Discriminant Analysis

```
library (MASS)
# reading in the data
wine = read.csv("wine.csv")
# selecting numeric variables
wine_numpred = c("ash", "ash_alkalinity", "nonflav_phenols", "proanth")
class = wine[, "vintage"]
# numeric variables and class
pre_and_class = wine[, c(wine_numpred, "vintage")]
```

1. LDA

```
# Training and prediction
lda.fit = lda(vintage~., data=pre_and_class, CV=TRUE)
ldapred_class = lda.fit$class
# Confusion matrix
cfmatrix = table(ldapred_class, class)
# Accuracy divides TN and TP against sum of samples
accuracy = sum(diag(cfmatrix))/sum(cfmatrix)
error = 1-accuracy
print(error)

## [1] 0.2542373

print(accuracy)

## [1] 0.7457627

show(cfmatrix)
```

```
## class
## ldapred_class A B C
## A 31 1 16
## B 1 53 7
## C 16 4 48
```

After fitting a LDA model using numerical variables as predictors for class=vintage we observe a 25.4% error rate and 74.6% accuracy rate. Noting in the confusion matrix what class values the LDA model has incorrectly classified.

2. QDA

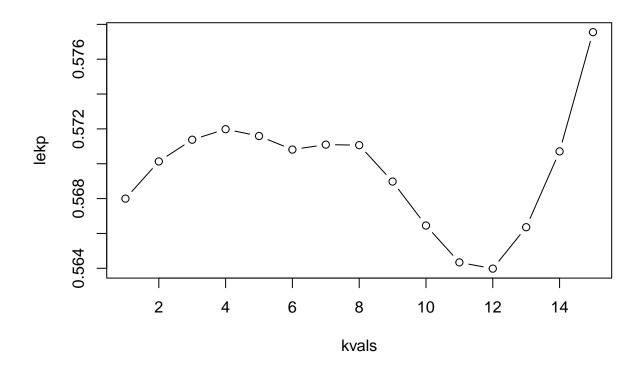
```
# Training and prediction
qda.fit = qda(vintage~., data=pre_and_class, CV=TRUE)
qdapred_class = qda.fit$class
accuracy = sum(diag(cfmatrix))/sum(cfmatrix)
error = 1-accuracy
print(error)
## [1] 0.2542373
print(accuracy)
## [1] 0.7457627
cfmatrix = table(qdapred_class, class)
show(cfmatrix)
##
                class
## qdapred_class A B C
##
               A 36
##
               В
                 1 50 8
               C 11 8 46
##
```

After fitting a QDA model using numerical variables as predictors for class=vintage we observe a 25.4% error rate and 74.6% accuracy rate. Noting in the confusion matrix what class values the LDA model has incorrectly classified. Interestingly, the accuracy of the model appears to be identical however, it's obvious from the confusion matrix that the QDA model has predicted different different values for classification than LDA. It's unclear whether the data set exhibits a more favourable linear, or quadratic spread of data- where the analyst may want to then consider the simpler model.

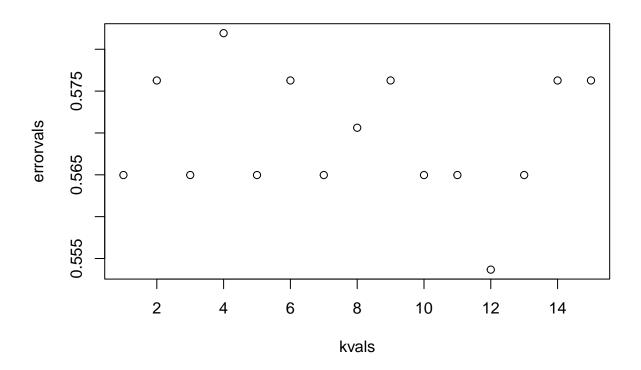
K Nearest Neighbours

3.

```
library(class)
# predictors (numeric only):
numeric_predictors = c("ash", "ash_alkalinity", "nonflav_phenols", "proanth")
# class labels
class = wine[,"vintage"]
Predictors = wine[, numeric_predictors]
# storing some values from the loop iterations
kvals = c()
errorvals = c()
accuracyvals = c()
\# performing a loop to evaluate \mathit{K=n} models
for (K in c(1:15)) {
  predicted_class = knn.cv(train=Predictors, cl=class, k=K) #associate the k=K class
  cm = table(predicted_class, class)
  accuracy = (cm[1,1]+cm[2,2])/sum(cm)
  error = 1 - accuracy
  kvals[K] = K
  errorvals[K] = error
 accuracyvals[K] = accuracy
  }
lek = loess(errorvals~kvals)
lekp = predict(lek)
plot(kvals, lekp, type="b")
```



plot(errorvals~kvals)



```
\# specify the k=n best performing K value to predict with most accuracy
predicted_class = knn.cv(train=Predictors, cl=class, k=12)
  cm = table(predicted_class, class)
  accuracy = (cm[1,1]+cm[2,2])/sum(cm)
  error = 1 - accuracy
  print(error)
## [1] 0.5649718
 print(accuracy)
## [1] 0.4350282
 print(cm)
##
                  class
## predicted_class A B C
##
                 A 33 2 19
                 B 2 44 16
##
```

We have designed a KNN (LOOCV) model with a loop of n=15. After fitting the model using numerical variables as predictors for class=vintage we observe that an optimal value for k is k=12 in the first chunk.

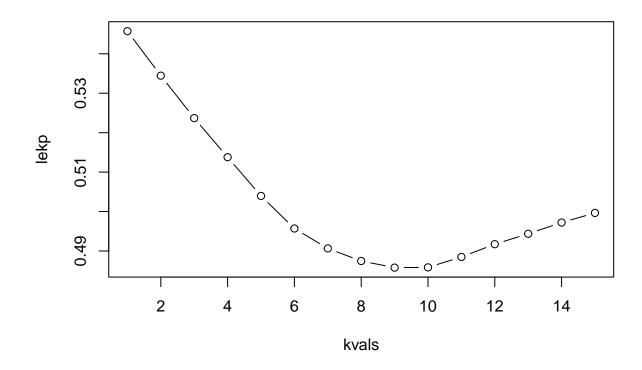
##

C 13 12 36

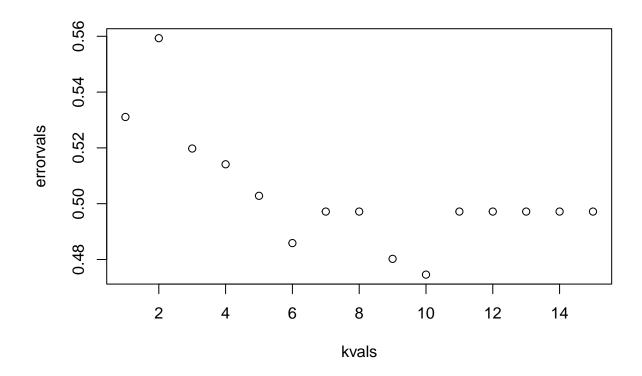
Separately, in the following chunk we recomputed the code with an optimal kvalue k=12 and observed an error rate of approximately 55% and an accuracy rate of approximately 45%. Noting in the confusion matrix what class values the LDA model has incorrectly classified. The KNN model is a non-parametric approach to classification that performs well for complex decision boundaries. Given the KNN (LOOCV) model has performed significantly worse than the QDA and LDA models, we can speculate that the true decision boundaries may be more linear.

4.

```
# predictors (numeric only):
numeric_predictors = c("ash", "ash_alkalinity", "nonflav_phenols", "proanth")
# class labels
class = wine[,"vintage"]
Predictors = wine[, numeric_predictors]
# scaling the predictors
Predictors = scale(Predictors)
kvals = c()
errorvals = c()
accuracyvals = c()
for (K in c(1:15)) {
  predicted_class = knn.cv(train=Predictors, cl=class, k=K) #associate the k=K class
  cm = table(predicted_class, class)
  accuracy = (cm[1,1]+cm[2,2])/sum(cm)
  error = 1 - accuracy
  kvals[K] = K
  errorvals[K] = error
  accuracyvals[K] = accuracy
 }
lek = loess(errorvals~kvals)
lekp = predict(lek)
plot(kvals, lekp, type="b")
```



plot(errorvals~kvals)



```
predicted_class = knn.cv(train=Predictors, cl=class, k=10)
cm = table(predicted_class, class)
accuracy = (cm[1,1]+cm[2,2])/sum(cm)
error = 1 - accuracy
print(error)

## [1] 0.4858757
print(accuracy)
```

```
## [1] 0.5141243
```

```
print(cm)
```

We have designed a KNN (LOOCV) model with a loop of n=15. After fitting the model using numerical variables as predictors for class=vintage and scaling the predictor variables, we observe that an optimal value for k is k=10. This is a value lower than the previous KNN (LOOCV) model without scaling, suggesting the

data without predictors scaled featured skewed predictor variable values. In the process of standardisation, we observe that the scale of values for "ash" and "proanth" to be similar. We can expect scaling to have introduced an increased influence on the model for predictor "nonflav_phenols" which was structured on a lower value scale and a reduced influence on the model for "ash_alkalinity" which was originally structured on a higher value scale.

Naive Bayes

5.

```
library(naivebayes)
## naivebayes 0.9.7 loaded
no_obs <- dim(pre_and_class)[1] # dataset size</pre>
Pred_class <- rep("", no_obs)</pre>
# LOOCV using loop less the one observation per loop:
for (i in 1:no_obs){
# fitting the naive bayes model
NB.fit <- naive_bayes(vintage ~., data = pre_and_class[-i, ])</pre>
# Predict the leftover:
Pred_class_test <- predict(NB.fit, newdata = pre_and_class[i,], type = "class")</pre>
Pred_class[i] <- as.character(Pred_class_test)</pre>
nbcm <- table(Pred_class, class)</pre>
accuracy <- sum(diag(nbcm))/sum(nbcm)</pre>
error <- 1 - accuracy
print(error)
## [1] 0.2824859
print(accuracy)
## [1] 0.7175141
print(nbcm)
##
              class
## Pred_class A B C
            A 38 1 21
##
            B 0 50 11
##
            C 10 7 39
```

After fitting a Naive Bayes Classifier model with a LOOCV loop across the total number of observations, using numerical variables as predictors for class=vintage, we observe a 28.2% error rate and 71.8% accuracy rate. Noting in the confusion matrix what class values the LDA model has incorrectly classified. Naive Bayes Classifer models the probability of a class using Baye's Rule making the assumption the features are independent. For our numeric predictors, this has not proven to be more effective than QDA and LDA models.

6.

```
library(naivebayes)
pre_and_class_col = wine[, c(wine_numpred, "colour", "vintage")]
no_obs <- dim(pre_and_class_col)[1]</pre>
Pred_class <- rep("", no_obs)</pre>
for (i in 1:no_obs){
# set laplace smoothing to 1
NB.fit <- naive_bayes(vintage ~., data = pre_and_class_col[-i, ], laplace=1)
Pred_class_test <- predict(NB.fit, newdata = pre_and_class_col[i, ], type = "class")</pre>
Pred_class[i] <- as.character(Pred_class_test)</pre>
}
nbcm <- table(Pred_class, class)</pre>
accuracy <- sum(diag(nbcm))/sum(nbcm)</pre>
error <- 1 - accuracy
print(error)
## [1] 0.180791
print(accuracy)
## [1] 0.819209
print(nbcm)
##
             class
## Pred_class A B C
##
            A 43
                   2 8
##
            B 0 46 7
            C 5 10 56
##
```

After fitting a Naive Bayes Classifier model with a LOOCV loop across the total number of observations, using numeric variables and categorical variable "Colour" as predictors for class=vintage, we observe an 18.1% error rate an 81.9% accuracy rate. The Naive Bayes Classifier model different to LDA & QDA can be modeled using categorical variables because of the assumptions made for independent variables. We observe the inclusion of just 1 categorical predictor "Colour" improve the performance of our model to perform better than QDA and LDA.

7.

```
library(naivebayes)
no_obs <- dim(wine)[1]</pre>
Pred_class <- rep("", no_obs)</pre>
for (i in 1:no_obs){
# fit all wine data with laplace smoothing
NB.fit <- naive_bayes(vintage ~., data = wine[-i, ], laplace=1)</pre>
Pred_class_test <- predict(NB.fit, newdata = wine[i, ], type = "class")</pre>
Pred_class[i] <- as.character(Pred_class_test)</pre>
}
nbcm <- table(Pred_class, class)</pre>
accuracy <- sum(diag(nbcm))/sum(nbcm)</pre>
error <- 1 - accuracy
print(error)
## [1] 0.1242938
print(accuracy)
## [1] 0.8757062
print(nbcm)
##
              class
## Pred_class A B C
##
            A 43 1 6
            B 0 50 3
##
            C 5 7 62
##
```

After fitting a Naive Bayes Classifier model with a LOOCV loop across the total number of observations, using all variables as predictors for class=vintage and a Laplace smoothing laplace=1, we observe a 12.4% error rate an 87.6% accuracy rate. Concluding this Naive Bayes (LOOCV) model to be the most accurate model out of those computed.

```
NB.fit$call
## naive_bayes.formula(formula = vintage ~ ., data = wine[-i, ],
## laplace = 1)

NB.fit$prior
##
## A B C
## 0.2670455 0.3295455 0.4034091
```

```
tables(NB.fit,)
```

```
##
 ::: ash (Gaussian)
##
## ash
     A B
##
  mean 2.4306383 2.4560345 2.2447887
  sd 0.1811486 0.2291245 0.3154673
##
## -----
 ::: ash alkalinity (Gaussian)
##
## ash_alkalinity A
                 В
  mean 21.351064 17.062069 20.238028
       sd 2.235861 2.561375 3.349770
##
##
## -----
## ::: magnesium (Gaussian)
## -----
##
## magnesium A B
    mean 99.38298 105.98276 94.54930
    sd 10.99714 10.22465 16.75350
##
##
## -----
## ::: nonflav_phenols (Gaussian)
##
## nonflav_phenols
               Α
   mean 0.44510638 0.29017241 0.36366197
##
##
        sd 0.12435700 0.07064841 0.12396128
##
## -----
## ::: proanth (Gaussian)
##
## proanth A
               В
   mean 1.1493617 1.8925862 1.6302817
##
   sd 0.4122178 0.4124193 0.6020678
##
##
 ::: colour (Categorical)
## ------
##
              В
## colour
         Α
  col1 0.21568627 0.06451613 0.42666667
##
  col2 0.74509804 0.20967742 0.04000000
##
  col3 0.01960784 0.43548387 0.02666667
##
  col4 0.01960784 0.29032258 0.50666667
##
```

$$P(Y = A, B, C)$$

$$P(X_{colour} = col1|Y)$$

```
# no_obs of class A
col1_pred_A = nrow(wine[which (wine$colour=='col1' & wine$vintage=='A'),])
# priors
vin_A = nrow(wine[which (wine$vintage=='A'),])
col1_pred_A_P = col1_pred_A / vin_A
# no_obs of class B
col1_pred_B = nrow(wine[which (wine$colour=='col1' & wine$vintage=='B'),])
# priors
vin_B = nrow(wine[which (wine$vintage=='B'),])
col1_pred_B_P = col1_pred_B / vin_B
# no_obs of class C
col1_pred_C = nrow(wine[which (wine$colour=='col1' & wine$vintage=='C'),])
# priors
vin_C = nrow(wine[which (wine$vintage=='C'),])
col1_pred_C_P = col1_pred_C / vin_C
print(col1_pred_A_P)
## [1] 0.2083333
print(col1_pred_B_P)
## [1] 0.05172414
print(col1_pred_C_P)
```

[1] 0.4366197

By taking the total observations where colour=col1 and vintage classes were either A, B or C respectively, then dividing colour+class observations by the total number of observations for each respective class, we are able to obtain the estimated probabilities for each of the classes given that colour is col1.