

Class 7: Machine Learning 1

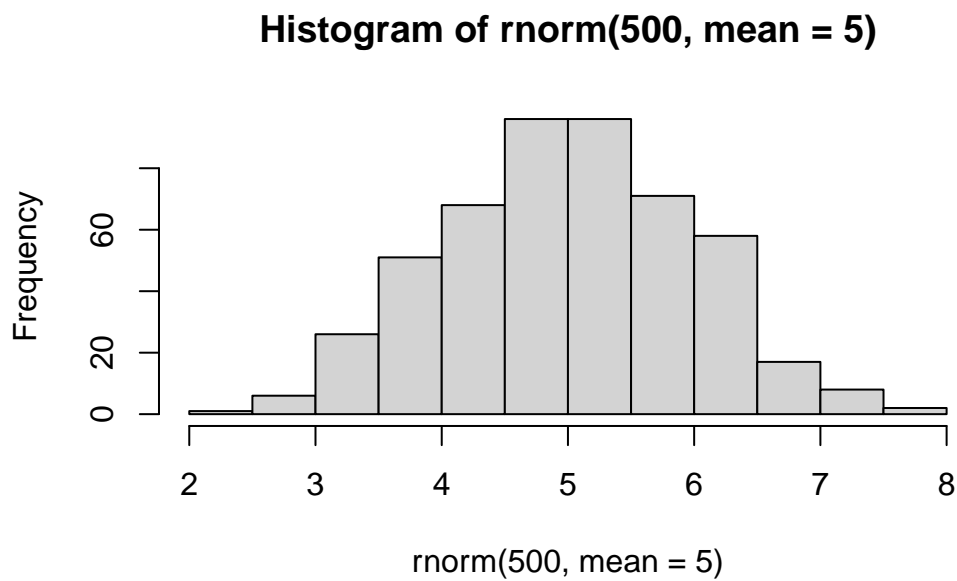
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Today we will explore some fundamental machine learning methods including clustering and dimensionality reduction.

K-means clustering

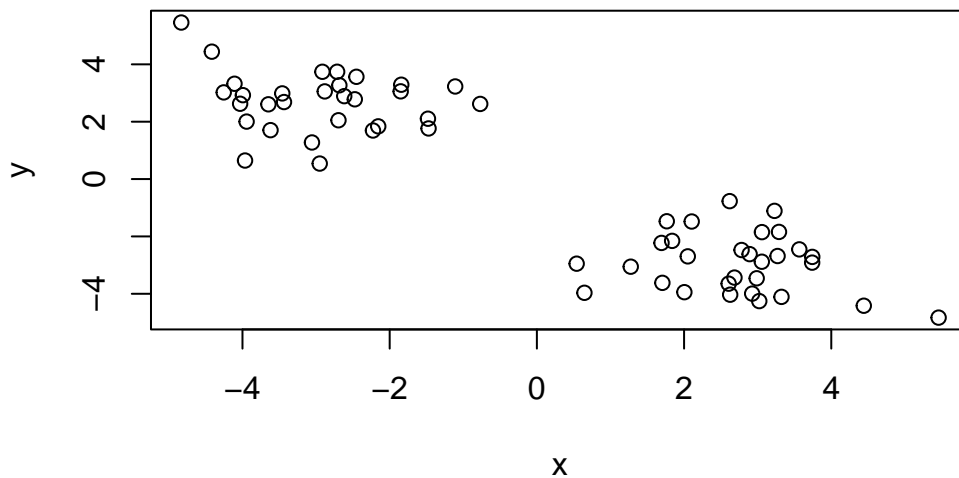
To see how this works let's first make up some data to cluster where we know what the answer should be. We can use the 'rnorm()' function to help here:

```
hist(rnorm(500,mean=5))
```



```
x<-c(rnorm(30,mean=-3), rnorm(30,mean=3))
y<-rev(x)
```

```
x<-cbind(x,y)
plot(x)
```



The function for K-means clustering in “base” R is ‘kmeans()’

```
k<-kmeans(x,centers=2)
k
```

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

Cluster means:

	x	y
1	2.697869	-2.935037
2	-2.935037	2.697869

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 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

Within cluster sum of squares by cluster:

```
[1] 62.5526 62.5526
(between_SS / total_SS = 88.4 %)
```

Available components:

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

To get the results of the returned list object we can dollar '\$' syntax

Q. How many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q. What 'component' of your result object details -cluster assignment/membership?
-cluster center?

```
k$cluster
```

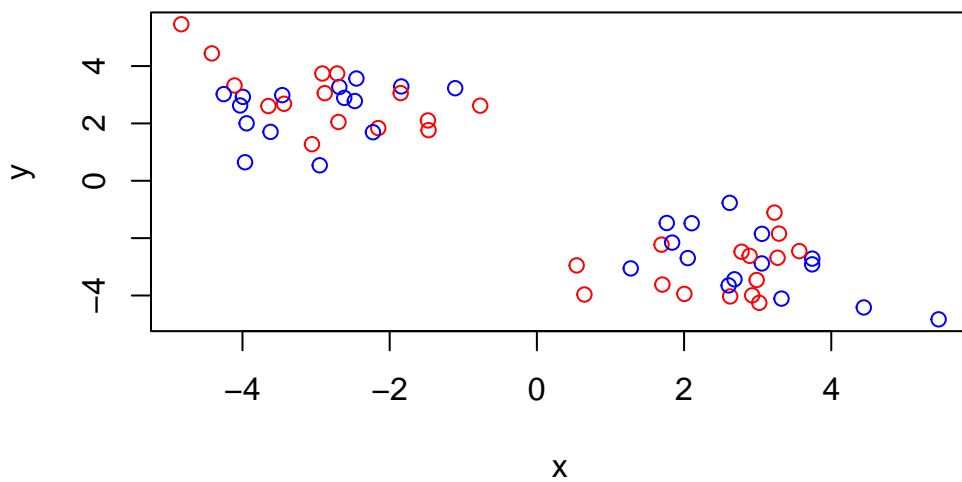
```
[1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
k$centers
```

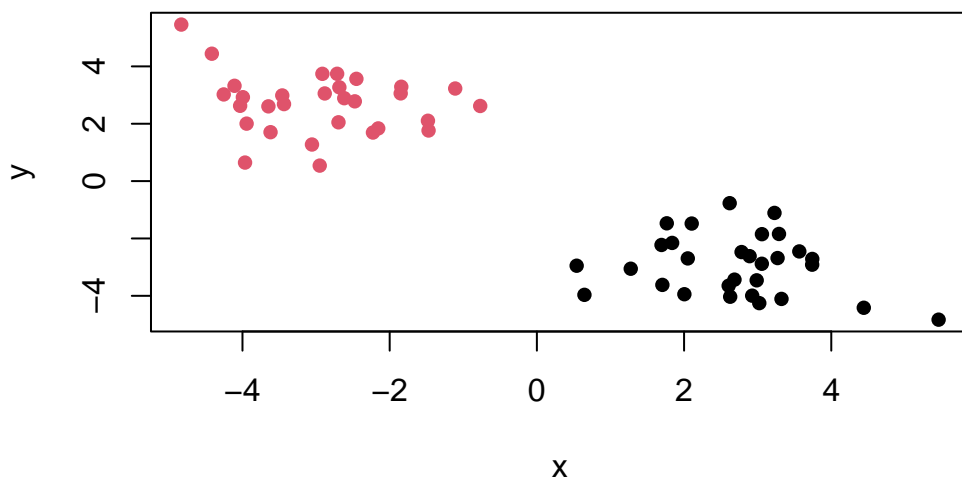
```
      x      y
1  2.697869 -2.935037
2 -2.935037  2.697869
```

Q. Make a clustering results figure of the data colored by cluster membership.

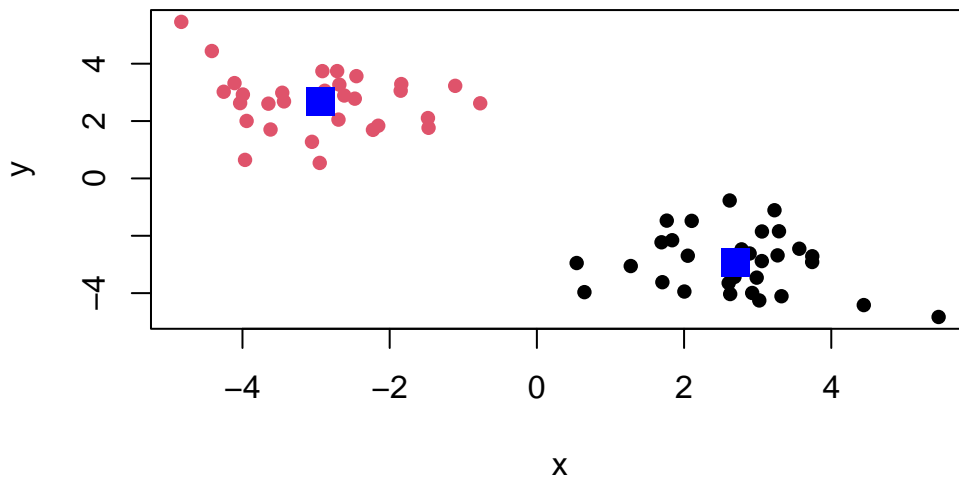
```
plot(x,col=c("red","blue"))
```



```
plot(x,col=k$cluster,pch=16)
```



```
plot(x,col=k$cluster,pch=16)
points(k$centers,col="blue",pch=15,cex=2)
```

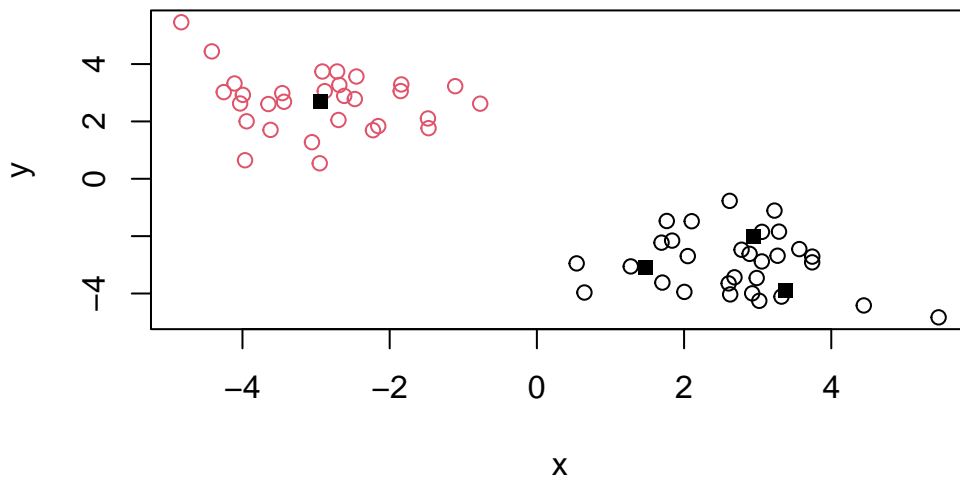


K-means clustering is very popular as its very fast and relatively straight forward: it takes numeric data as input and returns the cluster membership vector etc.

The “issue” is we tell ‘kmeans()’ how many clusters we want!

Q. Run kmeans again and cluster into 4 grps/clusters and plot the results like we did above?

```
k4<-kmeans(x,centers=4)
plot(x,col=k4$cluster)
points(k4$centers,pch=15)
```



Screeplot to pick k 'centers' value

Can do through brute force

```
c(k1<-kmeans(x,centers=1),
  k2<-kmeans(x,centers=2),
  k3<-kmeans(x,centers=3),
  k4<-kmeans(x,centers=4),
  k5<-kmeans(x,centers=5))
```

\$cluster

```
[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 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 1 1 1 1 1 1 1 1 1 1
```

\$centers

```
      x      y
1 -0.1185837 -0.1185837
```

\$totss

```
[1] 1076.994
```

\$withinss

```
[1] 1076.994
```

```
$tot.withinss
```

```
[1] 1076.994
```

```
$betweenss
```

```
[1] 0
```

```
$size
```

```
[1] 60
```

```
$iter
```

```
[1] 1
```

```
$ifault
```

```
NULL
```

```
$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 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 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
$centers
```

	x	y
1	2.697869	-2.935037
2	-2.935037	2.697869

```
$totss
```

```
[1] 1076.994
```

```
$withinss
```

```
[1] 62.5526 62.5526
```

```
$tot.withinss
```

```
[1] 125.1052
```

```
$betweenss
```

```
[1] 951.889
```

```
$size
```

```
[1] 30 30
```

```
$iter
```

```
[1] 1
```

```

$ifault
[1] 0

$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 2 2 1 3 3 3 3 1 1 3
[39] 3 3 3 1 1 1 1 1 1 1 3 1 1 3 1 1 3 3 3 3 1 3 1

$centers
      x      y
1  3.296805 -3.584584
2 -2.935037  2.697869
3  2.098934 -2.285489

$totss
[1] 1076.994

$withinss
[1] 17.09540 62.55260 22.03812

$tot.withinss
[1] 101.6861

$betweenss
[1] 975.308

$size
[1] 15 30 15

$iter
[1] 2

$ifault
[1] 0

$cluster
[1] 3 1 3 1 1 1 1 3 3 1 3 3 1 3 3 3 3 3 3 1 1 1 1 3 3 1 1 1 1 3 4 2 2 2 2 4 4 2
[39] 2 2 2 4 4 4 4 4 4 2 4 4 2 4 4 2 2 2 2 4 2 4

$centers
      x      y
1 -2.285489  2.098934
2  2.098934 -2.285489
3 -3.584584  3.296805

```



```
4 3.296805 -3.584584
```

```
$totss
```

```
[1] 1076.994
```

```
$withinss
```

```
[1] 22.03812 22.03812 17.09540 17.09540
```

```
$tot.withinss
```

```
[1] 78.26705
```

```
$betweeness
```

```
[1] 998.7271
```

```
$size
```

```
[1] 15 15 15 15
```

```
$iter
```

```
[1] 2
```

```
$ifault
```

```
[1] 0
```

```
$cluster
```

```
[1] 1 5 1 5 5 5 5 1 1 5 1 1 5 1 1 1 1 1 5 5 5 5 1 1 5 5 5 5 1 4 2 3 3 3 3 2 2  
[39] 3 3 2 4 4 4 4 3 3 3 3 4 2 4 4 3 2 2 2 4 3 4
```

```
$centers
```

	x	y
1	-3.584584	3.296805
2	1.469058	-3.076408
3	2.947425	-2.028868
4	3.381452	-3.909343
5	-2.285489	2.098934

```
$totss
```

```
[1] 1076.994
```

```
$withinss
```

```
[1] 17.095404 6.010551 9.042607 10.493127 22.038121
```

```
$tot.withinss
```

```
[1] 64.67981
```

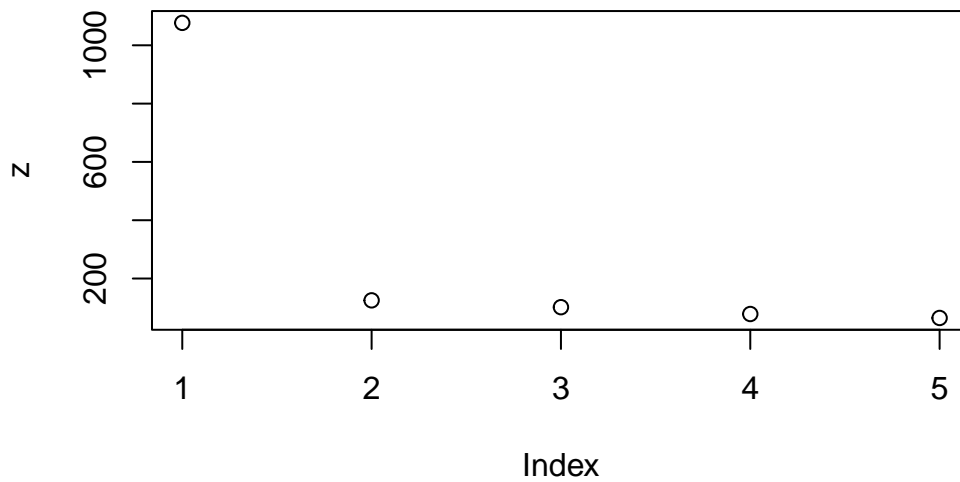
```
$betweenss  
[1] 1012.314
```

```
$size  
[1] 15  8 12 10 15
```

```
$iter  
[1] 2
```

```
$ifault  
[1] 0
```

```
z<-c(k1$tot.withinss,  
      k2$tot.withinss,  
      k3$tot.withinss,  
      k4$tot.withinss,  
      k5$tot.withinss)  
plot(z,)
```

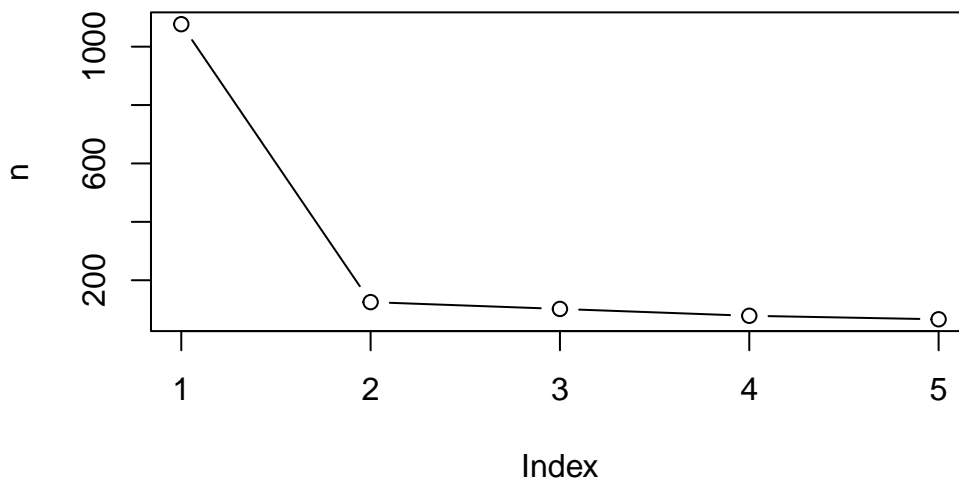


```
n<-NULL  
for(i in 1:5) {
```

```

  n<-c(n,kmeans(x,centers=i)$tot.withinss)
}
plot(n,typ="b")

```



##Hierarchial Clustering

The main “base” R function for Hierarchal Clustering is called ‘hclust()’. Here we can’t just input our data we need to first calculate a distance matrix (e.g. ‘dist()’) for our data and use this as input to ‘hclust()’

```

d<-dist(x)
hc<-hclust(d)
hc

```

Call:

```
hclust(d = d)
```

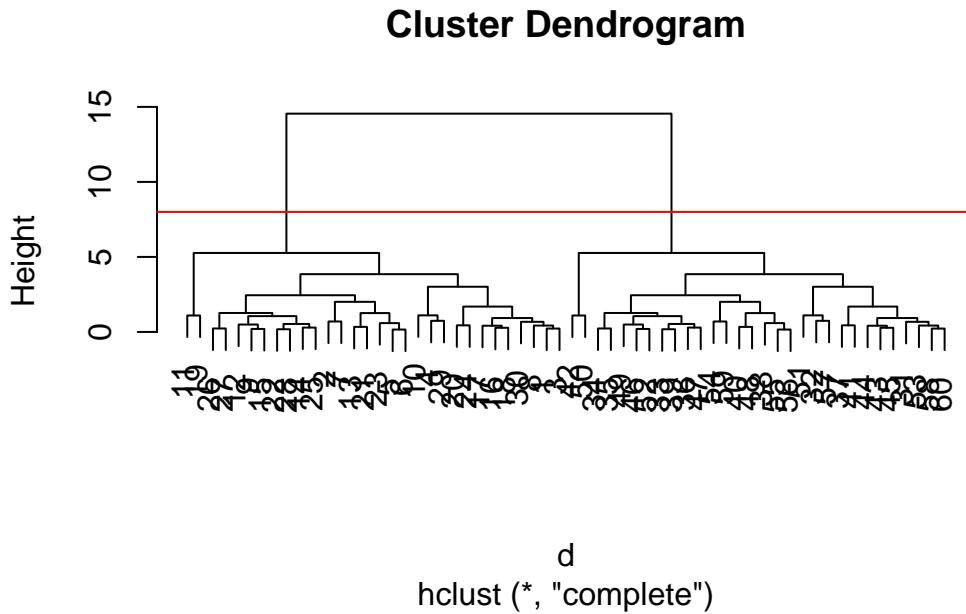
```

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

```

There is a plot method for hclust result lets try it, notice how the higher numbers are on the right side.

```
plot(hc)
abline(h=8,col="red")
```



```
cutree(hc, h=8)
```

[illegible]

To get our cluster “membership” vector (i.e. our main clustering result) we can “cut” the tree at a given height or at a height that yields a given “k” groups.

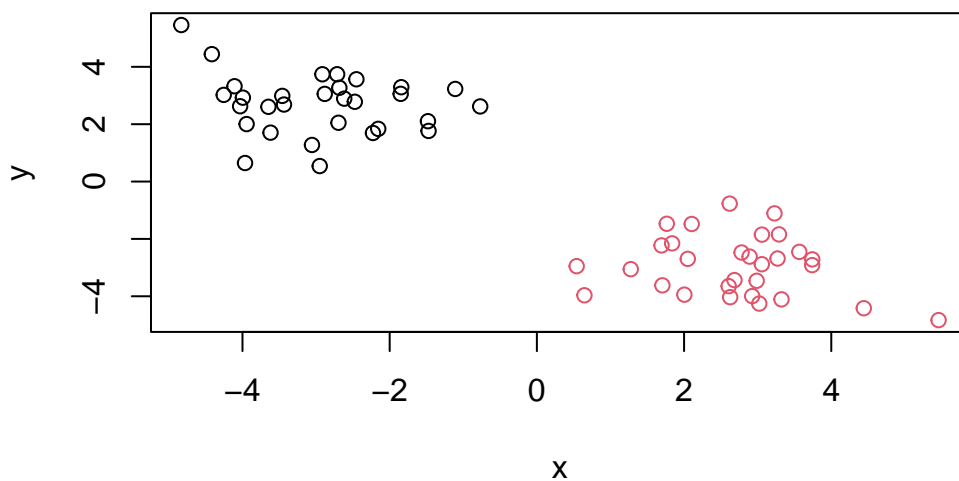
```
cutree(hc,h=8)
```

```
[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
```

```
grps<-cutree(hc,k=2)
```

Q. Plot the data with out hclust result coloring

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



#Principal Component Analysis (PCA)

##PCA of UK Food Data

Import food data from an online CSV file:"<https://tiny.url.com/UK-foods>"

```
url<-("https://bioboot.github.io/bggn213_f17/class-material/UK_foods.csv")
x <- read.csv(url)
head(x)
```

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

```
rownames(x)<-x[,1]
x<-x[,-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

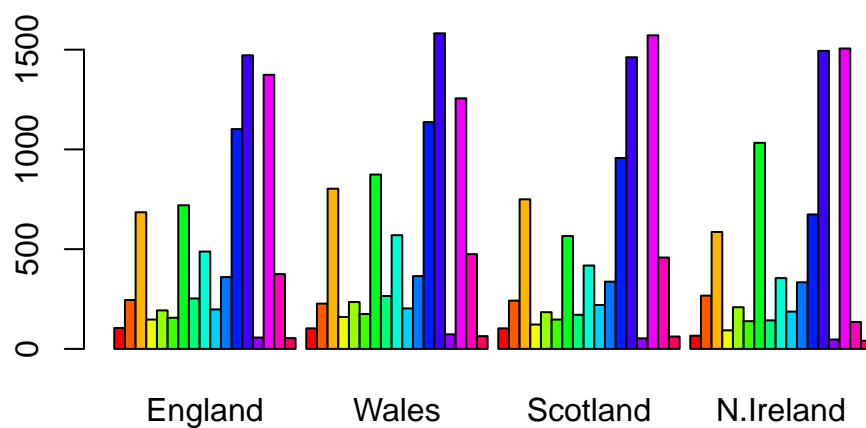
```
x<-read.csv(url,row.names=1)
x
```

	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

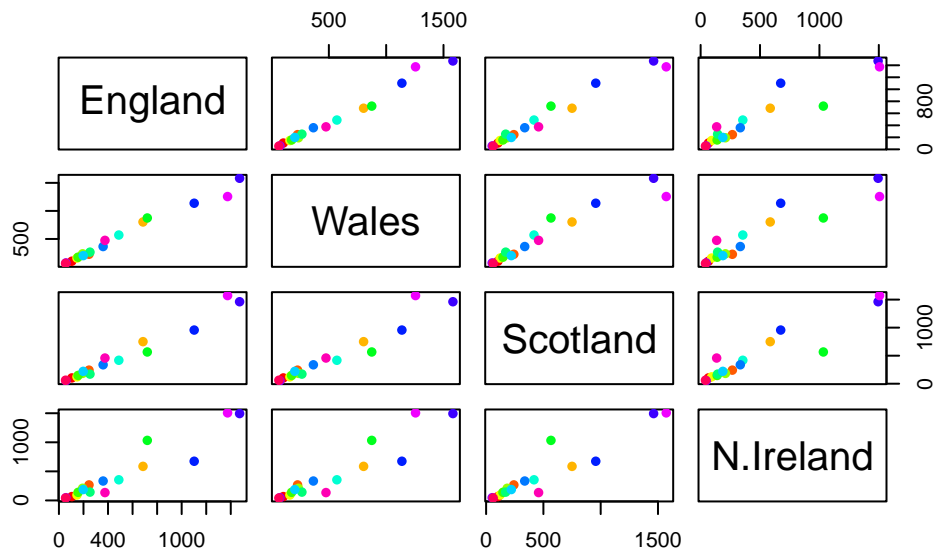
Some base figures

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



There is one plot that can be useful for small datasets:

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



Main point: It can be difficult to spot major trends and patterns even in relatively small multivariate datasets (here we only have 17 dimensions, typically we have 1000s).

##PCA will help

The main function in “base” R for PCA is called ‘prcomp()’ I will take transpose of our data so the “food” are in the columns:

```
pca<-prcomp(t(x))
summary(pca)
```

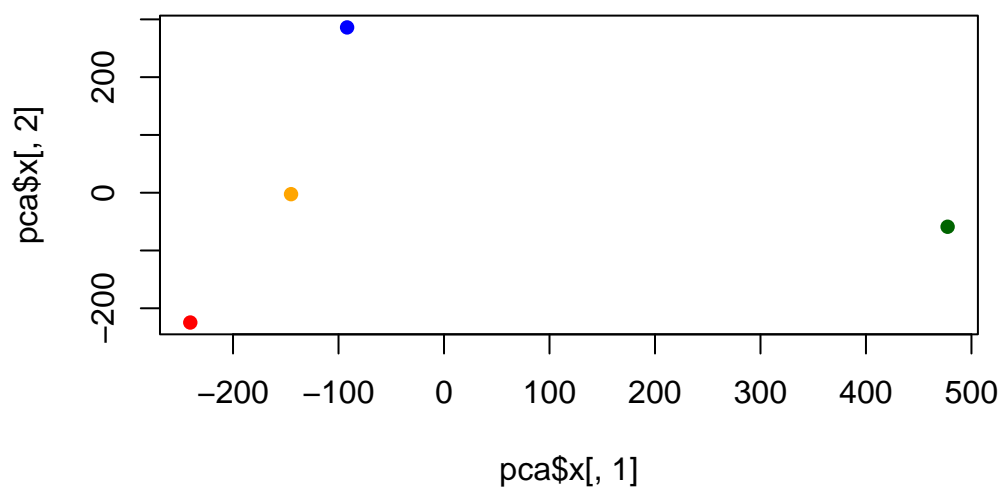
Importance of components:

	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

```
pca$x
```

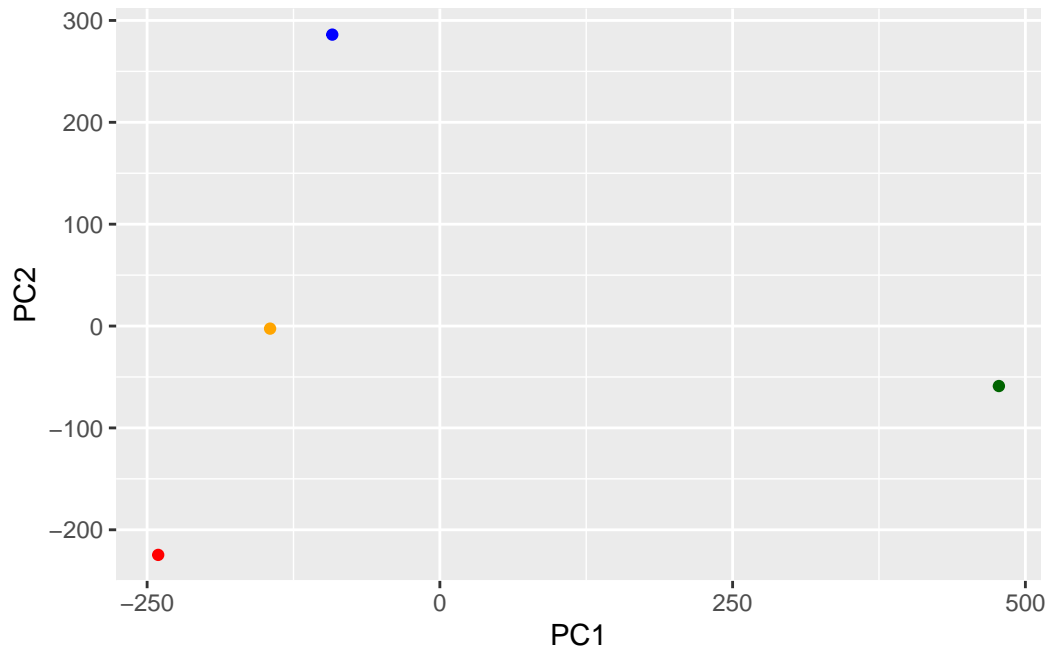

	PC1	PC2	PC3	PC4
England	-144.99315	-2.532999	105.768945	-9.152022e-15
Wales	-240.52915	-224.646925	-56.475555	5.560040e-13
Scotland	-91.86934	286.081786	-44.415495	-6.638419e-13
N.Ireland	477.39164	-58.901862	-4.877895	1.329771e-13

```
cols<-c("orange", "red","blue","darkgreen" )
plot(pca$x[,1],pca$x[,2],col=cols, pch=16)
```

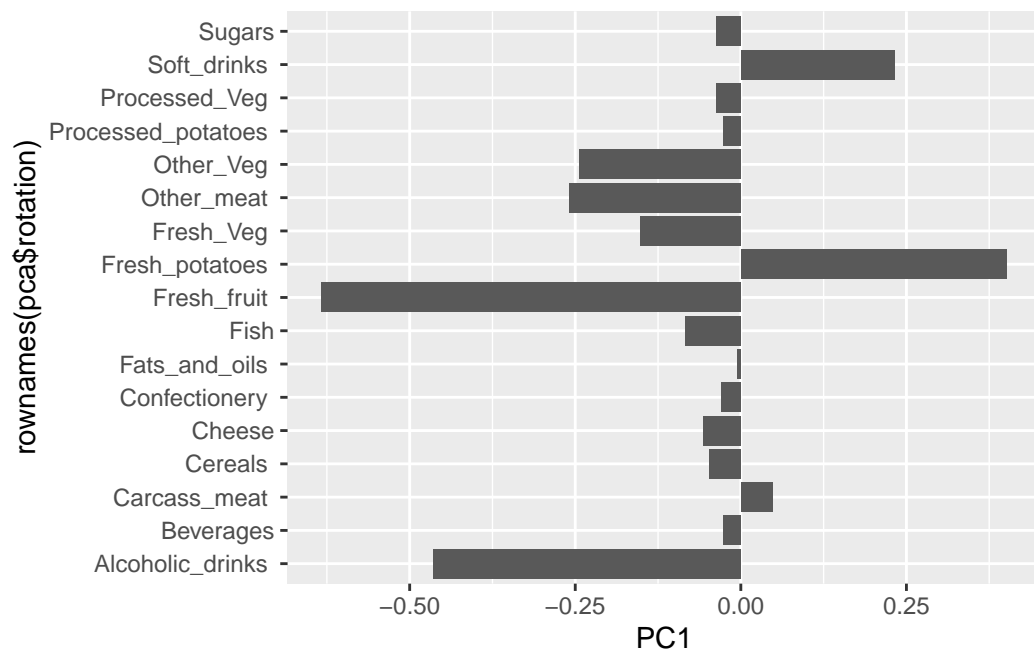


```
library(ggplot2)
```

```
ggplot(pca$x)+
  aes(PC1,PC2)+
  geom_point(col=cols)
```



```
ggplot(pca$rotation)+
  aes(PC1, rownames(pca$rotation))+
  geom_col()
```



PCA looks super useful and we will come back to describe this further the next day.