Class07: Machine Learning 1

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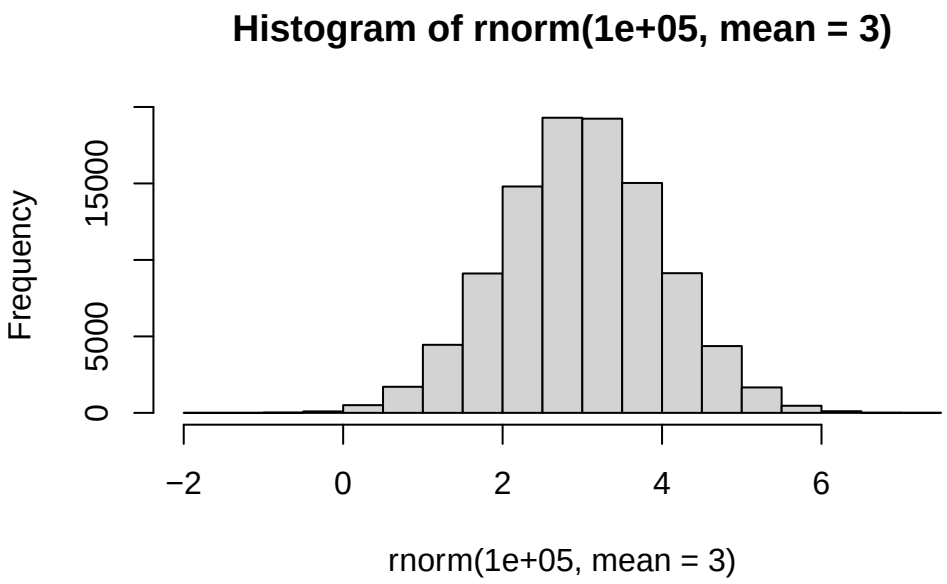
Today we will start our multi-part exploration of some keu machine learning methods. We will begin with clustering - finding groupings in data, and then dimensionallity reduction.

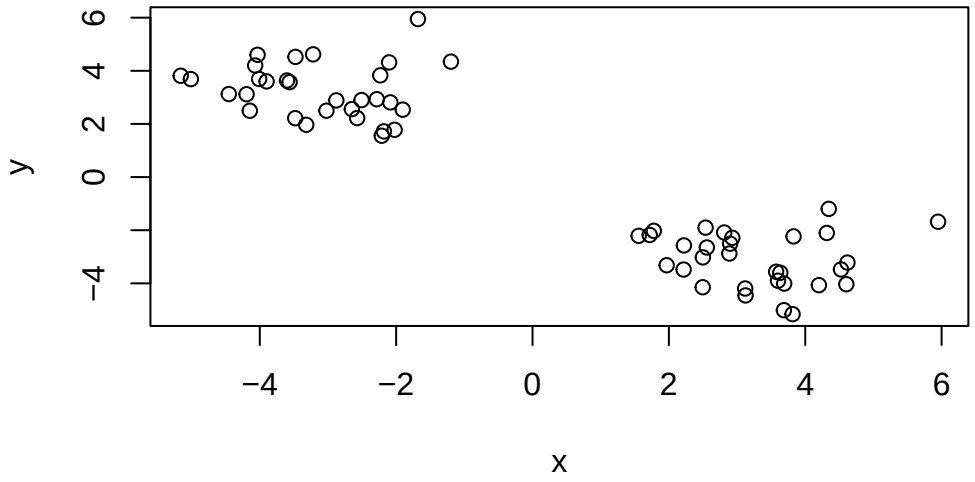
CLustering

Let's start with "k-means" clustering . The main function in base R for this `kmeans()`.

```
#Make up some data
hist(rnorm(100000, mean=3))
```



```r
tmp <- c(rnorm(30, -3), rnorm(30, +3))
x <- cbind(x=tmp, y=rev(tmp))
plot(x)
```



Now let's try out `kmeans()`

```r
km <- kmeans(x, centers=2)
km
```

```
K-means clustering with 2 clusters of sizes 30, 30

Cluster means:
          x         y
1  3.256896 -3.105346
2 -3.105346  3.256896

Clustering vector:
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

Within cluster sum of squares by cluster:
```

```
[1] 61.41485 61.41485
 (between_SS / total_SS =  90.8 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

```
attributes(km)
```

```
$names
[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"

$class
[1] "kmeans"
```

Q. How many points in each cluster?

```
km$size
```

```
[1] 30 30
```

Q. What component of your result object details cluster argument/membership?

```
km$cluster
```

```
 [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

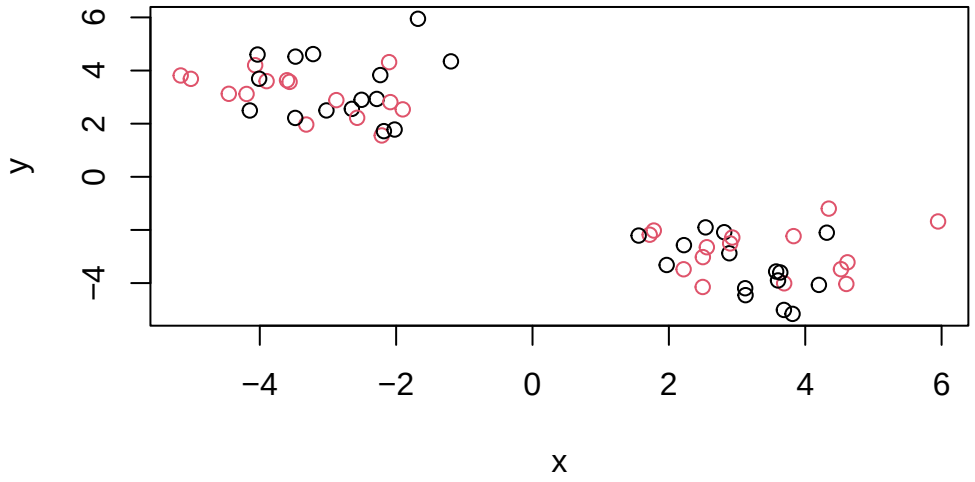
Q. What are centers/mean values of each cluster?

```
km$centers
```

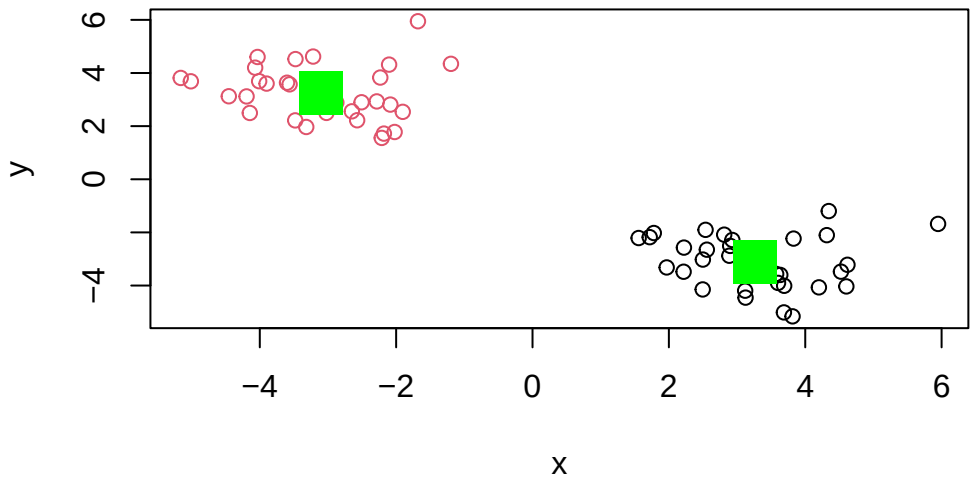
```
          x         y
1  3.256896 -3.105346
2 -3.105346  3.256896
```

Q. Make a plot of your data showing your clustering results.

```r
plot(x, col=c(1,2))
```




```r
#Selecting the cluster attribute vector from the the results of the kmeans() function we u
plot(x, col=km$cluster)
points(km$centers, col="green", pch=15, cex=3)
```



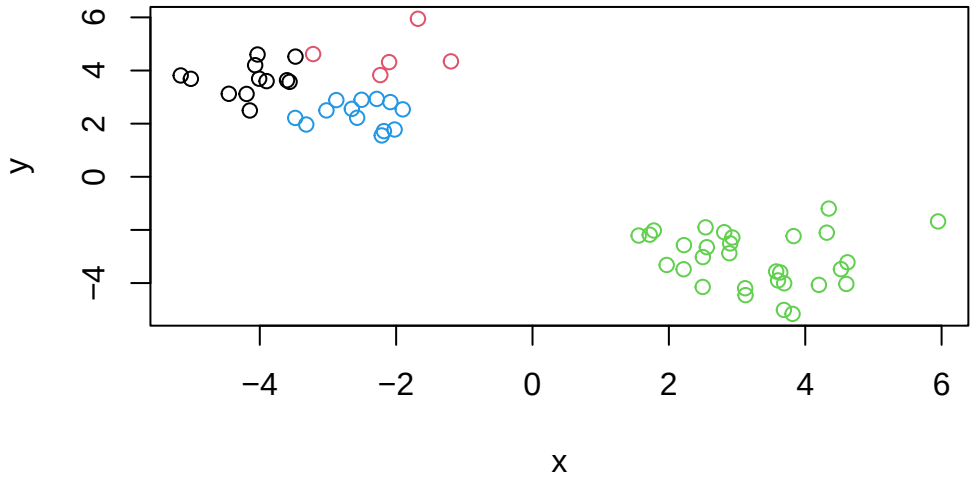
Q. Run `kmeans()` again and cluster in 4 groupsand plot the results.

```
km4 <- kmeans(x, centers=4)
km4
```

```
K-means clustering with 4 clusters of sizes 12, 5, 30, 13

Cluster means:
          x         y
1 -4.134665  3.672285
2 -2.086204  4.611556
3  3.256896 -3.105346
4 -2.547183  2.352437

Clustering vector:
 [1] 4 4 1 4 4 1 2 1 4 1 1 2 2 1 2 1 4 1 4 1 1 4 2 4 4 1 1 4 4 4 3 3 3 3 3 3 3 3
[39] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3

Within cluster sum of squares by cluster:
[1]  6.951537  4.817664 61.414853  5.807639
 (between_SS / total_SS =  94.1 %)
```

```
Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

```
plot(x, col=km4$cluster)
```



Hierarchical Clustering

This form of clustering aims to reveal the structure in your data by progressively grouping points into an ever smaller number of clusters.

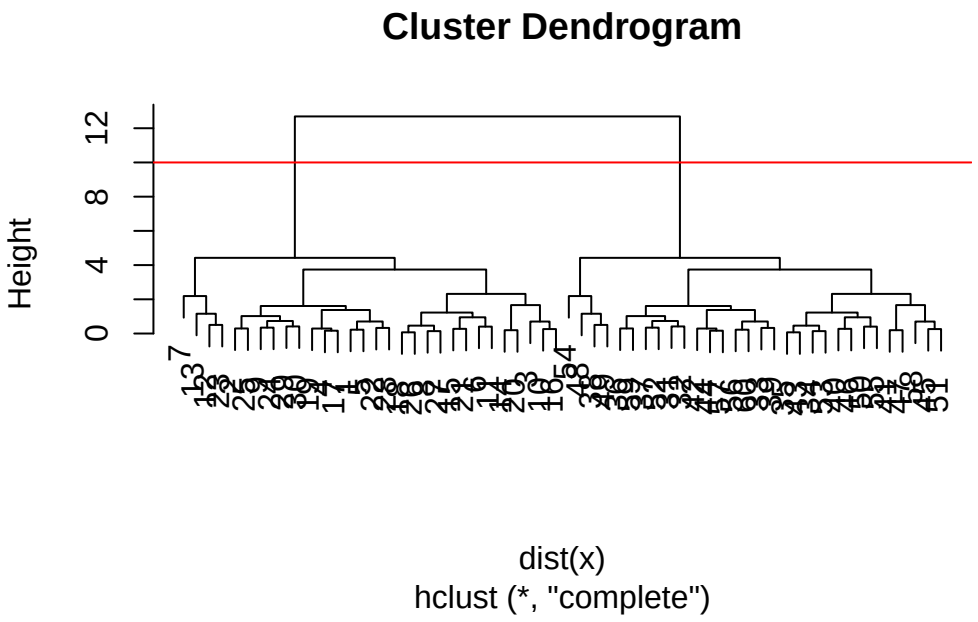
The main function in base R for this is called `hclust()`. This function does not take our input data directly but wants a "distance matrix" that details how (dis)similar all our input points are to each other.

```
#you can't just input x alone, hclust needs a distance matrix as it's input, which comes f
hc <- hclust(dist(x))
hc
```

```
Call:
hclust(d = dist(x))

Cluster method   : complete
Distance         : euclidean
Number of objects: 60
```

The printout above is not very useful (unlike the one from kmeans) but there is a useful `plot()` method.

```
plot(hc)
abline(h=10, col="red")
```

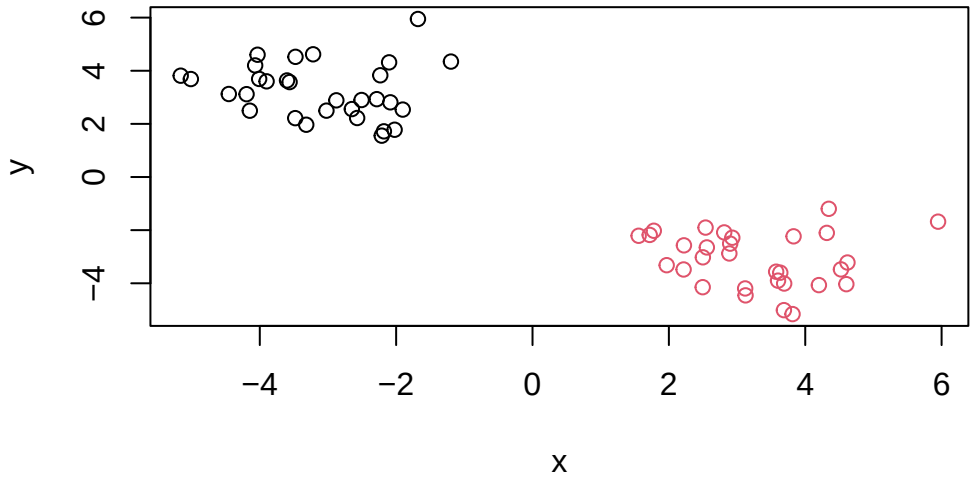


To get my main result (my cluster membership vector) I need to "cut" my tree using the function `cutree()`

```
grps <- cutree(hc, h=10)
grps
```

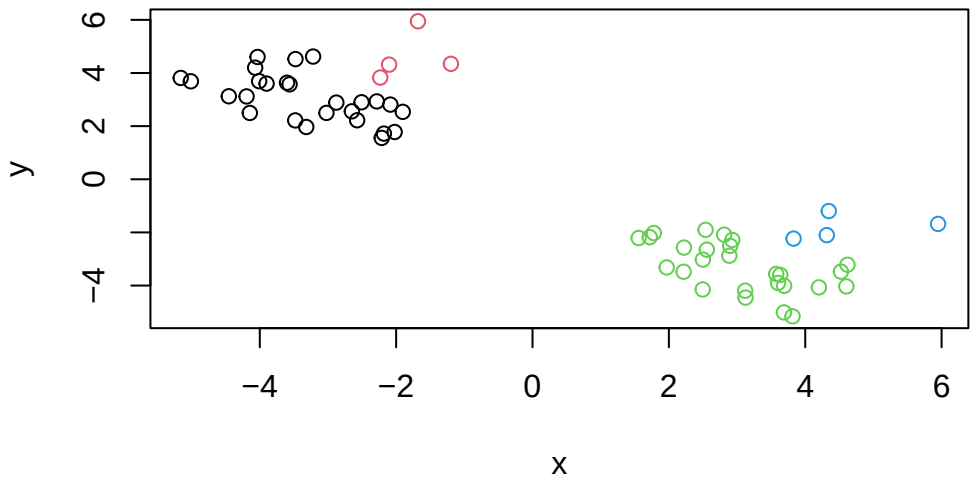
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

```
plot(x, col=grps)
```



Cutting the tree a second time at h=4, splits the plotted data into more than two clusters.

```
plot(x, col=cutree(hc, h=4))
```



#Principal Component Analysis (PCA)

The goal of PCA is to reduce the dimensionality of a data set down to a smaller subset of new variables (called PCs) that are a useful basis for further analysis, like visualization, clustering, etc.

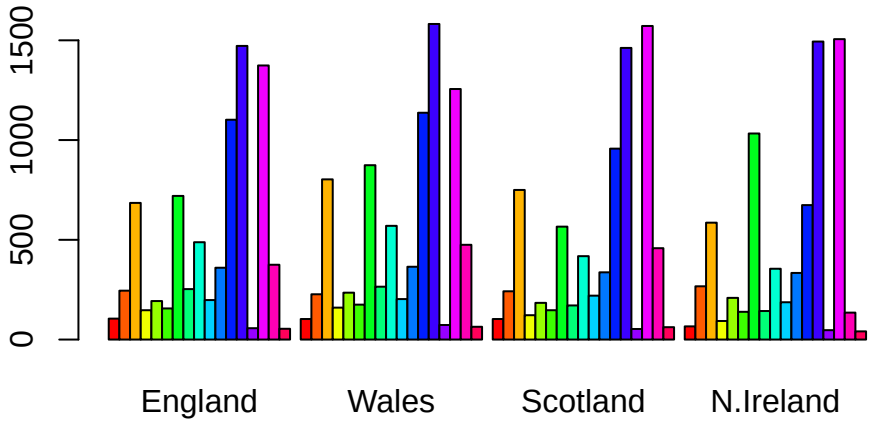
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
head(x)
```

```
              England Wales Scotland N.Ireland
Cheese            105   103      103        66
Carcass_meat      245   227      242       267
Other_meat        685   803      750       586
Fish              147   160      122        93
Fats_and_oils     193   235      184       209
Sugars            156   175      147       139
```

```
dim(x)
```

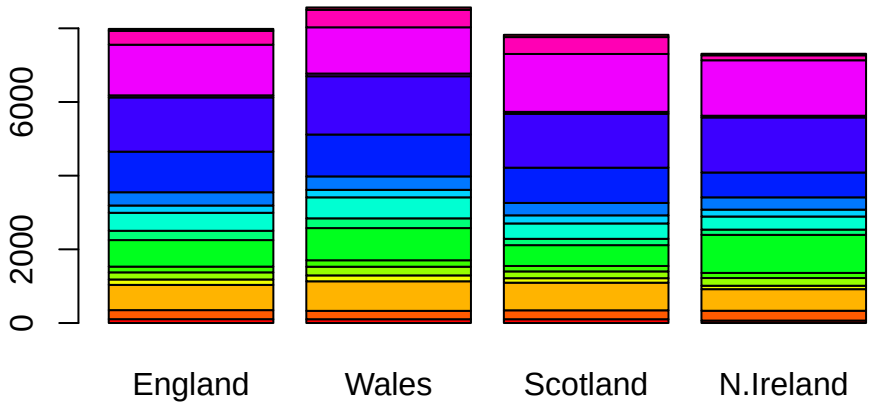
```
[1] 17  4
```

```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



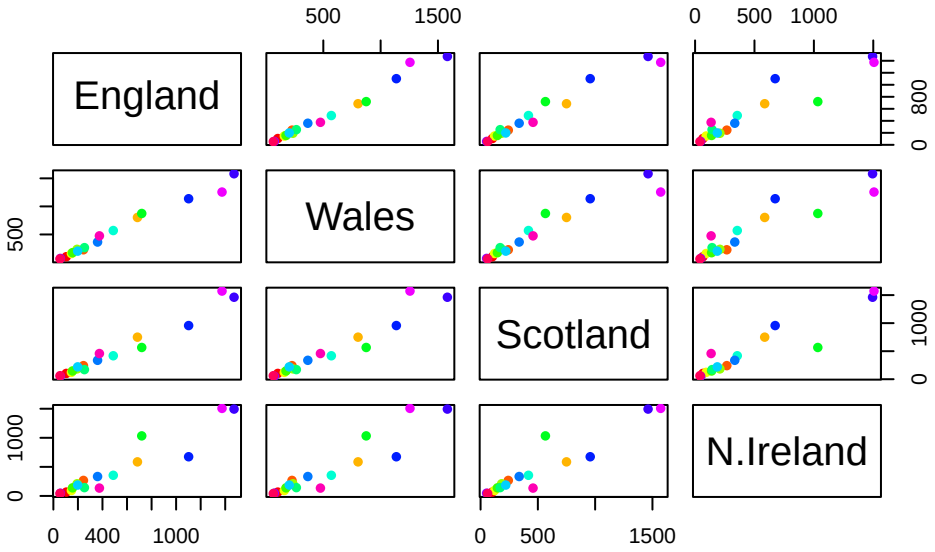
Changing the beside argument of the barplot() function changes the plot to be:

```
barplot(as.matrix(x), col=rainbow(nrow(x)))
```



The so-called "pairs" plot can be useful for small datasets:

```
pairs(x, col=rainbow(nrow(x)), pch=16)
```



These plots show each country in comparison to each other one - hence the title "pairs". You only need to look at half, the information is duplicated. Any departure from the straight diagnol line indicates a difference in the values between countries.

So the pairs plot is useful for small data sets but it can be a lot of work to interpret and gets untraceable for larger datasets.

PCA to the rescue...

The main function to do PCA in base R is called `prcomp()`. This functions wants the transpose of our data in this case.

```
#need to switch the data, we want foods as the columns for PCA
pca <- prcomp(t(x))
summary(pca)
```

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
attributes(pca)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

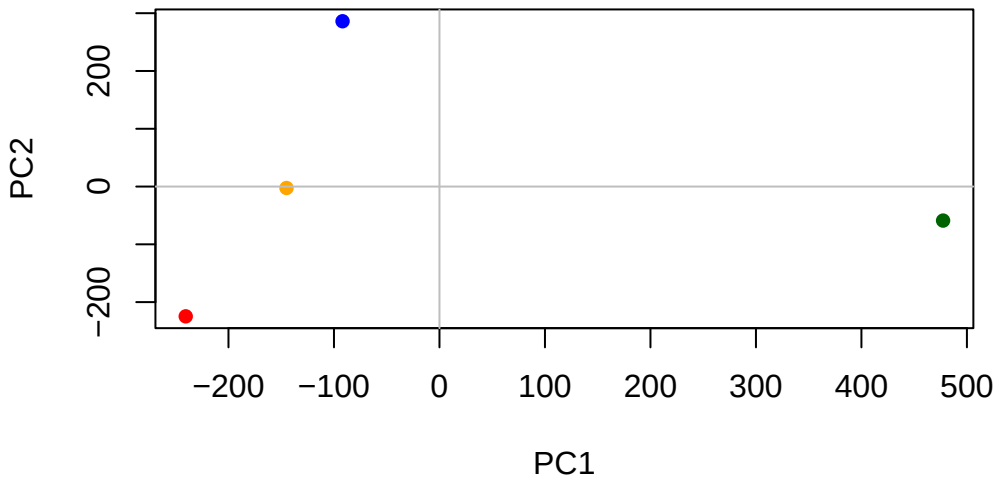
x shows how the data lies on the new axes

```
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -4.894696e-14
Wales     -240.52915 -224.646925 -56.475555  5.700024e-13
Scotland   -91.86934  286.081786 -44.415495 -7.460785e-13
N.Ireland  477.39164  -58.901862  -4.877895  2.321303e-13
```

A major PCA result viz is called a "PCA plot" (a.k.a. a score plot, bi-plot, PC1 vs PC2 plot, ordination plot)

```
mycols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col=mycols, pch=16,
     xlab="PC1", ylab="PC2")
abline(h=0, col="gray")
abline(v=0, col="gray")
```



Another important output from PCA is called the "loadings" vector or "rotation" component - this tells us how much the original variables (the foods in this case) contribute to the new PCs.

```
pca$rotation
```

	PC1	PC2	PC3	PC4
Cheese	-0.056955380	0.016012850	0.02394295	-0.694538519
Carcass_meat	0.047927628	0.013915823	0.06367111	0.489884628
Other_meat	-0.258916658	-0.015331138	-0.55384854	0.279023718
Fish	-0.084414983	-0.050754947	0.03906481	-0.008483145
Fats_and_oils	-0.005193623	-0.095388656	-0.12522257	0.076097502
Sugars	-0.037620983	-0.043021699	-0.03605745	0.034101334
Fresh_potatoes	0.401402060	-0.715017078	-0.20668248	-0.090972715
Fresh_Veg	-0.151849942	-0.144900268	0.21382237	-0.039901917
Other_Veg	-0.243593729	-0.225450923	-0.05332841	0.016719075
Processed_potatoes	-0.026886233	0.042850761	-0.07364902	0.030125166
Processed_Veg	-0.036488269	-0.045451802	0.05289191	-0.013969507
Fresh_fruit	-0.632640898	-0.177740743	0.40012865	0.184072217
Cereals	-0.047702858	-0.212599678	-0.35884921	0.191926714
Beverages	-0.026187756	-0.030560542	-0.04135860	0.004831876
Soft_drinks	0.232244140	0.555124311	-0.16942648	0.103508492

```
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.316290619
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001847469
```

PCA looks to be a super useful method for gaining some insight into high dimensional data that is difficult to examine in other ways.

PCA of RNAseq Data

```
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)
```

```
      wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
gene1  439 458  408  429 420  90  88  86  90  93
gene2  219 200  204  210 187 427 423 434 433 426
gene3 1006 989 1030 1017 973 252 237 238 226 210
gene4  783 792  829  856 760 849 856 835 885 894
gene5  181 249  204  244 225 277 305 272 270 279
gene6  460 502  491  491 493 612 594 577 618 638
```

```
## Again we have to take the transpose of our data
pca <- prcomp(t(rna.data), scale=TRUE)
```

```
summary(pca)
```

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     9.6237 1.5198 1.05787 1.05203 0.88062 0.82545 0.80111
Proportion of Variance 0.9262 0.0231 0.01119 0.01107 0.00775 0.00681 0.00642
Cumulative Proportion  0.9262 0.9493 0.96045 0.97152 0.97928 0.98609 0.99251
                           PC8     PC9      PC10
Standard deviation     0.62065 0.60342 3.457e-15
Proportion of Variance 0.00385 0.00364 0.000e+00
Cumulative Proportion  0.99636 1.00000 1.000e+00
```

Q. How many genes are in the data set?

```
nrow(rna.data)
```

```
[1] 100
```

```
attributes(pca)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```
head(pca$x)
```

```
          PC1        PC2        PC3        PC4        PC5        PC6
wt1 -9.697374  1.5233313 -0.2753567  0.7322391 -0.6749398  1.1823860
wt2 -9.138950  0.3748504  1.0867958 -1.9461655  0.7571209 -0.4369228
wt3 -9.054263 -0.9855163  0.4152966  1.4166028  0.5835918  0.6937236
wt4 -8.731483 -0.7468371  0.5875748  0.2268129 -1.5404775 -1.2723618
wt5 -9.006312 -0.2945307 -1.8498101 -0.4303812  0.8666124 -0.2496025
ko1  8.846999  2.2345475 -0.1462750 -1.1544333 -0.6947862  0.7128021
           PC7         PC8         PC9         PC10
wt1 -0.24446614  1.03519396  0.07010231 3.073930e-15
wt2 -0.03275370  0.26622249  0.72780448 1.963707e-15
wt3 -0.03578383 -1.05851494  0.52979799 2.893519e-15
wt4 -0.52795595 -0.20995085 -0.50325679 2.872702e-15
wt5  0.83227047 -0.05891489 -0.81258430 1.693090e-15
ko1 -0.07864392 -0.94652648 -0.24613776 4.052314e-15
```

```
kmeans(pca$x[,1], centers=2)
```

```
K-means clustering with 2 clusters of sizes 5, 5

Cluster means:
       [,1]
1 -9.125676
2  9.125676

Clustering vector:
wt1 wt2 wt3 wt4 wt5 ko1 ko2 ko3 ko4 ko5
```

```
  1   1   1   1   1   2   2   2   2   2

Within cluster sum of squares by cluster:
[1] 0.5017505 0.2648467
 (between_SS / total_SS =  99.9 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

I will make a main result figure using ggplot.

```
library(ggplot2)
```

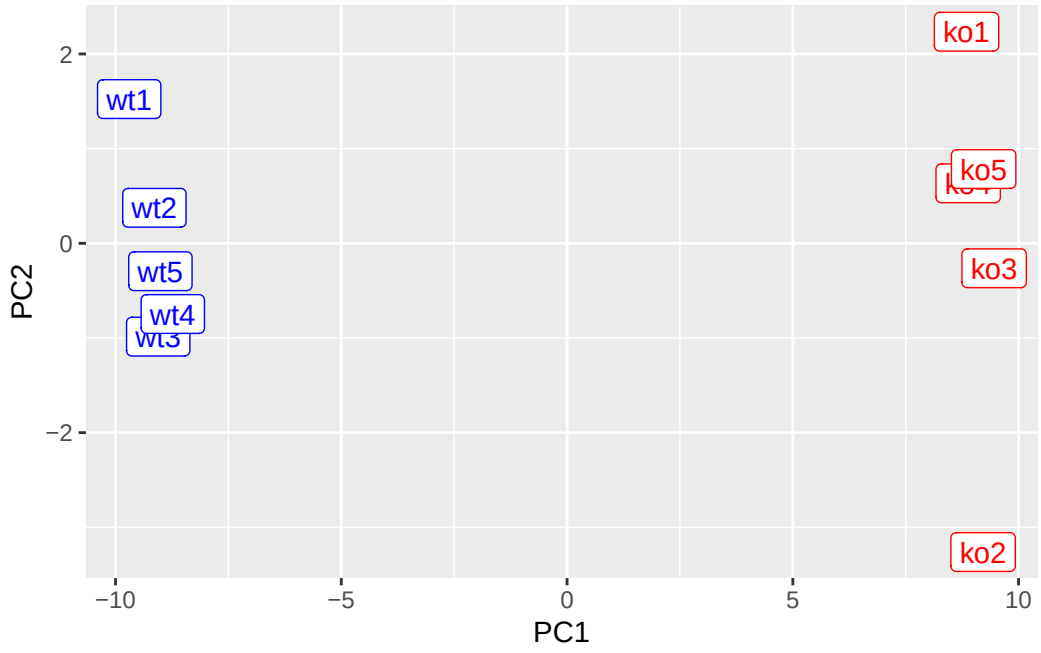
```
res <- as.data.frame(pca$x)
head(res)
```

```
          PC1        PC2        PC3        PC4        PC5        PC6
wt1 -9.697374  1.5233313 -0.2753567  0.7322391 -0.6749398  1.1823860
wt2 -9.138950  0.3748504  1.0867958 -1.9461655  0.7571209 -0.4369228
wt3 -9.054263 -0.9855163  0.4152966  1.4166028  0.5835918  0.6937236
wt4 -8.731483 -0.7468371  0.5875748  0.2268129 -1.5404775 -1.2723618
wt5 -9.006312 -0.2945307 -1.8498101 -0.4303812  0.8666124 -0.2496025
ko1  8.846999  2.2345475 -0.1462750 -1.1544333 -0.6947862  0.7128021
            PC7         PC8         PC9         PC10
wt1 -0.24446614  1.03519396  0.07010231 3.073930e-15
wt2 -0.03275370  0.26622249  0.72780448 1.963707e-15
wt3 -0.03578383 -1.05851494  0.52979799 2.893519e-15
wt4 -0.52795595 -0.20995085 -0.50325679 2.872702e-15
wt5  0.83227047 -0.05891489 -0.81258430 1.693090e-15
ko1 -0.07864392 -0.94652648 -0.24613776 4.052314e-15
```

```
mycols <- c(rep("blue", 5), rep("red", 5))
mycols
```

```
 [1] "blue" "blue" "blue" "blue" "blue" "red"  "red"  "red"  "red"  "red"
```

```
ggplot(res) +
  aes(x=PC1, y=PC2, label=row.names(res)) +
  geom_point(col=mycols) +
  geom_label(col=mycols)
```




```
colnames(rna.data)
```

```
[1] "wt1" "wt2" "wt3" "wt4" "wt5" "ko1" "ko2" "ko3" "ko4" "ko5"
```