Classification

S.Tonini, F. Chiaromonte (special thanks to J. Di Iorio and L. Insolia)

February 14th 2024

Contents

Introduction

Libraries

We are going to use:

- **tidyverse**: *Easily Install and Load the 'Tidyverse'*
- **caret**: *Classification and Regression Training*
- **MASS**: *Support Functions and Datasets for Venables and Ripley's MASS*
- **ggplot2**: *Create Elegant Data Visualisations Using the Grammar of Graphics*
- **readxl**: *Read Excel Files*

```
library(tidyverse)  # for data manipulation and visualization
library(caret)      # for statistical learning techniques
library(MASS)       # for AIC based stepwise regression
library(ggplot2)    # for plots
library(klaR)       # for LDA and QDA partition
library(readxl)     # for reading xlsx files
```

Data

Today we are going to use the **Titanic** data set.
It contains 1309 rows and 15 columns. Each row represents a passenger and the columns describe some of their attributes.

```r
df <- read_excel("Titanic.xlsx")
head(df, 10)
```

```
## # A tibble: 10 x 15
##    pclass survived Residence name    age sibsp parch ticket  fare cabin embarked
##     <dbl>    <dbl>     <dbl> <chr> <dbl> <dbl> <dbl> <chr>  <dbl> <chr> <chr>
##  1      3        0         0 Abbi~    42     0     0 C.A. ~  7.55 <NA>  S
##  2      3        0         0 Abbo~    13     0     2 C.A. ~ 20.2  <NA>  S
##  3      3        0         0 Abbo~    16     1     1 C.A. ~ 20.2  <NA>  S
##  4      3        1         0 Abbo~    35     1     1 C.A. ~ 20.2  <NA>  S
##  5      3        1         2 Abel~    16     0     0 348125  7.65 <NA>  S
##  6      3        1         0 Abel~    25     0     0 348122  7.65 F G63 S
##  7      2        0         2 Abel~    30     1     0 P/PP ~ 24    <NA>  C
##  8      2        1         2 Abel~    28     1     0 P/PP ~ 24    <NA>  C
##  9      3        1         2 Abra~    20     0     0 SOTON~  7.92 <NA>  S
## 10      3        1         2 Abra~    18     0     0 2657    7.23 <NA>  C
## # i 4 more variables: boat <chr>, body <dbl>, home.dest <chr>, Gender <dbl>
```

Let's see the internal data structure.

```r
str(df)
```

```
## tibble [1,309 x 15] (S3: tbl_df/tbl/data.frame)
##  $ pclass   : num [1:1309] 3 3 3 3 3 3 2 2 3 3 ...
##  $ survived : num [1:1309] 0 0 0 1 1 1 0 1 1 1 ...
##  $ Residence: num [1:1309] 0 0 0 0 2 0 2 2 2 2 ...
##  $ name     : chr [1:1309] "Abbing, Mr. Anthony" "Abbott, Master. Eugene Joseph" "Abbott, Mr. Rossmo
##  $ age      : num [1:1309] 42 13 16 35 16 25 30 28 20 18 ...
##  $ sibsp    : num [1:1309] 0 0 1 1 0 0 1 1 0 0 ...
##  $ parch    : num [1:1309] 0 2 1 1 0 0 0 0 0 0 ...
##  $ ticket   : chr [1:1309] "C.A. 5547" "C.A. 2673" "C.A. 2673" "C.A. 2673" ...
##  $ fare     : num [1:1309] 7.55 20.25 20.25 20.25 7.65 ...
##  $ cabin    : chr [1:1309] NA NA NA NA ...
##  $ embarked : chr [1:1309] "S" "S" "S" "S" ...
##  $ boat     : chr [1:1309] NA NA NA "A" ...
##  $ body     : num [1:1309] NA NA 190 NA NA NA NA NA NA NA ...
##  $ home.dest: chr [1:1309] NA "East Providence, RI" "East Providence, RI" "East Providence, RI" ...
##  $ Gender   : num [1:1309] 0 0 0 1 1 0 0 1 0 1 ...
```

The type of some variables is not the optimal one (e.g., gender as a numeric variable). We can change these through the **mutate** function in **dplyr**.

```r
df <- df %>%
  dplyr::mutate(across(c(pclass, survived,       # select features
                Residence, body, Gender),
                factor))                         # transform to factor

# this is the traditional approach through base R
# df$pclass     <- as.factor(df$pclass)
# df$survived   <- as.factor(df$survived)
# df$Residence  <- as.factor(df$Residence)
# df$body       <- as.factor(df$body)
# df$Gender     <- as.factor(df$Gender)
```

According to the column type, the function **summary** provides some summary statistics for each variable.

```
summary(df)
```

```
##  pclass  survived Residence     name                age
##  1:323   0:809    0:258     Length:1309        Min.   : 0.1667
##  2:277   1:500    1:302     Class :character   1st Qu.:21.0000
##  3:709            2:749     Mode  :character   Median :28.0000
##                                                Mean   :29.8811
##                                                3rd Qu.:39.0000
##                                                Max.   :80.0000
##                                                NA's   :263
##      sibsp            parch          ticket               fare
##  Min.   :0.0000   Min.   :0.000   Length:1309        Min.   :  0.000
##  1st Qu.:0.0000   1st Qu.:0.000   Class :character   1st Qu.:  7.896
##  Median :0.0000   Median :0.000   Mode  :character   Median : 14.454
##  Mean   :0.4989   Mean   :0.385                      Mean   : 33.295
##  3rd Qu.:1.0000   3rd Qu.:0.000                      3rd Qu.: 31.275
##  Max.   :8.0000   Max.   :9.000                      Max.   :512.329
##                                                     NA's   :1
##     cabin             embarked            boat                body
##  Length:1309        Length:1309        Length:1309        1      :   1
##  Class :character   Class :character   Class :character   4      :   1
##  Mode  :character   Mode  :character   Mode  :character   7      :   1
##                                                           9      :   1
##                                                           14     :   1
##                                                           (Other): 116
##                                                           NA's   :1188
##   home.dest         Gender
##  Length:1309        0:843
##  Class :character   1:466
##  Mode  :character
##
##
##
##
```

Now, we drop the columns having more than 50 percent of NAs, as well as the ones that will not be useful for our analysis.

We also drop all those rows without age information.

```
# selecting columns
df <- df %>%
  dplyr::select(-c(name,ticket, fare, cabin,
                   embarked, boat, body, home.dest))

# filtering out rows
df <- df %>% filter(!is.na(age))

# our "final" dataset
dim(df)
```

```
## [1] 1046    7
```

```
summary(df)
```

```
##  pclass  survived Residence      age              sibsp            parch
```

```
##  1:284   0:619    0:232     Min.   : 0.1667   Min.   :0.0000   Min.   :0.0000
##  2:261   1:427    1:248     1st Qu.:21.0000   1st Qu.:0.0000   1st Qu.:0.0000
##  3:501             2:566     Median :28.0000   Median :0.0000   Median :0.0000
##                              Mean   :29.8811   Mean   :0.5029   Mean   :0.4207
##                              3rd Qu.:39.0000   3rd Qu.:1.0000   3rd Qu.:1.0000
##                              Max.   :80.0000   Max.   :8.0000   Max.   :6.0000
##  Gender
##  0:658
##  1:388
##
##
##
##
```

Logistic Regression

To assess prediction accuracy, we split the data into training and testing sets (at random, with no replacement). These encompass 75 and 25 percent of the points, respectively.

```
set.seed(123)
# set.seed(1)               # try to re-run the analysis with this
training_samples <- df$survived %>%
  caret::createDataPartition(p = 0.75, list = FALSE)

train <- df[training_samples, ]
test  <- df[-training_samples, ]
```

Simple Logistic Regression

Using the training set, we build a simple logistic regression model using sex as the only explanatory variable of the survival status for each passenger.

```
simple_glm <- glm(survived ~ Gender,
                  data = train, family = 'binomial')
summary(simple_glm)
```

```
##
## Call:
## glm(formula = survived ~ Gender, family = "binomial", data = train)
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -1.3211     0.1109  -11.91   <2e-16 ***
## Gender1       2.3362     0.1719   13.59   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 1063.10  on 785  degrees of freedom
## Residual deviance:  847.53  on 784  degrees of freedom
## AIC: 851.53
##
## Number of Fisher Scoring iterations: 4
```

You can extract various inforation from the output object `simple_glm`, such as the regression coefficients:

```
simple_glm$coefficients
```

```
## (Intercept)     Gender1
##   -1.321108    2.336156
```

Our model is $log(\frac{p(x)}{1-p(x)}) = \beta_0 + \beta_1 Gender$, where $\beta_0 = Intercept$ and $\beta_1 = Gender1$. Therefore, $log(\frac{p(x)}{1-p(x)}) = Intercept + Gender1 \times Gender$.

Let's see predictive power of our model in terms of *accuracy* – i.e. the proportion of correct predictions, both true positives and true negatives, among the total number of cases examined.

Since our response (Survival) is a binary variable, we need to round the probabilities which are predicted by the logistic model.

```
# Test for accuracy: predict test data
predict_sex_survived <- predict(simple_glm, newdata = test,type = 'response')

# round up the predictions
predict_sex_survived <- ifelse(predict_sex_survived>0.5, 1, 0)

# calculate accuracy
accuracyRed <- mean(predict_sex_survived==test$survived)
accuracyRed
```

```
## [1] 0.8115385
```

Our result is "pretty good" and it is also consistent with the "women and children first" code of conduct/policy (you can find more details on Wikipedia).

Multiple Logistic Regression – Stepwise selection

We may try to improve predictive power by including more features into the model. Let us start with the full/saturated model (i.e., the one comprising all features).

```
glm_complete <- glm(survived ~ ., data=train, family = 'binomial')
summary(glm_complete)
```

```
##
## Call:
## glm(formula = survived ~ ., family = "binomial", data = train)
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)  1.638344   0.390539   4.195 2.73e-05 ***
## pclass2     -1.177714   0.291066  -4.046 5.21e-05 ***
## pclass3     -2.372486   0.296672  -7.997 1.27e-15 ***
## Residence1  -0.483365   0.307982  -1.569  0.11654
## Residence2  -0.125636   0.271809  -0.462  0.64392
## age         -0.044028   0.007677  -5.735 9.74e-09 ***
## sibsp       -0.384458   0.118970  -3.232  0.00123 **
## parch        0.145025   0.109662   1.322  0.18601
## Gender1      2.428404   0.199612  12.166  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
```

```
##
##     Null deviance: 1063.10  on 785  degrees of freedom
## Residual deviance:  729.57  on 777  degrees of freedom
## AIC: 747.57
##
## Number of Fisher Scoring iterations: 5
```

Let's see its predictive accuracy. Has it improved?

```
# Test for accuracy: predict test data
predict_sex_survived <- predict(glm_complete, newdata = test,type = 'response')

# round up the predictions
predict_sex_survived <- ifelse(predict_sex_survived>0.5, 1, 0)

# calculate accuracy
accuracySat <- mean(predict_sex_survived==test$survived)
accuracySat
```

```
## [1] 0.8
```

```
confusionMatrix(as.factor(predict_sex_survived), test$survived)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 132  30
##          1  22  76
##
##                Accuracy : 0.8
##                  95% CI : (0.7461, 0.8469)
##     No Information Rate : 0.5923
##     P-Value [Acc > NIR] : 8.187e-13
##
##                   Kappa : 0.581
##
##  Mcnemar's Test P-Value : 0.3317
##
##             Sensitivity : 0.8571
##             Specificity : 0.7170
##          Pos Pred Value : 0.8148
##          Neg Pred Value : 0.7755
##              Prevalence : 0.5923
##          Detection Rate : 0.5077
##    Detection Prevalence : 0.6231
##       Balanced Accuracy : 0.7871
##
##        'Positive' Class : 0
##
```

Moreover, we notice that some features result as non-significant according to their p-values (last column of the previous table). We can select "relevant" predictors through stepwise regression, and then compute an information criterion such as AIC to compare different sub-models and pick the "best" one (e.g. minimizing the AIC).

```r
glm_stepwise <- glm_complete %>%
  MASS::stepAIC(direction='both', trace = T)
```

```
## Start:  AIC=747.57
## survived ~ pclass + Residence + age + sibsp + parch + Gender
##
##             Df Deviance    AIC
## - Residence  2   732.48 746.48
## - parch      1   731.31 747.31
## <none>           729.57 747.57
## - sibsp      1   741.04 757.04
## - age        1   766.10 782.10
## - pclass     2   804.71 818.71
## - Gender     1   907.90 923.90
##
## Step:  AIC=746.48
## survived ~ pclass + age + sibsp + parch + Gender
##
##             Df Deviance    AIC
## - parch      1   734.08 746.08
## <none>           732.48 746.48
## + Residence  2   729.57 747.57
## - sibsp      1   744.58 756.58
## - age        1   770.62 782.62
## - pclass     2   836.37 846.37
## - Gender     1   916.05 928.05
##
## Step:  AIC=746.08
## survived ~ pclass + age + sibsp + Gender
##
##             Df Deviance    AIC
## <none>           734.08 746.08
## + parch      1   732.48 746.48
## + Residence  2   731.31 747.31
## - sibsp      1   744.61 754.61
## - age        1   773.15 783.15
## - pclass     2   837.71 845.71
## - Gender     1   932.11 942.11
```

```r
summary(glm_stepwise)
```

```
##
## Call:
## glm(formula = survived ~ pclass + age + sibsp + Gender, family = "binomial",
##     data = train)
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)  1.619044   0.364356   4.444 8.85e-06 ***
## pclass2     -1.383870   0.263438  -5.253 1.50e-07 ***
## pclass3     -2.469957   0.264871  -9.325  < 2e-16 ***
## age         -0.045191   0.007606  -5.942 2.82e-09 ***
## sibsp       -0.346727   0.111916  -3.098  0.00195 **
## Gender1      2.496307   0.196409  12.710  < 2e-16 ***
```

```
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 1063.10  on 785  degrees of freedom
## Residual deviance:  734.08  on 780  degrees of freedom
## AIC: 746.08
##
## Number of Fisher Scoring iterations: 4
```

A comparison of the simple, saturated and the selected model using AIC indicate that the latter is a good compromise between the two. It should have a "comparable" predictive power but a lower complexity compared to the saturated one.

```
AIC(simple_glm, glm_complete, glm_stepwise)
```

```
##              df      AIC
## simple_glm    2 851.5342
## glm_complete  9 747.5722
## glm_stepwise  6 746.0796
```

Using the selected model, we compute again the probability for survival on the test set, and the overall prediction accuracy.

```
predict_sex_survived <- predict(glm_stepwise, newdata = test,type = 'response')

predict_sex_survived <- ifelse(predict_sex_survived>0.5, 1, 0)

accuracy <- mean(predict_sex_survived==test$survived)
accuracy
```

```
## [1] 0.8038462
```

We can create also a confusion matrix (and statistics) to compare our predictions for the test set.

```
confusionMatrix(as.factor(predict_sex_survived), test$survived)
```

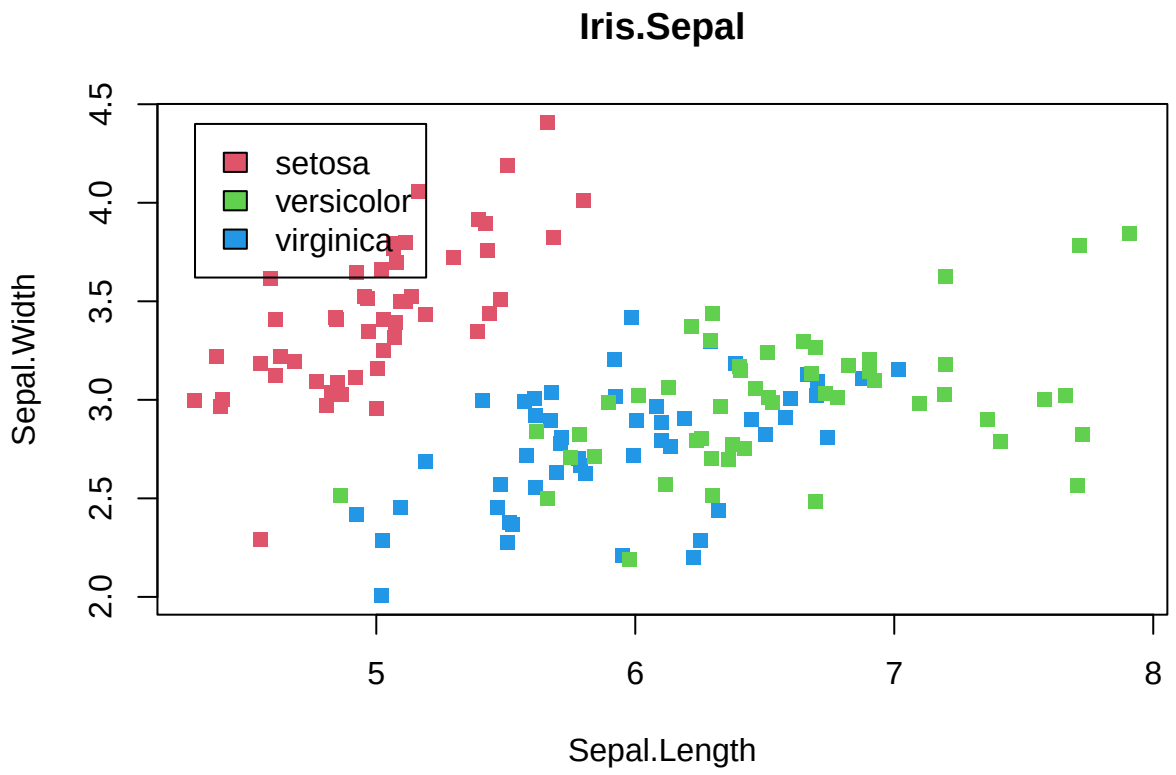
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 133  30
##          1  21  76
##
##                Accuracy : 0.8038
##                  95% CI : (0.7503, 0.8503)
##     No Information Rate : 0.5923
##     P-Value [Acc > NIR] : 2.921e-13
##
##                   Kappa : 0.5884
##
##  Mcnemar's Test P-Value : 0.2626
##
##             Sensitivity : 0.8636
##             Specificity : 0.7170
##          Pos Pred Value : 0.8160
##          Neg Pred Value : 0.7835
```

```
##              Prevalence : 0.5923
##          Detection Rate : 0.5115
##    Detection Prevalence : 0.6269
##       Balanced Accuracy : 0.7903
##
##        'Positive' Class : 0
##
```

LDA and QDA

Let us apply LDA and QDA to a multi label dataset such as **iris**. We are going to use just the first two columns with a gaussian noise.

```
iris2 <- iris[,c(1,2,5)]
species_name <- iris$Species
iris2[,1] <- iris2[,1] + rnorm(150, sd=0.025)
iris2[,2] <- iris2[,2] + rnorm(150, sd=0.025)

plot(iris2[,1:2], main='Iris.Sepal', xlab='Sepal.Length', ylab='Sepal.Width', pch=15)
points(iris2[1:50,], col=2, pch=15)
points(iris2[51:100,], col=4, pch=15)
points(iris2[101:150,], col=3, pch=15)
legend(min(iris[,1]), max(iris[,2]), legend=levels(species_name), fill=c(2,3,4))
```



Once again we create a train set and a test set.

```r
set.seed(123)
training.samples <- species_name %>%
  createDataPartition(p = 0.8, list = FALSE)
train <- iris2[training.samples, ]
test <- iris2[-training.samples, ]
```

It is generally recommended to standardize/normalize continuous predictor before the analysis.

```r
help(preProcess)

# Estimate preprocessing parameters
preproc.param <- train %>%
  preProcess(method = c("center", "scale"))
# Transform the data using the estimated parameters
train_transformed <- preproc.param %>% predict(train)
test_transformed <- preproc.param %>% predict(test)
```

LDA

Before performing LDA, consider:

- Inspecting the univariate distributions of each variable and check whether they are normally distributed. If not, you can transform them using log and root for exponential distributions and Box-Cox for skewed distributions.
- Standardize the variables to make their scale comparable.
- Be careful for the possible presence of outliers, and remember: "*any reasonable, formal or informal, procedure for rejecting outliers will prevent the worst*" (P.J. Huber).

```r
help(lda)

lda.iris <- lda(factor(Species)~ Sepal.Length + Sepal.Width, data=train_transformed)
lda.iris
```

```
## Call:
## lda(factor(Species) ~ Sepal.Length + Sepal.Width, data = train_transformed)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width
## setosa       -1.0120940  0.77319367
## versicolor    0.1004989 -0.68484625
## virginica     0.9115952 -0.08834742
##
## Coefficients of linear discriminants:
##                     LD1        LD2
## Sepal.Length -1.775634 -0.6120093
## Sepal.Width   1.086270 -0.9378600
##
## Proportion of trace:
##    LD1    LD2
## 0.9493 0.0507
```

In the output above, aside from prior provability and group means, we have:

- *Coefficients of linear discriminants*: the linear combination of predictor variables that are used to form the LDA decision rule.
- *Proportion of trace*: the separation achieved by each discriminant function (in percentage).

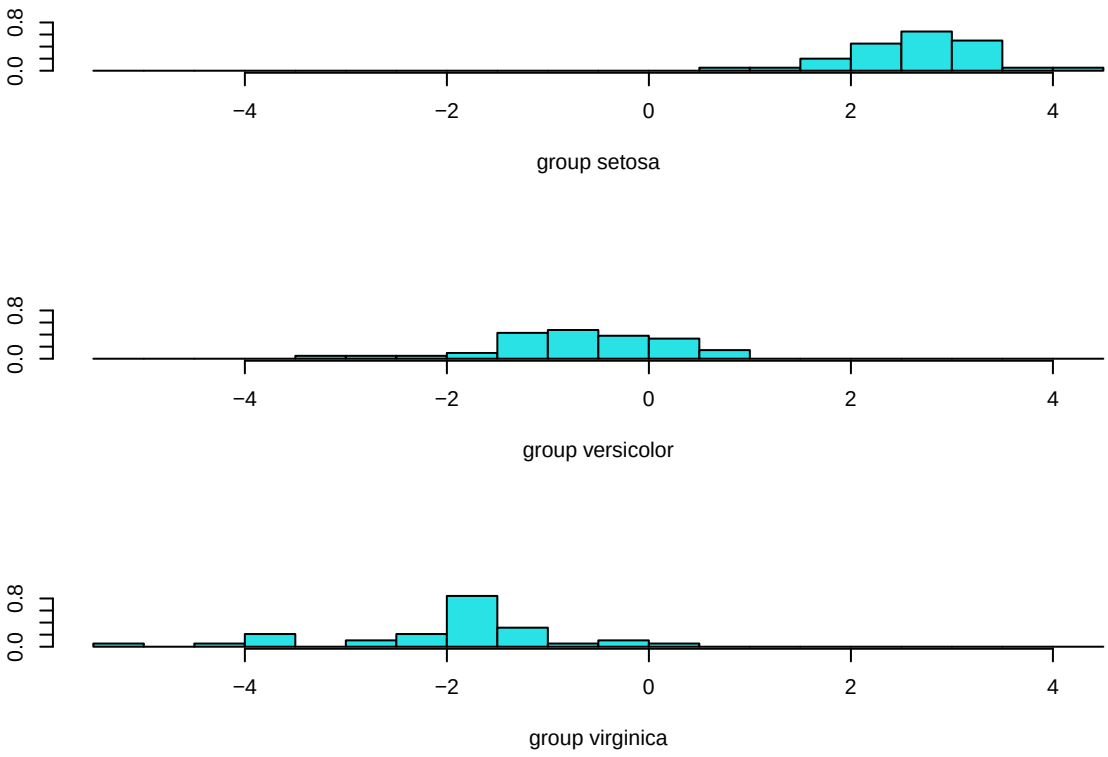
Here is the model accuracy on training data.

```
predmodel.train.lda = predict(lda.iris, data=train_transformed)
confusionMatrix(as.factor(predmodel.train.lda$class), train_transformed$Species)
```

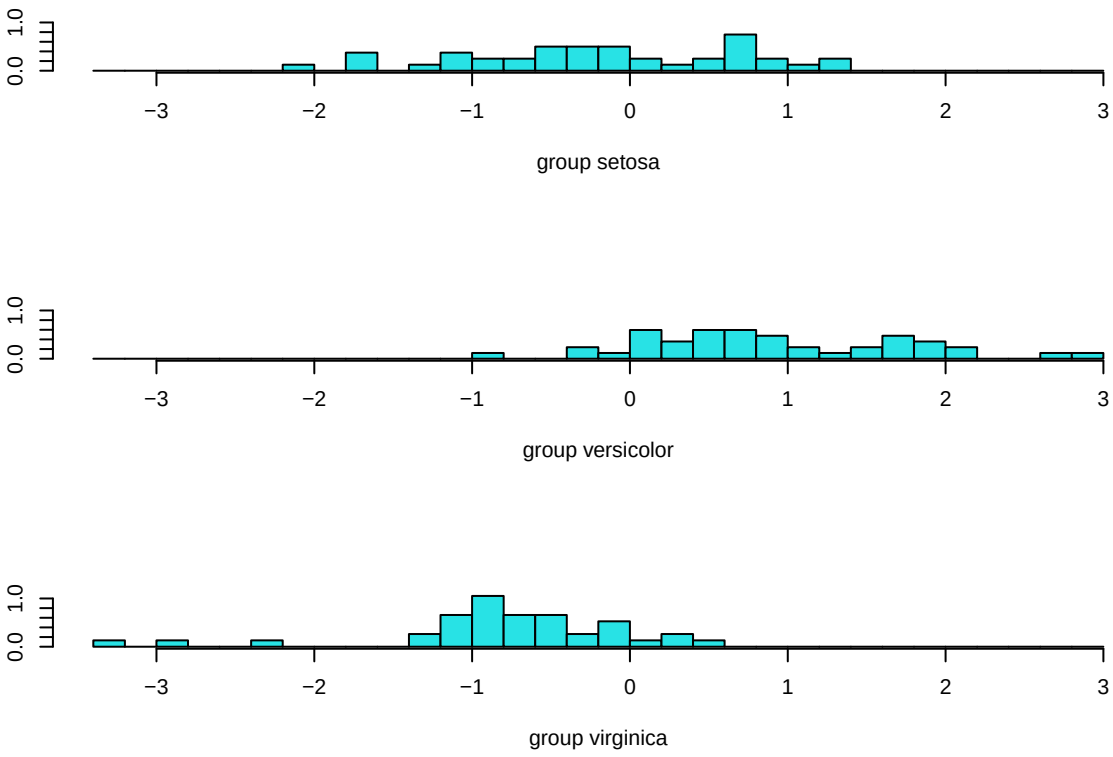
```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         39          1         0
##   versicolor      1         29        12
##   virginica       0         10        28
##
## Overall Statistics
##
##                Accuracy : 0.8
##                  95% CI : (0.7172, 0.8675)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.7
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 0.9750            0.7250           0.7000
## Specificity                 0.9875            0.8375           0.8750
## Pos Pred Value              0.9750            0.6905           0.7368
## Neg Pred Value              0.9875            0.8590           0.8537
## Prevalence                  0.3333            0.3333           0.3333
## Detection Rate              0.3250            0.2417           0.2333
## Detection Prevalence        0.3333            0.3500           0.3167
## Balanced Accuracy           0.9812            0.7812           0.7875
```

The plot below shows how the response class has been classified by the LDA classifier. The x-axis shows the value of the line defined by the coefficient of linear discriminant for LDA. Groups are the ones in the response classes.

```
# first discriminant
ldahist(predmodel.train.lda$x[,1], g= predmodel.train.lda$class)
```

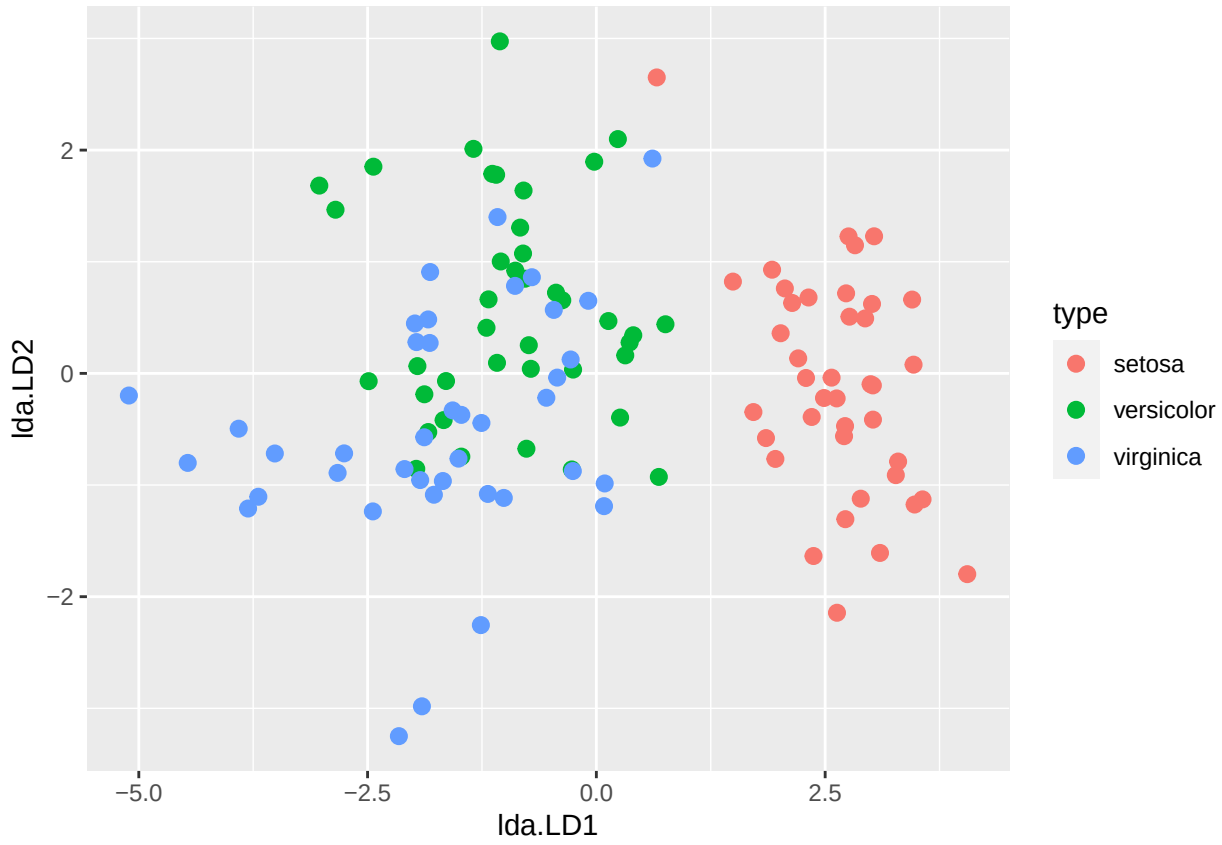



```
# second discriminant
ldahist(predmodel.train.lda$x[,2], g= predmodel.train.lda$class)
```



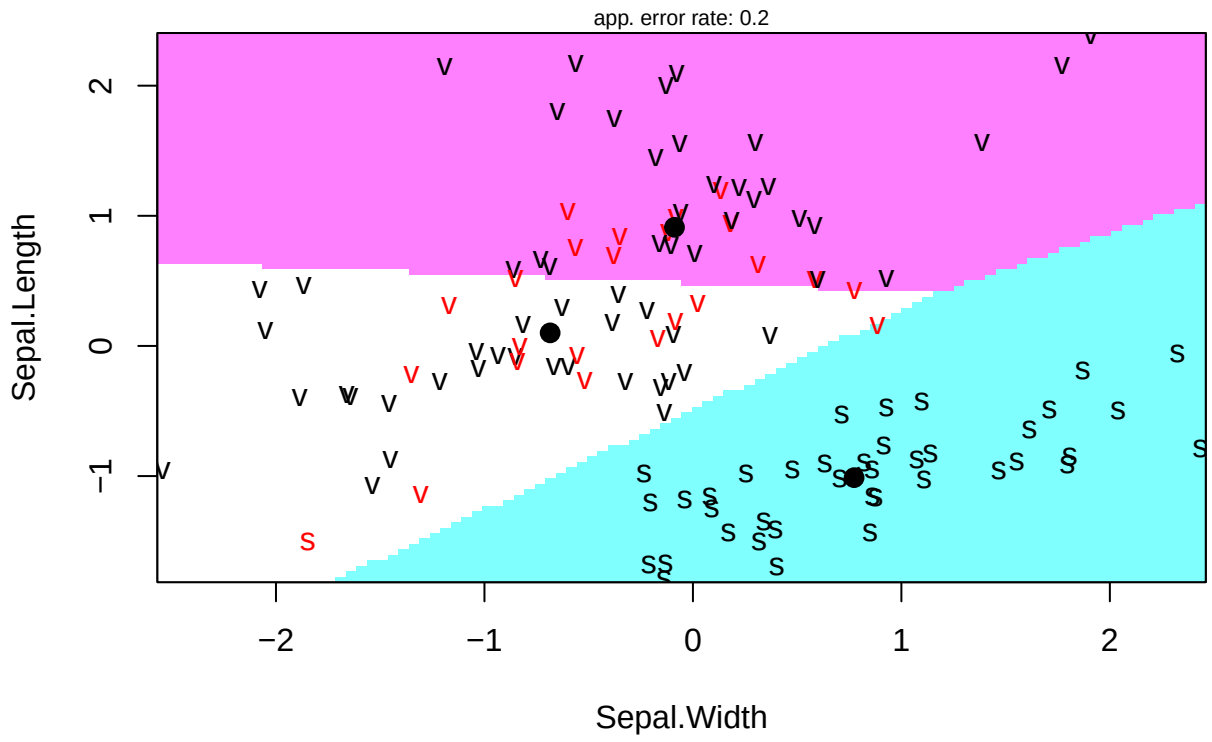
See new x with original labels

```
#convert to data frame
newdata <- data.frame(type = train_transformed$Species, lda = predmodel.train.lda$x)
library(ggplot2)
ggplot(newdata) + geom_point(aes(lda.LD1, lda.LD2, colour = type), size = 2.5)
```



See geometric division

```
# library(klaR)
partimat(factor(Species)~ Sepal.Length + Sepal.Width,
         data=train_transformed, method = "lda")
```



Now we check the model accuracy on test data.

```
predmodel.test.lda = predict(lda.iris, newdata=test_transformed)
confusionMatrix(as.factor(predmodel.test.lda$class), test_transformed$Species)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0          8         4
##   virginica       0          2         6
##
## Overall Statistics
##
##                Accuracy : 0.8
##                  95% CI : (0.6143, 0.9229)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : 2.09e-07
##
##                   Kappa : 0.7
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
```

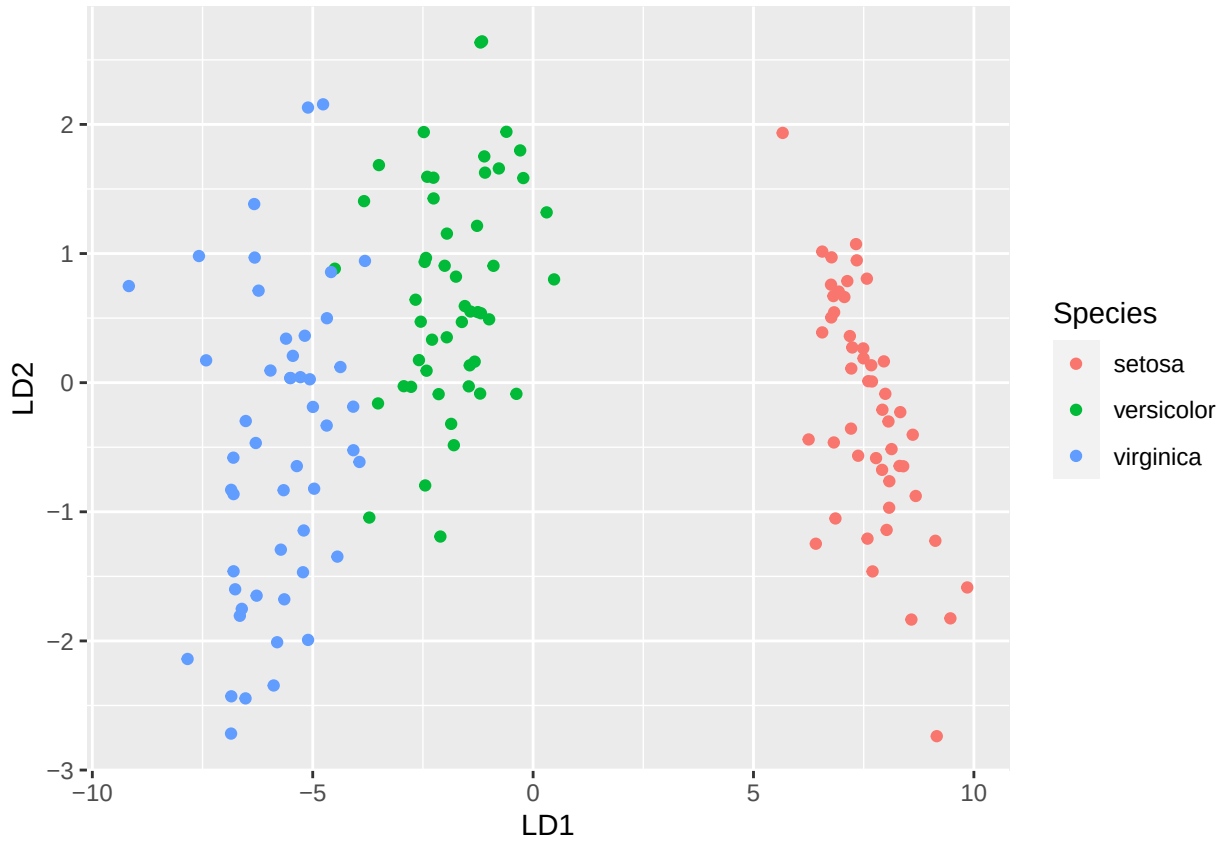
```
## Sensitivity                 1.0000           0.8000           0.6000
## Specificity                 1.0000           0.8000           0.9000
## Pos Pred Value              1.0000           0.6667           0.7500
## Neg Pred Value              1.0000           0.8889           0.8182
## Prevalence                  0.3333           0.3333           0.3333
## Detection Rate              0.3333           0.2667           0.2000
## Detection Prevalence        0.3333           0.4000           0.2667
## Balanced Accuracy           1.0000           0.8000           0.7500
```

Let's try LDA with all variables in iris data:

```
irisLda <- lda(Species~.,data=iris)
irisLda
```

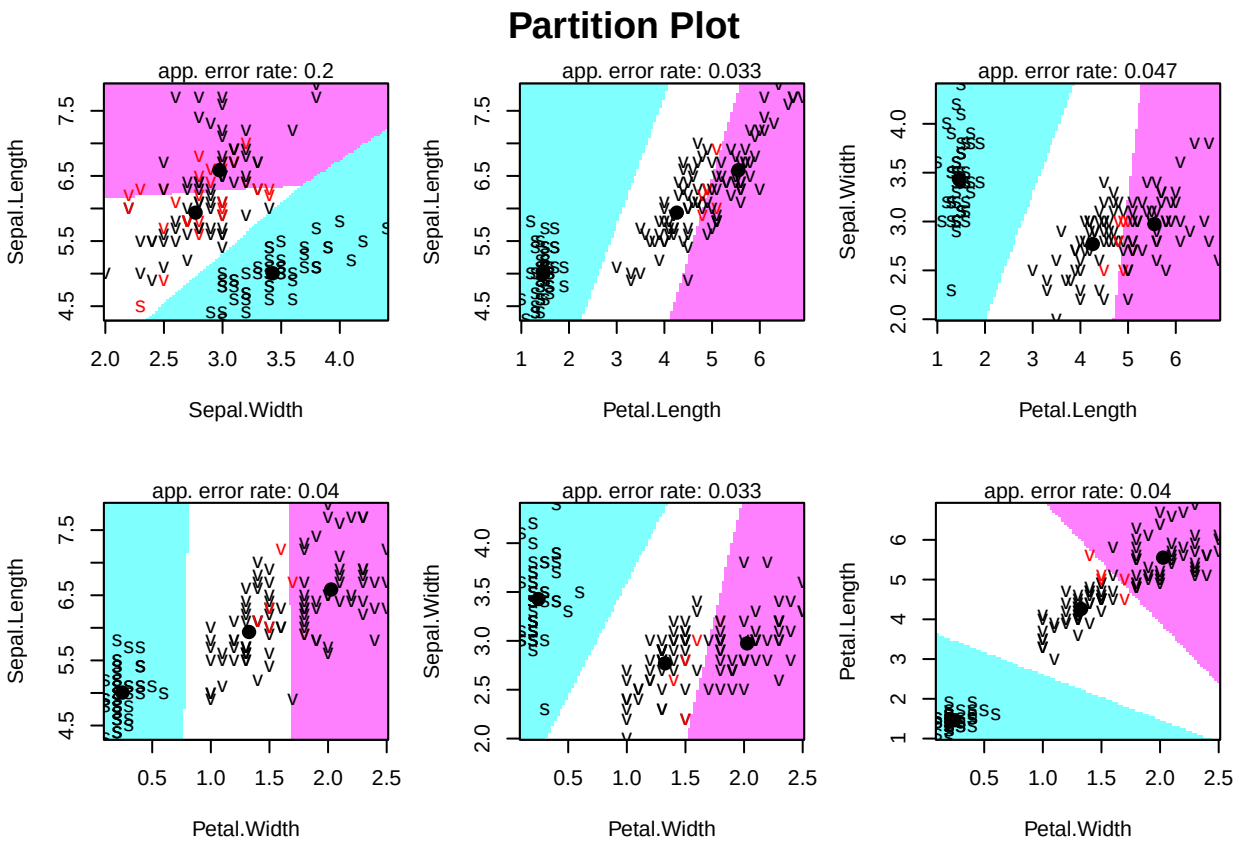
```
## Call:
## lda(Species ~ ., data = iris)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width Petal.Length Petal.Width
## setosa            5.006       3.428        1.462       0.246
## versicolor        5.936       2.770        4.260       1.326
## virginica         6.588       2.974        5.552       2.026
##
## Coefficients of linear discriminants:
##                     LD1         LD2
## Sepal.Length  0.8293776 -0.02410215
## Sepal.Width   1.5344731 -2.16452123
## Petal.Length -2.2012117  0.93192121
## Petal.Width  -2.8104603 -2.83918785
##
## Proportion of trace:
##    LD1    LD2
## 0.9912 0.0088
```

```
scalIris <- scale(as.matrix(iris[,-5]),scale=FALSE)

irisProjection <- cbind(scalIris %*% irisLda$scaling, iris[,5,drop=FALSE])

p <- ggplot(data=irisProjection,aes(x=LD1,y=LD2,col=Species))
p + geom_point()
```



Geometric division

```
partimat(factor(Species)~.,
         data=iris, method = "lda")
```



QDA

Next we will fit the model trough QDA The command is similar to LDA and it outputs the prior probabilities and Group means. Note that "Prior Probabilities" and "Group Means" values are same as of LDA.

```
qda.iris <- qda(factor(Species)~ Sepal.Length + Sepal.Width, data=train_transformed)
qda.iris
```

```
## Call:
## qda(factor(Species) ~ Sepal.Length + Sepal.Width, data = train_transformed)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width
## setosa       -1.0120940  0.77319367
## versicolor    0.1004989 -0.68484625
## virginica     0.9115952 -0.08834742
```

We will find the model accuracy for training data.

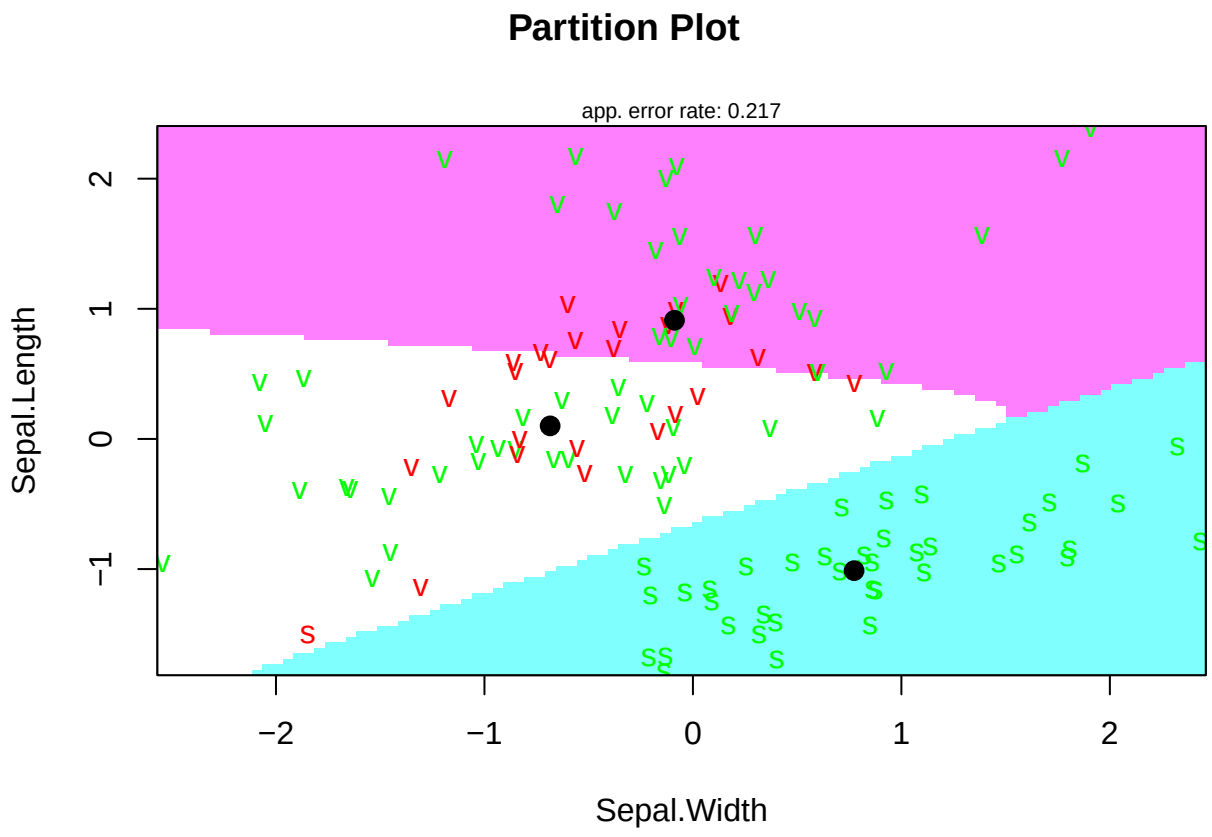
```
predmodel.train.qda = predict(qda.iris, data=train_transformed)
confusionMatrix(as.factor(predmodel.train.qda$class), train_transformed$Species)
```

```
## Confusion Matrix and Statistics
##
```

```
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         39          0         0
##   versicolor      1         30        15
##   virginica       0         10        25
##
## Overall Statistics
##
##                Accuracy : 0.7833
##                  95% CI : (0.6989, 0.8533)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.675
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 0.9750            0.7500           0.6250
## Specificity                 1.0000            0.8000           0.8750
## Pos Pred Value              1.0000            0.6522           0.7143
## Neg Pred Value              0.9877            0.8649           0.8235
## Prevalence                  0.3333            0.3333           0.3333
## Detection Rate              0.3250            0.2500           0.2083
## Detection Prevalence        0.3250            0.3833           0.2917
## Balanced Accuracy           0.9875            0.7750           0.7500
```

We can see the geometric partition

```
# library(klaR)
partimat(factor(Species) ~ Sepal.Length + Sepal.Width,
         data=train_transformed, method = "qda",
         col.correct='green', col.wrong='red')
```

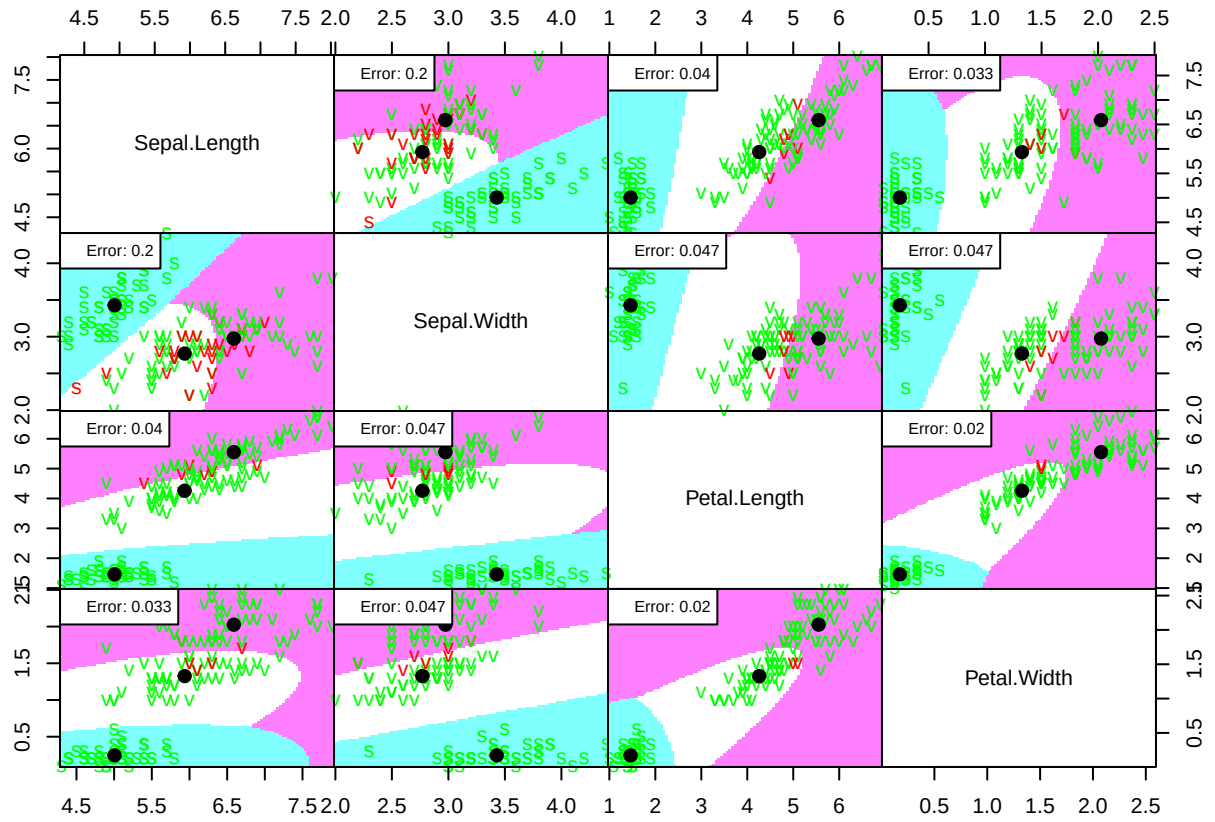


Let's also try QDA on all original variables

```
irisQda <- qda(Species~.,data=iris)
irisQda
```

```
## Call:
## qda(Species ~ ., data = iris)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width Petal.Length Petal.Width
## setosa            5.006       3.428        1.462       0.246
## versicolor        5.936       2.770        4.260       1.326
## virginica         6.588       2.974        5.552       2.026
```

```
partimat(Species ~ ., data = iris, method = "qda",
         plot.matrix = TRUE, col.correct='green', col.wrong='red')
```



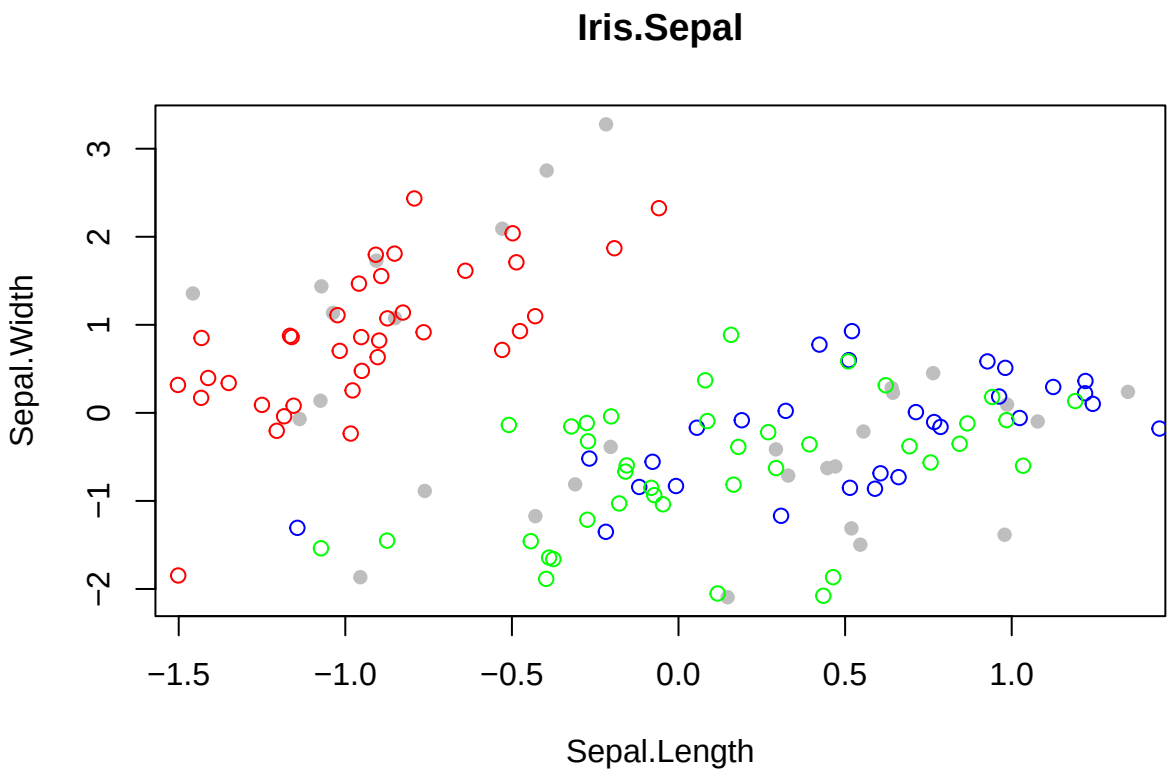
kNN

We are going to use the **knn3()** function within **caret** package on the iris2 data (i.e. working on 2 dimensions). Let's train the knn with $k = 1, 2, 3, 10$

```
set.seed(123)
knn_iris1  <- knn3(factor(Species) ~ Sepal.Length + Sepal.Width,
                   data=train_transformed, k = 1)
knn_iris2  <- knn3(factor(Species) ~ Sepal.Length + Sepal.Width,
                   data=train_transformed, k = 2)
knn_iris3  <- knn3(factor(Species) ~ Sepal.Length + Sepal.Width,
                   data=train_transformed, k = 3)
knn_iris10 <- knn3(factor(Species) ~ Sepal.Length + Sepal.Width,
                   data=train_transformed, k = 10)
```

Hand-made KNN:

```
plot(test_transformed[,1:2], main='Iris.Sepal',
     xlab='Sepal.Length', ylab='Sepal.Width',pch=16, col='grey')
points(train_transformed[which(train_transformed$Species=="setosa"),1:2],
       col='red', pch=1)
points(train_transformed[which(train_transformed$Species=="virginica"),1:2],
       col='blue', pch=1)
points(train_transformed[which(train_transformed$Species=="versicolor"),1:2],
       col='green', pch=1)
```



And now let us predict new points labels in the test set. Using $k = 1$:

```
predict(knn_iris1, test_transformed, type='prob')
```

```
##       setosa versicolor virginica
##  [1,]      1          0         0
##  [2,]      1          0         0
##  [3,]      1          0         0
##  [4,]      1          0         0
##  [5,]      1          0         0
##  [6,]      1          0         0
##  [7,]      1          0         0
##  [8,]      1          0         0
##  [9,]      1          0         0
## [10,]      1          0         0
## [11,]      0          0         1
## [12,]      0          0         1
## [13,]      0          1         0
## [14,]      0          1         0
## [15,]      0          1         0
## [16,]      0          0         1
## [17,]      0          1         0
## [18,]      0          1         0
## [19,]      0          0         1
## [20,]      0          1         0
## [21,]      0          1         0
## [22,]      0          0         1
```

```
## [23,]      0          1         0
## [24,]      0          0         1
## [25,]      0          1         0
## [26,]      0          1         0
## [27,]      0          1         0
## [28,]      0          0         1
## [29,]      0          1         0
## [30,]      0          0         1
```

```
predict_test_knn1 <- predict(knn_iris1, test_transformed, type='class')
confusionMatrix(predict_test_knn1, test_transformed$Species)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0          6         6
##   virginica       0          4         4
##
## Overall Statistics
##
##                Accuracy : 0.6667
##                  95% CI : (0.4719, 0.8271)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : 0.0001938
##
##                   Kappa : 0.5
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.6000           0.4000
## Specificity                 1.0000            0.7000           0.8000
## Pos Pred Value              1.0000            0.5000           0.5000
## Neg Pred Value              1.0000            0.7778           0.7273
## Prevalence                  0.3333            0.3333           0.3333
## Detection Rate              0.3333            0.2000           0.1333
## Detection Prevalence        0.3333            0.4000           0.2667
## Balanced Accuracy           1.0000            0.6500           0.6000
```

Using $k = 2$:

```
predict(knn_iris2, test_transformed, type='prob')
```

```
##       setosa versicolor virginica
##  [1,]      1        0.0       0.0
##  [2,]      1        0.0       0.0
##  [3,]      1        0.0       0.0
##  [4,]      1        0.0       0.0
##  [5,]      1        0.0       0.0
##  [6,]      1        0.0       0.0
##  [7,]      1        0.0       0.0
##  [8,]      1        0.0       0.0
```

```
##  [9,]      1        0.0       0.0
## [10,]      1        0.0       0.0
## [11,]      0        0.0       1.0
## [12,]      0        0.5       0.5
## [13,]      0        1.0       0.0
## [14,]      0        0.5       0.5
## [15,]      0        1.0       0.0
## [16,]      0        0.5       0.5
## [17,]      0        0.5       0.5
## [18,]      0        1.0       0.0
## [19,]      0        0.5       0.5
## [20,]      0        0.5       0.5
## [21,]      0        1.0       0.0
## [22,]      0        0.0       1.0
## [23,]      0        0.5       0.5
## [24,]      0        0.5       0.5
## [25,]      0        0.5       0.5
## [26,]      0        1.0       0.0
## [27,]      0        0.5       0.5
## [28,]      0        0.5       0.5
## [29,]      0        0.5       0.5
## [30,]      0        0.0       1.0
```

```
predict_test_knn2 <- predict(knn_iris2, test_transformed, type='class')
confusionMatrix(predict_test_knn2, test_transformed$Species)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0          5         3
##   virginica       0          5         7
##
## Overall Statistics
##
##                Accuracy : 0.7333
##                  95% CI : (0.5411, 0.8772)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : 8.752e-06
##
##                   Kappa : 0.6
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.5000           0.7000
## Specificity                 1.0000            0.8500           0.7500
## Pos Pred Value              1.0000            0.6250           0.5833
## Neg Pred Value              1.0000            0.7727           0.8333
## Prevalence                  0.3333            0.3333           0.3333
## Detection Rate              0.3333            0.1667           0.2333
## Detection Prevalence        0.3333            0.2667           0.4000
```

```
## Balanced Accuracy           1.0000            0.6750           0.7250
```

Using $k = 3$:

```
# k=3
predict(knn_iris3, test_transformed, type='prob')
```

```
##          setosa versicolor virginica
##  [1,] 1.0000000  0.0000000 0.0000000
##  [2,] 1.0000000  0.0000000 0.0000000
##  [3,] 1.0000000  0.0000000 0.0000000
##  [4,] 1.0000000  0.0000000 0.0000000
##  [5,] 1.0000000  0.0000000 0.0000000
##  [6,] 1.0000000  0.0000000 0.0000000
##  [7,] 1.0000000  0.0000000 0.0000000
##  [8,] 1.0000000  0.0000000 0.0000000
##  [9,] 1.0000000  0.0000000 0.0000000
## [10,] 1.0000000  0.0000000 0.0000000
## [11,] 0.0000000  0.0000000 1.0000000
## [12,] 0.0000000  0.6666667 0.3333333
## [13,] 0.0000000  1.0000000 0.0000000
## [14,] 0.0000000  0.6666667 0.3333333
## [15,] 0.0000000  0.6666667 0.3333333
## [16,] 0.0000000  0.3333333 0.6666667
## [17,] 0.0000000  0.6666667 0.3333333
## [18,] 0.3333333  0.6666667 0.0000000
## [19,] 0.0000000  0.6666667 0.3333333
## [20,] 0.0000000  0.3333333 0.6666667
## [21,] 0.0000000  0.6666667 0.3333333
## [22,] 0.0000000  0.3333333 0.6666667
## [23,] 0.0000000  0.3333333 0.6666667
## [24,] 0.0000000  0.6666667 0.3333333
## [25,] 0.0000000  0.6666667 0.3333333
## [26,] 0.0000000  1.0000000 0.0000000
## [27,] 0.0000000  0.3333333 0.6666667
## [28,] 0.0000000  0.3333333 0.6666667
## [29,] 0.0000000  0.6666667 0.3333333
## [30,] 0.0000000  0.0000000 1.0000000
```

```
predict_test_knn3 <- predict(knn_iris3, test_transformed, type='class')
confusionMatrix(predict_test_knn3, test_transformed$Species)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0          7         5
##   virginica       0          3         5
##
## Overall Statistics
##
##                Accuracy : 0.7333
##                  95% CI : (0.5411, 0.8772)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : 8.752e-06
```

```
##
##                   Kappa : 0.6
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.7000           0.5000
## Specificity                 1.0000            0.7500           0.8500
## Pos Pred Value              1.0000            0.5833           0.6250
## Neg Pred Value              1.0000            0.8333           0.7727
## Prevalence                  0.3333            0.3333           0.3333
## Detection Rate              0.3333            0.2333           0.1667
## Detection Prevalence        0.3333            0.4000           0.2667
## Balanced Accuracy           1.0000            0.7250           0.6750
```

Using $k = 10$

```
# k=10
predict(knn_iris10, test_transformed, type='prob')
```

```
##       setosa versicolor virginica
##  [1,]    1.0        0.0       0.0
##  [2,]    1.0        0.0       0.0
##  [3,]    1.0        0.0       0.0
##  [4,]    1.0        0.0       0.0
##  [5,]    1.0        0.0       0.0
##  [6,]    1.0        0.0       0.0
##  [7,]    1.0        0.0       0.0
##  [8,]    1.0        0.0       0.0
##  [9,]    1.0        0.0       0.0
## [10,]    1.0        0.0       0.0
## [11,]    0.0        0.2       0.8
## [12,]    0.0        0.7       0.3
## [13,]    0.0        0.6       0.4
## [14,]    0.0        0.5       0.5
## [15,]    0.0        0.5       0.5
## [16,]    0.0        0.4       0.6
## [17,]    0.0        0.8       0.2
## [18,]    0.1        0.7       0.2
## [19,]    0.0        0.6       0.4
## [20,]    0.0        0.7       0.3
## [21,]    0.0        0.5       0.5
## [22,]    0.0        0.5       0.5
## [23,]    0.0        0.3       0.7
## [24,]    0.0        0.5       0.5
## [25,]    0.0        0.3       0.7
## [26,]    0.0        0.8       0.2
## [27,]    0.0        0.6       0.4
## [28,]    0.0        0.6       0.4
## [29,]    0.0        0.4       0.6
## [30,]    0.0        0.4       0.6
```

```
predict_test_knn10 <- predict(knn_iris10, test_transformed, type='class')
confusionMatrix(predict_test_knn10, test_transformed$Species)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0          8         3
##   virginica       0          2         7
##
## Overall Statistics
##
##                Accuracy : 0.8333
##                  95% CI : (0.6528, 0.9436)
##     No Information Rate : 0.3333
##     P-Value [Acc > NIR] : 2.444e-08
##
##                   Kappa : 0.75
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.8000           0.7000
## Specificity                 1.0000            0.8500           0.9000
## Pos Pred Value              1.0000            0.7273           0.7778
## Neg Pred Value              1.0000            0.8947           0.8571
## Prevalence                  0.3333            0.3333           0.3333
## Detection Rate              0.3333            0.2667           0.2333
## Detection Prevalence        0.3333            0.3667           0.3000
## Balanced Accuracy           1.0000            0.8250           0.8000
```