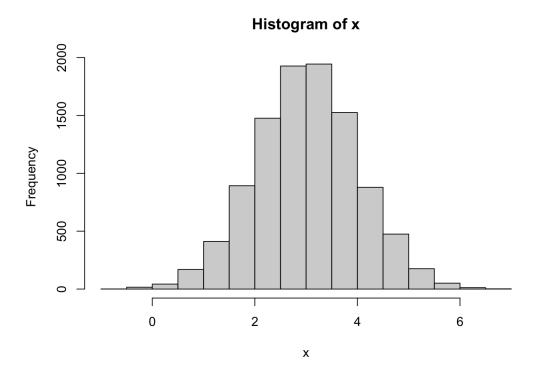
Class 7

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Clustering we will start today's lab with clustering methods, in particular so-called K-means. The main function for this in R is kmeans() Let's try it on some made up data where we know that what the answer should be.

```
x <- rnorm(10000, mean=3)
hist(x)</pre>
```



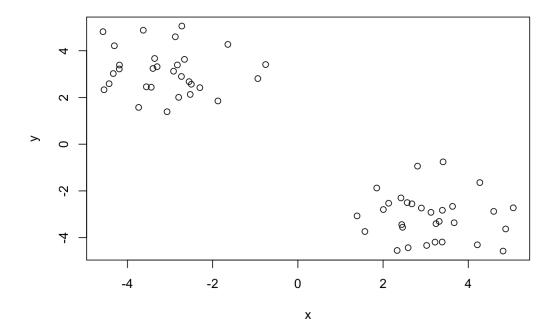
```
tmp <- c(rnorm(30, mean=3), rnorm(30, mean=-3))
x <- cbind(x=tmp, y=rev(tmp))
x</pre>
```

```
Х
 [1,] 1.5730617 -3.7374268
 [2,] 2.0059203 -2.7983824
 [3,] 4.8776676 -3.6285281
 [4,] 2.3305371 -4.5500263
 [5,] 3.3872891 -4.1880801
 [6,] 2.4381875 -3.4417533
 [7,] 3.1238067 -2.9183922
 [8,] 5.0561355 -2.7236296
 [9,] 3.3918173 -2.8282738
[10,] 3.0228338 -4.3334883
[11,] 2.5655748 -2.5006622
[12,] 3.6298575 -2.6619461
[13,] 2.5880133 -4.4307532
[14,] 4.2711998 -1.6431886
[15,] 2.6769813 -2.5530005
[16,] 3.4084627 -0.7565067
[17,] 3.6684502 -3.3627415
[18,] 1.3894406 -3.0703916
[19,] 2.4567153 -3.5570015
```

```
[20,] 2.4196013 -2.2999740
[21,] 4.8162607 -4.5744524
[22,] 3.2417289 -3.4015945
[23,] 1.8513929 -1.8763947
[24,] 2.1305445 -2.5276290
[25,] 4.5969326 -2.8761861
[26,] 3.3170021 -3.3040674
[27,] 3.2194570 -4.1922045
[28,] 2.8989878 -2.7332841
[29,] 4.2126782 -4.3076060
[30,] 2.8085571 -0.9398339
[31,] -0.9398339 2.8085571
[32,] -4.3076060 4.2126782
[33,] -2.7332841
                 2.8989878
[34,] -4.1922045 3.2194570
[35,] -3.3040674 3.3170021
[36,] -2.8761861 4.5969326
[37,] -2.5276290 2.1305445
[38,] -1.8763947
                 1.8513929
[39,] -3.4015945
                 3.2417289
[40,] -4.5744524 4.8162607
[41,] -2.2999740 2.4196013
[42,] -3.5570015 2.4567153
[43,] -3.0703916 1.3894406
[44,] -3.3627415 3.6684502
[45,] -0.7565067
                 3.4084627
[46,] -2.5530005 2.6769813
[47,] -1.6431886 4.2711998
[48,] -4.4307532 2.5880133
[49,] -2.6619461
                 3.6298575
[50,] -2.5006622
                 2.5655748
[51,] -4.3334883 3.0228338
[52,] -2.8282738 3.3918173
[53,] -2.7236296 5.0561355
[54,] -2.9183922 3.1238067
[55,] -3.4417533 2.4381875
[56,] -4.1880801 3.3872891
[57,] -4.5500263 2.3305371
[58,] -3.6285281
                 4.8776676
[59,] -2.7983824
                 2.0059203
[60,] -3.7374268 1.5730617
```

We can pass this to the base R plot() function for a quick plot

plot(x)



```
k <- kmeans(x, centers=2, nstart=20)
k</pre>
```

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

Cluster means:

x y 1 3.112503 -3.090580 2 -3.090580 3.112503

Clustering vector:

Within cluster sum of squares by cluster:

[1] 56.18001 56.18001 (between_SS / total_SS = 91.1 %)

Available components:

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

k\$size

[1] 30 30

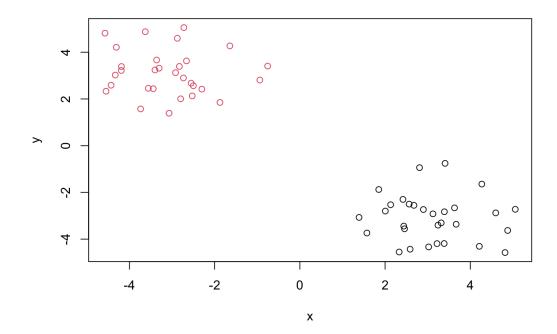
k\$cluster

k\$centers

```
x y
1 3.112503 -3.090580
2 -3.090580 3.112503
```

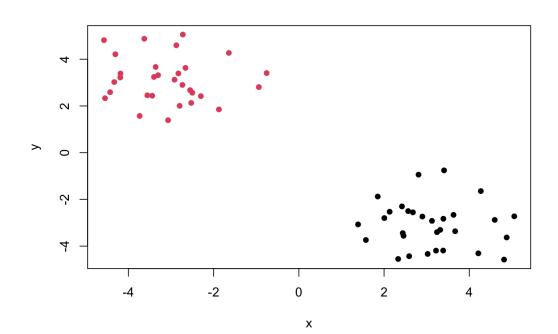
Now we got to the main results let's use them to plot our data with the kmeans result.

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



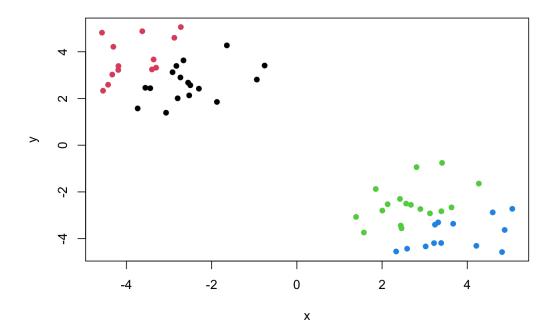
Q4.Plot x colored by the kmeans cluster assignment and add cluster centers as blue points

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



Q5. Cluster the data again with kmeans() into 4 groups and plot the results.

```
k4 <- kmeans(x, center= 4, nstart=20)
plot(x, col=k4$cluster, pch=16)</pre>
```



K-means is very popular mostly because it is fast and relatively straight forward to run and understand. It has a big limitation in that you need to tell it how many groups (k, or centers) you want. #Hierarchical clustering The main function in base R is called 'hclust()'. You have to pass it in a "distance matrix" not just your input data. you can generate a distance matrix with the "dist()"

```
hc <- hclust( dist(x))
hc</pre>
```

Call:
hclust(d = dist(x))

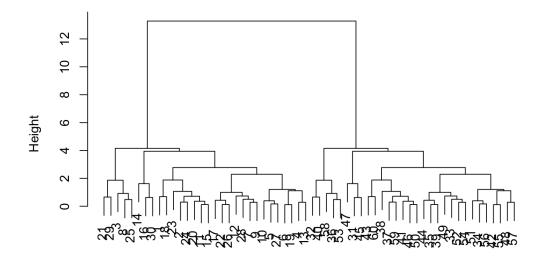
Cluster method : complete
Distance : euclidean

Number of objects: 60

Q6. Plot our hclust results.

plot(hc)

Cluster Dendrogram

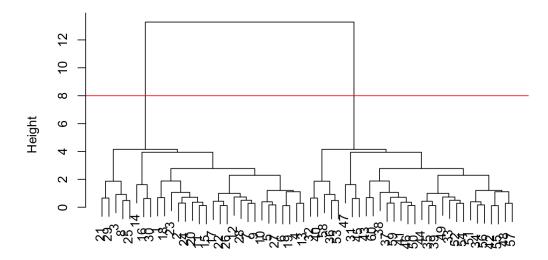


dist(x) hclust (*, "complete")

To find the cluster(cluster membership vector)from a 'hclust()' result we can "cut" the tree at a certain height

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

Cluster Dendrogram



dist(x) hclust (*, "complete")

```
grps <- cutree(hc, h=8)
table(grps)</pre>
```

Principal Component Analysis PCA of UK food data Read data showing the consumption in grams (per person, per week) of 17 different types of food-stuff measured and averaged in the four countries of the United kingdom. Let's see how PCA can help us but first we can try conventional analysis.

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
x</pre>
```

	Х	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
7	Fresh_potatoes	720	874	566	1033
8	Fresh_Veg	253	265	171	143
9	Other_Veg	488	570	418	355
10	Processed_potatoes	198	203	220	187
11	Processed_Veg	360	365	337	334
12	Fresh_fruit	1102	1137	957	674
13	Cereals	1472	1582	1462	1494
14	Beverages	57	73	53	47
15	Soft_drinks	1374	1256	1572	1506
16	Alcoholic_drinks	375	475	458	135
17	Confectionery	54	64	62	41

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
rownames(x) <- x[ ,1]
x <-x[, -1]
head(x)</pre>
```

	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

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() give both rows and coloumns, there are 17 rows and 4 columns.

```
## Complete the following code to find out how many rows and columns are in x? \dim(x)
```

[1] 17 4

```
x <- read.csv(url, row.names=1)
head(x)</pre>
```

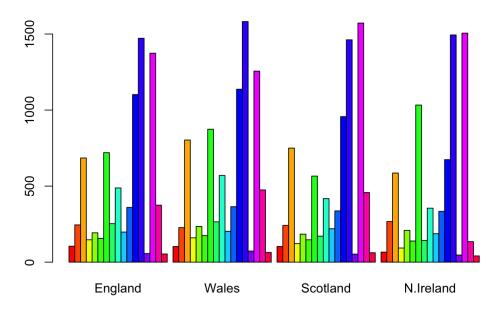
	England	Wales	Scotland	N.Ireland
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139

dim(x)

[1] 17 4

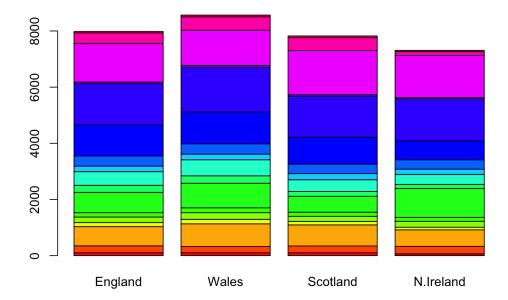
Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances? Everytime run x <- x[,-1] the first row is gone. I would prefer x <- read.csv(url, row.names=1)

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



Q3: Changing what optional argument in the above barplot() function results in the following plot? Change beside to False.

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

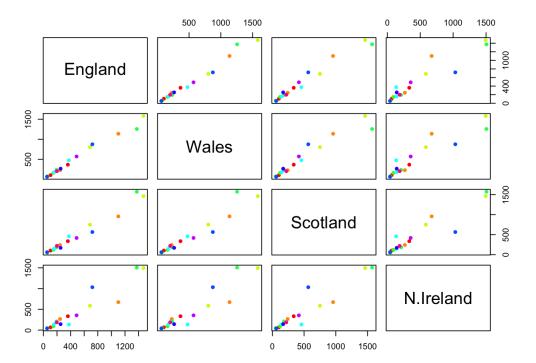


Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot? Each row and column of the matrix corresponds to a dataset, which seems to be named after regions/countries: England, Wales, Scotland, and N.Ireland.

The points in the scatterplots are colored using the rainbow function with 10 different colors, as indicated in the provided code. This means that there are likely 10 different categories or groups in the dataset, possibly representing time points, groups, or other categorizations.

The pairwise scatterplots provide insights into how the datasets relate to each other. For example, if these datasets represent yearly measurements of a specific parameter (like GDP or population) for the four regions, then a point lying on the diagonal in the scatterplot comparing "England" and "Wales" would mean that in that specific year, both England and Wales had the same measurement value.

pairs(x, col=rainbow(10), pch=16)



Principal Component Analysis(PCA) PCA can help us make sense of these types of datasets. Let's see how it works. The main function in "base" R is called 'prcomp()'. In this case we want to first take the teanspose of our input 'x' so the columns are the food types and the countries are the rows.

```
head( t(x) )
```

	Cheese Carcass	_meat	Other_	meat	Fish	Fats_and_	_oils	Sugars
England	105	245		685	147		193	156
Wales	103	227		803	160		235	175
Scotland	103	242		750	122		184	147
N.Ireland	66	267		586	93		209	139
	Fresh_potatoes	Fresh	_Veg	Other_	_Veg	Processed	d_pota	toes
England	72	10	253		488			198
Wales	87	4	265		570			203
Scotland	56	6	171		418			220
N.Ireland	103	3	143		355			187
	Processed_Veg	Fresh_	fruit	Cerea	als	Beverages	Soft_d	drinks
England	360)	1102	:	1472	57		1374
Wales	365	i	1137	:	1582	73		1256
Scotland	337	,	957	:	1462	53		1572
N.Ireland	334	ļ	674	:	1494	47		1506
	Alcoholic_drin	ıks Con	fectio	nery				
England		375		54				
Wales		475		64				
Scotland		458		62				
N.Ireland		135		41				

```
pca <- prcomp( t(x) )
summary(pca)</pre>
```

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	1.0000+00

```
PC1 PC2 PC3 PC4

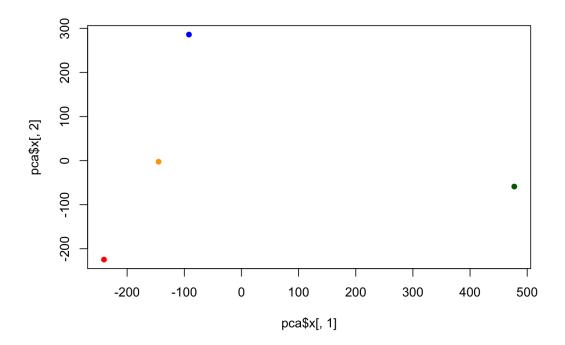
England -144.99315 -2.532999 105.768945 -4.894696e-14

Wales -240.52915 -224.646925 -56.475555 5.700024e-13

Scotland -91.86934 286.081786 -44.415495 -7.460785e-13

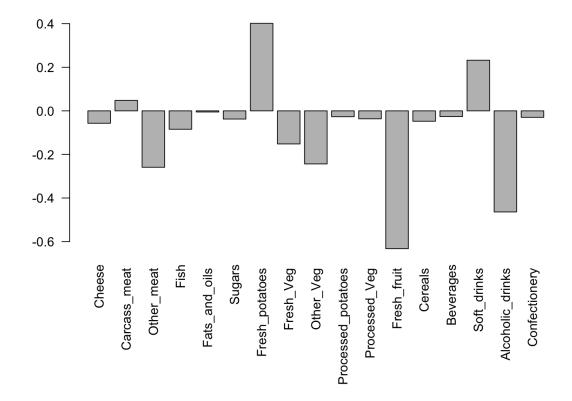
N.Ireland 477.39164 -58.901862 -4.877895 2.321303e-13

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



The "loadings" tells us how much the origional variables (in our case the foods) contribute to the new variables i.e. the PCs.

```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



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
                   -0.084414983 -0.050754947
Fish
                                              0.03906481 -0.008483145
Fats_and_oils
                   -0.005193623 -0.095388656 -0.12522257
                                                          0.076097502
                   -0.037620983 -0.043021699 -0.03605745
Sugars
                                                          0.034101334
Fresh_potatoes
                    0.401402060 -0.715017078 -0.20668248 -0.090972715
                   -0.151849942 -0.144900268 0.21382237 -0.039901917
Fresh_Veg
Other_Veg
                   -0.243593729 -0.225450923 -0.05332841
                                                          0.016719075
                   Processed_potatoes
                                                          0.030125166
Processed_Veg
                   -0.036488269 -0.045451802 0.05289191 -0.013969507
                   -0.632640898 -0.177740743 0.40012865
                                                          0.184072217
Fresh_fruit
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
```

The inbuilt biplot() can be useful for small datasets biplot(pca)

