Class07: Machine learning 1

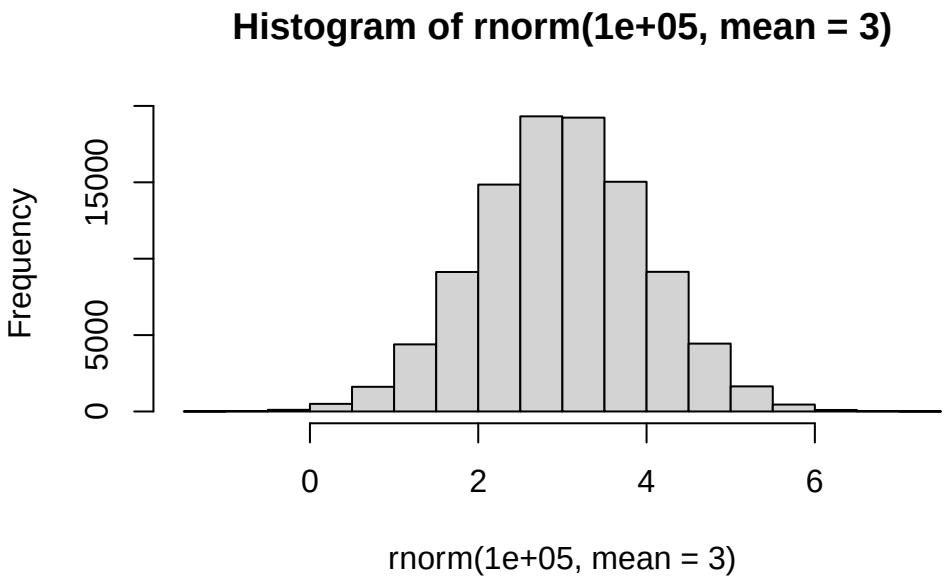
Kalisa Kang (PID: A16741690)

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

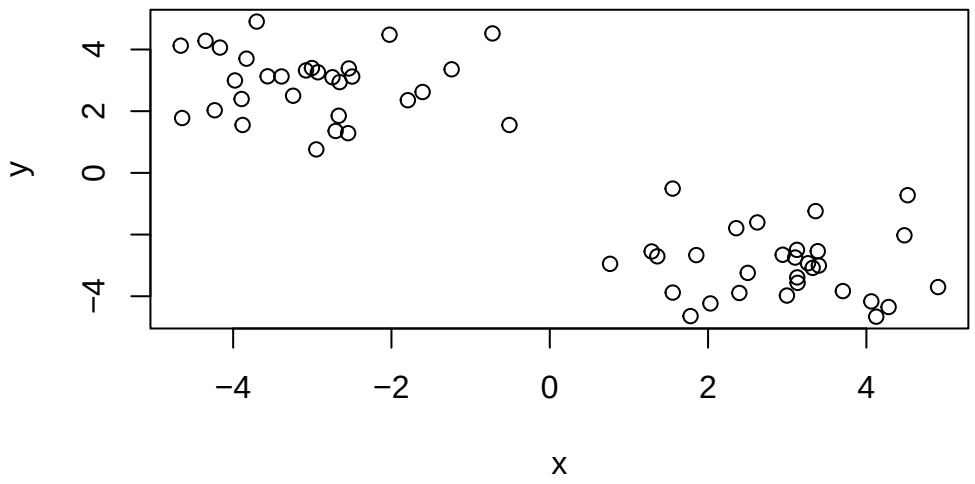
Clustering

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

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



```r
# rnorm(30, -3) gives 30 points of a normal distribution and centers it at -3
# c() puts things in a vector form
# rev() gives the +3 values first, then -3 values next

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  2.908928 -2.991688
2 -2.991688  2.908928

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] 67.14413 67.14413
 (between_SS / total_SS =  88.6 %)

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 assignment/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
```

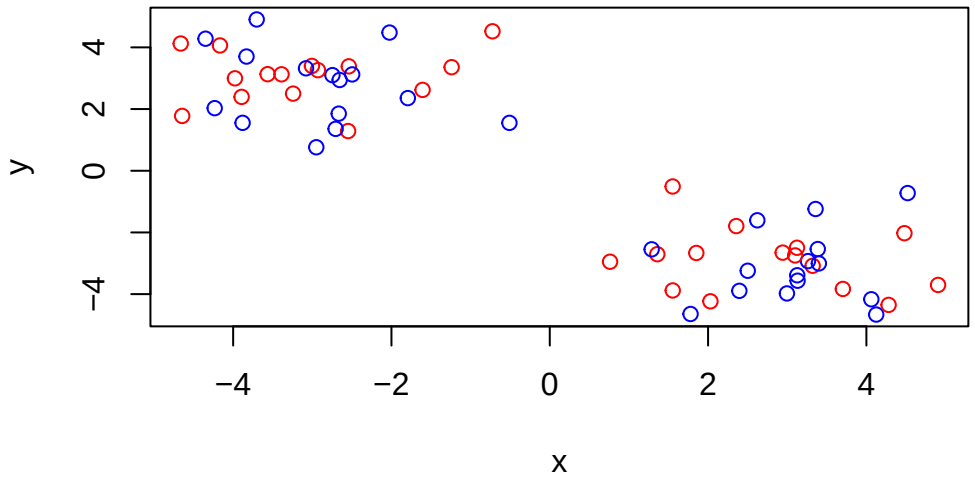
Q. What are centers/mean values of each cluster?

```
km$centers
```

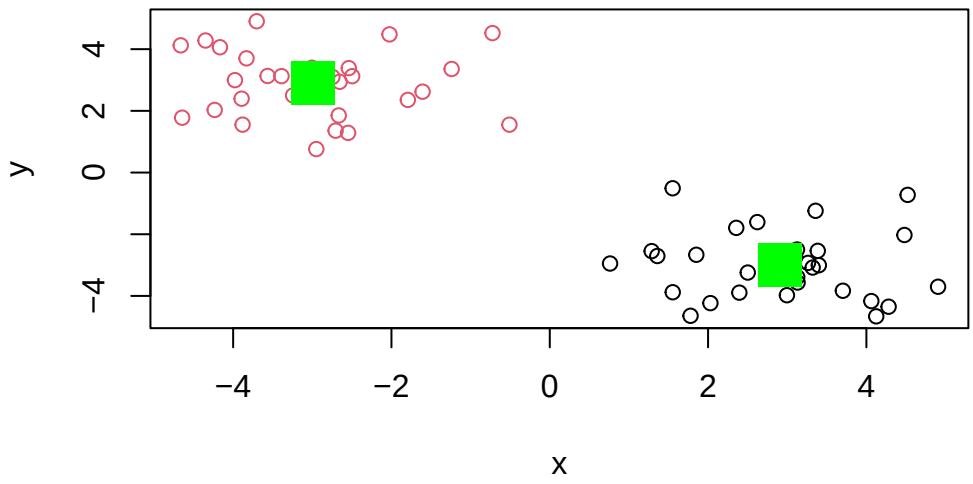
```
          x         y
1  2.908928 -2.991688
2 -2.991688  2.908928
```

Q. Make a plot of your data showing your clustering results (groupings/clusters and cluster centers).

```
plot(x, col=c("red","blue"))
```

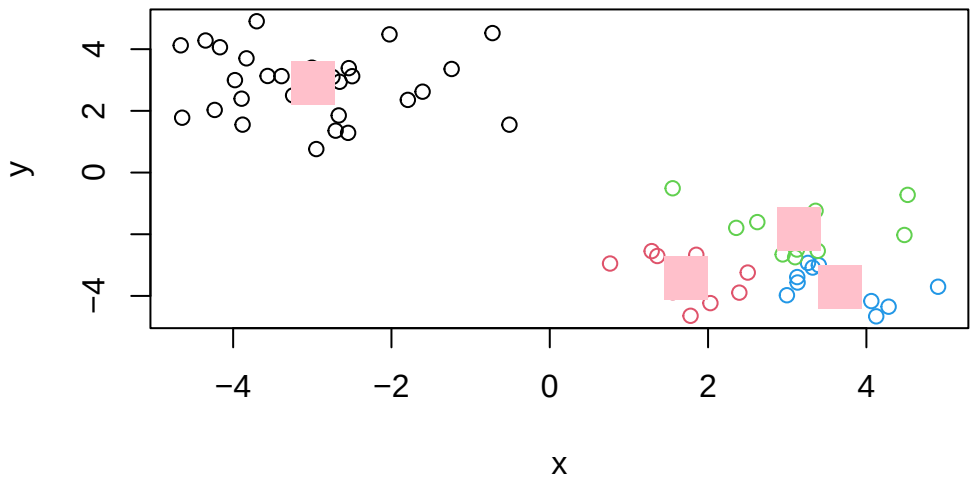



```
# plot(x, col(1,2)) will give a plot of alternating blacks and red points. But we don't wa

# points() adds a point to the plot. `pch` changes the point size and `cex` changes the po
plot(x, col= km$cluster)
points(km$centers, col= "green", pch=15, cex=3)
```



Q. Run `kmeans()` again and clusterin 4 groups and plot the results.

```
km4 <- kmeans(x, centers=4)
plot(x, col= km4$cluster)
points(km4$centers, col="pink", pch=15, cex=3)
```



Hierarchical clustering

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

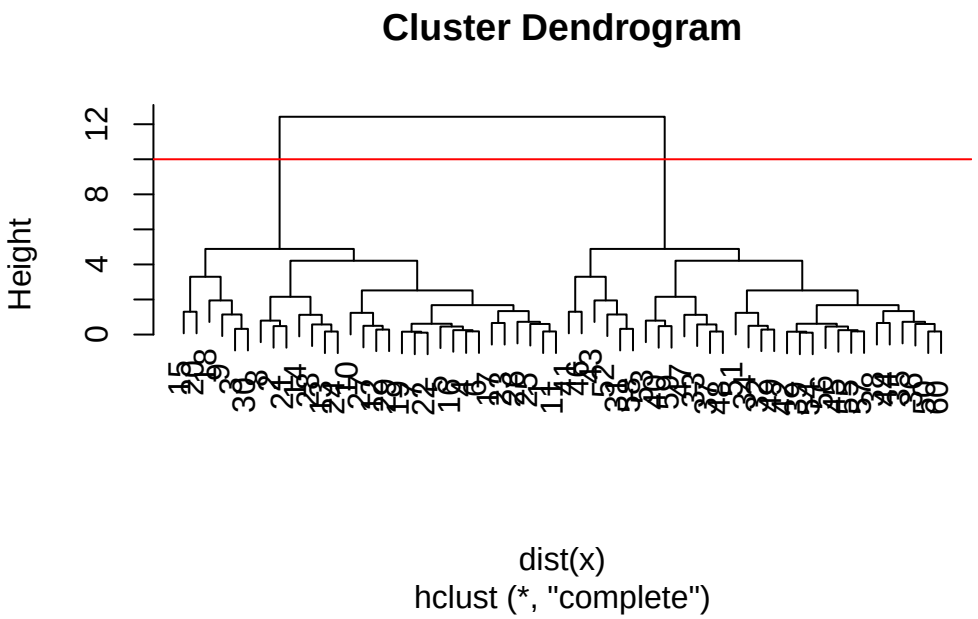
The main function in base R for this is called `hclust()`. This function does not take our input data directly, but wants a "distance matrix" that details how (dis)similar all our input points are to each other.

```
# `dist(x)` is the distance matrix
hc <- hclust(dist(x))
hc
```

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

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

The print out above is not very useful (unlike that of kmeans), but there is a useful `plot()` method.

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

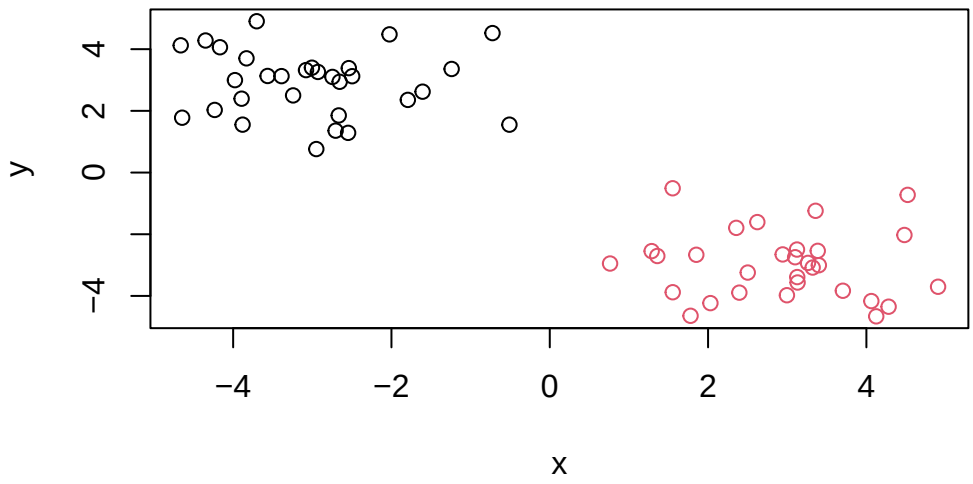


To get my main result (i.e., my cluster membership vector), I need to "cut" my tree using the function `cutree()`

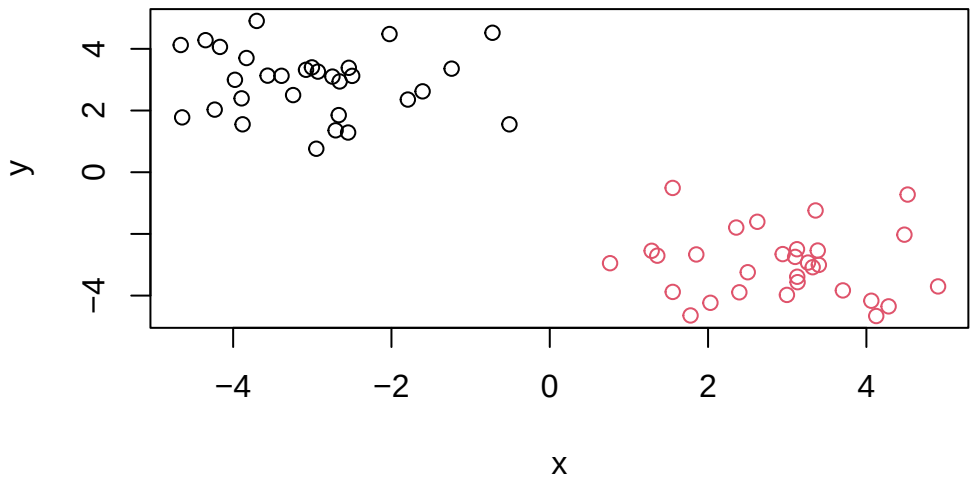
```
grps <- cutree(hc, h=10)
grps
```

```
 [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 2 2
```

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




```
# I cut at height 7 to get 3 groups now.
plot(x, col=cutree(hc, h=7))
```



Principal Component Analysis

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

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
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
Fresh_potatoes	720	874	566	1033
Fresh_Veg	253	265	171	143
Other_Veg	488	570	418	355
Processed_potatoes	198	203	220	187
Processed_Veg	360	365	337	334
Fresh_fruit	1102	1137	957	674
Cereals	1472	1582	1462	1494
Beverages	57	73	53	47
Soft_drinks	1374	1256	1572	1506
Alcoholic_drinks	375	475	458	135
Confectionery	54	64	62	41

> Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this questions?

```
dim(x)
```

```
[1] 17  4
```

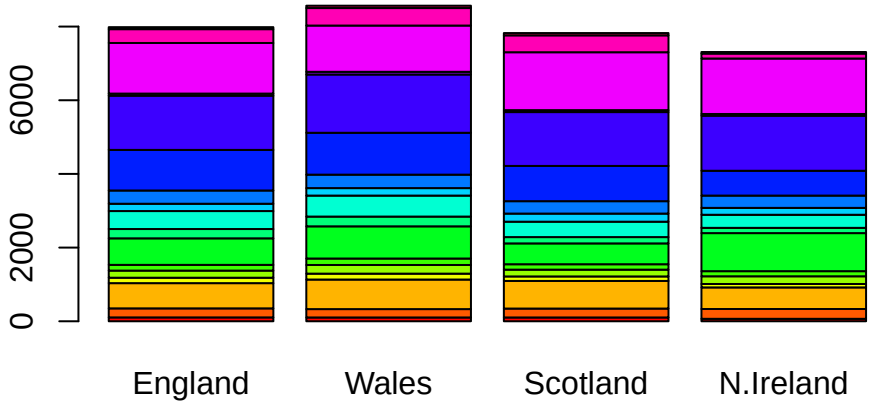
17 rows and 4 columns.

> Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

I prefer using the row.names argument because it is more robust in ensuring that the number of columns corresponds to the actual dataset rather than the names of the rows.

> Q3: Changing what optional argument in the above barplot() function results in the following plot?

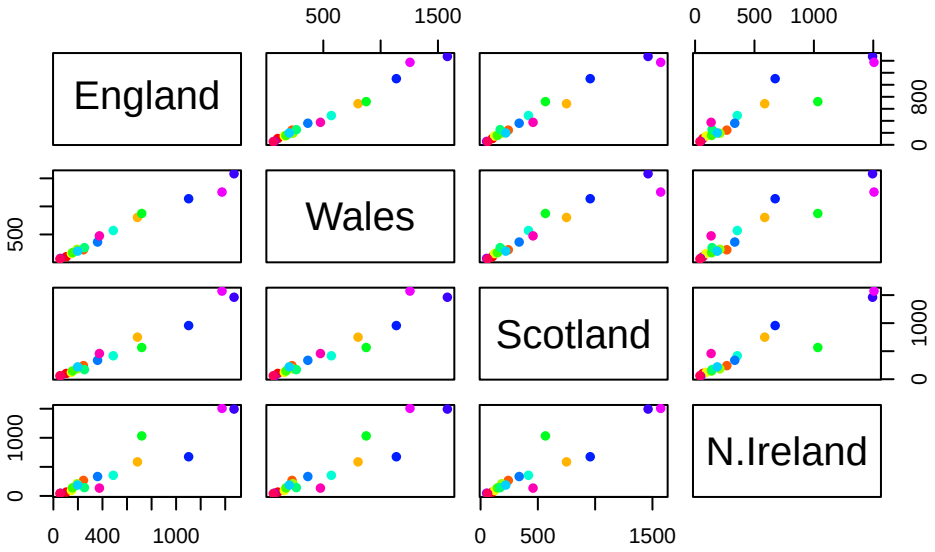
```
# Changing beside=T to beside=F
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



> Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

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

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



Diagonal boxes containing the country names is the x and y axes of the plots, so we only need to read half of the plots (eg top diagonal half or bottom diagonal half). If points lie on the straight line, then that means the values are similar. Departure from the straight line means that the values are more different.

So the pairs plot is useful for small datasets, but it can be lots of work to interpret and gets intractable for larger datasets.

So PCA to the rescue!

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

```
# t(x) transposes the data
pca <-prcomp(t(x))
summary(pca)
```

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 2.921e-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)
```

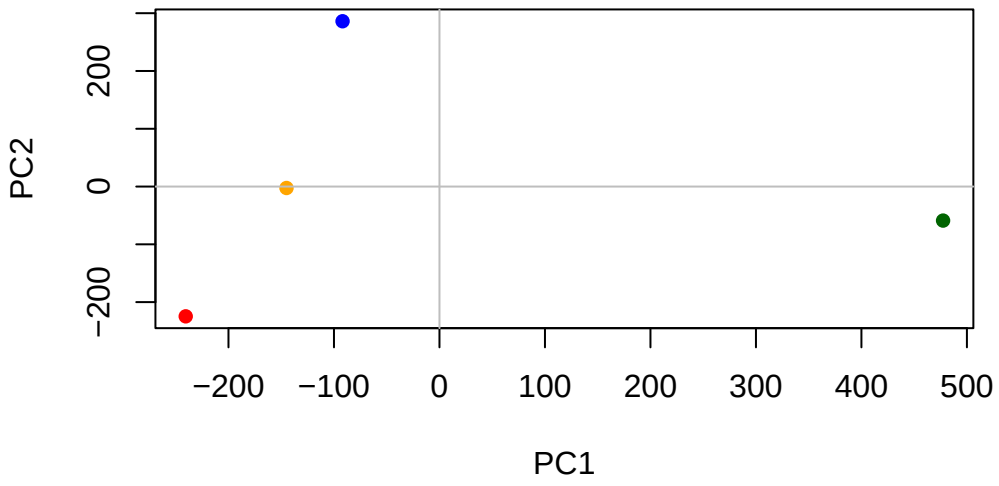
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

```
pca$x
```

```
                PC1         PC2        PC3           PC4
England   -144.99315   -2.532999 105.768945 -9.152022e-15
Wales     -240.52915 -224.646925 -56.475555  5.560040e-13
Scotland   -91.86934  286.081786 -44.415495 -6.638419e-13
N.Ireland  477.39164  -58.901862  -4.877895  1.329771e-13
```

A major PCA result visualization is called a "PCA plot" (aka a score plot, biplot, 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 the "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	-0.409382587
Carcass_meat	0.047927628	0.013915823	0.06367111	0.729481922
Other_meat	-0.258916658	-0.015331138	-0.55384854	0.331001134
Fish	-0.084414983	-0.050754947	0.03906481	0.022375878
Fats_and_oils	-0.005193623	-0.095388656	-0.12522257	0.034512161
Sugars	-0.037620983	-0.043021699	-0.03605745	0.024943337
Fresh_potatoes	0.401402060	-0.715017078	-0.20668248	0.021396007
Fresh_Veg	-0.151849942	-0.144900268	0.21382237	0.001606882
Other_Veg	-0.243593729	-0.225450923	-0.05332841	0.031153231
Processed_potatoes	-0.026886233	0.042850761	-0.07364902	-0.017379680
Processed_Veg	-0.036488269	-0.045451802	0.05289191	0.021250980
Fresh_fruit	-0.632640898	-0.177740743	0.40012865	0.227657348
Cereals	-0.047702858	-0.212599678	-0.35884921	0.100043319
Beverages	-0.026187756	-0.030560542	-0.04135860	-0.018382072
Soft_drinks	0.232244140	0.555124311	-0.16942648	0.222319484

```
Alcoholic_drinks    -0.463968168  0.113536523 -0.49858320 -0.273126013
Confectionery       -0.029650201  0.005949921 -0.05232164  0.001890737
```

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