Classification Example with 3 Groups: Iris Dataset

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 $The following example is mainly taken from \ https://daviddalpiaz.github.io/r4sl/generative-models.html$

Example of LDA With 3 Classes

There is "famous" dataset in R called the "Iris".

There are three iris flowers from three different species.

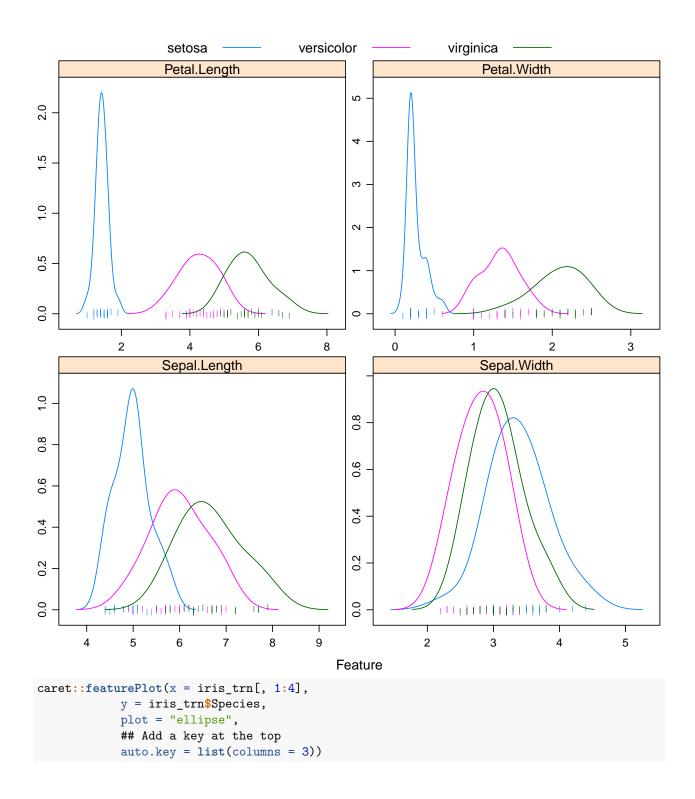
- 1. Iris-setosa
- 2. Iris-versicolor
- 3. Iris-virginica

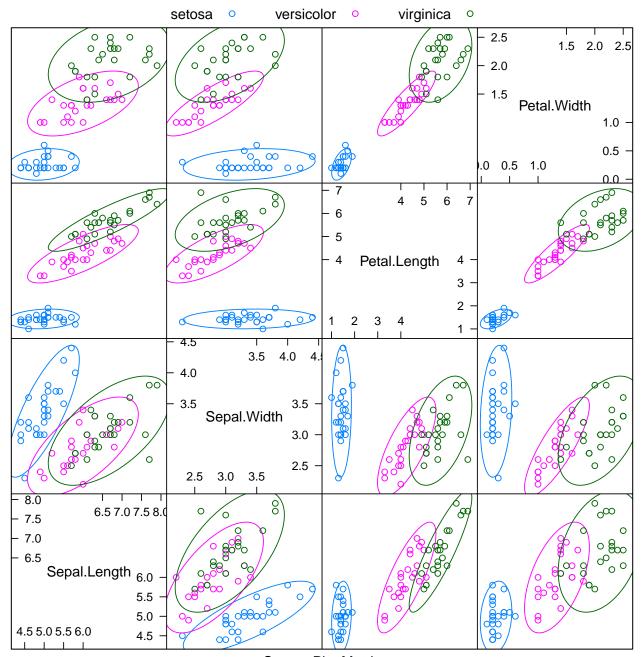
There are four features for predicting the species of flower.

- 1. Sepal length (cm)
- 2. Sepal width (cm)
- 3. Petal length (cm)
- 4. Petal width (cm)

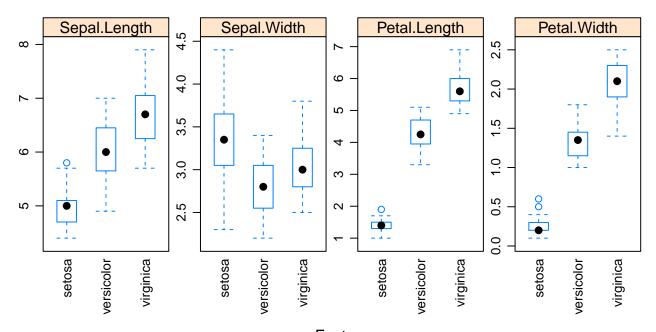
Investigating the Data

```
set.seed(430)
iris_obs = nrow(iris)
iris_idx = sample(iris_obs, size = trunc(0.50 * iris_obs))
# iris_index = sample(iris_obs, size = trunc(0.10 * iris_obs))
iris_trn = iris[iris_idx, ]
iris_tst = iris[-iris_idx, ]
caret::featurePlot(x = iris_trn[, c("Sepal.Length", "Sepal.Width",
                                     "Petal.Length", "Petal.Width")],
                   y = iris_trn$Species,
                   plot = "density",
                   scales = list(x = list(relation = "free"),
                                 y = list(relation = "free")),
                   adjust = 1.5,
                   pch = "|",
                   layout = c(2, 2),
                   auto.key = list(columns = 3))
```





Scatter Plot Matrix



Feature

What is a good classifier?

Using LDA

```
library(MASS)
iris_lda = lda(Species ~ ., data = iris_trn)
iris_lda
## Call:
## lda(Species ~ ., data = iris_trn)
##
## Prior probabilities of groups:
##
       setosa versicolor virginica
   0.3733333  0.3200000  0.3066667
##
##
## Group means:
##
              Sepal.Length Sepal.Width Petal.Length Petal.Width
                  4.978571
                              3.378571
                                            1.432143
                                                       0.2607143
## setosa
## versicolor
                  5.995833
                              2.808333
                                            4.254167
                                                       1.3333333
                              3.065217
                  6.669565
                                            5.717391
                                                       2.0956522
## virginica
##
## Coefficients of linear discriminants:
##
                       LD1
## Sepal.Length 0.7100013 -0.8446128
## Sepal.Width
                 1.2435532
                           2.4773120
## Petal.Length -2.3419418 -0.4065865
## Petal.Width -1.8502355 2.3234441
##
## Proportion of trace:
##
      LD1
             LD2
## 0.9908 0.0092
```

```
Here we see the estimated \hat{\pi}_k and \hat{\mu}_k for each class.
```

```
is.list(predict(iris_lda, iris_trn))
## [1] TRUE
names(predict(iris_lda, iris_trn))
## [1] "class"
                   "posterior" "x"
head(predict(iris_lda, iris_trn)$class, n = 10)
##
   [1] setosa
                   virginica setosa
                                         setosa
                                                     virginica setosa
## [7] virginica setosa
                              versicolor setosa
## Levels: setosa versicolor virginica
head(predict(iris_lda, iris_trn)$posterior, n = 10)
##
                      versicolor
             setosa
                                    virginica
## 23 1.000000e+00 1.517145e-21 1.717663e-41
## 106 2.894733e-43 1.643603e-06 9.999984e-01
## 37 1.000000e+00 2.169066e-20 1.287216e-40
## 40 1.000000e+00 3.979954e-17 8.243133e-36
## 145 1.303566e-37 4.335258e-06 9.999957e-01
## 36 1.000000e+00 1.947567e-18 5.996917e-38
## 119 2.220147e-51 9.587514e-09 1.000000e+00
## 16 1.000000e+00 5.981936e-23 1.344538e-42
## 94 1.599359e-11 9.999999e-01 1.035129e-07
## 27 1.000000e+00 8.154612e-15 4.862249e-32
Getting Predictions and Error Rates
iris_lda_trn_pred = predict(iris_lda, iris_trn)$class
iris_lda_tst_pred = predict(iris_lda, iris_tst)$class
We store the predictions made on the train and test sets.
calc_class_err = function(actual, predicted) {
  mean(actual != predicted)
calc_class_err(predicted = iris_lda_trn_pred, actual = iris_trn$Species)
## [1] 0.04
calc_class_err(predicted = iris_lda_tst_pred, actual = iris_tst$Species)
## [1] 0.01333333
As expected, LDA performs well on both the train and test data.
table(predicted = iris_lda_tst_pred, actual = iris_tst$Species)
##
               actual
## predicted
                setosa versicolor virginica
##
     setosa
                    22
                                0
                                          0
##
     versicolor
                     0
                               26
                                          1
##
    virginica
                     0
                                0
                                         26
```

QDA

```
Guess what?! There is a qda function. Yay!
iris_qda = qda(Species ~ ., data = iris_trn)
iris_qda
## Call:
## qda(Species ~ ., data = iris_trn)
## Prior probabilities of groups:
##
       setosa versicolor virginica
   0.3733333  0.3200000  0.3066667
##
## Group means:
##
              Sepal.Length Sepal.Width Petal.Length Petal.Width
## setosa
                  4.978571
                               3.378571
                                            1.432143
                                                        0.2607143
                  5.995833
                               2.808333
                                            4.254167
                                                        1.3333333
## versicolor
## virginica
                  6.669565
                               3.065217
                                            5.717391
                                                        2.0956522
iris_qda_trn_pred = predict(iris_qda, iris_trn)$class
iris_qda_tst_pred = predict(iris_qda, iris_tst)$class
The predict() function operates the same as the predict() function for LDA.
calc_class_err(predicted = iris_qda_trn_pred, actual = iris_trn$Species)
## [1] 0.01333333
calc_class_err(predicted = iris_qda_tst_pred, actual = iris_tst$Species)
## [1] 0.04
table(predicted = iris_qda_tst_pred, actual = iris_tst$Species)
##
               actual
## predicted
                setosa versicolor virginica
                    22
     setosa
                                0
##
                     0
                                23
                                           0
     versicolor
     virginica
                     0
                                 3
                                          27
```

Logistic Regression

In lecture, you were told that Logistic Regression does not get used for more than 2 groups all that much. Let's see how it performs anyway.

In this case, the glm function cannot be used. Instead a function from the nnet packages will be used.

```
library(nnet)
iris_log=multinom(Species~., data=iris_trn)

## # weights: 18 (10 variable)
## initial value 82.395922
## iter 10 value 6.164184
## iter 20 value 3.952967
## iter 30 value 3.887791
## iter 40 value 3.826736
```

```
## iter 50 value 3.766389
## iter 60 value 3.755861
## iter 70 value 3.747011
## iter 80 value 3.746702
## iter 90 value 3.745246
## final value 3.745179
## converged
summary(iris log)
## Call:
## multinom(formula = Species ~ ., data = iris_trn)
## Coefficients:
##
              (Intercept) Sepal.Length Sepal.Width Petal.Length Petal.Width
                             -6.983313
                                                        20.35750
## versicolor
                 26.81602
                                          -16.24574
                                                                    3.218787
## virginica
                -34.24228
                             -8.398869
                                          -17.03985
                                                        31.94659
                                                                   11.594518
##
## Std. Errors:
##
              (Intercept) Sepal.Length Sepal.Width Petal.Length Petal.Width
                              226.5881
                                                        67.37825
## versicolor
                  74.3553
                                           115.8998
                                                                    16.14625
                                                                    16.04269
                  76.2057
                                                        66.96215
## virginica
                              226.6131
                                           115.6749
## Residual Deviance: 7.490358
## AIC: 27.49036
iris_log_trn_pred = predict(iris_log, iris_trn, "class")
iris_log_tst_pred = predict(iris_log, iris_tst, "class")
The predict() function operates the same as the predict() function for LDA.
calc_class_err(predicted = iris_log_trn_pred, actual = iris_trn$Species)
## [1] 0.04
calc_class_err(predicted = iris_log_tst_pred, actual = iris_tst$Species)
## [1] 0.06666667
table(predicted = iris_log_tst_pred, actual = iris_tst$Species)
##
               actual
## predicted
                setosa versicolor virginica
##
     setosa
                    22
                                0
                                           0
                                           5
##
                               26
     versicolor
                     0
     virginica
                     0
                                0
                                          22
```

KNN

```
library(class)

kmax = 100
err = double(kmax)
for(ii in 1:kmax){
   pk = knn.cv(iris_trn[,-5],iris_trn$Species, k=ii) # does leave one out CV
   err[ii] = mean(pk != iris_trn$Species)
```

```
ggplot(data.frame(k=1:kmax,error=err), aes(k,error)) +
  geom_line(color=red)
 0.6 -
 0.4 -
 0.2 -
  0.0 -
                           25
                                                                    75
                                                                                        100
                                                50
best.k <- max(which(err == min(err)))</pre>
best.k
## [1] 17
iris_knn_trn_pred = knn(iris_trn[,-5], iris_trn[,-5], iris_trn$Species, k = best.k)
iris_knn_tst_pred = knn(iris_trn[,-5], iris_tst[,-5], iris_trn$Species, k = best.k)
calc_class_err(predicted = iris_knn_trn_pred, actual = iris_trn$Species)
## [1] 0.02666667
calc_class_err(predicted = iris_knn_tst_pred, actual = iris_tst$Species)
```

[1] 0.06666667