

Chapter 16

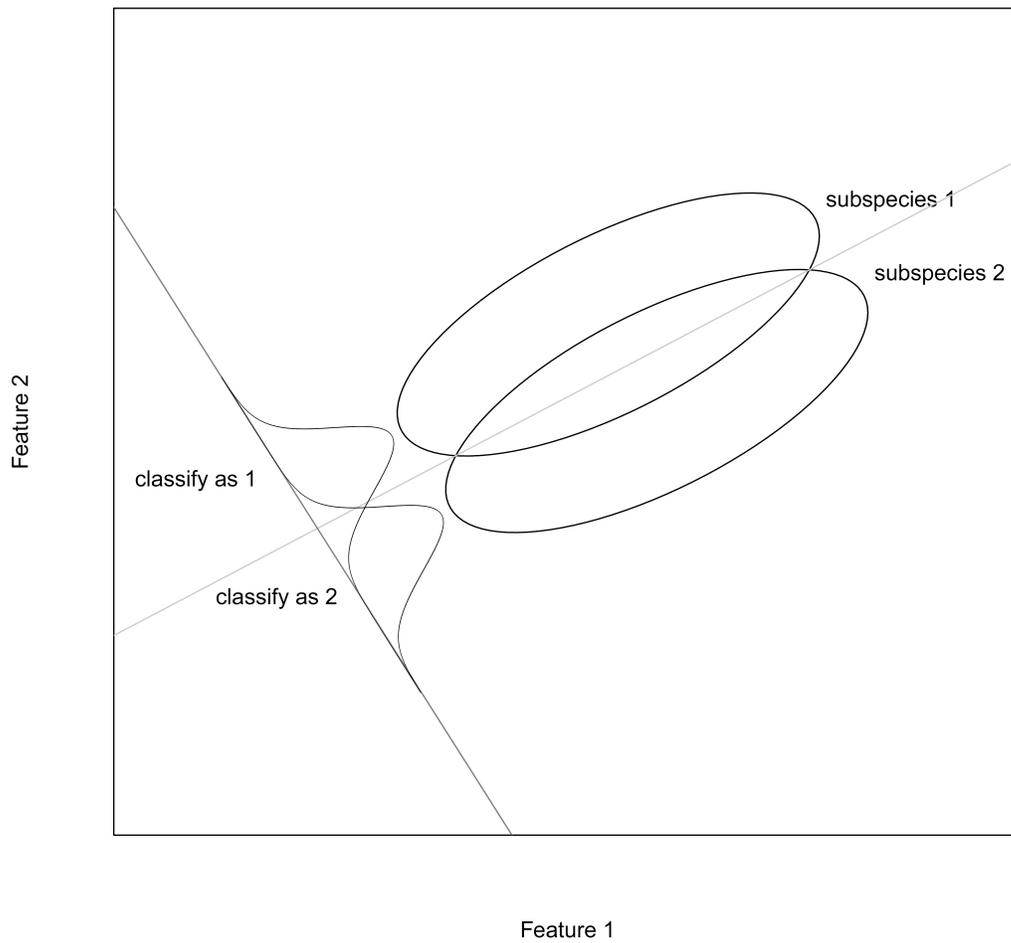
Discriminant Analysis

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A researcher collected data on two external features for two (known) sub-species of an insect. She can use **discriminant analysis** to find linear combinations of the features that best distinguish the sub-species. The analysis can then be used to classify insects with unknown sub-species origin into one of the two sub-species based on their external features.

To see how this might be done, consider the following data plot. Can1 is the linear combination of the two features that best distinguishes or discriminates the two sub-species. The value of Can1 could be used to classify insects into one of the two groups, as illustrated.



The method generalizes to more than two features and sub-species.

16.1 Canonical Discriminant Analysis

While there's a connection between **canonical discriminant analysis** and **canonical correlation**, I prefer to emphasize the connection between canonical discriminant analysis and MANOVA because these techniques are essentially identical.

Assume that you have representative samples from k groups, strata, or subpopulations. Each selected individual is measured on p features (measurements) X_1, X_2, \dots, X_p . As in MANOVA, canonical discriminant analysis assumes you have independent samples from multivariate normal populations with identical variance-covariance matrices.

Canonical discriminant analysis computes $r = \min(p, k - 1)$ linear combinations of the features with the following properties. The first linear combination, called the **first linear discriminant function**

$$\text{Can1} = a_{11}X_1 + a_{12}X_2 + \cdots + a_{1p}X_p$$

gives the most significant F -test for a null hypothesis of no group differences in a one-way ANOVA, among all linear combinations of the features. The second linear combination or the **second linear discriminant function**:

$$\text{Can2} = a_{21}X_1 + a_{22}X_2 + \cdots + a_{2p}X_p$$

gives the most significant F -test for no group differences in a one-way ANOVA, among all linear combinations of the features that are uncorrelated (adjusting for groups) with Can1. In general, the j^{th} linear combination Can j ($j = 1, 2, \dots, r$) gives the most significant F -test for no group differences in a one-way ANOVA, among all linear combinations of the features that are uncorrelated with Can1, Can2, \dots , Can($j - 1$).

The coefficients in the canonical discriminant functions can be multiplied by a constant, or all the signs can be changed (that is, multiplied by the constant -1), without changing their properties or interpretations.

16.2 Example: Owners of riding mowers

The manufacturer of a riding lawn mower wishes to identify the best prospects for buying their product using data on the incomes (X_1) and lot sizes (X_2) of homeowners (Johnson and Wichern, 1988). The data below are the incomes and lot sizes from independent random samples of 12 current owners and 12 non-owners of the mowers.

```
library(tidyverse)

# load ada functions
source("ada_functions.R")

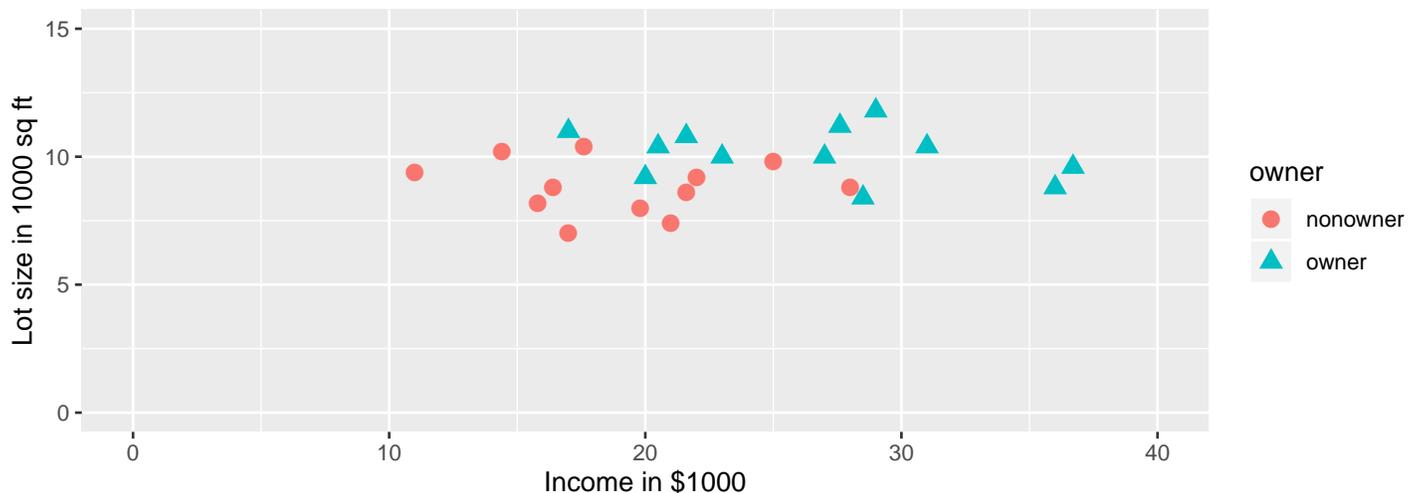
#### Example: Riding mowers
dat_mower <-
  read_table2(
    "http://statacumen.com/teach/ADA2/notes/ADA2_notes_Ch16_mower.dat"
  )

## Parsed with column specification:
## cols(
##   income = col_double(),
##   lotsize = col_double(),
##   owner = col_character()
## )
# income = income in £1000
# lotsize = lot size in 1000 sq ft
# owner = nonowners or owners
str(dat_mower)

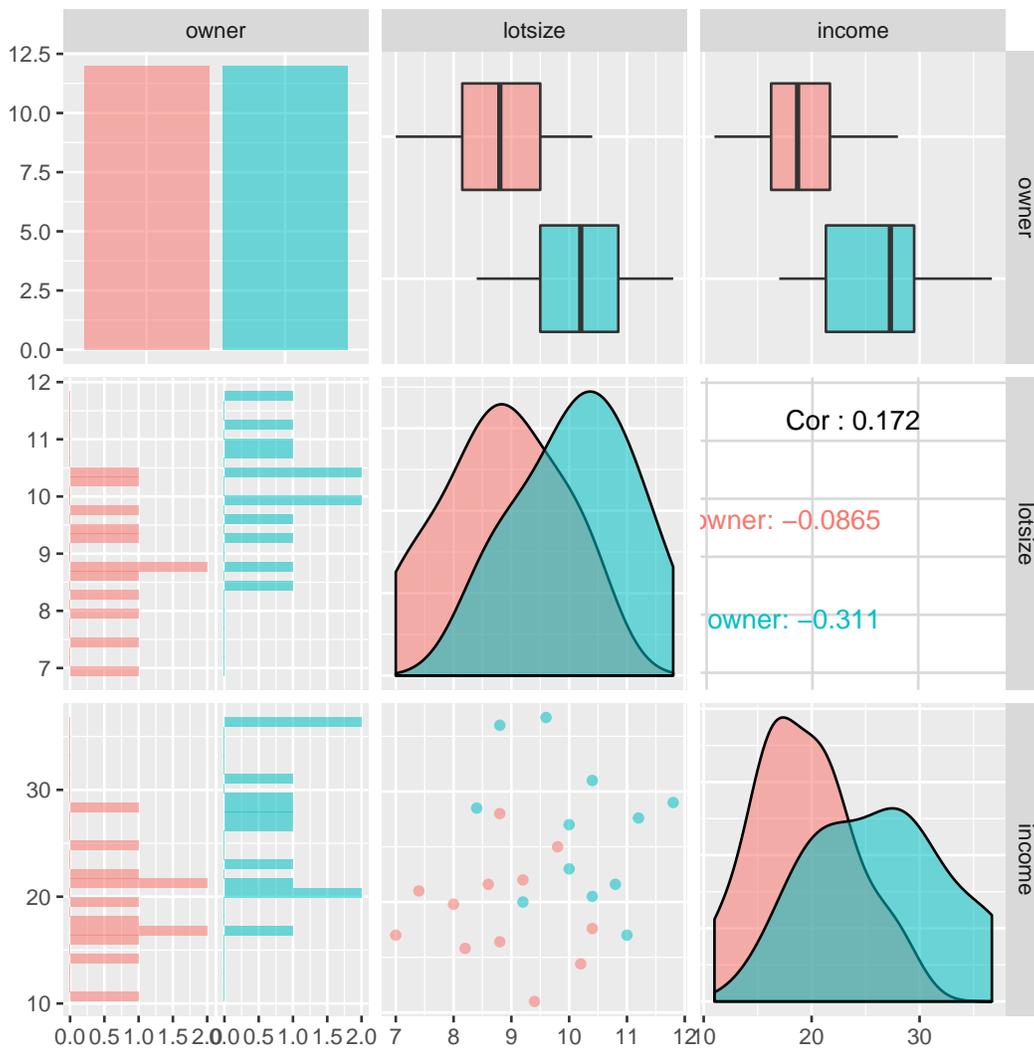
## Classes 'spec_tbl_df', 'tbl_df', 'tbl' and 'data.frame': 24 obs. of 3 variables:
## $ income : num 20 28.5 21.6 20.5 29 36.7 36 27.6 23 31 ...
## $ lotsize: num 9.2 8.4 10.8 10.4 11.8 9.6 8.8 11.2 10 10.4 ...
## $ owner : chr "owner" "owner" "owner" "owner" ...
## - attr(*, "spec")=
## .. cols(
## .. income = col_double(),
## .. lotsize = col_double(),
## .. owner = col_character()
## .. )
```

	income	lotsize	owner		income	lotsize	owner
1	20.00	9.20	owner	1	25.00	9.80	nonowner
2	28.50	8.40	owner	2	17.60	10.40	nonowner
3	21.60	10.80	owner	3	21.60	8.60	nonowner
4	20.50	10.40	owner	4	14.40	10.20	nonowner
5	29.00	11.80	owner	5	28.00	8.80	nonowner
6	36.70	9.60	owner	6	19.80	8.00	nonowner
7	36.00	8.80	owner	7	22.00	9.20	nonowner
8	27.60	11.20	owner	8	15.80	8.20	nonowner
9	23.00	10.00	owner	9	11.00	9.40	nonowner
10	31.00	10.40	owner	10	17.00	7.00	nonowner
11	17.00	11.00	owner	11	16.40	8.80	nonowner
12	27.00	10.00	owner	12	21.00	7.40	nonowner

```
library(ggplot2)
p <- ggplot(dat_mower, aes(x = income, y = lotsize, shape = owner, colour = owner))
p <- p + geom_point(size = 3)
p <- p + scale_y_continuous(limits = c(0, 15))
p <- p + scale_x_continuous(limits = c(0, 40))
p <- p + coord_fixed(ratio = 1) # square axes (for perp lines)
p <- p + xlab("Income in $1000")
p <- p + ylab("Lot size in 1000 sq ft")
print(p)
```



```
library(GGally)
p <-
  ggpairs(
    rev(dat_mower)
    , mapping = ggplot2::aes(colour = owner, alpha = 0.5)
    , progress = FALSE
  )
print(p)
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```



Although the two groups overlap, the owners tend to have higher incomes and larger lots than the non-owners. Income seems to distinguish owners and non-owners better than lot size, but both variables seem to be useful for discriminating between groups.

Qualitatively, one might classify prospects based on their location relative to a roughly vertical line on the scatter plot. A discriminant analysis gives similar results to this heuristic approach because the Can1 scores will roughly correspond to the projection of the two features onto a line perpendicular to the hypothetical vertical line. `candisc()` computes one discriminant function here because $p = 2$ and $k = 2$ gives $r = \min(p, k - 1) = \min(2, 1) = 1$.

Below we first fit a `lm()` and use that object to compare populations. First we compare using univariate ANOVAs. The p-values are for one-way ANOVA comparing owners to non-owners and both income and lotsize features are im-

portant individually for distinguishing between the groups.

```
# first fit lm() with formula = continuous variables ~ factor variables
lm_mower <-
  lm(
    cbind(income, lotsize) ~ owner
    , data = dat_mower
  )

# univariate ANOVA tests
summary(lm_mower)

## Response income :
##
## Call:
## lm(formula = income ~ owner, data = dat_mower)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -9.4917 -3.8021  0.5875  2.5979 10.2083
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   19.133      1.601  11.954 4.28e-11 ***
## ownerowner     7.358      2.264   3.251 0.00367 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.545 on 22 degrees of freedom
## Multiple R-squared:  0.3245, Adjusted R-squared:  0.2938
## F-statistic: 10.57 on 1 and 22 DF,  p-value: 0.003665
##
##
## Response lotsize :
##
## Call:
## lm(formula = lotsize ~ owner, data = dat_mower)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.81667 -0.66667 -0.01667  0.71667  1.66667
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    8.8167     0.2984  29.55 < 2e-16 ***
## ownerowner     1.3167     0.4220   3.12 0.00498 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.034 on 22 degrees of freedom
```

```
## Multiple R-squared:  0.3068, Adjusted R-squared:  0.2753
## F-statistic: 9.736 on 1 and 22 DF,  p-value: 0.004983
```

Second, the MANOVA indicates the multivariate means are different indicating both income and lotsize features taken together are important for distinguishing between the groups.

```
# test whether the multivariate means of the two populations are different
library(car)
man_mower <- Manova(lm_mower)
summary(man_mower)

##
## Type II MANOVA Tests:
##
## Sum of squares and products for error:
##      income  lotsize
## income  676.31583 -26.41333
## lotsize -26.41333  23.50333
##
## -----
##
## Term: owner
##
## Sum of squares and products for the hypothesis:
##      income  lotsize
## income  324.87042 58.13083
## lotsize  58.13083 10.40167
##
## Multivariate Tests: owner
##      Df test stat approx F num Df den Df      Pr(>F)
## Pillai      1 0.5386044 12.25704      2      21 0.00029701 ***
## Wilks       1 0.4613956 12.25704      2      21 0.00029701 ***
## Hotelling-Lawley 1 1.1673374 12.25704      2      21 0.00029701 ***
## Roy         1 1.1673374 12.25704      2      21 0.00029701 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Finally, we fit the canonical discriminant function with `candisc()`. The LR (likelihood ratio) p-values below correspond to tests of no differences between groups on the canonical discriminant functions. There is only one canonical discriminant function here. The tests of no differences based on the first canonical discriminant function is equivalent to Roy's MANOVA test.

```
# perform canonical discriminant analysis
library(car)
can_mower <- candisc(lm_mower)
```

```

can_mower
##
## Canonical Discriminant Analysis for owner:
##
##   CanRsq Eigenvalue Difference Percent Cumulative
## 1 0.5386      1.1673           100         100
##
## Test of H0: The canonical correlations in the
## current row and all that follow are zero
##
##   LR test stat approx F numDF denDF Pr(> F)
## 1      0.4614           2

```

The objects available from the `candisc()` object are named below, and we'll soon use a few. There are also a few plots available, but I'll be creating other plots shortly.

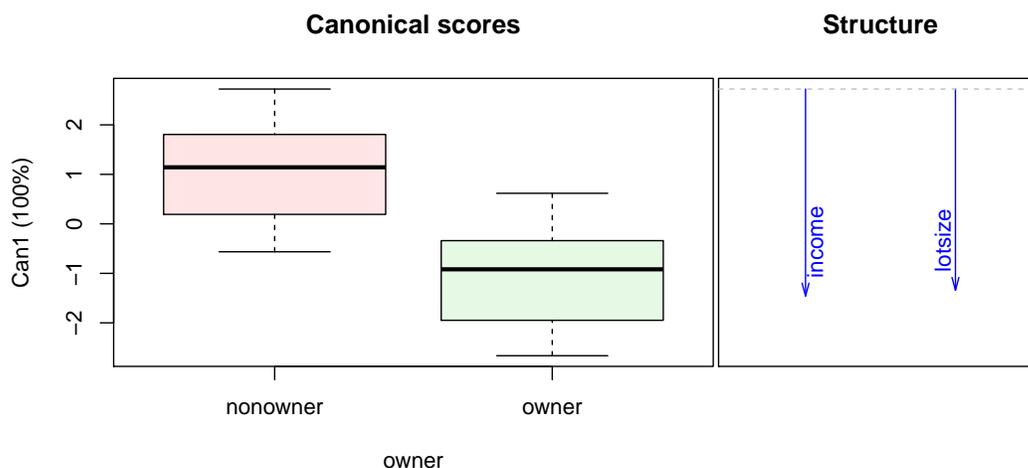
```

names(can_mower) # list of objects in can_mower
## [1] "dfh"      "dfe"      "eigenvalues" "canrsq"
## [5] "pct"      "rank"     "ndim"       "means"
## [9] "factors"  "term"     "terms"      "coeffs.raw"
## [13] "coeffs.std" "structure" "scores"

plot(can_mower) # boxplots with proportional contribution of each variable to Can1

### can also plot 2D plots when have more than two groups (will use later)
## library(heplots)
#heplot(can_mower, scale=6, fill=TRUE)
#heplot3d(can_mower, scale=6, fill=TRUE)

```



The raw canonical coefficients define the canonical discriminant variables and are identical to the feature loadings in a one-way MANOVA, except for an unimportant multiplicative factor. Only Can1 is generated here.

```
can_mower$coeffs.raw
##           Can1
## income  -0.1453404
## lotsize  -0.7590457
```

The means output gives the mean score on the canonical discriminant variables by group, after centering the scores to have mean zero over all groups. These are in order of the owner factor levels (nonowner, owner).

```
can_mower$means
## [1]  1.034437 -1.034437
```

The linear combination of income and lotsize that best distinguishes owners from non-owners

$$\text{Can1} = -0.1453 \text{ INCOME} + -0.759 \text{ LOTSIZ}$$

is a weighted average of income and lotsize.

In the scatterplot below, Can1 is the direction indicated by the dashed line.

```
library(ggplot2)

# Scatterplots with Can1 line overlaid
p <- ggplot(dat_mower, aes(x = income, y = lotsize, shape = owner, colour = owner))
p <- p + geom_point(size = 3)

# use a little algebra to determine the intercept and slopes of the
# Can1 line and a line perpendicular to it.

# dashed line of Can1
b1 <- can_mower$coeffs.raw[1]/can_mower$coeffs.raw[2] # slope
a1 <- mean(dat_mower$lotsize) - b1 * mean(dat_mower$income) - 3.5 # intercept
p <- p + geom_abline(intercept = a1, slope = b1, linetype = 2)
p <- p + annotate("text", x = 10, y = 6, label = "Can1"
, hjust = 0, vjust = 1, size = 4)

# solid line to separate groups (perpendicular to Can1)
b2 <- -can_mower$coeffs.raw[2]/can_mower$coeffs.raw[1] # slope
a2 <- mean(dat_mower$lotsize) - b2 * mean(dat_mower$income) - 4.5 # intercept
p <- p + geom_abline(intercept = a2, slope = b2, linetype = 1, alpha = 0.5)
p <- p + annotate("text", x = 22, y = 15, label = "Perp to Can1 for discrim"
, hjust = 0, vjust = 1, size = 4)

p <- p + scale_y_continuous(limits = c(0, 15))
p <- p + scale_x_continuous(limits = c(0, 40))
p <- p + coord_fixed(ratio = 1) # square axes (for perp lines)
```

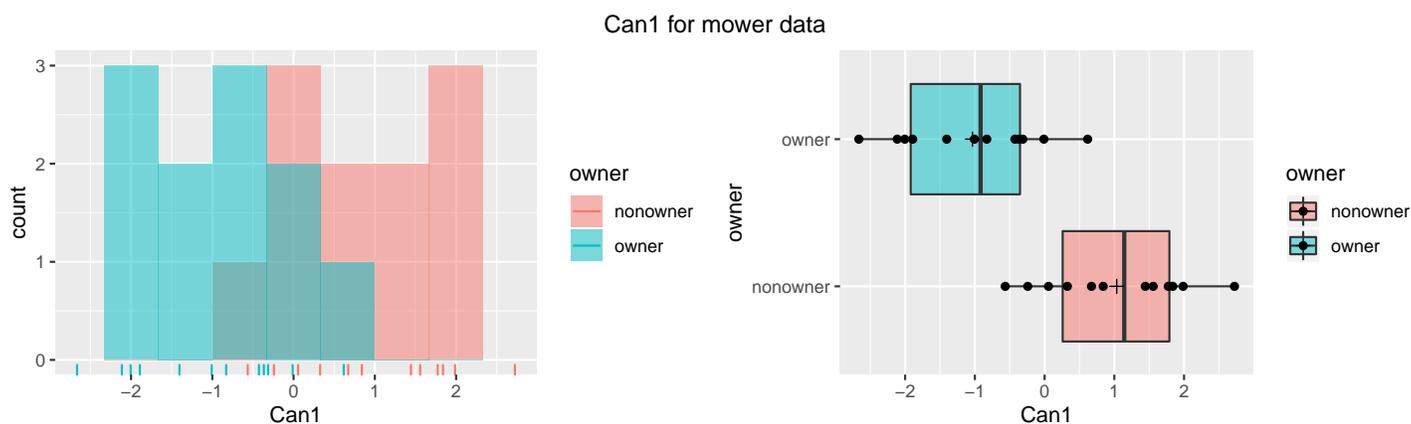
```
p <- p + labs(x = "Income in $1000"
             , y = "Lot size in 1000 sq ft"
             , caption = "Dashed line is Can1"
             )
print(p)
```



```
# Plots of Can1
p1 <- ggplot(can_mower$scores, aes(x = Can1, fill = owner))
p1 <- p1 + geom_histogram(binwidth = 2/3, alpha = 0.5, position="identity")
p1 <- p1 + scale_x_continuous(limits = c(min(can_mower$scores$Can1), max(can_mower$scores$Can1)))
p1 <- p1 + geom_rug(aes(colour = owner))
#p1 <- p1 + labs(title = "Can1 for mower data")
#print(p1)

p2 <- ggplot(can_mower$scores, aes(y = Can1, x = owner, fill = owner))
p2 <- p2 + geom_boxplot(alpha = 0.5)
# add a "+" at the mean
p2 <- p2 + stat_summary(fun.y = mean, geom = "point", shape = 3, size = 2)
p2 <- p2 + geom_point()
p2 <- p2 + coord_flip()
p2 <- p2 + scale_y_continuous(limits = c(min(can_mower$scores$Can1), max(can_mower$scores$Can1)))
#p2 <- p2 + labs(title = "Can1 for mower data")
#print(p2)

library(gridExtra)
grid.arrange(grobs = list(p1, p2), ncol=2, top = "Can1 for mower data")
## Warning: Removed 4 rows containing missing values (geom.bar).
```



The standardized coefficients (use the pooled within-class coefficients) in-

dicating the relative contributions of the features to the discrimination. The standardized coefficients are roughly equal, which suggests that income and lotsize contribute similarly to distinguishing the owners from non-owners.

```
can_mower$coeffs.std
##           Can1
## income -0.8058419
## lotsize -0.7845512
```

The p-value of 0.0004 on the likelihood ratio test indicates that Can1 strongly distinguishes between owners and non-owners. This is consistent with the separation between owners and non-owners in the boxplot of Can1 scores.

I noted above that Can1 is essentially the same linear combination given in a MANOVA comparison of owners to non-owners. Here is some `Manova()` output to support this claim. The MANOVA test p-values agree with the `candisc` output (as we saw earlier). The first characteristic vector from the MANOVA is given here.

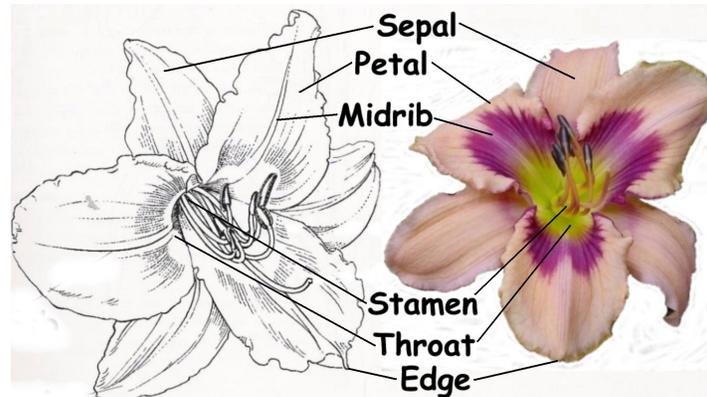
```
## For Roy's characteristic Root and vector
H <- man_mower$SSP$owner # H = hypothesis matrix
E <- man_mower$SSPE      # E = error matrix
# characteristic roots of (E inverse * H)
EinvH <- solve(E) %*% H # solve() computes the matrix inverse
ev <- eigen(EinvH)      # eigenvalue/eigenvectors
ev
## eigen() decomposition
## $values
## [1] 1.167337 0.000000
##
## $vectors
##           [,1]      [,2]
## [1,] 0.1880613 -0.1761379
## [2,] 0.9821573  0.9843655
mult_char_can_disc <- can_mower$coeffs.raw[1] / ev$vectors[1,1]
mult_char_can_disc
## [1] -0.7728352
```

The first canonical discriminant function is obtained by multiplying the first characteristic vector given in MANOVA by -0.7728:

$$\begin{aligned} \text{Can1} &= -0.1453 \text{ INCOME} + -0.759 \text{ LOTSIZ} \\ &= -0.7728 (0.1881 \text{ INCOME} + 0.9822 \text{ LOTSIZ}) \end{aligned}$$

16.3 Discriminant Analysis on Fisher's Iris Data

Fisher's iris data consists of samples of 50 flowers from each of three species of iris: Setosa, Versicolor, and Virginica. Four measurements (in mm) were taken on each flower: sepal length, sepal width, petal length, and petal width.



The plots show big differences between Setosa and the other two species. The differences between Versicolor and Virginica are smaller, and appear to be mostly due to differences in the petal widths and lengths.

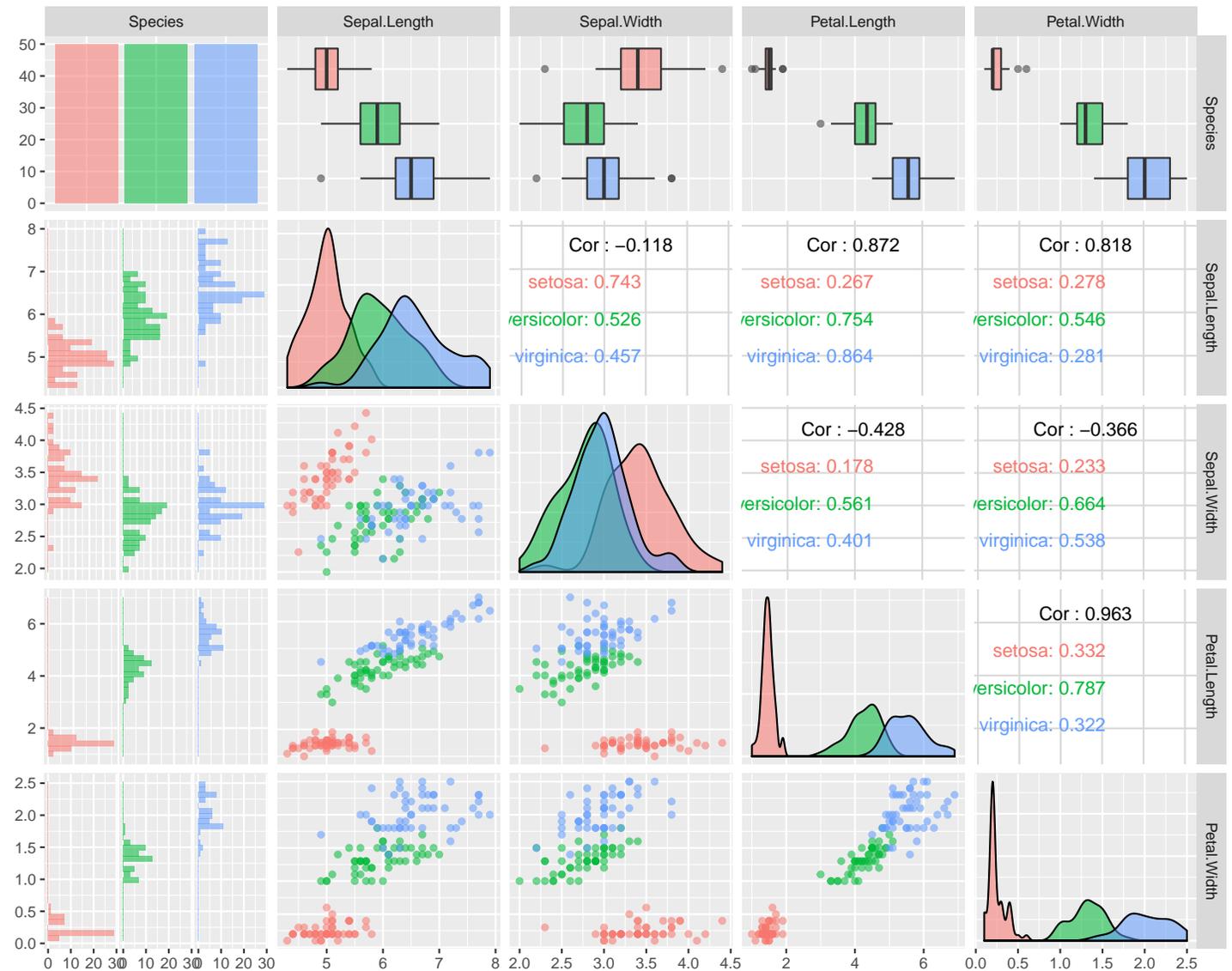
```
#### Example: Fisher's iris data
# The "iris" dataset is included with R in the library(datasets)
data(iris)
str(iris)

## 'data.frame': 150 obs. of 5 variables:
## $ Sepal.Length: num  5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
## $ Sepal.Width : num  3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
## $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
## $ Petal.Width : num  0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
## $ Species      : Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 1 ...

## Scatterplot matrix
library(ggplot2)
library(GGally)
p <-
  ggpairs(
    iris[,c(5,1,2,3,4)]
    , mapping = ggplot2::aes(colour = Species, alpha = 0.5)
    , progress = FALSE
  )
print(p)

## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```

```
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```



```
## parallel coordinate plot
library(ggplot2)
library(GGally)
```

```
# univariate min/max scaling
```

```
p1 <- ggparcoord(
  data = iris
  , columns = 1:4
  , groupColumn = 5
  , order = "anyClass"
  , scale = "uniminmax" # "uniminmax". "globalminmax"
  , showPoints = FALSE
  , title = "uniminmax scaling"
  , alphaLines = 1/3
  #, shadeBox = "white"
```

```

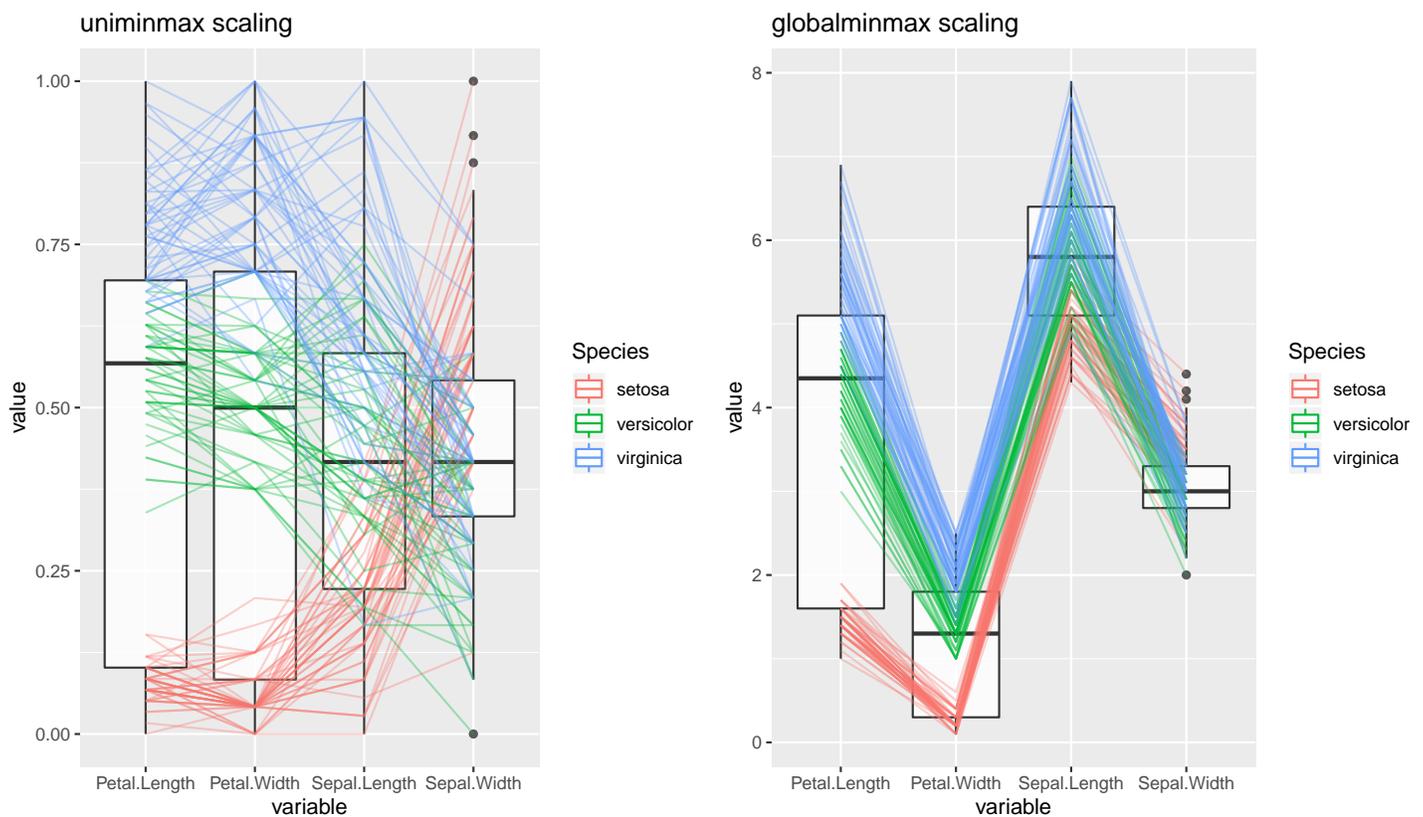
, boxplot = TRUE
) #+ theme_bw()

# global min/max scaling
p2 <- ggparcoord(
  data = iris
, columns = 1:4
, groupColumn = 5
, order = "anyClass"
, scale = "globalminmax" # "uniminmax". "globalminmax"
, showPoints = FALSE
, title = "globalminmax scaling"
, alphaLines = 1/3
#, shadeBox = "white"
, boxplot = TRUE
) #+ theme_bw()

library(gridExtra)
grid.arrange(grobs = list(p1, p2), ncol=2, top = "Parallel Coordinate Plots of Iris data")

```

Parallel Coordinate Plots of Iris data



`candisc` was used to discriminate among species. There are $k = 3$ species and $p = 4$ features, so the number of discriminant functions is 2 (the minimum of 4 and $3 - 1$).

```

# first fit lm() with formula = continuous variables ~ factor variables
lm_iris <-
  lm(
    cbind(Sepal.Length, Sepal.Width, Petal.Length, Petal.Width) ~ Species
    , data = iris
  )

## univariate ANOVA tests
#summary(lm_iris)
## test whether the multivariate means of the two populations are different
#library(car)
#man_mower <- Manova(lm_iris)
#summary(man_mower)
# perform canonical discriminant analysis

library(candisc)
can_iris <- candisc(lm_iris)
can_iris$coeffs.raw

##              Can1          Can2
## Sepal.Length -0.8293776  0.02410215
## Sepal.Width  -1.5344731  2.16452123
## Petal.Length  2.2012117 -0.93192121
## Petal.Width   2.8104603  2.83918785

```

Can1 is a comparison of petal and sepal measurements (from Raw Canonical Coefficients):

$$\text{Can1} = -0.8294 \text{ sepalL} + -1.534 \text{ sepalW} + 2.201 \text{ petalL} + 2.81 \text{ petalW}.$$

Can2 is not easily interpreted, though perhaps a comparison of lengths and widths ignoring sepalL:

$$\text{Can2} = 0.0241 \text{ sepalL} + 2.165 \text{ sepalW} + -0.9319 \text{ petalL} + 2.839 \text{ petalW}.$$

The canonical directions provide a maximal separation the species. Two lines across Can1 will provide a classification rule.

```

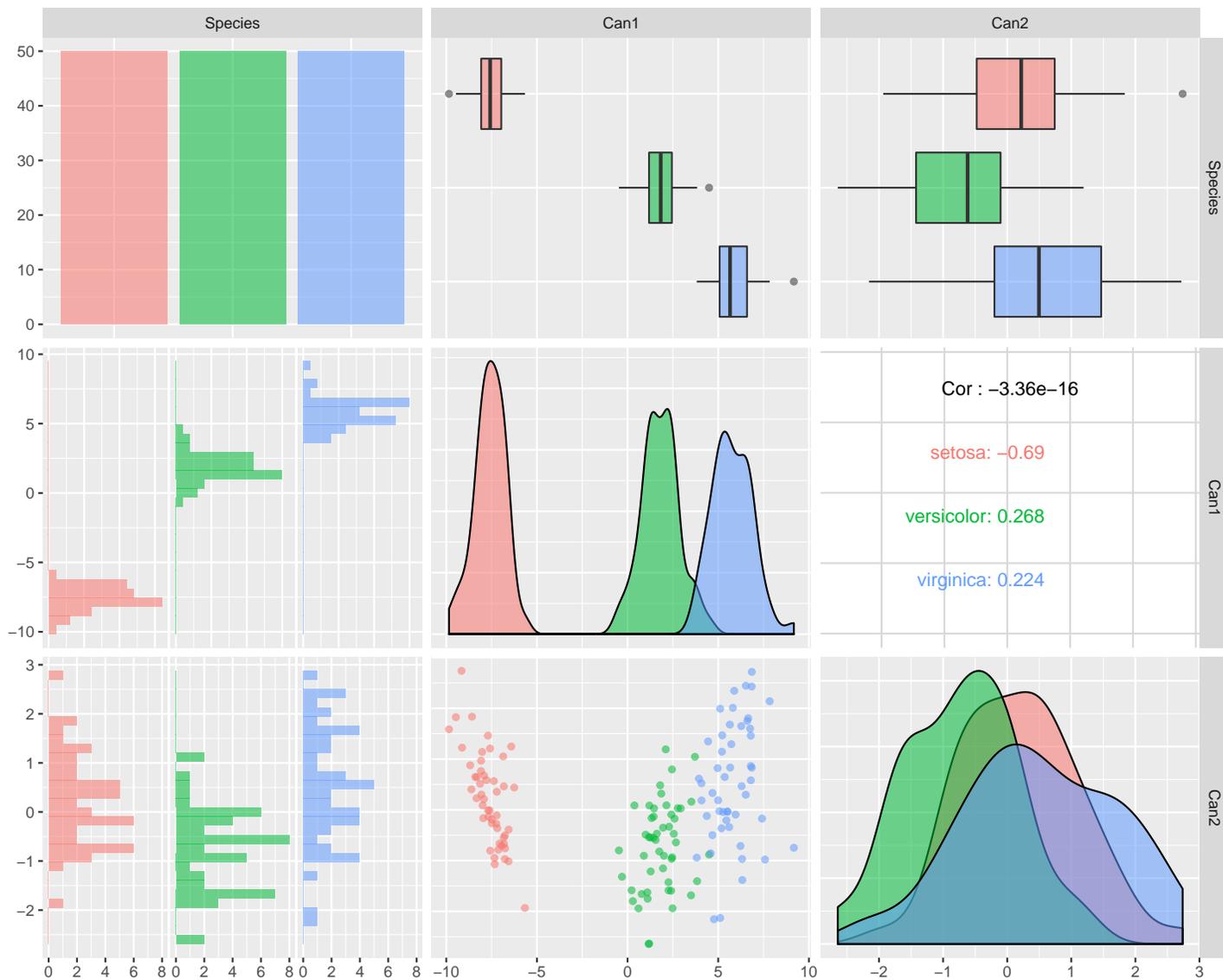
## Scatterplot matrix
library(ggplot2)
library(GGally)
p <-
  ggpairs(
    can_iris$scores
    , mapping = ggplot2::aes(colour = Species, alpha = 0.5)
    , progress = FALSE
  )

```

```
)
print(p)
```

```
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```

```
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```



There are significant differences among species on both discriminant functions; see the p-values under the likelihood ratio tests. Of course, Can1 produces the largest differences — the overlap among species on Can1 is small. Setosa has the lowest Can1 scores because this species has the smallest petal measurements relative to its sepal measurements. Virginica has the highest Can1 scores.

```
can_iris
##
## Canonical Discriminant Analysis for Species:
```

```
##
##      CanRsq Eigenvalue Difference   Percent Cumulative
## 1 0.96987   32.19193    31.907 99.12126    99.121
## 2 0.22203    0.28539    31.907  0.87874   100.000
##
## Test of H0: The canonical correlations in the
## current row and all that follow are zero
##
##      LR test stat approx F numDF denDF   Pr(> F)
## 1      0.02344  199.145     8   288 < 2.2e-16 ***
## 2      0.77797   13.794     3   145 5.794e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Questions:

1. What is the most striking feature of the plot of the Can1 scores?
2. Does the assumption of equal population covariance matrices across species seem plausible?
3. How about multivariate normality?

```
# Covariance matrices by species
by(iris[,1:4], iris$Species, cov)
## iris$Species: setosa
##           Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length  0.12424898 0.099216327  0.016355102 0.010330612
## Sepal.Width   0.09921633 0.143689796  0.011697959 0.009297959
## Petal.Length  0.01635510 0.011697959  0.030159184 0.006069388
## Petal.Width   0.01033061 0.009297959  0.006069388 0.011106122
## -----
## iris$Species: versicolor
##           Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length  0.26643265 0.08518367  0.18289796  0.05577959
## Sepal.Width   0.08518367 0.09846939  0.08265306  0.04120408
## Petal.Length  0.18289796 0.08265306  0.22081633  0.07310204
## Petal.Width   0.05577959 0.04120408  0.07310204  0.03910612
## -----
## iris$Species: virginica
##           Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length  0.40434286 0.09376327  0.30328980  0.04909388
## Sepal.Width   0.09376327 0.10400408  0.07137959  0.04762857
## Petal.Length  0.30328980 0.07137959  0.30458776  0.04882449
## Petal.Width   0.04909388 0.04762857  0.04882449  0.07543265
```

```
# Test multivariate normality using the Shapiro-Wilk test for multivariate normality
library(mvnormtest)
```

```

# The data needs to be transposed t() so each variable is a row
# with observations as columns.

mshapiro.test(t(iris[iris$Species == "setosa" , 1:4]))
##
## Shapiro-Wilk normality test
##
## data: Z
## W = 0.95878, p-value = 0.07906
mshapiro.test(t(iris[iris$Species == "versicolor", 1:4]))
##
## Shapiro-Wilk normality test
##
## data: Z
## W = 0.93043, p-value = 0.005739
mshapiro.test(t(iris[iris$Species == "virginica" , 1:4]))
##
## Shapiro-Wilk normality test
##
## data: Z
## W = 0.93414, p-value = 0.007955

# Graphical Assessment of Multivariate Normality
par(mfrow=c(1,3))
f_mnv_norm_qqplot(iris[iris$Species == "setosa" , 1:4], "setosa" )
f_mnv_norm_qqplot(iris[iris$Species == "versicolor", 1:4], "versicolor")
f_mnv_norm_qqplot(iris[iris$Species == "virginica" , 1:4], "virginica" )
par(mfrow=c(1,1))

```

