Multivariate Analysis using R

In my next series of articles, I will demonstrate how to use the R statistical software to carry out some simple multivariate analyses, with a focus on principal components analysis (PCA) and linear discriminant analysis (LDA). PCA and LDA, will constitute parts II and III, respectively.

The first thing that you will want to do to analyze your multivariate data will be to load it into R, and to plot the data. You can load dataset into R using the require(rattle), 'wine' is a data set in this package. The dataset 'wine' contains data on concentrations of 13 different chemicals in wines grown in the same region in Italy that are derived from three different cultivars.

There is one row per wine sample. The first column contains the cultivar of a wine sample (labelled 1, 2 or 3), and the following thirteen columns contain the concentrations of the 13 different chemicals in that sample. The columns are separated by commas. We can load in the file using the require() function as follows:

```
require(rattle)
wine # a dataset in the rattle package
     V1    V2   V3   V4   V5  V6   V7   V8   V9  V10       V11   V12  V13  V14
 1    1 14.23 1.71 2.43 15.6 127 2.80 3.06 0.28 2.29  5.640000 1.040 3.92 1065
 2    1 13.20 1.78 2.14 11.2 100 2.65 2.76 0.26 1.28  4.380000 1.050 3.40 1050
 3    1 13.16 2.36 2.67 18.6 101 2.80 3.24 0.30 2.81  5.680000 1.030 3.17 1185
 4    1 14.37 1.95 2.50 16.8 113 3.85 3.49 0.24 2.18  7.800000 0.860 3.45 1480
 5    1 13.24 2.59 2.87 21.0 118 2.80 2.69 0.39 1.82  4.320000 1.040 2.93  735
 ...
 176  3 13.27 4.28 2.26 20.0 120 1.59 0.69 0.43 1.35 10.200000 0.590 1.56  835
 177  3 13.17 2.59 2.37 20.0 120 1.65 0.68 0.53 1.46  9.300000 0.600 1.62  840
 178  3 14.13 4.10 2.74 24.5  96 2.05 0.76 0.56 1.35  9.200000 0.610 1.60  560
```

In this case the data on 178 samples of wine has been read into the variable 'wine'.

Plotting Multivariate Data

Once you have read a multivariate data set into R, the next step is usually to make a plot of the data.

A Matrix Scatterplot

One common way of plotting multivariate data is to make a "matrix scatterplot", showing each pair of variables plotted against each other. We can use the "scatterplotMatrix()" function from the "car" R package to do this. To use this function, we first need to install the "car" R package (for instructions on how to install an R package, see How to install an R package).

Once you have installed the "car" R package, you can load the "car" R package by typing:

```
> library("car")
```

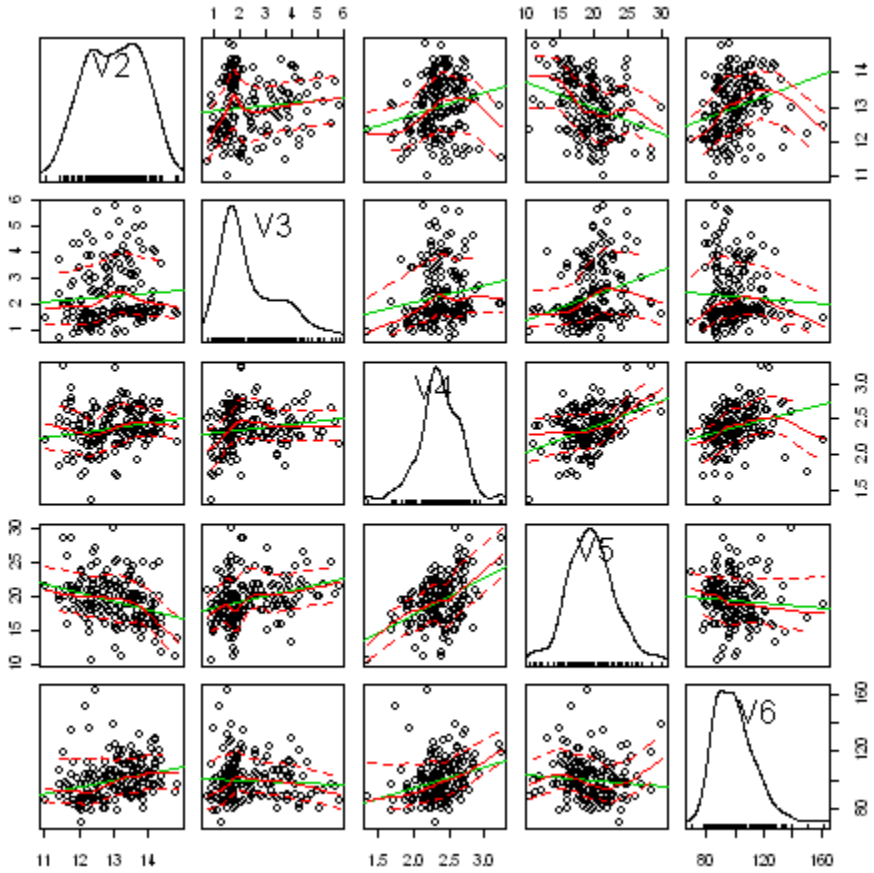
You can then use the "scatterplotMatrix()" function to plot the multivariate data.

To use the scatterplotMatrix() function, you need to give it as its input the variables that you want included in the plot. Say for example, that we just want to include the variables corresponding to the concentrations of the first five chemicals. These are stored in columns 2-6 of the variable "wine". We can extract just these columns from the variable "wine" by typing:

```
> wine[2:6]
         V2   V3   V4   V5  V6
  1   14.23 1.71 2.43 15.6 127
  2   13.20 1.78 2.14 11.2 100
  3   13.16 2.36 2.67 18.6 101
  4   14.37 1.95 2.50 16.8 113
  5   13.24 2.59 2.87 21.0 118
  ...
```

To make a matrix scatterplot of just these 13 variables using the scatterplotMatrix() function we type:

```
> scatterplotMatrix(wine[2:6])
```



In this matrix scatterplot, the diagonal cells show histograms of each of the variables, in this case the concentrations of the first five chemicals (variables V2, V3, V4, V5, V6).

Each of the off-diagonal cells is a scatterplot of two of the five chemicals, for example, the second cell in the first row is a scatterplot of V2 (y-axis) against V3 (x-axis).

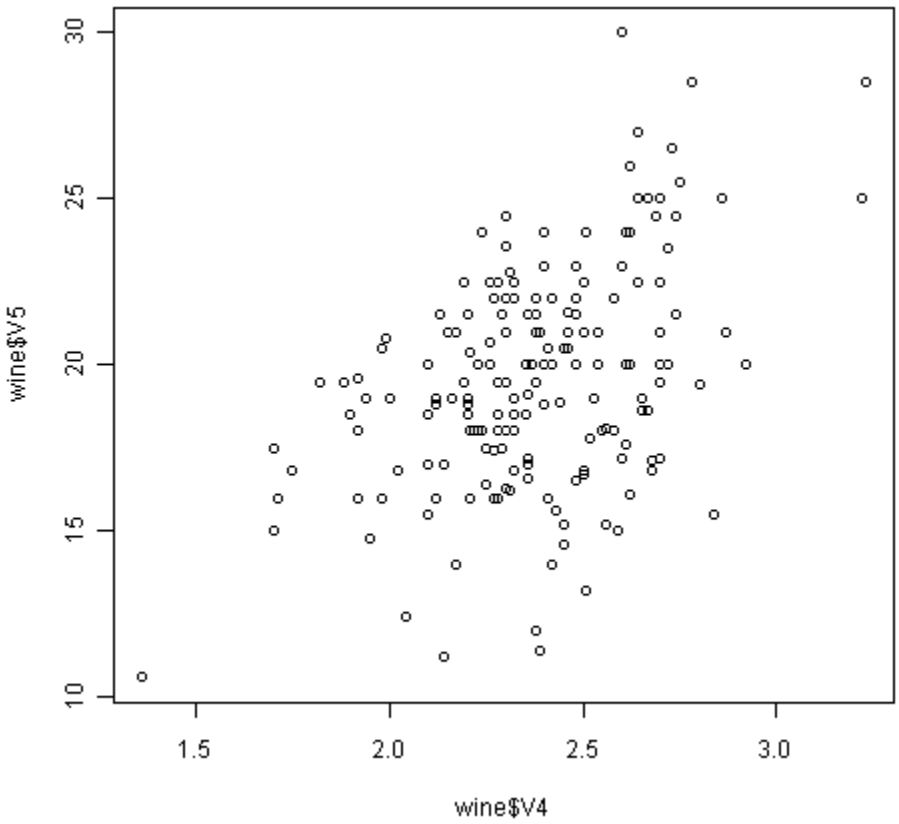
A Scatterplot with the Data Points Labelled by their Group

If you see an interesting scatterplot for two variables in the matrix scatterplot, you may want to plot that scatterplot in more detail, with the data points labelled by their group (their cultivar in this case).

For example, in the matrix scatterplot above, the cell in the third column of the fourth row down is a scatterplot of V5 (x-axis) against V4 (y-axis). If you look at this scatterplot, it appears that there may be a positive relationship between V5 and V4.

We may therefore decide to examine the relationship between V5 and V4 more closely, by plotting a scatterplot of these two variable, with the data points labelled by their group (their cultivar). To plot a scatterplot of two variables, we can use the "plot" R function. The V4 and V5 variables are stored in the columns V4 and V5 of the variable "wine", so can be accessed by typing wine$V4 or wine$V5. Therefore, to plot the scatterplot, we type:

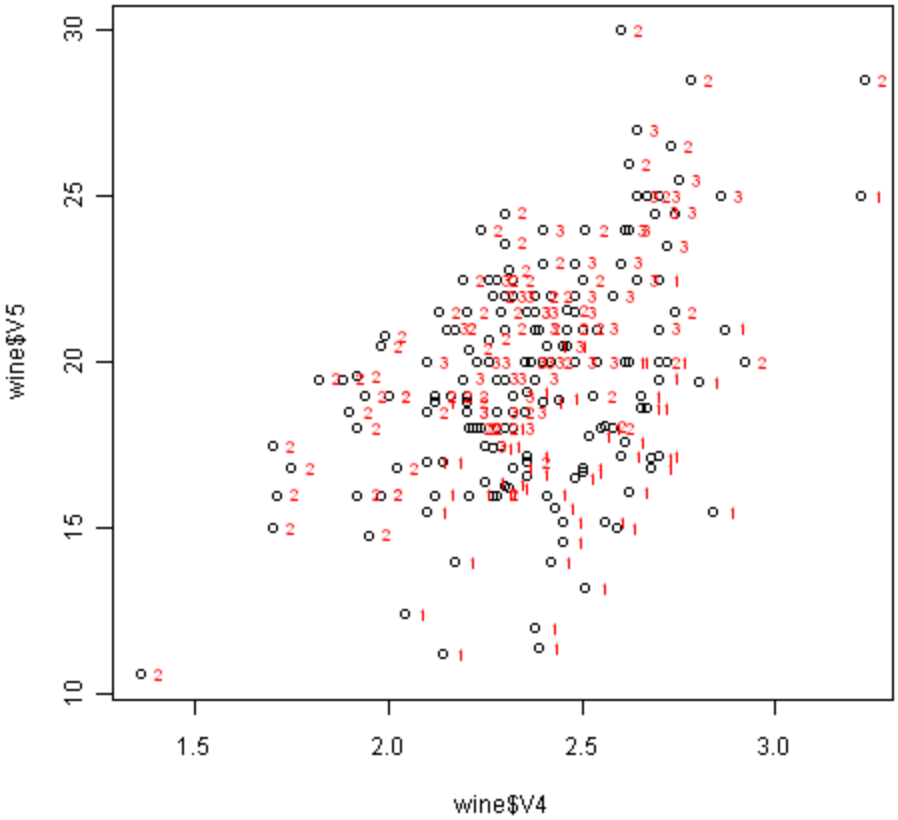
```
> plot(wine$V4, wine$V5)
```



If we want to label the data points by their group (the cultivar of wine here), we can use the "text" function in R to plot some text beside every data point. In this case, the cultivar of wine is stored in the column V1 of the variable "wine", so we type:

```
> text(wine$V4, wine$V5, wine$V1, cex=0.7, pos=4, col="red")
```

If you look at the help page for the "text" function, you will see that "pos=4" will plot the text just to the right of the symbol for a data point. The "cex=0.5" option will plot the text at half the default size, and the "col=red" option will plot the text in red. This gives us the following plot:



We can see from the scatterplot of V4 versus V5 that the wines from cultivar 2 seem to have lower values of V4 compared to the wines of cultivar 1.

A Profile Plot

Another type of plot that is useful is a "profile plot", which shows the variation in each of the variables, by plotting the value of each of the variables for each of the samples.

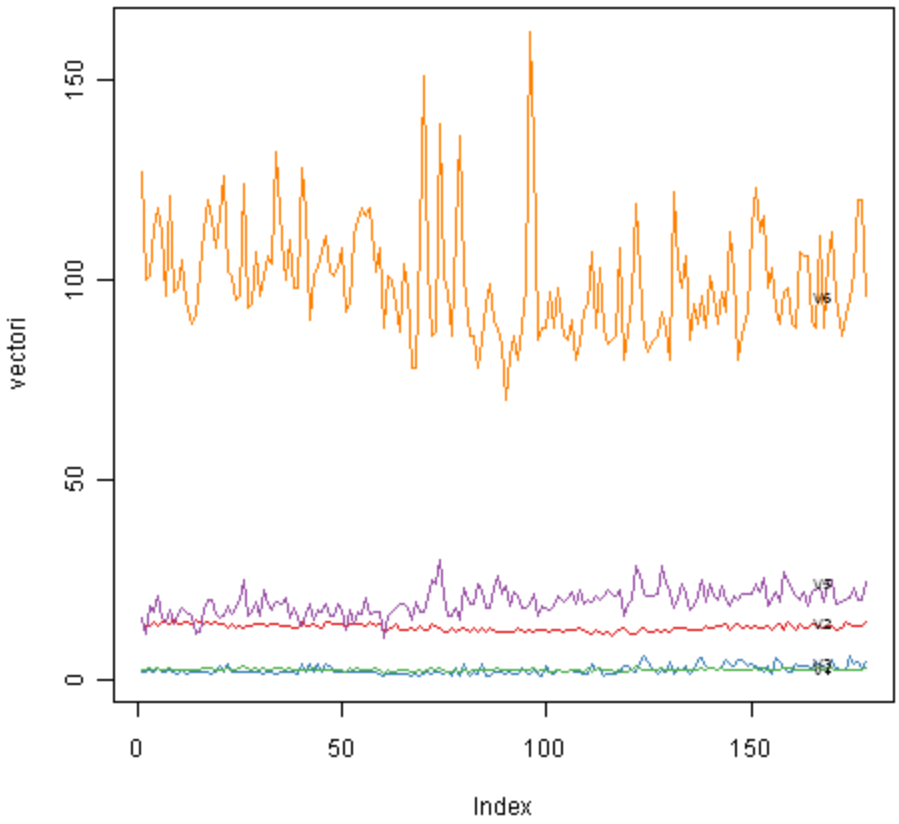
The function "makeProfilePlot()" below can be used to make a profile plot. This function requires the "RColorBrewer" library. To use this function, we first need to install the "RColorBrewer" R package (for instructions on how to install an R package, see How to install an R package).

```
> makeProfilePlot <- function(mylist,names)
  {
     require(RColorBrewer)
     # find out how many variables we want to include
     numvariables <- length(mylist)
     # choose 'numvariables' random colors
     colors <- brewer.pal(numvariables,"Set1")
     # find out the minimum and maximum values of the variables:
     mymin <- 1e+20
     mymax <- 1e-20
     for (i in 1:numvariables)
     {
        vectori <- mylist[[i]]
        mini <- min(vectori)
        maxi <- max(vectori)
        if (mini < mymin) { mymin <- mini }
        if (maxi > mymax) { mymax <- maxi }
     }
     # plot the variables
     for (i in 1:numvariables)
     {
        vectori <- mylist[[i]]
        namei <- names[i]
        colori <- colors[i]
        if (i == 1) { plot(vectori,col=colori,type="l",ylim=c(mymin,mymax)) }
        else         { points(vectori, col=colori,type="l") }
        lastxval <- length(vectori)
        lastyval <- vectori[length(vectori)]
        text((lastxval-10),(lastyval),namei,col="black",cex=0.6)
     }
  }
```

To use this function, you first need to copy and paste it into R. The arguments to the function are a vector containing the names of the varibles that you want to plot, and a list variable containing the variables themselves.

For example, to make a profile plot of the concentrations of the first five chemicals in the wine samples (stored in columns V2, V3, V4, V5, V6 of variable “wine”), we type:

```
> library(RColorBrewer)
> names <- c("V2","V3","V4","V5","V6")
> mylist <- list(wine$V2,wine$V3,wine$V4,wine$V5,wine$V6)
> makeProfilePlot(mylist,names)
```



It is clear from the profile plot that the mean and standard deviation for V6 is quite a lot higher than that for the other variables.

Calculating Summary Statistics for Multivariate Data

Another thing that you are likely to want to do is to calculate summary statistics such as the mean and standard deviation for each of the variables in your multivariate data set.

sapply

The “sapply()” function can be used to apply some other function to each column in a data frame, eg. sapply(mydataframe,sd) will calculate the standard deviation of each column in a dataframe “mydataframe”.

This is easy to do, using the “mean()” and “sd()” functions in R. For example, say we want to calculate the mean and standard deviations of each of the 13 chemical concentrations in the wine samples. These are stored in columns 2-14 of the variable “wine”. So we type:

```
> sapply(wine[2:14],mean)
         V2          V3          V4          V5          V6          V7
 13.0006180   2.3363483   2.3665169  19.4949438  99.7415730   2.2951124
         V8          V9         V10         V11         V12         V13
  2.0292697   0.3618539   1.5908989   5.0580899   0.9574494   2.6116854
         V14
746.8932584
```

This tells us that the mean of variable V2 is 13.0006180, the mean of V3 is 2.3363483, and so on.

Similarly, to get the standard deviations of the 13 chemical concentrations, we type:

```
> sapply(wine[2:14],sd)
         V2          V3          V4          V5          V6          V7
  0.8118265   1.1171461   0.2743440   3.3395638  14.2824835   0.6258510
         V8          V9         V10         V11         V12         V13
  0.9988587   0.1244533   0.5723589   2.3182859   0.2285716   0.7099904
         V14
  314.9074743
```

We can see here that it would make sense to standardize in order to compare the variables because the variables have very different standard deviations - the standard deviation of V14 is 314.9074743, while the standard deviation of V9 is just 0.1244533. Thus, in order to compare the variables, we need to standardize each variable so that it has a sample variance of 1 and sample mean of 0. We will explain below how to standardize the variables.

Means and Variances Per Group

It is often interesting to calculate the means and standard deviations for just the samples from a particular group, for example, for the wine samples from each cultivar. The cultivar is stored in the column "V1" of the variable "wine".

To extract out the data for just cultivar 2, we can type:

```
> cultivar2wine <- wine[wine$V1=="2",]
```

We can then calculate the mean and standard deviations of the 13 chemicals' concentrations, for just the cultivar 2 samples:

```
> sapply(cultivar2wine[2:14],mean)
    V2         V3         V4         V5         V6         V7         V8
 12.278732   1.932676   2.244789  20.238028  94.549296   2.258873   2.080845
    V9        V10        V11        V12        V13        V14
  0.363662   1.630282   3.086620   1.056282   2.785352 519.507042
> sapply(cultivar2wine[2:14])
    V2          V3          V4          V5          V6          V7          V8
 0.5379642   1.0155687   0.3154673   3.3497704  16.7534975   0.5453611   0.7057008
    V9         V10         V11         V12         V13         V14
 0.1239613   0.6020678   0.9249293   0.2029368   0.4965735 157.2112204
```

You can calculate the mean and standard deviation of the 13 chemicals' concentrations for just cultivar 1 samples, or for just cultivar 3 samples, in a similar way.

However, for convenience, you might want to use the function "printMeanAndSdByGroup()" below, which prints out the mean and standard deviation of the variables for each group in your data set:

```
> printMeanAndSdByGroup <- function(variables,groupvariable)
  {
     # find the names of the variables
     variablenames <- c(names(groupvariable),names(as.data.frame(variables)))
     # within each group, find the mean of each variable
     groupvariable <- groupvariable[,1] # ensures groupvariable is not a list
     means <- aggregate(as.matrix(variables) ~ groupvariable, FUN = mean)
     names(means) <- variablenames
     print(paste("Means:"))
     print(means)
     # within each group, find the standard deviation of each variable:
     sds <- aggregate(as.matrix(variables) ~ groupvariable, FUN = sd)
     names(sds) <- variablenames
     print(paste("Standard deviations:"))
     print(sds)
     # within each group, find the number of samples:
     samplesizes <- aggregate(as.matrix(variables) ~ groupvariable, FUN = length)
     names(samplesizes) <- variablenames
     print(paste("Sample sizes:"))
     print(samplesizes)
  }
```

To use the function "printMeanAndSdByGroup()", you first need to copy and paste it into R. The arguments of the function are the variables that you want to calculate means and standard deviations for, and the variable containing the group of each sample. For example, to calculate the mean and standard deviation for each of the 13 chemical concentrations, for each of the three different wine cultivars, we type:

```
> printMeanAndSdByGroup(wine[2:14],wine[1])
  [1] "Means:"
    V1       V2       V3       V4       V5       V6       V7        V8       V9
  1  1 13.74475 2.010678 2.455593 17.03729 106.3390 2.840169 2.9823729 0.290000
  2  2 12.27873 1.932676 2.244789 20.23803  94.5493 2.258873 2.0808451 0.363662
  3  3 13.15375 3.333750 2.437083 21.41667  99.3125 1.678750 0.7814583 0.447500
       V10      V11       V12      V13       V14
  1.899322 5.528305 1.0620339 3.157797 1115.7119
  1.630282 3.086620 1.0562817 2.785352  519.5070
  1.153542 7.396250 0.6827083 1.683542  629.8958
  [1] "Standard deviations:"
    V1       V2       V3       V4      V5       V6       V7       V8         V9
  1  1 0.462125 0.688549 0.227166 2.54632 10.49895 0.338961 0.397494 0.07004924
  2  2 0.537964 1.015569 0.315467 3.34977 16.75350 0.545361 0.705701 0.12396128
  3  3 0.530241 1.087906 0.184690 2.25816 10.89047 0.356971 0.293504 0.12413959
        V10       V11       V12       V13      V14
  0.4121092 1.2385728 0.1164826 0.3570766 221.5208
  0.6020678 0.9249293 0.2029368 0.4965735 157.2112
  0.4088359 2.3109421 0.1144411 0.2721114 115.0970
  [1] "Sample sizes:"
    V1 V2 V3 V4 V5 V6 V7 V8 V9 V10 V11 V12 V13 V14
  1  1 59 59 59 59 59 59 59 59  59  59  59  59  59
  2  2 71 71 71 71 71 71 71 71  71  71  71  71  71
  3  3 48 48 48 48 48 48 48 48  48  48  48  48  48
```

The function "printMeanAndSdByGroup()" also prints out the number of samples in each group. In this case, we see that there are 59 samples of cultivar 1, 71 of cultivar 2, and 48 of cultivar 3.

Between-groups Variance and Within-groups Variance for a Variable

If we want to calculate the within-groups variance for a particular variable (for example, for a particular chemical's concentration), we can use the function "calcWithinGroupsVariance()" below:

```
> calcWithinGroupsVariance <- function(variable,groupvariable)
  {
     # find out how many values the group variable can take
     groupvariable2 <- as.factor(groupvariable[[1]])
     levels <- levels(groupvariable2)
     numlevels <- length(levels)
     # get the mean and standard deviation for each group:
     numtotal <- 0
     denomtotal <- 0
     for (i in 1:numlevels)
     {
        leveli <- levels[i]
        levelidata <- variable[groupvariable==leveli,]
        levelilength <- length(levelidata)
        # get the standard deviation for group i:
        sdi <- sd(levelidata)
        numi <- (levelilength - 1)*(sdi * sdi)
        denomi <- levelilength
        numtotal <- numtotal + numi
        denomtotal <- denomtotal + denomi
     }
     # calculate the within-groups variance
     Vw <- numtotal / (denomtotal - numlevels)
     return(Vw)
  }
```

You will need to copy and paste this function into R before you can use it. For example, to calculate the within-groups variance of the variable V2 (the concentration of the first chemical), we type:

```
> calcWithinGroupsVariance(wine[2],wine[1])
  [1] 0.2620525
```

Thus, the within-groups variance for V2 is 0.2620525.

We can calculate the between-groups variance for a particular variable (eg. V2) using the function "calcBetweenGroupsVariance()" below:

```
> calcBetweenGroupsVariance <- function(variable,groupvariable)
  {
     # find out how many values the group variable can take
     groupvariable2 <- as.factor(groupvariable[[1]])
     levels <- levels(groupvariable2)
     numlevels <- length(levels)
     # calculate the overall grand mean:
     grandmean <- mean(variable)
     # get the mean and standard deviation for each group:
     numtotal <- 0
     denomtotal <- 0
     for (i in 1:numlevels)
     {
        leveli <- levels[i]
        levelidata <- variable[groupvariable==leveli,]
        levelilength <- length(levelidata)
        # get the mean and standard deviation for group i:
        meani <- mean(levelidata)
        sdi <- sd(levelidata)
        numi <- levelilength * ((meani - grandmean)^2)
        denomi <- levelilength
        numtotal <- numtotal + numi
        denomtotal <- denomtotal + denomi
     }
     # calculate the between-groups variance
     Vb <- numtotal / (numlevels - 1)
     Vb <- Vb[[1]]
     return(Vb)
  }
```

Once you have copied and pasted this function into R, you can use it to calculate the between-groups variance for a variable such as V2:

```
> calcBetweenGroupsVariance (wine[2],wine[1])
  [1] 35.39742
```

Thus, the between-groups variance of V2 is 35.39742.

We can calculate the “separation” achieved by a variable as its between-groups variance devided by its within-groups variance. Thus, the separation achieved by V2 is calculated as:

```
> 35.39742/0.2620525
  [1] 135.0776
```

If you want to calculate the separations achieved by all of the variables in a multivariate data set, you can use the function “calcSeparations()” below:

```
> calcSeparations <- function(variables,groupvariable)
  {
     # find out how many variables we have
     variables <- as.data.frame(variables)
     numvariables <- length(variables)
     # find the variable names
     variablenames <- colnames(variables)
     # calculate the separation for each variable
     for (i in 1:numvariables)
     {
        variablei <- variables[i]
        variablename <- variablenames[i]
        Vw <- calcWithinGroupsVariance(variablei, groupvariable)
        Vb <- calcBetweenGroupsVariance(variablei, groupvariable)
        sep <- Vb/Vw
        print(paste("variable",variablename,"Vw=",Vw,"Vb=",Vb,"separation=",sep))
     }
  }
```

For example, to calculate the separations for each of the 13 chemical concentrations, we type:

```
> calcSeparations(wine[2:14],wine[1])
  [1] "variable  V2 Vw= 0.262052469154 Vb= 35.3974249603 separation= 135.07762424"
  [1] "variable  V3 Vw= 0.887546796747 Vb= 32.7890184870 separation= 36.943424963"
  [1] "variable  V4 Vw= 0.066072101343 Vb= 0.87961135725 separation= 13.312901199"
  [1] "variable  V5 Vw= 8.006811181212 Vb= 286.416746363 separation= 35.771637407"
  [1] "variable  V6 Vw= 180.6577731644 Vb= 2245.50102789 separation= 12.429584338"
  [1] "variable  V7 Vw= 0.191270475225 Vb= 17.9283572943 separation= 93.733009620"
  [1] "variable  V8 Vw= 0.274707514338 Vb= 64.2611950236 separation= 233.92587268"
  [1] "variable  V9 Vw= 0.011911702213 Vb= 0.32847015746 separation= 27.575417147"
  [1] "variable V10 Vw= 0.246172943796 Vb= 7.45199550778 separation= 30.271383170"
  [1] "variable V11 Vw= 2.284923081334 Vb= 275.708000822 separation= 120.66401844"
  [1] "variable V12 Vw= 0.024487646943 Vb= 2.48100991494 separation= 101.31679539"
  [1] "variable V13 Vw= 0.160778729561 Vb= 30.5435083544 separation= 189.97232058"
  [1] "variable V14 Vw= 29707.68187052 Vb= 6176832.32228 separation= 207.92037390"
```

Thus, the individual variable which gives the greatest separations between the groups (the wine cultivars) is V8 (separation 233.9). As we will discuss below, the purpose of linear discriminant analysis (LDA) is to find the linear combination of the individual variables that will give the greatest separation between the groups (cultivars here). This hopefully will give a better separation than the best separation achievable by any individual variable (233.9 for V8 here).

Between-groups Covariance and Within-groups Covariance for Two Variables

If you have a multivariate data set with several variables describing sampling units from different groups, such as the wine samples from different cultivars, it is often of interest to calculate the within-groups covariance and between-groups variance for pairs of the variables.

This can be done using the following functions, which you will need to copy and paste into R to use them:

```
> calcWithinGroupsCovariance <- function(variable1,variable2,groupvariable)
  {
     # find out how many values the group variable can take
     groupvariable2 <- as.factor(groupvariable[[1]])
     levels <- levels(groupvariable2)
     numlevels <- length(levels)
```

```
    # get the covariance of variable 1 and variable 2 for each group:
    Covw <- 0
    for (i in 1:numlevels)
    {
       leveli <- levels[i]
       levelidata1 <- variable1[groupvariable==leveli,]
       levelidata2 <- variable2[groupvariable==leveli,]
       mean1 <- mean(levelidata1)
       mean2 <- mean(levelidata2)
       levelilength <- length(levelidata1)
       # get the covariance for this group:
       term1 <- 0
       for (j in 1:levelilength)
       {
          term1 <- term1 + ((levelidata1[j] - mean1)*(levelidata2[j] - mean2))
       }
       Cov_groupi <- term1 # covariance for this group
       Covw <- Covw + Cov_groupi
    }
    totallength <- nrow(variable1)
    Covw <- Covw / (totallength - numlevels)
    return(Covw)
  }
```

For example, to calculate the within-groups covariance for variables V8 and V11, we type:

```
> calcWithinGroupsCovariance(wine[8],wine[11],wine[1])
  [1] 0.2866783
> calcBetweenGroupsCovariance <- function(variable1,variable2,groupvariable)
  {
     # find out how many values the group variable can take
     groupvariable2 <- as.factor(groupvariable[[1]])
     levels <- levels(groupvariable2)
     numlevels <- length(levels)
     # calculate the grand means
     variable1mean <- mean(variable1)
     variable2mean <- mean(variable2)
     # calculate the between-groups covariance
     Covb <- 0
     for (i in 1:numlevels)
     {
        leveli <- levels[i]
        levelidata1 <- variable1[groupvariable==leveli,]
        levelidata2 <- variable2[groupvariable==leveli,]
        mean1 <- mean(levelidata1)
        mean2 <- mean(levelidata2)
        levelilength <- length(levelidata1)
        term1 <- (mean1 - variable1mean)*(mean2 - variable2mean)*(levelilength)
        Covb <- Covb + term1
     }
     Covb <- Covb / (numlevels - 1)
     Covb <- Covb[[1]]
     return(Covb)
  }
```

For example, to calculate the between-groups covariance for variables V8 and V11, we type:

```
> calcBetweenGroupsCovariance(wine[8],wine[11],wine[1])
  [1] -60.41077
```

Thus, for V8 and V11, the between-groups covariance is -60.41 and the within-groups covariance is 0.29. Since the within-groups covariance is positive (0.29), it means V8 and V11 are positively related within groups: for individuals from the same group, individuals with a high value of V8 tend to have a high value of V11, and vice versa. Since the between-groups covariance is negative (-60.41), V8 and V11 are negatively related between groups: groups with a high mean value of V8 tend to have a low mean value of V11, and vice versa.

Calculating Correlations for Multivariate Data

It is often of interest to investigate whether any of the variables in a multivariate data set are significantly correlated.

To calculate the linear (Pearson) correlation coefficient for a pair of variables, you can use the "cor.test()" function in R. For example, to calculate the correlation coefficient for the first two chemicals' concentrations, V2 and V3, we type:

```
> cor.test(wine$V2, wine$V3)
  Pearson's product-moment correlation
  data:  wine$V2 and wine$V3
  t = 1.2579, df = 176, p-value = 0.2101
  alternative hypothesis: true correlation is not equal to 0
  95 percent confidence interval:
  -0.05342959  0.23817474
  sample estimates:
   cor
  0.09439694
```

This tells us that the correlation coefficient is about 0.094, which is a very weak correlation. Furthermore, the P-value for the statistical test of whether the correlation coefficient is significantly different from zero is 0.21. This is much greater than 0.05 (which we can use here as a cutoff for statistical significance), so there is very weak evidence that that the correlation is non-zero.

If you have a lot of variables, you can use "cor.test()" to calculate the correlation coefficient for each pair of variables, but you might be just interested in finding out what are the most highly correlated pairs of variables. For this you can use the function "mosthighlycorrelated()" below.

The function "mosthighlycorrelated()" will print out the linear correlation coefficients for each pair of variables in your data set, in order of the correlation coefficient. This lets you see very easily which pair of variables are most highly correlated.

```
> mosthighlycorrelated <- function(mydataframe,numtoreport)
  {
     # find the correlations
     cormatrix <- cor(mydataframe)
     # set the correlations on the diagonal or lower triangle to zero,
     # so they will not be reported as the highest ones:
     diag(cormatrix) <- 0
     cormatrix[lower.tri(cormatrix)] <- 0
     # flatten the matrix into a dataframe for easy sorting
     fm <- as.data.frame(as.table(cormatrix))
     # assign human-friendly names
     names(fm) <- c("First.Variable", "Second.Variable","Correlation")
     # sort and print the top n correlations
     head(fm[order(abs(fm$Correlation),decreasing=T),],n=numtoreport)
  }
```

To use this function, you will first have to copy and paste it into R. The arguments of the function are the variables that you want to calculate the correlations for, and the number of top correlation coefficients to print out (for example, you can tell it to print out the largest ten correlation coefficients, or the largest 20).

For example, to calculate correlation coefficients between the concentrations of the 13 chemicals in the wine samples, and to print out the top 10 pairwise correlation coefficients, you can type:

```
> mosthighlycorrelated(wine[2:14], 10)
     First.Variable Second.Variable Correlation
84               V7              V8   0.8645635
150              V8             V13   0.7871939
149              V7             V13   0.6999494
111              V8             V10   0.6526918
157              V2             V14   0.6437200
110              V7             V10   0.6124131
154             V12             V13   0.5654683
132              V3             V12  -0.5612957
118              V2             V11   0.5463642
137              V8             V12   0.5434786
```

This tells us that the pair of variables with the highest linear correlation coefficient are V7 and V8 (correlation = 0.86 approximately).

Standardizing Variables

If you want to compare different variables that have different units, are very different variances, it is a good idea to first standardize the variables.

For example, we found above that the concentrations of the 13 chemicals in the wine samples show a wide range of standard deviations, from 0.1244533 for V9 (variance 0.01548862) to 314.9074743 for V14 (variance 99166.72). This is a range of approximately 6,402,554-fold in the variances.

As a result, it is not a good idea to use the unstandardized chemical concentrations as the input for a principal component analysis (PCA, see below) of the wine samples, as if you did that, the first principal component would be dominated by the variables which show the largest variances, such as V14.

Thus, it would be a better idea to first standardize the variables so that they all have variance 1 and mean 0, and to then carry out the principal component analysis on the standardized data. This would allow us to find the principal components that provide the best low-dimensional representation of the variation in the original data, without being overly biased by those variables that show the most variance in the original data.

You can standardize variables in R using the "scale()" function.

For example, to standardize the concentrations of the 13 chemicals in the wine samples, we type:

```
> standardizedconcentrations <- as.data.frame(scale(wine[2:14]))
```

Note that we use the "as.data.frame()" function to convert the output of "scale()" into a "data frame", which is the same type of R variable that the "wine" variable.

We can check that each of the standardized variables stored in "standardizedconcentrations" has a mean of 0 and a standard deviation of 1 by typing:

```
> sapply(standardizedconcentrations,mean)
            V2             V3             V4             V5             V6
 -8.591766e-16 -6.776446e-17  8.045176e-16 -7.720494e-17 -4.073935e-17
            V7             V8             V9            V10            V11
 -1.395560e-17  6.958263e-17 -1.042186e-16 -1.221369e-16  3.649376e-17
           V12            V13            V14
  2.093741e-16  3.003459e-16 -1.034429e-16
> sapply(standardizedconcentrations,sd)
 V2  V3  V4  V5  V6  V7  V8  V9 V10 V11 V12 V13 V14
  1   1   1   1   1   1   1   1   1   1   1   1   1
```

We see that the means of the standardized variables are all very tiny numbers and so are essentially equal to 0, and the standard deviations of the standardized variables are all equal to 1.

Principal Component Analysis

The purpose of principal component analysis is to find the best low-dimensional representation of the variation in a multivariate data set. For example, in the case of the wine data set, we have 13 chemical concentrations describing wine samples from three different cultivars. We can carry out a principal component analysis to investigate whether we can capture most of the variation between samples using a smaller number of new variables (principal components), where each of these new variables is a linear combination of all or some of the 13 chemical concentrations.

To carry out a principal component analysis (PCA) on a multivariate data set, the first step is often to standardize the variables under study using the "scale()" function (see above). This is necessary if the input variables have very different variances, which is true in this case as the concentrations of the 13 chemicals have very different variances (see above).

Once you have standardized your variables, you can carry out a principal component analysis using the "prcomp()" function in R.

For example, to standardize the concentrations of the 13 chemicals in the wine samples, and carry out a principal components analysis on the standardized concentrations, we type:

```
> standardizedconcentrations <- as.data.frame(scale(wine[2:14])) # standardize the variables
> wine.pca <- prcomp(standardizedconcentrations)                 # do a PCA
```

You can get a summary of the principal component analysis results using the "summary()" function on the output of "prcomp()":

```
> summary(wine.pca)
  Importance of components:
                          PC1   PC2   PC3    PC4    PC5    PC6    PC7    PC8    PC9   PC10
  Standard deviation     2.169 1.580 1.203 0.9586 0.9237 0.8010 0.7423 0.5903 0.5375 0.5009
  Proportion of Variance 0.362 0.192 0.111 0.0707 0.0656 0.0494 0.0424 0.0268 0.0222 0.0193
  Cumulative Proportion  0.362 0.554 0.665 0.7360 0.8016 0.8510 0.8934 0.9202 0.9424 0.9617
                          PC11   PC12    PC13
```

```
  Standard deviation     0.4752 0.4108 0.32152
  Proportion of Variance 0.0174 0.0130 0.00795
  Cumulative Proportion  0.9791 0.9920 1.00000
```

This gives us the standard deviation of each component, and the proportion of variance explained by each component. The standard deviation of the components is stored in a named element called "sdev" of the output variable made by "prcomp":

```
> wine.pca$sdev
  [1] 2.1692972 1.5801816 1.2025273 0.9586313 0.9237035 0.8010350 0.7423128 0.5903367
  [9] 0.5374755 0.5009017 0.4751722 0.4108165 0.3215244
```

The total variance explained by the components is the sum of the variances of the components:

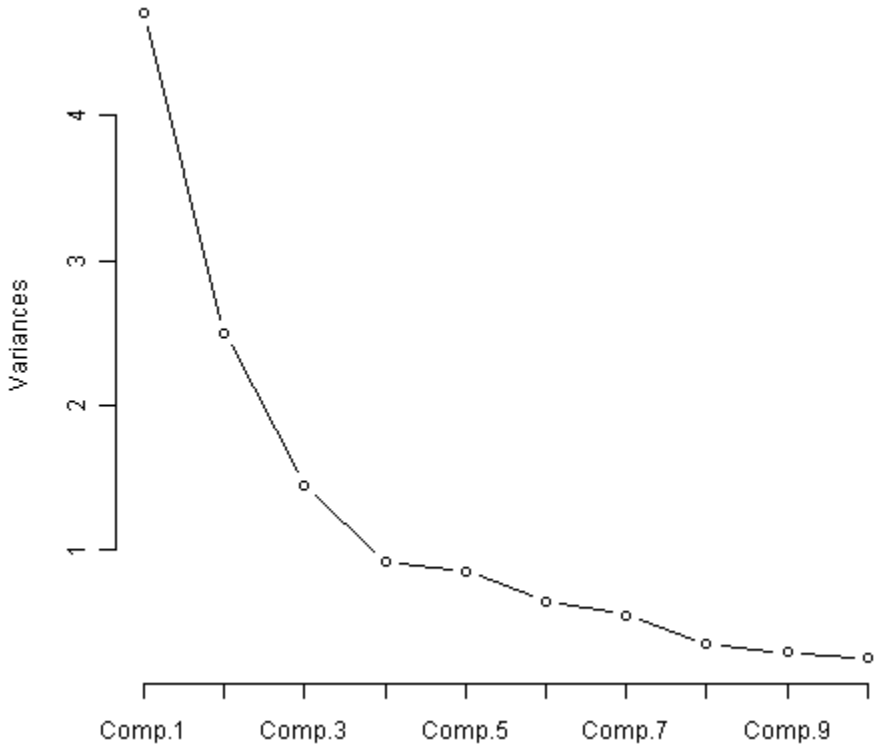
```
> sum((wine.pca$sdev)^2)
  [1] 13
```

In this case, we see that the total variance is 13, which is equal to the number of standardized variables (13 variables). This is because for standardized data, the variance of each standardized variable is 1. The total variance is equal to the sum of the variances of the individual variables, and since the variance of each standardized variable is 1, the total variance should be equal to the number of variables (13 here).

Deciding How Many Principal Components to Retain

In order to decide how many principal components should be retained, it is common to summarize the results of a principal components analysis by making a scree plot, which we can do in R using the "screeplot()" function:

```
> screeplot(wine.pca, type="lines")
```



The most obvious change in slope in the scree plot occurs at component 4, which is the "elbow" of the scree plot. Therefore, it could be argued based on the basis of the scree plot that the first three components should be retained.

Another way of deciding how many components to retain is to use Kaiser's criterion: that we should only retain principal components for which the variance is above 1 (when principal component analysis was applied to standardized data). We can check this by finding the variance of each of the principal components:

```
> (wine.pca$sdev)^2
  [1] 4.7058503 2.4969737 1.4460720 0.9189739 0.8532282 0.6416570 0.5510283 0.3484974
  [9] 0.2888799 0.2509025 0.2257886 0.1687702 0.1033779
```

We see that the variance is above 1 for principal components 1, 2, and 3 (which have variances 4.71, 2.50, and 1.45, respectively). Therefore, using Kaiser's criterion, we would retain the first three principal components.

A third way to decide how many principal components to retain is to decide to keep the number of components required to explain at least some minimum amount of the total variance. For example, if it is important to explain at least 80% of the variance, we would retain the first five principal components, as we can see from the output of "summary(wine.pca)" that the first five principal components explain 80.2% of the variance (while the first four components explain just 73.6%, so are not sufficient).

Loadings for the Principal Components

The loadings for the principal components are stored in a named element "rotation" of the variable returned by "prcomp()". This contains a matrix with the loadings of each principal component, where the first column in the matrix contains the loadings for the first principal component, the second column contains the loadings for the second principal component, and so on.

Therefore, to obtain the loadings for the first principal component in our analysis of the 13 chemical concentrations in wine samples, we type:

```
> wine.pca$rotation[,1]
           V2           V3           V4           V5           V6           V7
-0.144329395  0.245187580  0.002051061  0.239320405 -0.141992042 -0.394660845
           V8           V9          V10          V11          V12          V13
-0.422934297  0.298533103 -0.313429488  0.088616705 -0.296714564 -0.376167411
          V14
-0.286752227
```

This means that the first principal component is a linear combination of the variables: -0.144*Z2 + 0.245*Z3 + 0.002*Z4 + 0.239*Z5 - 0.142*Z6 - 0.395*Z7 - 0.423*Z8 + 0.299*Z9 -0.313*Z10 + 0.089*Z11 - 0.297*Z12 - 0.376*Z13 - 0.287*Z14, where Z2, Z3, Z4...Z14 are the standardized versions of the variables V2, V3, V4...V14 (that each have mean of 0 and variance of 1).

Note that the square of the loadings sum to 1, as this is a constraint used in calculating the loadings:

```
> sum((wine.pca$rotation[,1])^2)
  [1] 1
```

To calculate the values of the first principal component, we can define our own function to calculate a principal component given the loadings and the input variables' values:

```
> calcpc <- function(variables,loadings)
  {
     # find the number of samples in the data set
     as.data.frame(variables)
     numsamples <- nrow(variables)
     # make a vector to store the component
     pc <- numeric(numsamples)
     # find the number of variables
     numvariables <- length(variables)
```

```
    # calculate the value of the component for each sample
    for (i in 1:numsamples)
    {
       valuei <- 0
       for (j in 1:numvariables)
       {
          valueij <- variables[i,j]
          loadingj <- loadings[j]
          valuei <- valuei + (valueij * loadingj)
       }
       pc[i] <- valuei
    }
    return(pc)
  }
```

We can then use the function to calculate the values of the first principal component for each sample in our wine data:

```
> calcpc(standardizedconcentrations, wine.pca$rotation[,1])
  [1]  -3.30742097 -2.20324981 -2.50966069 -3.74649719 -1.00607049 -3.04167373 -2.44220051
  [8]  -2.05364379 -2.50381135 -2.74588238 -3.46994837 -1.74981688 -2.10751729 -3.44842921
  [15] -4.30065228 -2.29870383 -2.16584568 -1.89362947 -3.53202167 -2.07865856 -3.11561376
  [22] -1.08351361 -2.52809263 -1.64036108 -1.75662066 -0.98729406 -1.77028387 -1.23194878
  [29] -2.18225047 -2.24976267 -2.49318704 -2.66987964 -1.62399801 -1.89733870 -1.40642118
  [36] -1.89847087 -1.38096669 -1.11905070 -1.49796891 -2.52268490 -2.58081526 -0.66660159
  ...
```

In fact, the values of the first principal component are stored in the variable wine.pca$x[,1] that was returned by the "prcomp()" function, so we can compare those values to the ones that we calculated, and they should agree:

```
> wine.pca$x[,1]
  [1]  -3.30742097 -2.20324981 -2.50966069 -3.74649719 -1.00607049 -3.04167373 -2.44220051
  [8]  -2.05364379 -2.50381135 -2.74588238 -3.46994837 -1.74981688 -2.10751729 -3.44842921
  [15] -4.30065228 -2.29870383 -2.16584568 -1.89362947 -3.53202167 -2.07865856 -3.11561376
  [22] -1.08351361 -2.52809263 -1.64036108 -1.75662066 -0.98729406 -1.77028387 -1.23194878
  [29] -2.18225047 -2.24976267 -2.49318704 -2.66987964 -1.62399801 -1.89733870 -1.40642118
  [36] -1.89847087 -1.38096669 -1.11905070 -1.49796891 -2.52268490 -2.58081526 -0.66660159
  ...
```

We see that they do agree.

The first principal component has highest (in absolute value) loadings for V8 (-0.423), V7 (-0.395), V13 (-0.376), V10 (-0.313), V12 (-0.297), V14 (-0.287), V9 (0.299), V3 (0.245), and V5 (0.239). The loadings for V8, V7, V13, V10, V12 and V14 are negative, while those for V9, V3, and V5 are positive. Therefore, an interpretation of the first principal component is that it represents a contrast between the concentrations of V8, V7, V13, V10, V12, and V14, and the concentrations of V9, V3 and V5.

Similarly, we can obtain the loadings for the second principal component by typing:

```
> wine.pca$rotation[,2]
          V2           V3           V4           V5           V6           V7
 0.483651548  0.224930935  0.316068814 -0.010590502  0.299634003  0.065039512
          V8           V9          V10          V11          V12          V13
-0.003359812  0.028779488  0.039301722  0.529995672 -0.279235148 -0.164496193
         V14
 0.364902832
```

This means that the second principal component is a linear combination of the variables: 0.484*Z2 + 0.225*Z3 + 0.316*Z4 - 0.011*Z5 + 0.300*Z6 + 0.065*Z7 - 0.003*Z8 + 0.029*Z9 + 0.039*Z10 + 0.530*Z11 - 0.279*Z12 - 0.164*Z13 + 0.365*Z14, where Z1, Z2, Z3...Z14 are the standardized versions of variables V2, V3, ... V14 that each have mean 0 and variance 1.

Note that the square of the loadings sum to 1, as above:

```
> sum((wine.pca$rotation[,2])^2)
  [1] 1
```

The second principal component has highest loadings for V11 (0.530), V2 (0.484), V14 (0.365), V4 (0.316), V6 (0.300), V12 (-0.279), and V3 (0.225). The loadings for V11, V2, V14, V4, V6 and V3 are positive, while the loading for V12 is negative. Therefore, an interpretation of the second principal component is that it represents a contrast between the concentrations of V11, V2, V14, V4, V6 and V3, and the concentration of V12. Note that the loadings for V11 (0.530) and V2 (0.484) are the largest, so the contrast is mainly between the concentrations of V11 and V2, and the concentration of V12.

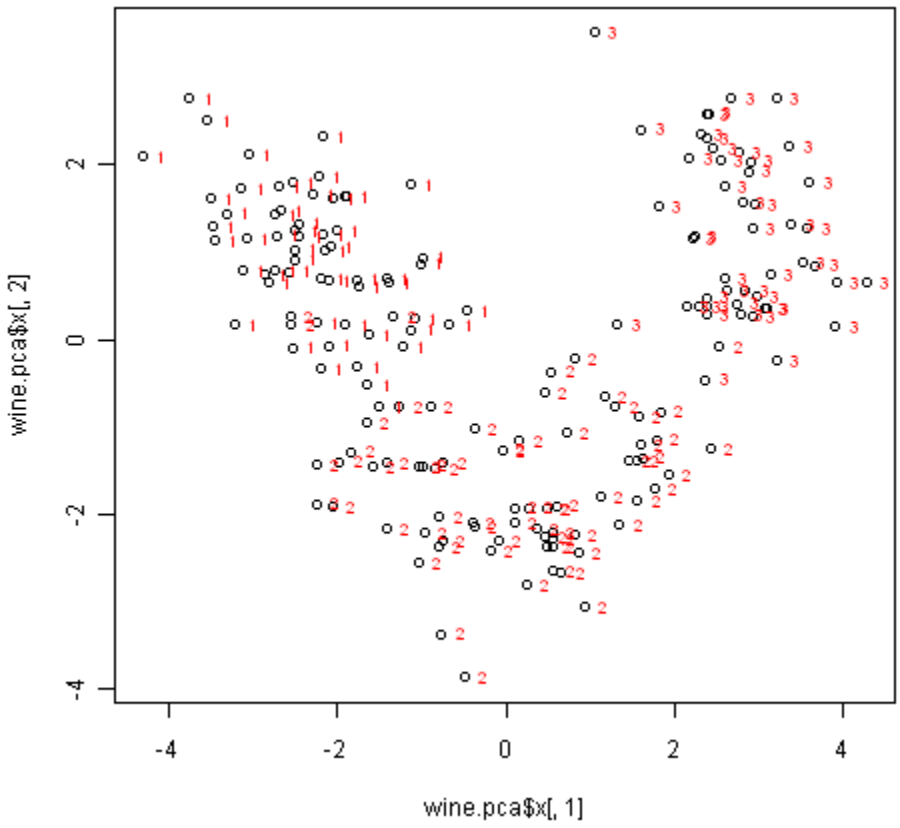
Scatterplots of the Principal Components

The values of the principal components are stored in a named element “x” of the variable returned by “prcomp()”. This contains a matrix with the principal components, where the first column in the matrix contains the first principal component, the second column the second component, and so on.

Thus, in our example, “wine.pca$x[,1]” contains the first principal component, and “wine.pca$x[,2]” contains the second principal component.

We can make a scatterplot of the first two principal components, and label the data points with the cultivar that the wine samples come from, by typing:

```
> plot(wine.pca$x[,1],wine.pca$x[,2]) # make a scatterplot
> text(wine.pca$x[,1],wine.pca$x[,2], wine$V1, cex=0.7, pos=4, col="red") # add labels
```



The scatterplot shows the first principal component on the x-axis, and the second principal component on the y-axis. We can see from the scatterplot that wine samples of cultivar 1 have much lower values of the first principal component than wine samples of cultivar 3. Therefore, the first principal component separates wine samples of cultivars 1 from those of cultivar 3.

We can also see that wine samples of cultivar 2 have much higher values of the second principal component than wine samples of cultivars 1 and 3. Therefore, the second principal component separates samples of cultivar 2 from samples of cultivars 1 and 3.

Therefore, the first two principal components are reasonably useful for distinguishing wine samples of the three different cultivars.

Above, we interpreted the first principal component as a contrast between the concentrations of V8, V7, V13, V10, V12, and V14, and the concentrations of V9, V3 and V5. We can check whether this makes sense in terms of the concentrations of these chemicals in the different cultivars, by printing out the means of the standardized concentration variables in each cultivar, using the “printMeanAndSdByGroup()” function (see above):

```
> printMeanAndSdByGroup(standardizedconcentrations,wine[1])
  [1] "Means:"
    V1         V2         V3         V4         V5          V6          V7          V8
  1  1  0.9166093 -0.2915199  0.3246886 -0.7359212  0.46192317  0.87090552  0.95419225
  2  2 -0.8892116 -0.3613424 -0.4437061  0.2225094 -0.36354162 -0.05790375  0.05163434
  3  3  0.1886265  0.8928122  0.2572190  0.5754413 -0.03004191 -0.98483874 -1.24923710
         V9        V10        V11        V12        V13        V14
-0.57735640  0.5388633  0.2028288  0.4575567  0.7691811  1.1711967
 0.01452785  0.0688079 -0.8503999  0.4323908  0.2446043 -0.7220731
 0.68817813 -0.7641311  1.0085728 -1.2019916 -1.3072623 -0.3715295
```

Does it make sense that the first principal component can separate cultivar 1 from cultivar 3? In cultivar 1, the mean values of V8 (0.954), V7 (0.871), V13 (0.769), V10 (0.539), V12 (0.458) and V14 (1.171) are very high compared to the mean values of V9 (-0.577), V3 (-0.292) and V5 (-0.736). In cultivar 3, the mean values of V8 (-1.249), V7 (-0.985), V13 (-1.307), V10 (-0.764), V12 (-1.202) and V14 (-0.372) are very low compared to the mean values of V9 (0.688), V3 (0.893) and V5 (0.575). Therefore, it does make sense that principal component 1 is a contrast between the concentrations of V8, V7, V13, V10, V12, and V14, and the concentrations of V9, V3 and V5; and that principal component 1 can separate cultivar 1 from cultivar 3.

Above, we intepreted the second principal component as a contrast between the concentrations of V11, V2, V14, V4, V6 and V3, and the concentration of V12. In the light of the mean values of these variables in the different cultivars, does it make sense that the second principal component can separate cultivar 2 from cultivars 1 and 3? In cultivar 1, the mean values of V11 (0.203), V2 (0.917), V14 (1.171), V4 (0.325), V6 (0.462) and V3 (-0.292) are not very different from the mean value of V12 (0.458). In cultivar 3, the mean values of V11 (1.009), V2 (0.189), V14 (-0.372), V4 (0.257), V6 (-0.030) and V3 (0.893) are also not very different from the mean value of V12 (-1.202). In contrast, in cultivar 2, the mean values of V11 (-0.850), V2 (-0.889), V14 (-0.722), V4 (-0.444), V6 (-0.364) and V3 (-0.361) are much less than the mean value of V12 (0.432). Therefore, it makes sense that principal component is a contrast between the concentrations of V11, V2, V14, V4, V6 and V3, and the concentration of V12; and that principal component 2 can separate cultivar 2 from cultivars 1 and 3.

Linear Discriminant Analysis

The purpose of principal component analysis is to find the best low-dimensional representation of the variation in a multivariate data set. For example, in the wine data set, we have 13 chemical concentrations describing wine samples from three cultivars. By carrying out a principal component analysis, we found that most of the variation in the chemical concentrations between the samples can be captured using the first two principal components, where each of the principal components is a particular linear combination of the 13 chemical concentrations.

The purpose of linear discriminant analysis (LDA) is to find the linear combinations of the original variables (the 13 chemical concentrations here) that gives the best possible separation between the groups (wine cultivars here) in our data set. Linear discriminant analysis is also known as “canonical discriminant analysis”, or simply “discriminant analysis”.

If we want to separate the wines by cultivar, the wines come from three different cultivars, so the number of groups (G) is 3, and the number of variables is 13 (13 chemicals’ concentrations; p = 13). The maximum number of useful discriminant functions that can separate the wines by cultivar is the minimum of G-1 and p, and so in this case it is the minimum of 2 and 13, which is 2. Thus, we can find at most 2 useful discriminant functions to separate the wines by cultivar, using the 13 chemical concentration variables.

You can carry out a linear discriminant analysis using the “lda()” function from the R “MASS” package. To use this function, we first need to install the “MASS” R package (for instructions on how to install an R package, see How to install an R package).

For example, to carry out a linear discriminant analysis using the 13 chemical concentrations in the wine samples, we type:

```
> library("MASS") # load the MASS package
> wine.lda <- lda(wine$V1 ~ wine$V2 + wine$V3 + wine$V4 + wine$V5 + wine$V6 +
                            wine$V7 + wine$V8 + wine$V9 + wine$V10 + wine$V11 +
                            wine$V12 + wine$V13 + wine$V14)
```

Loadings for the Discriminant Functions

To get the values of the loadings of the discriminant functions for the wine data, we can type:

```
> wine.lda
  Coefficients of linear discriminants:
              LD1           LD2
  wine$V2  -0.403399781  0.8717930699
  wine$V3   0.165254596  0.3053797325
  wine$V4  -0.369075256  2.3458497486
  wine$V5   0.154797889 -0.1463807654
  wine$V6  -0.002163496 -0.0004627565
  wine$V7   0.618052068 -0.0322128171
  wine$V8  -1.661191235 -0.4919980543
  wine$V9  -1.495818440 -1.6309537953
  wine$V10  0.134092628 -0.3070875776
  wine$V11  0.355055710  0.2532306865
  wine$V12 -0.818036073 -1.5156344987
  wine$V13 -1.157559376  0.0511839665
  wine$V14 -0.002691206  0.0028529846
```

This means that the first discriminant function is a linear combination of the variables: -0.403*V2 + 0.165*V3 - 0.369*V4 + 0.155*V5 - 0.002*V6 + 0.618*V7 - 1.661*V8 - 1.496*V9 + 0.134*V10 + 0.355*V11 - 0.818*V12 - 1.158*V13 - 0.003*V14, where V2, V3, ... V14 are the concentrations of the 14 chemicals found in the wine samples. For convenience, the value for each discriminant function (eg. the first discriminant function) are scaled so that their mean value is zero (see below).

Note that these loadings are calculated so that the within-group variance of each discriminant function for each group (cultivar) is equal to 1, as will be demonstrated below.

These scalings are also stored in the named element "scaling" of the variable returned by the lda() function. This element contains a matrix, in which the first column contains the loadings for the first discriminant function, the second column contains the loadings for the second discriminant function and so on. For example, to extract the loadings for the first discriminant function, we can type:

```
> wine.lda$scaling[,1]
   wine$V2      wine$V3      wine$V4      wine$V5      wine$V6      wine$V7
 -0.403399781  0.165254596 -0.369075256  0.154797889 -0.002163496  0.618052068
   wine$V8      wine$V9     wine$V10     wine$V11     wine$V12     wine$V13
 -1.661191235 -1.495818440  0.134092628  0.355055710 -0.818036073 -1.157559376
  wine$V14
 -0.002691206
```

To calculate the values of the first discriminant function, we can define our own function "calclda()":

```
> calclda <- function(variables,loadings)
  {
     # find the number of samples in the data set
     as.data.frame(variables)
     numsamples <- nrow(variables)
     # make a vector to store the discriminant function
     ld <- numeric(numsamples)
     # find the number of variables
     numvariables <- length(variables)
     # calculate the value of the discriminant function for each sample
     for (i in 1:numsamples)
     {
        valuei <- 0
        for (j in 1:numvariables)
        {
           valueij <- variables[i,j]
           loadingj <- loadings[j]
           valuei <- valuei + (valueij * loadingj)
        }
        ld[i] <- valuei
     }
     # standardize the discriminant function so that its mean value is 0:
     ld <- as.data.frame(scale(ld, center=TRUE, scale=FALSE))
     ld <- ld[[1]]
     return(ld)
  }
```

The function calclda() simply calculates the value of a discriminant function for each sample in the data set, for example, for the first disriminant function, for each sample we calculate the value using the equation -0.403*V2 - 0.165*V3 - 0.369*V4 + 0.155*V5 - 0.002*V6 + 0.618*V7 - 1.661*V8 - 1.496*V9 + 0.134*V10 + 0.355*V11 - 0.818*V12 - 1.158*V13 - 0.003*V14. Furthermore, the "scale()" command is used within the calclda() function in order to standardize the value of a discriminant function (eg. the first discriminant function) so that its mean value (over all the wine samples) is 0.

We can use the function calclda() to calculate the values of the first discriminant function for each sample in our wine data:

```
> calclda(wine[2:14], wine.lda$scaling[,1])
  [1] -4.70024401 -4.30195811 -3.42071952 -4.20575366 -1.50998168 -4.51868934
  [7] -4.52737794 -4.14834781 -3.86082876 -3.36662444 -4.80587907 -3.42807646
  [13] -3.66610246 -5.58824635 -5.50131449 -3.18475189 -3.28936988 -2.99809262
  [19] -5.24640372 -3.13653106 -3.57747791 -1.69077135 -4.83515033 -3.09588961
  [25] -3.32164716 -2.14482223 -3.98242850 -2.68591432 -3.56309464 -3.17301573
  [31] -2.99626797 -3.56866244 -3.38506383 -3.52753750 -2.85190852 -2.79411996
  ...
```

In fact, the values of the first linear discriminant function can be calculated using the "predict()" function in R, so we can compare those to the ones that we calculated, and they should agree:

```
> wine.lda.values <- predict(wine.lda, wine[2:14])
> wine.lda.values$x[,1] # contains the values for the first discriminant function
      1           2           3           4           5           6
 -4.70024401 -4.30195811 -3.42071952 -4.20575366 -1.50998168 -4.51868934
      7           8           9          10          11          12
 -4.52737794 -4.14834781 -3.86082876 -3.36662444 -4.80587907 -3.42807646
     13          14          15          16          17          18
 -3.66610246 -5.58824635 -5.50131449 -3.18475189 -3.28936988 -2.99809262
     19          20          21          22          23          24
 -5.24640372 -3.13653106 -3.57747791 -1.69077135 -4.83515033 -3.09588961
     25          26          27          28          29          30
 -3.32164716 -2.14482223 -3.98242850 -2.68591432 -3.56309464 -3.17301573
     31          32          33          34          35          36
 -2.99626797 -3.56866244 -3.38506383 -3.52753750 -2.85190852 -2.79411996
 ...
```

We see that they do agree.

It doesn't matter whether the input variables for linear discriminant analysis are standardized or not, unlike for principal components analysis in which it is often necessary to standardize the input variables. However, using standardized variables in linear discriminant analysis makes it easier to interpret the loadings in a linear discriminant function.

In linear discriminant analysis, the standardized version of an input variable is defined so that it has mean zero and within-groups variance of 1. Thus, we can calculate the "group-standardized" variable by subtracting the mean from each value of the variable, and dividing by the within-groups standard deviation. To calculate the group-standardized version of a set of variables, we can use the function "groupStandardize()" below:

```
> groupStandardize <- function(variables, groupvariable)
  {
     # find out how many variables we have
     variables <- as.data.frame(variables)
     numvariables <- length(variables)
     # find the variable names
     variablenames <- colnames(variables)
     # calculate the group-Standardized version of each variable
     for (i in 1:numvariables)
     {
        variablei <- variables[i]
        variablei_name <- variablenames[i]
        variablei_Vw <- calcWithinGroupsVariance(variablei, groupvariable)
        variablei_mean <- mean(variablei)
        variablei_new <- (variablei - variablei_mean)/(sqrt(variablei_Vw))
        data_length <- nrow(variablei)
        if (i == 1) { variables_new <- data.frame(row.names=seq(1,data_length)) }
        variables_new[`variablei_name`] <- variablei_new
     }
     return(variables_new)
  }
```

For example, we can use the "groupStandardize()" function to calculate the group-standardized versions of the chemical concentrations in wine samples:

```
> groupstandardizedconcentrations <- groupStandardize(wine[2:14], wine[1])
```

We can then use the lda() function to perform linear discriminant analysis on the group-standardized variables:

```
> wine.lda2 <- lda(wine$V1 ~ groupstandardizedconcentrations$V2 +
groupstandardizedconcentrations$V3 +
                            groupstandardizedconcentrations$V4 +
groupstandardizedconcentrations$V5 +
                            groupstandardizedconcentrations$V6 +
groupstandardizedconcentrations$V7 +
                            groupstandardizedconcentrations$V8 +
groupstandardizedconcentrations$V9 +
                            groupstandardizedconcentrations$V10 +
groupstandardizedconcentrations$V11 +
                            groupstandardizedconcentrations$V12 +
groupstandardizedconcentrations$V13 +
                            groupstandardizedconcentrations$V14)
> wine.lda2
  Coefficients of linear discriminants:
                                            LD1          LD2
  groupstandardizedconcentrations$V2  -0.20650463  0.446280119
  groupstandardizedconcentrations$V3   0.15568586  0.287697336
  groupstandardizedconcentrations$V4  -0.09486893  0.602988809
  groupstandardizedconcentrations$V5   0.43802089 -0.414203541
  groupstandardizedconcentrations$V6  -0.02907934 -0.006219863
  groupstandardizedconcentrations$V7   0.27030186 -0.014088108
  groupstandardizedconcentrations$V8  -0.87067265 -0.257868714
  groupstandardizedconcentrations$V9  -0.16325474 -0.178003512
  groupstandardizedconcentrations$V10  0.06653116 -0.152364015
  groupstandardizedconcentrations$V11  0.53670086  0.382782544
  groupstandardizedconcentrations$V12 -0.12801061 -0.237174509
  groupstandardizedconcentrations$V13 -0.46414916  0.020523349
  groupstandardizedconcentrations$V14 -0.46385409  0.491738050
```

It makes sense to interpret the loadings calculated using the group-standardized variables rather than the loadings for the original (unstandardized) variables.

In the first discriminant function calculated for the group-standardized variables, the largest loadings (in absolute) value are given to V8 (-0.871), V11 (0.537), V13 (-0.464), V14 (-0.464), and V5 (0.438). The loadings for V8, V13 and V14 are negative, while those for V11 and V5 are positive. Therefore, the discriminant function seems to represent a contrast between the concentrations of V8, V13 and V14, and the concentrations of V11 and V5.

We saw above that the individual variables which gave the greatest separations between the groups were V8 (separation 233.93), V14 (207.92), V13 (189.97), V2 (135.08) and V11 (120.66). These were mostly the same variables that had the largest loadings in the linear discriminant function (loading for V8: -0.871, for V14: -0.464, for V13: -0.464, for V11: 0.537).

We found above that variables V8 and V11 have a negative between-groups covariance (-60.41) and a positive within-groups covariance (0.29). When the between-groups covariance and within-groups covariance for two variables have opposite signs, it indicates that a better separation between groups can be obtained by using a linear combination of those two variables than by using either variable on its own.

Thus, given that the two variables V8 and V11 have between-groups and within-groups covariances of opposite signs, and that these are two of the variables that gave the greatest separations between groups when used individually, it is not surprising that these are the two variables that have the largest loadings in the first discriminant function.

Note that although the loadings for the group-standardized variables are easier to interpret than the loadings for the unstandardized variables, the values of the discriminant function are the same regardless of whether we standardize the input variables or not. For example, for wine data, we can calculate the value of the first discriminant function calculated using the unstandardized and group-standardized variables by typing:

```
> wine.lda.values <- predict(wine.lda, wine[2:14])
```

```
> wine.lda.values$x[,1]
# values for the first discriminant function, using the unstandardized data
      1           2           3           4           5           6
  -4.70024401 -4.30195811 -3.42071952 -4.20575366 -1.50998168 -4.51868934
      7           8           9          10          11          12
  -4.52737794 -4.14834781 -3.86082876 -3.36662444 -4.80587907 -3.42807646
     13          14          15          16          17          18
  -3.66610246 -5.58824635 -5.50131449 -3.18475189 -3.28936988 -2.99809262
     19          20          21          22          23          24
  -5.24640372 -3.13653106 -3.57747791 -1.69077135 -4.83515033 -3.09588961
  ...
> wine.lda.values2 <- predict(wine.lda2, groupstandardizedconcentrations)
> wine.lda.values2$x[,1]
# values for the first discriminant function, using the standardized data
      1           2           3           4           5           6
  -4.70024401 -4.30195811 -3.42071952 -4.20575366 -1.50998168 -4.51868934
      7           8           9          10          11          12
  -4.52737794 -4.14834781 -3.86082876 -3.36662444 -4.80587907 -3.42807646
     13          14          15          16          17          18
  -3.66610246 -5.58824635 -5.50131449 -3.18475189 -3.28936988 -2.99809262
     19          20          21          22          23          24
  -5.24640372 -3.13653106 -3.57747791 -1.69077135 -4.83515033 -3.09588961
  ...
```

We can see that although the loadings are different for the first discriminant functions calculated using unstandardized and group-standardized data, the actual values of the first discriminant function are the same.

Separation Achieved by the Discriminant Functions

To calculate the separation achieved by each discriminant function, we first need to calculate the value of each discriminant function, by substituting the variables' values into the linear combination for the discriminant function (eg. -0.403*V2 - 0.165*V3 - 0.369*V4 + 0.155*V5 - 0.002*V6 + 0.618*V7 - 1.661*V8 - 1.496*V9 + 0.134*V10 + 0.355*V11 - 0.818*V12 - 1.158*V13 - 0.003*V14 for the first discriminant function), and then scaling the values of the discriminant function so that their mean is zero.

As mentioned above, we can do this using the "predict()" function in R. For example, to calculate the value of the discriminant functions for the wine data, we type:

```
> wine.lda.values <- predict(wine.lda, standardizedconcentrations)
```

The returned variable has a named element "x" which is a matrix containing the linear discriminant functions: the first column of x contains the first discriminant function, the second column of x contains the second discriminant function, and so on (if there are more discriminant functions).

We can therefore calculate the separations achieved by the two linear discriminant functions for the wine data by using the "calcSeparations()" function (see above), which calculates the separation as the ratio of the between-groups variance to the within-groups variance:

```
> calcSeparations(wine.lda.values$x,wine[1])
  [1] "variable LD1 Vw= 1 Vb= 794.652200566216 separation= 794.652200566216"
  [1] "variable LD2 Vw= 1 Vb= 361.241041493455 separation= 361.241041493455"
```

As mentioned above, the loadings for each discriminant function are calculated in such a way that the within-group variance (Vw) for each group (wine cultivar here) is equal to 1, as we see in the output from calcSeparations() above.

The output from calcSeparations() tells us that the separation achieved by the first (best) discriminant function is 794.7, and the separation achieved by the second (second best) discriminant function is 361.2.

Therefore, the total separation is the sum of these, which is (794.652200566216+361.241041493455=1155.893) 1155.89, rounded to two decimal places. Therefore, the "percentage separation" achieved by the first discriminant function is (794.652200566216*100/1155.893=) 68.75%, and the percentage separation achieved by the second discriminant function is (361.241041493455*100/1155.893=) 31.25%.

The "proportion of trace" that is printed when you type "wine.lda" (the variable returned by the lda() function) is the percentage separation achieved by each discriminant function. For example, for the wine data we get the same values as just calculated (68.75% and 31.25%):

```
> wine.lda
  Proportion of trace:
    LD1    LD2
  0.6875 0.3125
```

Therefore, the first discriminant function does achieve a good separation between the three groups (three cultivars), but the second discriminant function does improve the separation of the groups by quite a large amount, so is it worth using the second discriminant function as well. Therefore, to achieve a good separation of the groups (cultivars), it is necessary to use both of the first two discriminant functions.

We found above that the largest separation achieved for any of the individual variables (individual chemical concentrations) was 233.9 for V8, which is quite a lot less than 794.7, the separation achieved by the first discriminant function. Therefore, the effect of using more than one variable to calculate the discriminant function is that we can find a discriminant function that achieves a far greater separation between groups than achieved by any one variable alone.

The variable returned by the lda() function also has a named element "svd", which contains the ratio of between- and within-group standard deviations for the linear discriminant variables, that is, the square root of the "separation" value that we calculated using calcSeparations() above. When we calculate the square of the value stored in "svd", we should get the same value as found using calcSeparations():

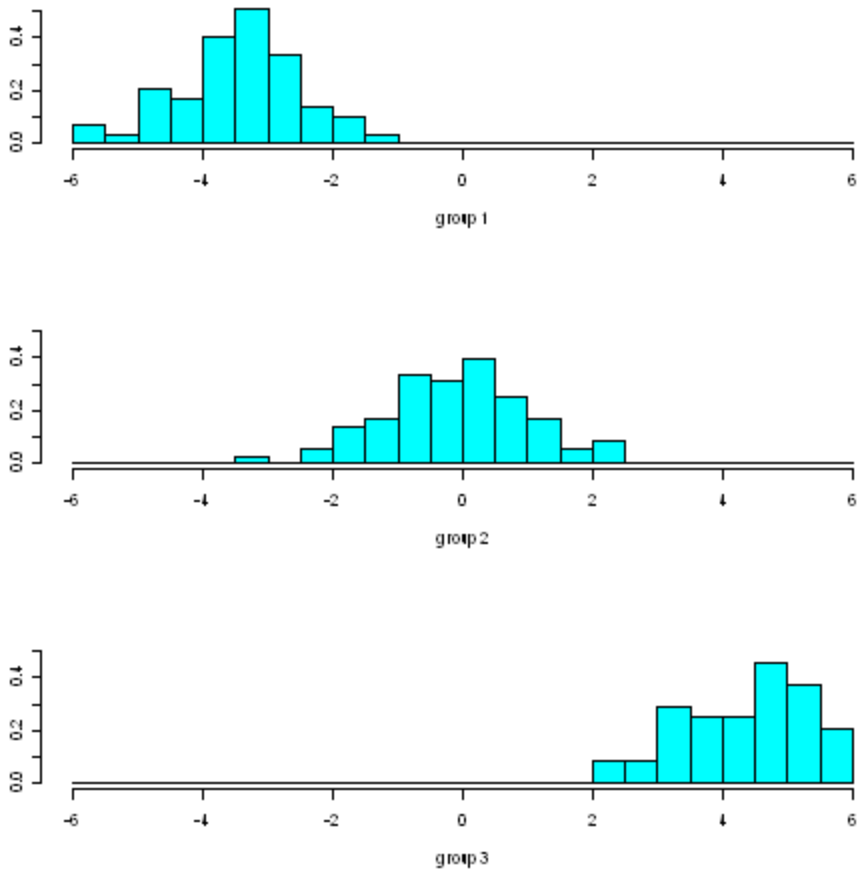
```
> (wine.lda$svd)^2
  [1] 794.6522 361.2410
```

A Stacked Histogram of the LDA Values

A nice way of displaying the results of a linear discriminant analysis (LDA) is to make a stacked histogram of the values of the discriminant function for the samples from different groups (different wine cultivars in our example).

We can do this using the "ldahist()" function in R. For example, to make a stacked histogram of the first discriminant function's values for wine samples of the three different wine cultivars, we type:

```
> ldahist(data = wine.lda.values$x[,1], g=wine$V1)
```



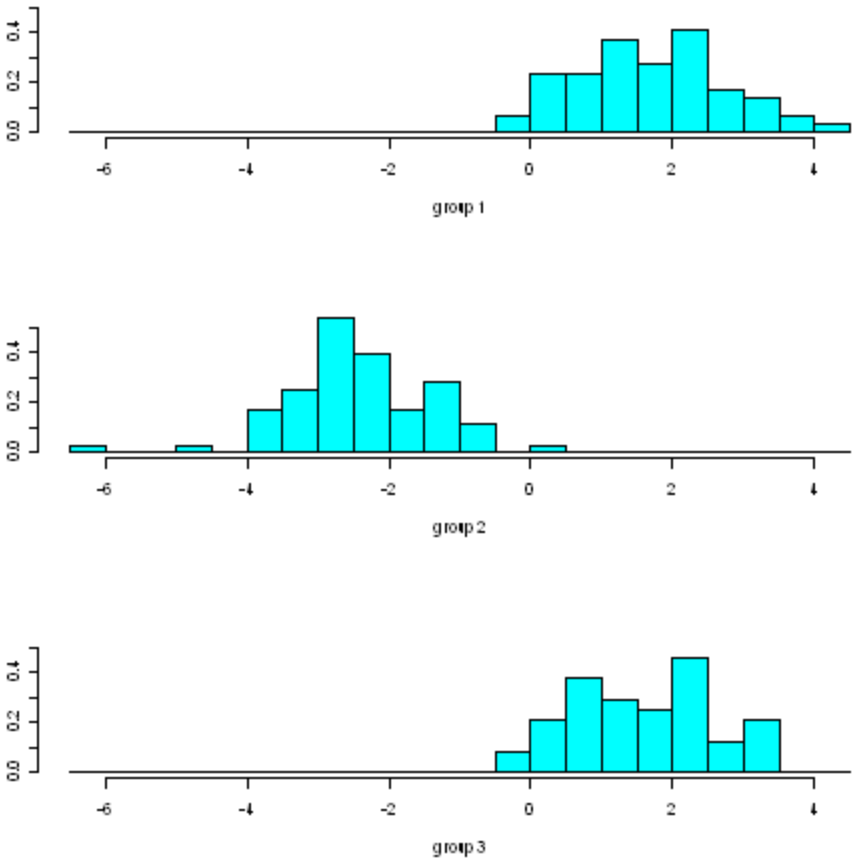
We can see from the histogram that cultivars 1 and 3 are well separated by the first discriminant function, since the values for the first cultivar are between -6 and -1, while the values for cultivar 3 are between 2 and 6, and so there is no overlap in values.

However, the separation achieved by the linear discriminant function on the training set may be an overestimate. To get a more accurate idea of how well the first discriminant function separates the groups, we would need to see a stacked histogram of the values for the three cultivars using some unseen “test set”, that is, using a set of data that was not used to calculate the linear discriminant function.

We see that the first discriminant function separates cultivars 1 and 3 very well, but does not separate cultivars 1 and 2, or cultivars 2 and 3, so well.

We therefore investigate whether the second discriminant function separates those cultivars, by making a stacked histogram of the second discriminant function’s values:

```
> ldahist(data = wine.lda.values$x[,2], g=wine$V1)
```



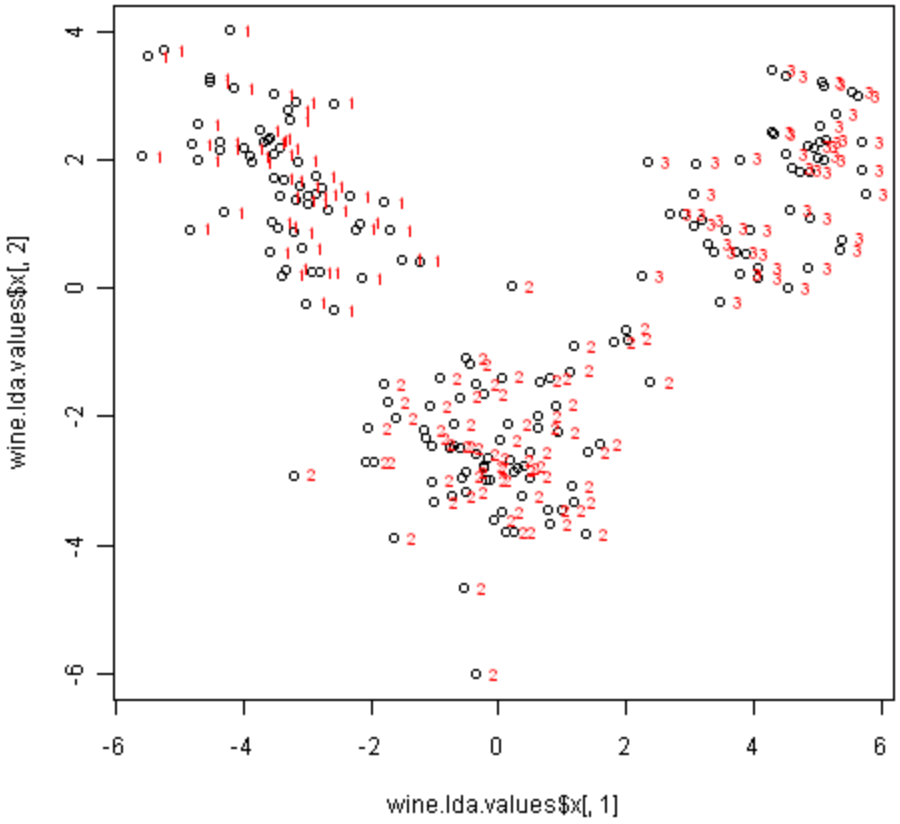
We see that the second discriminant function separates cultivars 1 and 2 quite well, although there is a little overlap in their values. Furthermore, the second discriminant function also separates cultivars 2 and 3 quite well, although again there is a little overlap in their values so it is not perfect.

Thus, we see that two discriminant functions are necessary to separate the cultivars, as was discussed above (see the discussion of percentage separation above).

Scatterplots of the Discriminant Functions

We can obtain a scatterplot of the best two discriminant functions, with the data points labelled by cultivar, by typing:

```
> plot(wine.lda.values$x[,1],wine.lda.values$x[,2]) # make a scatterplot
> text(wine.lda.values$x[,1],wine.lda.values$x[,2],wine$V1,cex=0.7,pos=4,col="red")
# add labels
```



From the scatterplot of the first two discriminant functions, we can see that the wines from the three cultivars are well separated in the scatterplot. The first discriminant function (x-axis) separates cultivars 1 and 3 very well, but doesn't not perfectly separate cultivars 1 and 3, or cultivars 2 and 3.

The second discriminant function (y-axis) achieves a fairly good separation of cultivars 1 and 3, and cultivars 2 and 3, although it is not totally perfect.

To achieve a very good separation of the three cultivars, it would be best to use both the first and second discriminant functions together, since the first discriminant function can separate cultivars 1 and 3 very well, and the second discriminant function can separate cultivars 1 and 2, and cultivars 2 and 3, reasonably well.

Allocation Rules and Misclassification Rate

We can calculate the mean values of the discriminant functions for each of the three cultivars using the "printMeanAndSdByGroup()" function (see above):

```
> printMeanAndSdByGroup(wine.lda.values$x,wine[1])
  [1] "Means:"
     V1         LD1       LD2
   1  1 -3.42248851  1.691674
   2  2 -0.07972623 -2.472656
   3  3  4.32473717  1.578120
```

We find that the mean value of the first discriminant function is -3.42248851 for cultivar 1, -0.07972623 for cultivar 2, and 4.32473717 for cultivar 3. The mid-way point between the mean values for cultivars 1 and 2 is (-3.42248851-0.07972623)/2=-1.751107, and the mid-way point between the mean values for cultivars 2 and 3 is (-0.07972623+4.32473717)/2 = 2.122505.

Therefore, we can use the following allocation rule:

- if the first discriminant function is <= -1.751107, predict the sample to be from cultivar 1
- if the first discriminant function is > -1.751107 and <= 2.122505, predict the sample to be from cultivar 2

- if the first discriminant function is > 2.122505, predict the sample to be from cultivar 3

We can examine the accuracy of this allocation rule by using the "calcAllocationRuleAccuracy()" function below:

```
> calcAllocationRuleAccuracy <- function(ldavalue, groupvariable, cutoffpoints)
  {
     # find out how many values the group variable can take
     groupvariable2 <- as.factor(groupvariable[[1]])
     levels <- levels(groupvariable2)
     numlevels <- length(levels)
     # calculate the number of true positives and false negatives for each group
     numlevels <- length(levels)
     for (i in 1:numlevels)
     {
        leveli <- levels[i]
        levelidata <- ldavalue[groupvariable==leveli]
        # see how many of the samples from this group are classified in each group
        for (j in 1:numlevels)
        {
           levelj <- levels[j]
           if (j == 1)
           {
              cutoff1 <- cutoffpoints[1]
              cutoff2 <- "NA"
              results <- summary(levelidata <= cutoff1)
           }
           else if (j == numlevels)
           {
              cutoff1 <- cutoffpoints[(numlevels-1)]
              cutoff2 <- "NA"
              results <- summary(levelidata > cutoff1)
           }
           else
           {
              cutoff1 <- cutoffpoints[(j-1)]
              cutoff2 <- cutoffpoints[(j)]
              results <- summary(levelidata > cutoff1 & levelidata <= cutoff2)
           }
           trues <- results["TRUE"]
           trues <- trues[[1]]
           print(paste("Number of samples of group",leveli,"classified as group",
              levelj,":",trues,"(cutoffs:",cutoff1,",",cutoff2,")"))
        }
     }
  }
```

For example, to calculate the accuracy for the wine data based on the allocation rule for the first `discriminant function, we type:`

```
> calcAllocationRuleAccuracy(wine.lda.values$x[,1], wine[1], c(-1.751107,
2.122505))
  [1] "Number of samples of group 1 classified as group 1:56 (cutoffs:-1.7511, NA)"
  [1] "Number of samples of group 1 classified as group 2:3 (cutoffs:-1.7511,
2.1225)"
  [1] "Number of samples of group 1 classified as group 3:NA (cutoffs:2.1225, NA)"
  [1] "Number of samples of group 2 classified as group 1:5 (cutoffs:-1.7511, NA)"
  [1] "Number of samples of group 2 classified as group 2:65 (cutoffs:-1.7511,
2.1225)"
  [1] "Number of samples of group 2 classified as group 3:1 (cutoffs:2.1225, NA)"
  [1] "Number of samples of group 3 classified as group 1:NA (cutoffs:-1.7511, NA)"
  [1] "Number of samples of group 3 classified as group 2:NA (cutoffs:-1.7511,
2.1225)"
  [1] "Number of samples of group 3 classified as group 3:48 (cutoffs:2.1225, NA)"
```

This can be displayed in a “confusion matrix”:

	Allocated to group 1	Allocated to group 2	Allocated to group 3
Is group 1	56	3	0
Is group 2	5	65	1
Is group 3	0	0	48

There are 3+5+1=9 wine samples that are misclassified, out of (56+3+5+65+1+48=) 178 wine samples: 3 samples from cultivar 1 are predicted to be from cultivar 2, 5 samples from cultivar 2 are predicted to be from cultivar 1, and 1 sample from cultivar 2 is predicted to be from cultivar 3. Therefore, the misclassification rate is 9/178, or 5.1%. The misclassification rate is quite low, and therefore the accuracy of the allocation rule appears to be relatively high.

However, this is probably an underestimate of the misclassification rate, as the allocation rule was based on this data (this is the “training set”). If we calculated the misclassification rate for a separate “test set” consisting of data other than that used to make the allocation rule, we would probably get a higher estimate of the misclassification rate.