

Class 7: Machine Learning 1

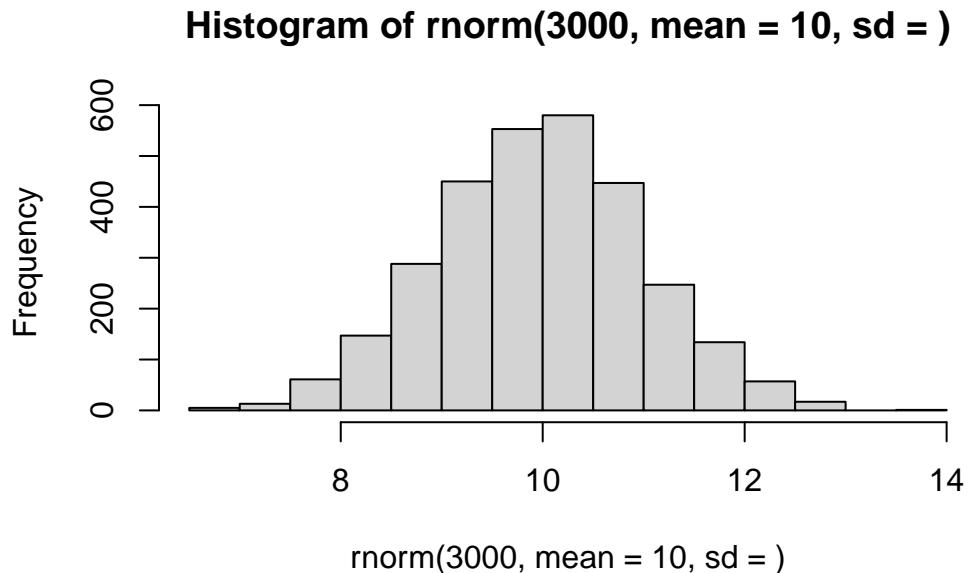
Jacob Hizon A17776679

Background

Today we will begin our exploration of important machine learning methods with a focus on **clustering** and **dimensionality reduction**.

To start testing these methods let's make up some sample data to cluster where we know what the answer should be.

```
hist( rnorm(3000, mean = 10, sd = ) )
```



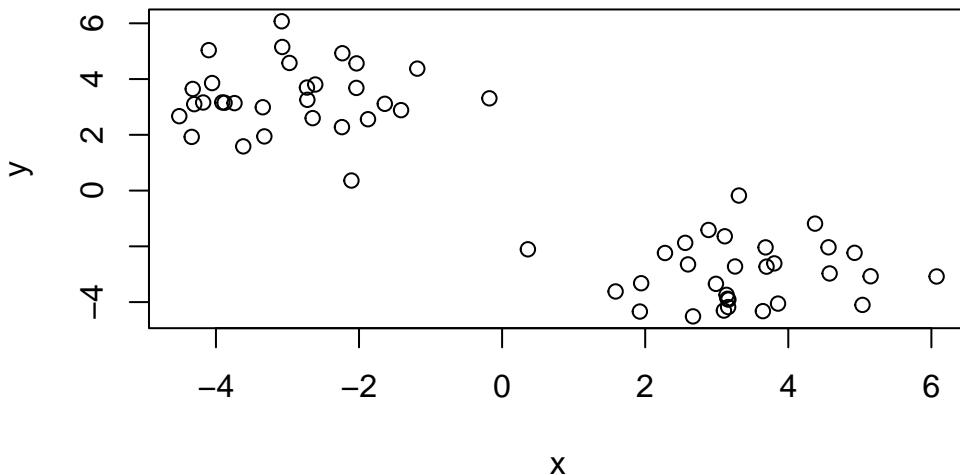
Q. Can you generate 30 numbers centered at +3 and 30 numbers at -3 taken at random from a normal distribution?

```

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

plot(x)

```



K-means clustering

The main function in “base R” for K-means clustering is called `kmeans()`, let’s try it out:

```

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

```

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

Cluster means:

	x	y
1	3.352206	-2.946797
2	-2.946797	3.352206

Clustering vector:

```
Within cluster sum of squares by cluster:  
[1] 75.36336 75.36336  
  (between_SS / total_SS =  88.8 %)
```

Available components:

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

Q. What component of your kmeans result object has the cluster centers?

k\$centers

```

          x      y
1  3.352206 -2.946797
2 -2.946797  3.352206

```

Q. What component of your kmeans result object has the cluster size (i.e. the main clustering result: which points are in which cluster)?

k\$size

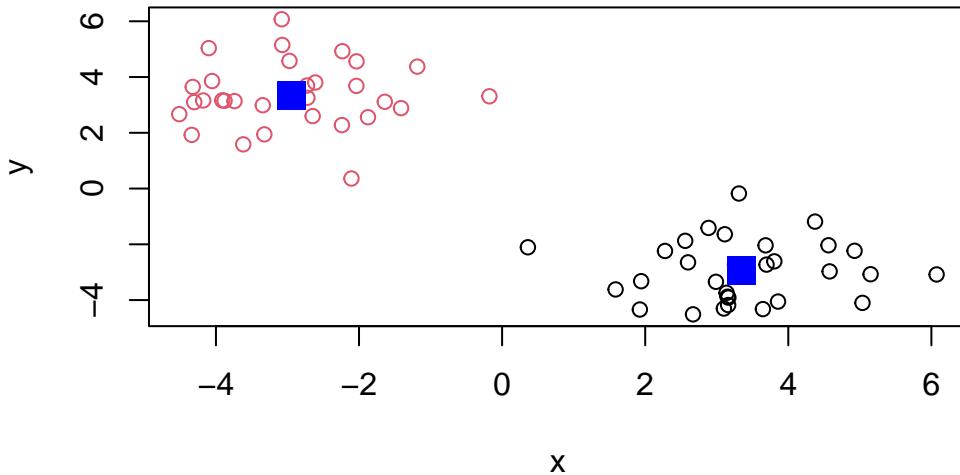
[1] 30 30

Q. What component of your kmeans result object has the cluster membership vector (i.e. the main clustering result: which points are in which cluster)?

k\$cluster

Q. Plot the results of clustering (i.e. our data colored by the clustering result) along with the cluster centers.

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



Q. Can you run `kmeans()` again and cluster `x` into 4 centers and plot the results just like we did above with coloring by cluster and the cluster centers shown in blue?

```
k4 <- kmeans(x, centers = 4)
k4
```

K-means clustering with 4 clusters of sizes 9, 12, 30, 9

Cluster means:

	x	y
1	4.689122	-2.668827
2	2.860328	-3.960674
3	-2.946797	3.352206
4	2.671126	-1.872931

Clustering vector:

```
[1] 4 4 1 1 4 4 1 4 2 4 1 1 2 2 1 2 2 4 4 2 2 1 1 2 1 2 2 2 2 4 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 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
```

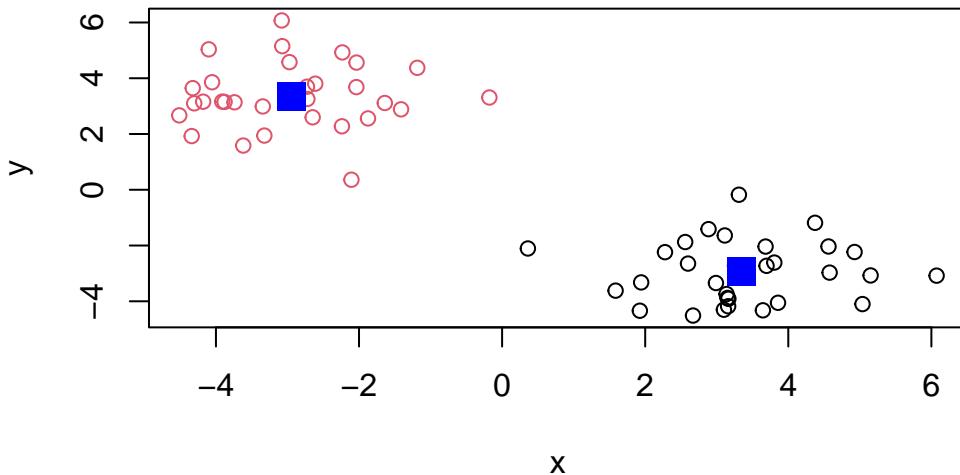
Within cluster sum of squares by cluster:

```
[1] 9.475399 7.111014 75.363361 12.203229
(between_SS / total_SS = 92.2 %)
```

```
Available components:
```

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

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



Key-point: Kmeans will always return the clustering that we ask for (this is the “K” or “centers” in K-means)!

```
k$tot.withinss
```

```
[1] 150.7267
```

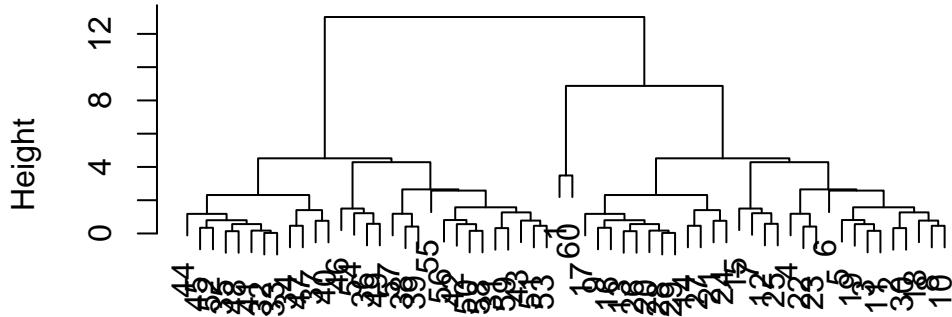
Hierarchical clustering

The main function Hierarchical clustering in base R is called `hclust()`.

One of the main differences with respect to the `kmeans()` function is that you cannot just pass your input data directly to `hclust()` - it needs a “distance matrix” as input. We can get this from lot’s of places including the `dist()` function.

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

Cluster Dendrogram

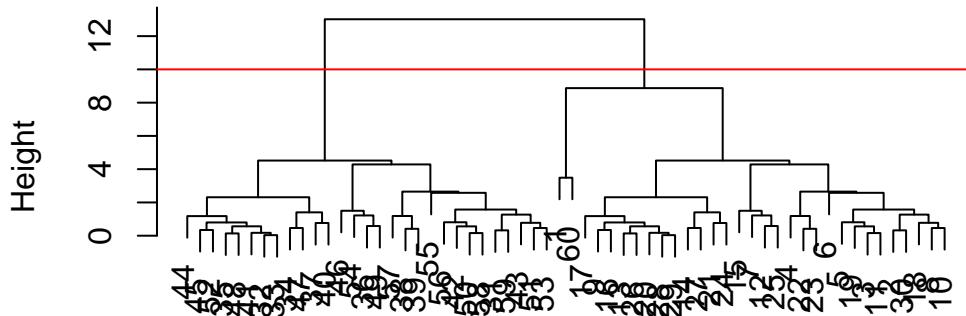


```
d
hclust (*, "complete")
```

We can “cut” the dendrogram or tree at a given height to yield our “clusters”. For this we use the function `cutree()`

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

Cluster Dendrogram



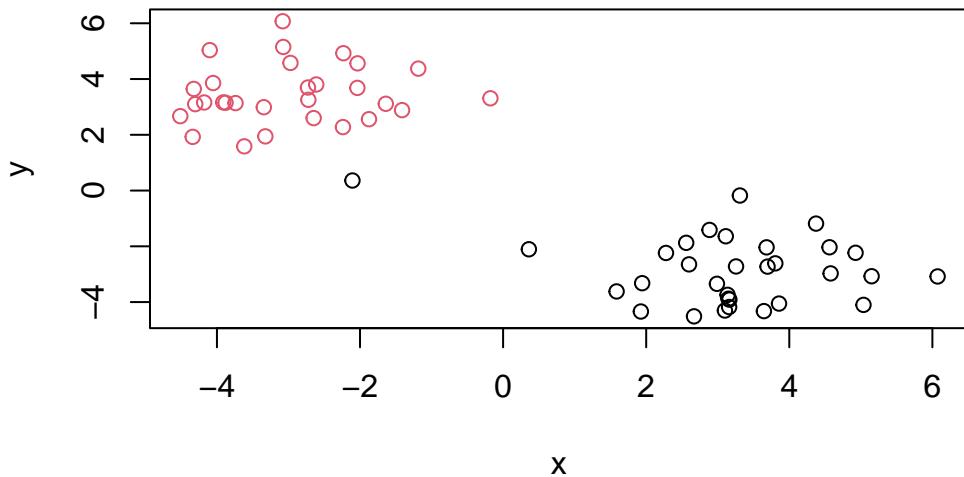
```
d  
hclust (*, "complete")
```

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

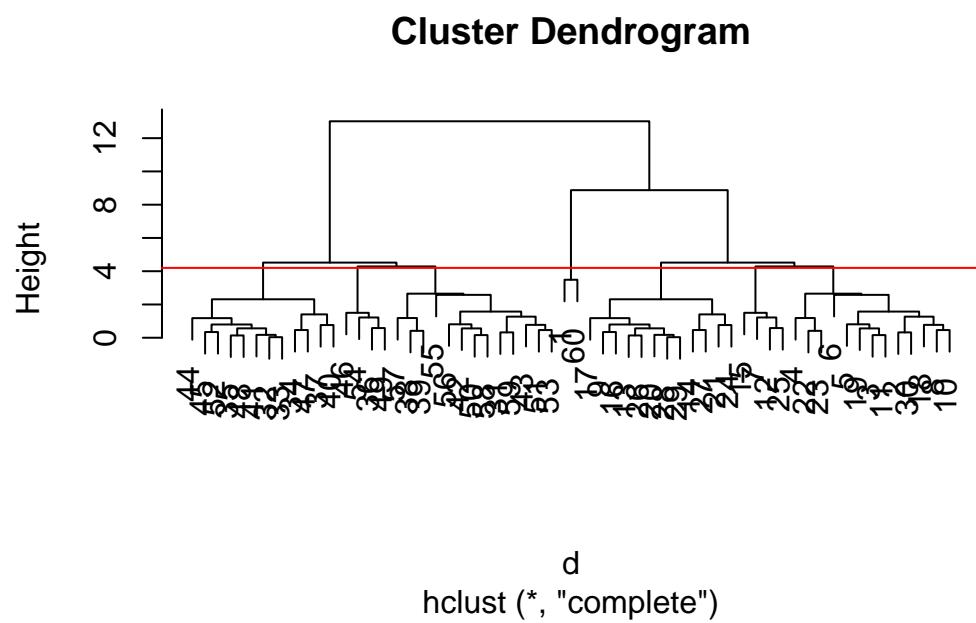
grps

Q. Plot our data `x` colored by the clusterinv result from `hclust()` and `cutree()`?

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



```
plot(hc)
abline( h =4.2, col = "red")
```



```
grps <- cutree(hc, h = 4.2)
```

Principal Component Analysis (PCA)

PCA is a popular dimensionality reduction technique that is widely used in bioinformatics.

PCA of UK food data

#Read in the data

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

It looks like the row names are not set up properly. We can fix this

```
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
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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

A better way to do this is fix row names assignment at import time:

```
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
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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?

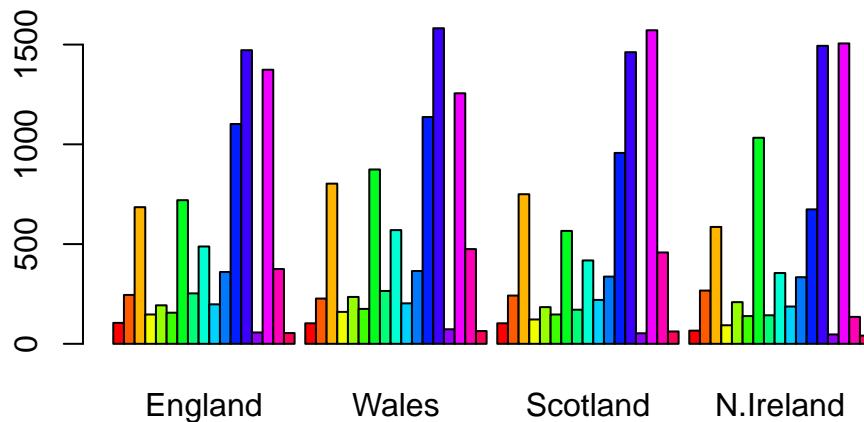
```
dim(x)
```

```
[1] 17 4
```

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 like making the change when you first read in the csv.

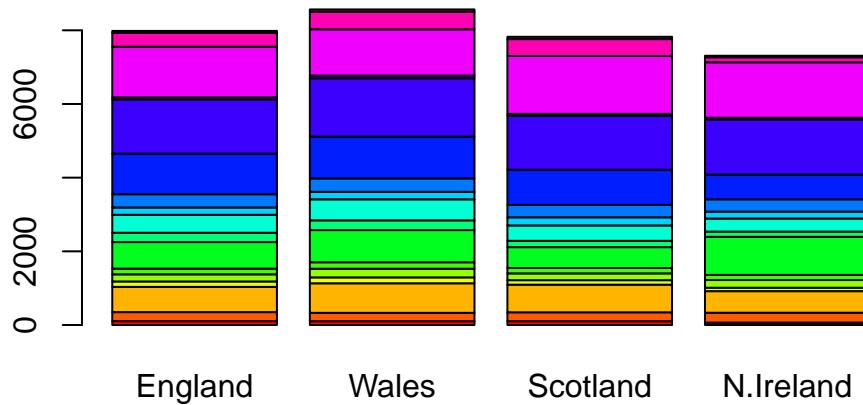
```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



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

By making the argument `beside=F`

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

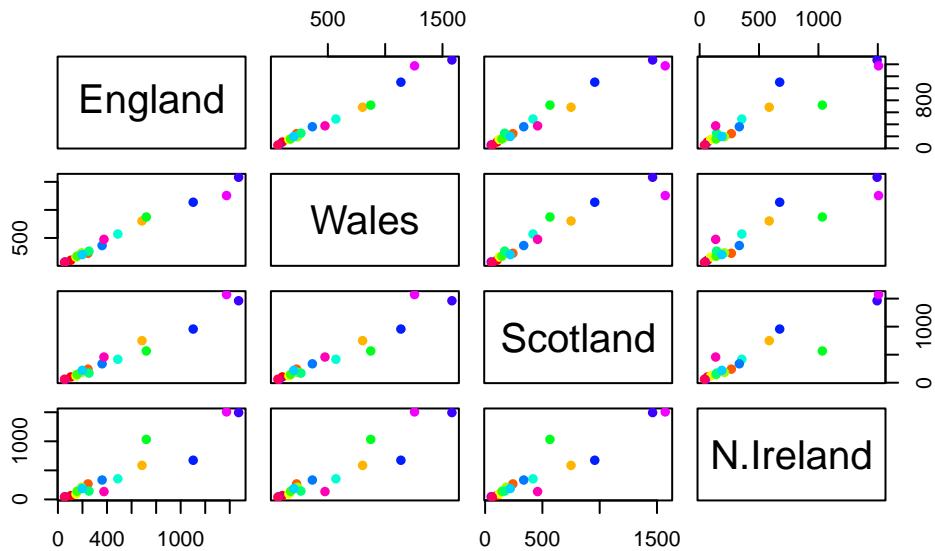


Pairs plots and heatmaps

Q4 is missing

Q5: We can use the `pairs()` function to generate all pairwise plots for our countries. 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?

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

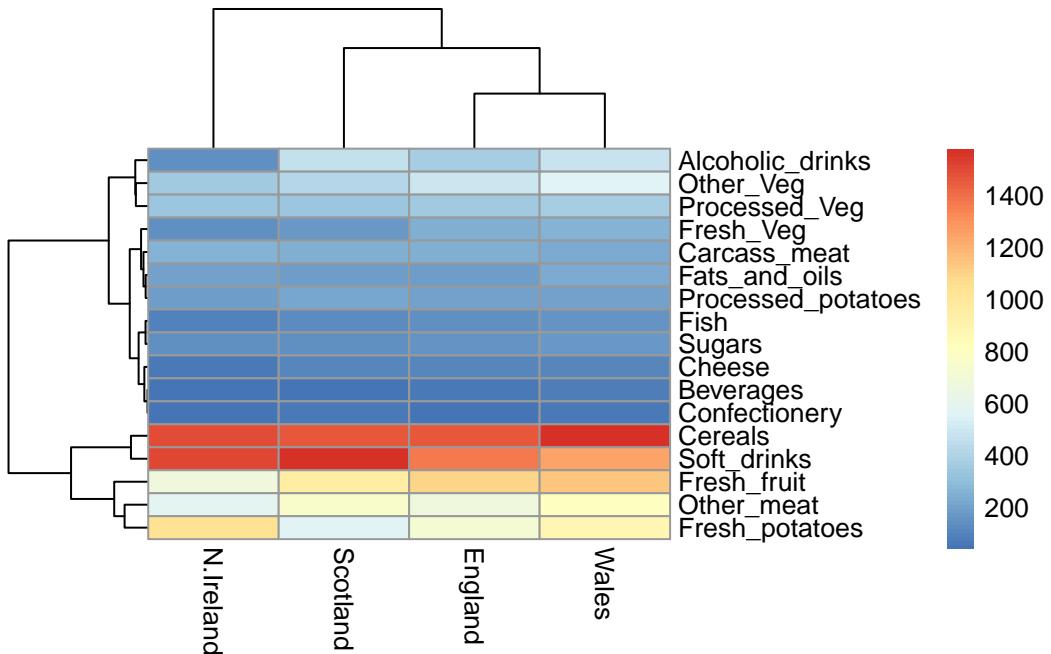


It shows a pairwise comparison between each country/territory with each territory in their own respective horizontal x axis. Similarity in consumption would lie perfectly on the diagonal and any spatial deviation represents dissimilarity in consumption in a specific food category.

Heatmap

We can install the `pheatmap` package with the `install.packages()` command that we used previously. Remember that we always run this in the console and not a code chunk in the quarto document.

```
library(pheatmap)  
pheatmap( as.matrix(x) )
```



Of all these plots really only the `pairs()` plot was useful. This however took a bit of work to interpret and will of scale when I am looking at much bigger data sets.

Q6. Based on the pairs and heatmap figures, which countries cluster together and what does this suggest about their food consumption patterns? Can you easily tell what the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

Consumption patterns are roughly the same visually. No we cannot easily see the difference it looks less quantified.

PCA to the rescue

The main function in “base R” for PCA is called `prcomp()`.

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

Importance of components:

	PC1	PC2	PC3	PC4
Standard deviation	324.1502	212.7478	73.87622	2.7e-14
Proportion of Variance	0.6744	0.2905	0.03503	0.0e+00
Cumulative Proportion	0.6744	0.9650	1.00000	1.0e+00

Q. How much variance is captured in the first PC?

67.44%

Q. How many PCs do I need to capture at least 90% of the total variance in the dataset?

2 PCs capture 96.5% of the total variance.

Q Plot our main PCA result. Folks can call this different things depending on their field of study e.g. “PC plot”, or “ordination plot”, “score plot”, “PC1 vs PC 2 plot”...

```
attributes(pca)
```

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

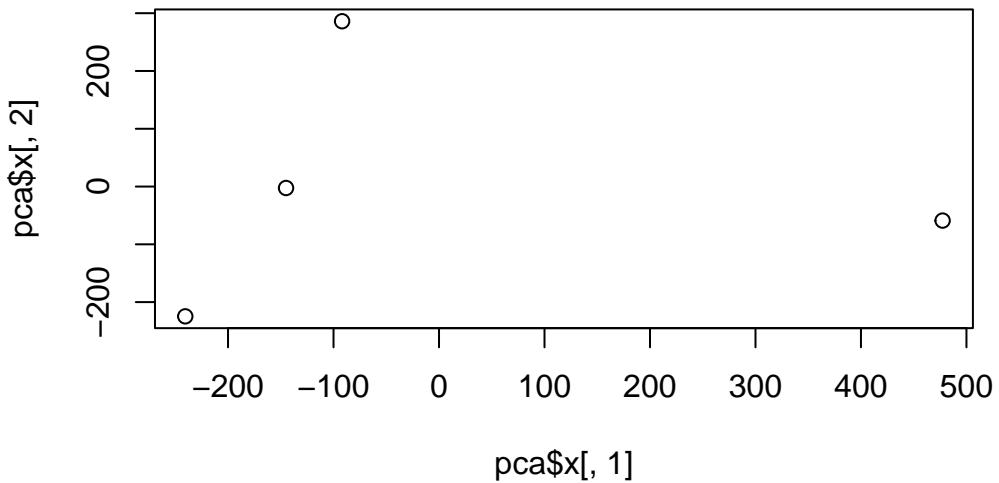
$class
[1] "prcomp"
```

To generate a PCA score plot we want the `pca$x` component of the result object

```
pca$x
```

	PC1	PC2	PC3	PC4
England	-144.99315	-2.532999	105.768945	1.612425e-14
Wales	-240.52915	-224.646925	-56.475555	4.751043e-13
Scotland	-91.86934	286.081786	-44.415495	-6.044349e-13
N.Ireland	477.39164	-58.901862	-4.877895	1.145386e-13

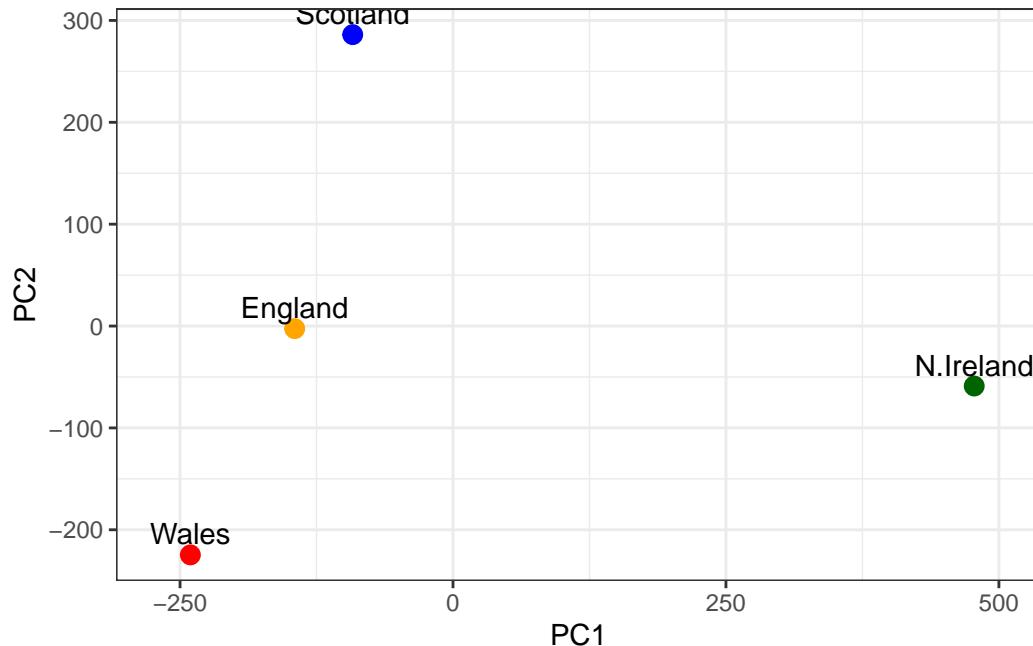
```
plot(pca$x[,1], pca$x[,2])
```



```
my_cols <- c("orange", "red", "blue", "darkgreen")
```

```
library(ggplot2)

ggplot(pca$x) +
  aes(x = PC1, y = PC2, label = rownames(pca$x)) +
  geom_point(size = 3, color = my_cols) +
  geom_text(vjust = -0.5) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



```
my_cols <- c("orange", "red", "blue", "darkgreen")
```

Digging deeper (variable loadings)

How do the original variables (i.e. the 17 different foods) contribute to our new PCs?

```
ggplot(pca$rotation) +
  aes(x = PC1,
      y = reorder(rownames(pca$rotation), PC1)) +
  geom_col(fill = "steelblue") +
  xlab("PC1 Loading Score") +
  ylab("") +
  theme_bw() +
  theme(axis.text.y = element_text(size = 9))
```

