

Class07

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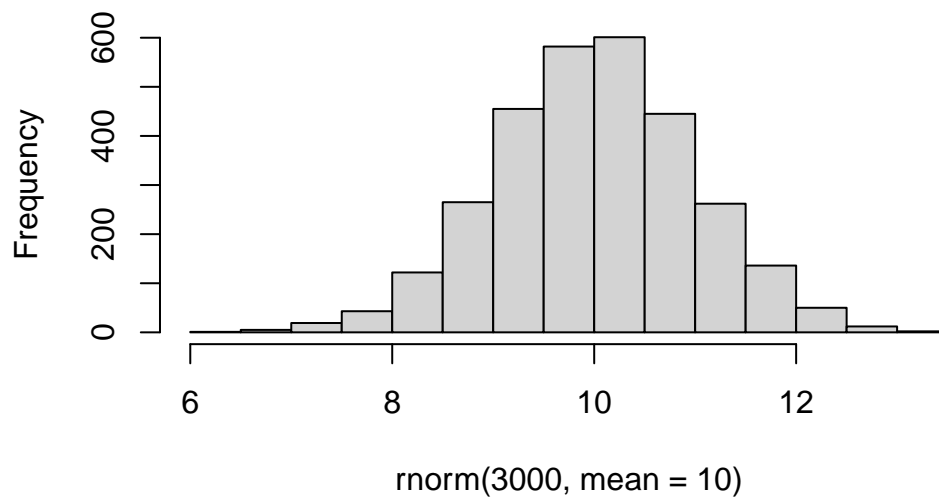
Background

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.

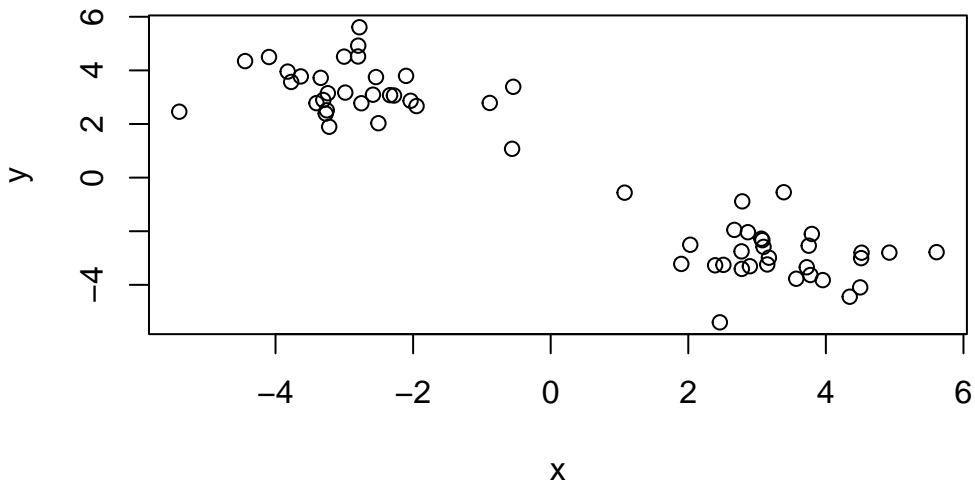
```
hist(rnorm(3000,mean=10))
```

Histogram of rnorm(3000, mean = 10)



Q. Can you generate 30 numbers centered at $+3/-3$ taken 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 `kmeans()`:

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

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

Cluster means:

	x	y
1	-2.854845	3.301629
2	3.301629	-2.854845

Clustering vector:

[illegible]

Within cluster sum of squares by cluster:

```
[1] 59.02758 59.02758
(between_SS / total_SS = 90.6 %)
```

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 -2.854845  3.301629
2  3.301629 -2.854845
```

Q. What component of your kmeans result object has the cluster size (i.e. how many points are in each cluster)?

```
k$size
```

```
[1] 30 30
```

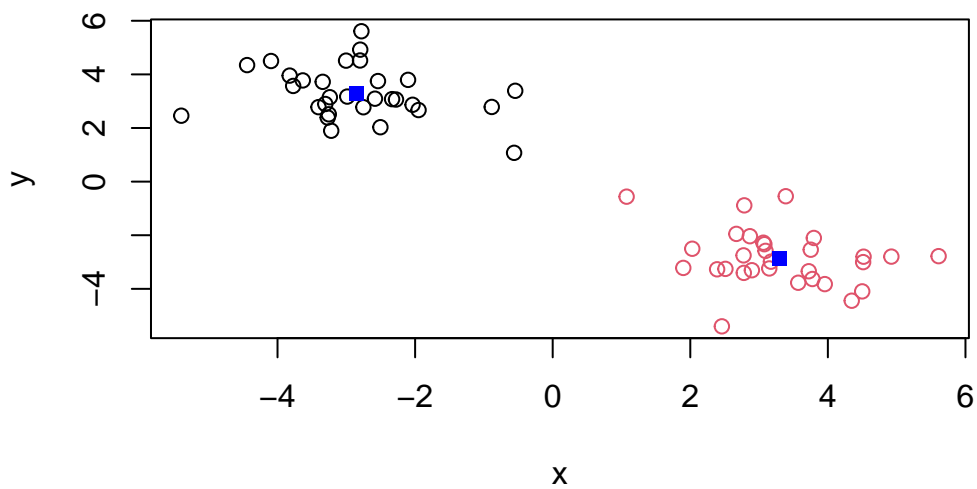
Q. What component of your kmeans result object has the cluster membership vector (i.e. the main clustering result: which points are in which cluster)?

```
k$cluster
```

```
[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 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
```

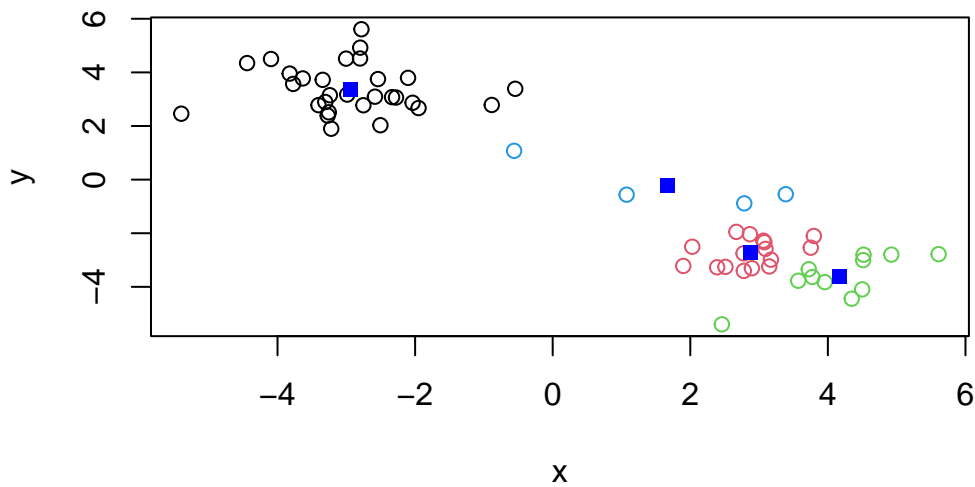
Q. Plot the results of clustering (i.e. our data colored by the clustering result) along with the cluster centers.

```
plot(x,col=k$cluster)
points(k$centers,col='blue',pch=15,cex=1)
```



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

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



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

```
k$tot.withinss
```

```
[1] 118.0552
```

```
k4$tot.withinss
```

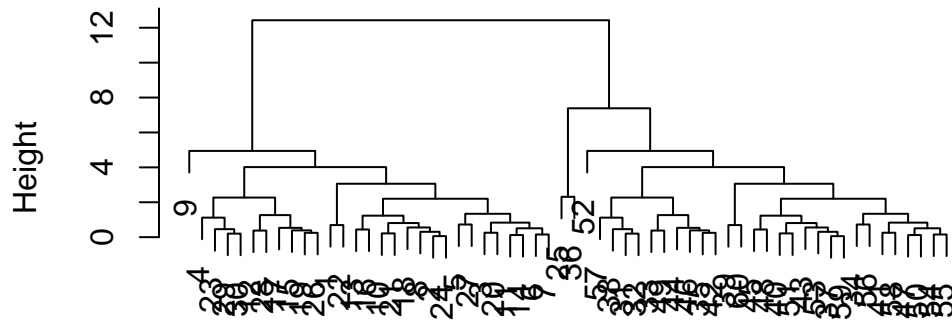
```
[1] 81.54265
```

Hierarchical clustering

The main function for hierarchical clustering in base R is called `hclust()`. One of the main differences with respect to the `kmeans()` function is that you can not 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

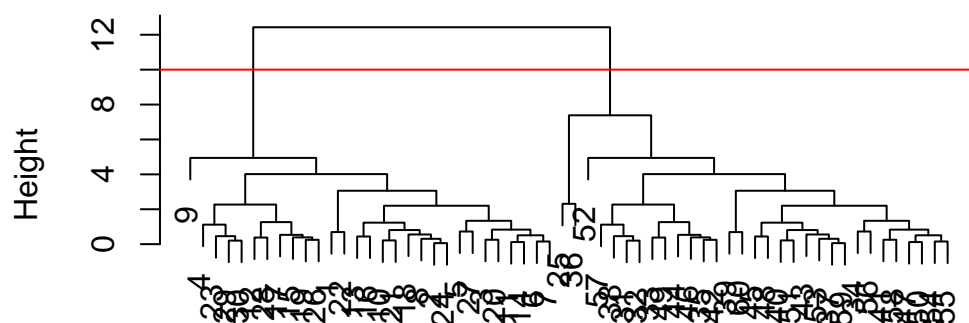


d
hclust (*, "complete")

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

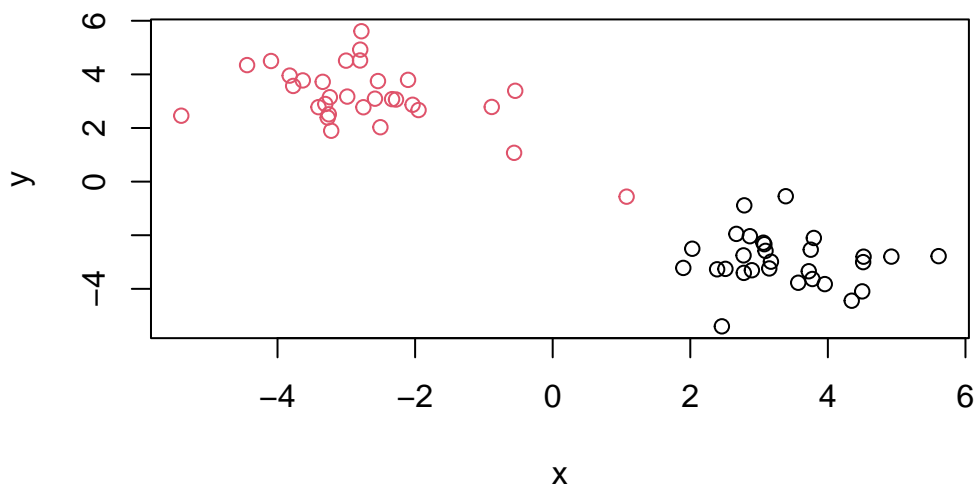


d
hclust (*, "complete")

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

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

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

Principal Component Analysis (PCA)

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

PCA of UK food data

Read data on food consumption in the UK

```
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 name are not set 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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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

But since this will overwrite x everytime

A better way to do this is fix the 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
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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)
```

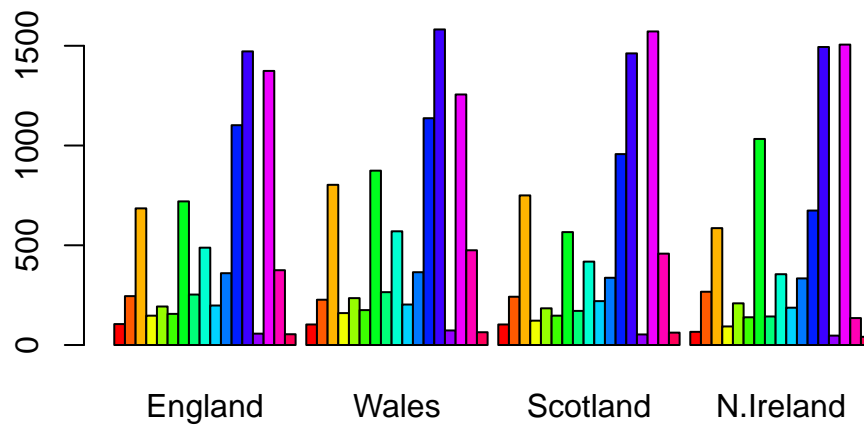
```
[1] 17  4
```

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?

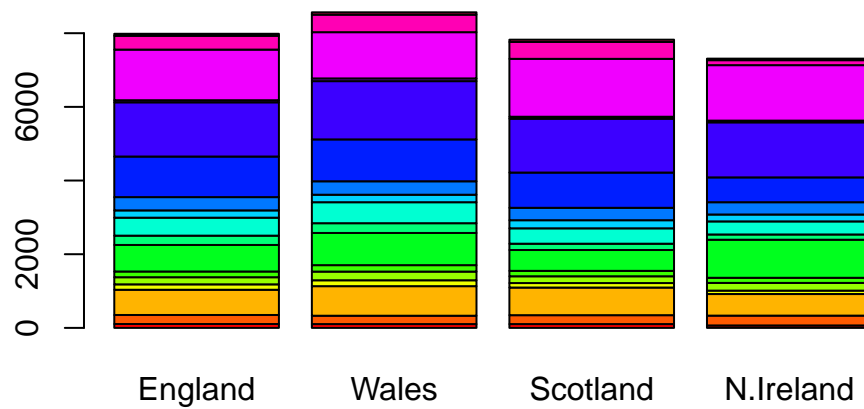
`x <- read.csv(url,row.names=1)` is preferred. For the first method, every time you run the code `x <- x[,-1]`, it rewrites `x` so you will lose another column.

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

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



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



Q4: Changing what optional argument in the above `ggplot()` code results in a stacked barplot figure?

```
library(tidyr)

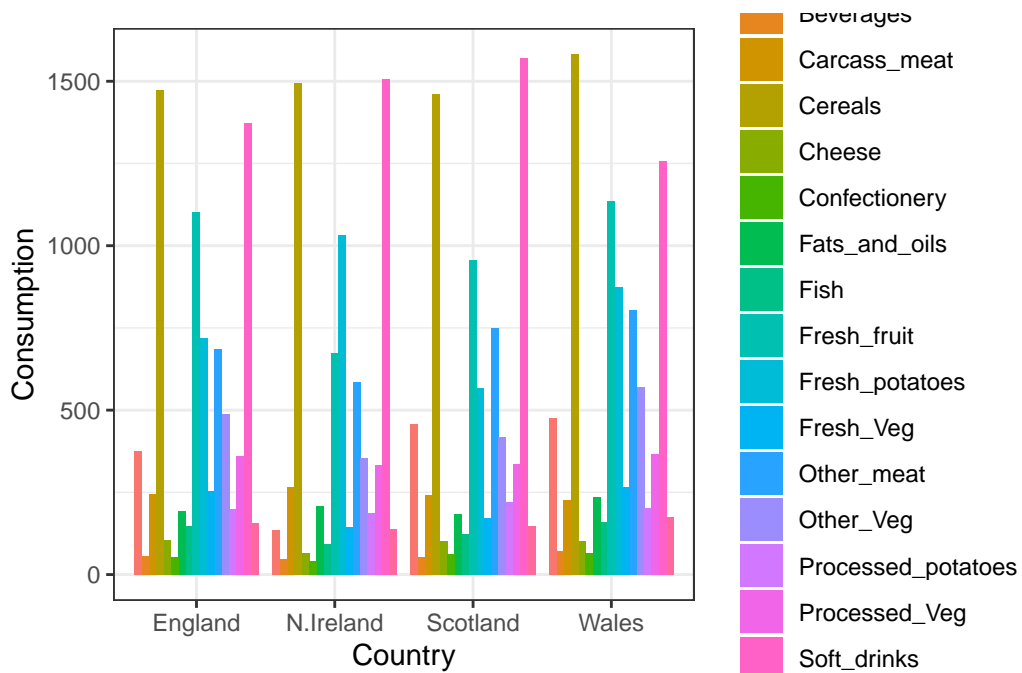
# Convert data to long format for ggplot with `pivot_longer()`
x_long <- x |>
  tibble::rownames_to_column("Food") |>
  pivot_longer(cols = -Food,
               names_to = "Country",
               values_to = "Consumption")

dim(x_long)
```

```
[1] 68 3
```

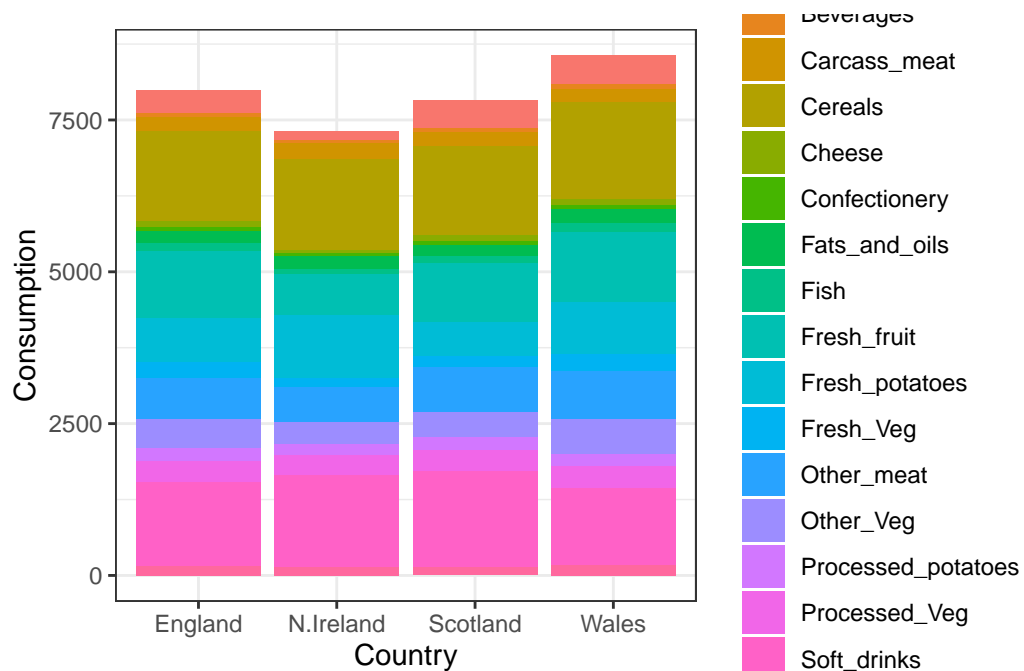
```
library(ggplot2)

ggplot(x_long) +
  aes(x = Country, y = Consumption, fill = Food) +
  geom_col(position = "dodge") +
  theme_bw()
```



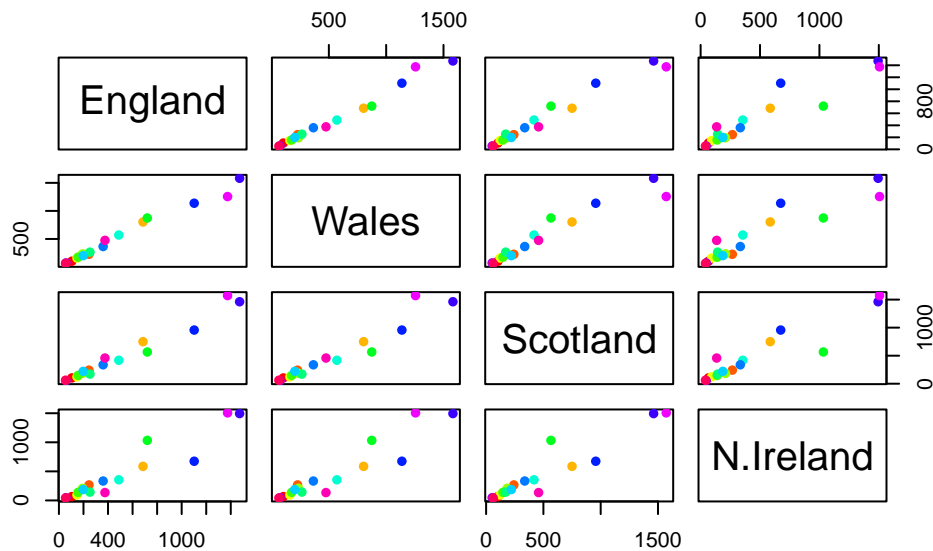
```
library(ggplot2)

ggplot(x_long) +
  aes(x = Country, y = Consumption, fill = Food) +
  geom_col(position = "stack") +
  theme_bw()
```



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)
```



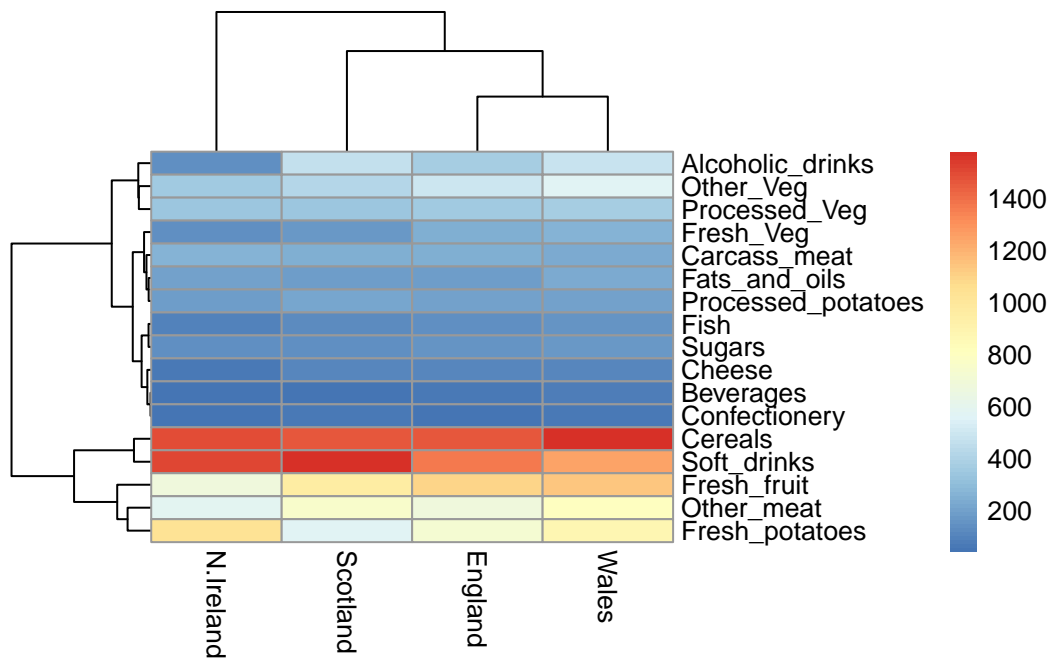
If a given point lies on the diagonal for a given plot, it means that the two countries have the same consumption on the food that point represents.

Heatmap

We can install **pheatmap** package with the `install.packages()` command that we used previously.

```
library(pheatmap)

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



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?

Based on the pairs, it seems like England and Wales have similar food consumption pattern, while England and N.Ireland have distinct food consumption pattern. It's hard to tell the main differences between N. Ireland and the other countries of the UK based on the heatmap.

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

PCA 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:PC1+PC2 (96.50%)

Q. Plot our main PCA result, Folks can call this different things depending on their field of study e.g. “PC plot”, “ordination plot”, “Score plot”, “PC1 vs PC2 plot”...

```
attributes(pca)
```

```
$names
```

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

```
$class
```

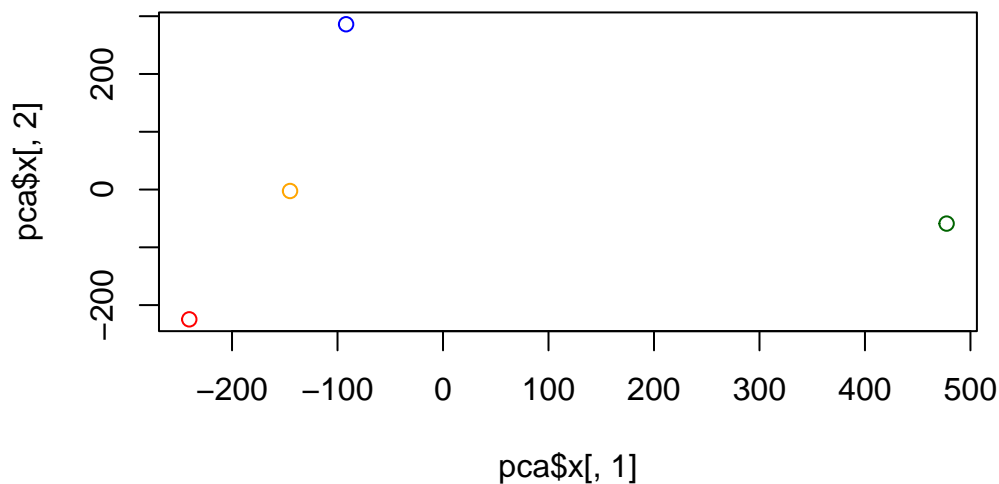
```
[1] "prcomp"
```

To generate our 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

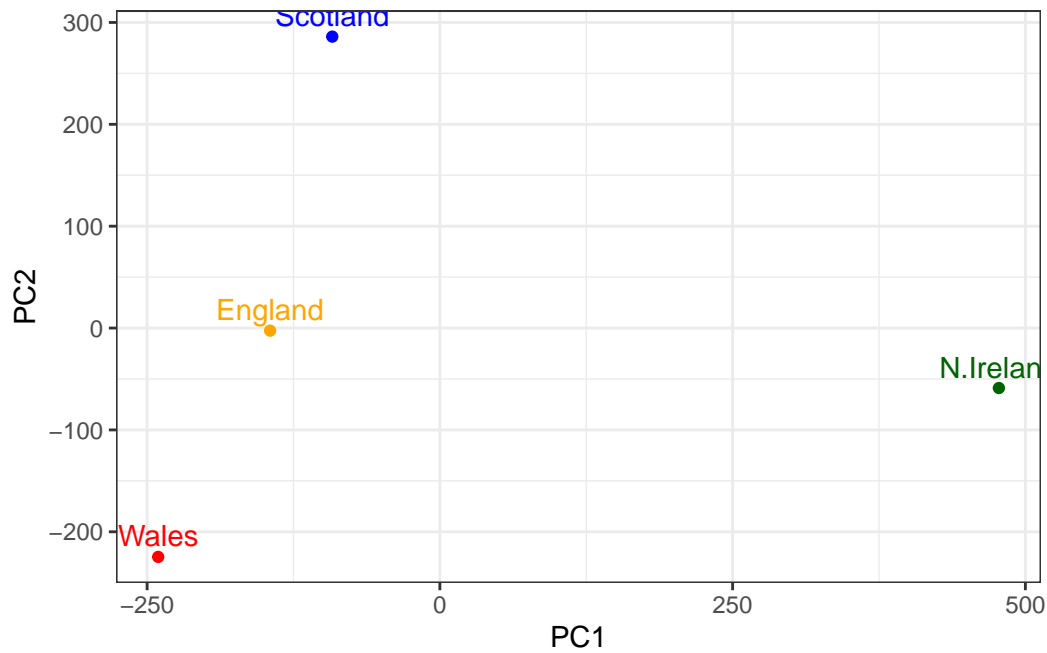
```
my_cols <- c('orange','red','blue','darkgreen')  
plot(pca$x[,1],pca$x[,2],col=my_cols)
```



Q7 & Q8. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

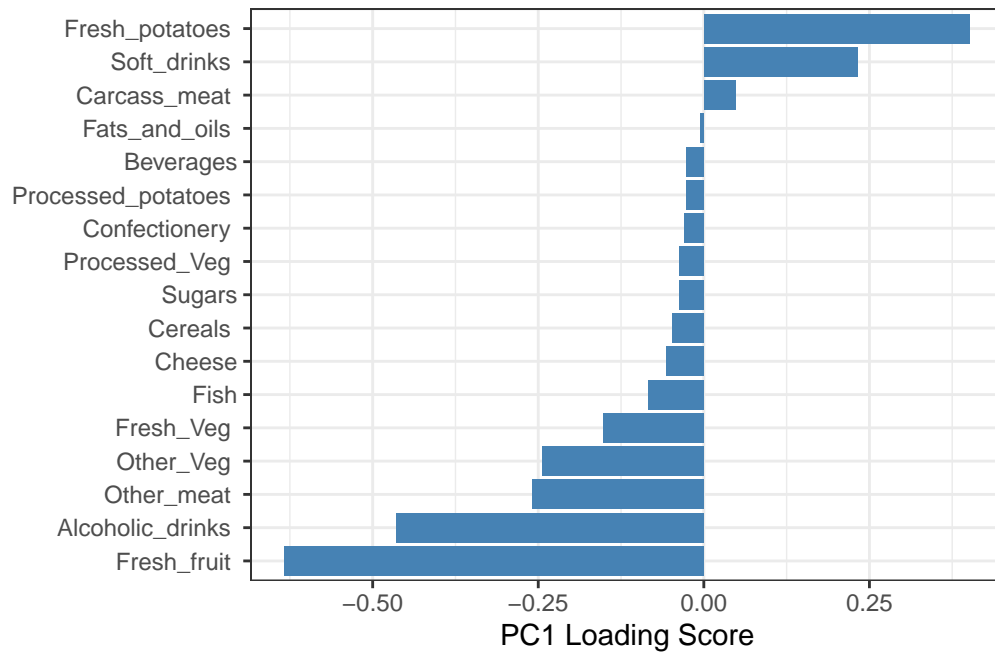
```
ggplot(pca$x)+
  aes(PC1,PC2,label=rownames(pca$x))+
  geom_point(col=my_cols)+
  geom_text(vjust = -0.5,col=my_cols)+
  theme_bw()
```



Digging deeper (variable loadings)

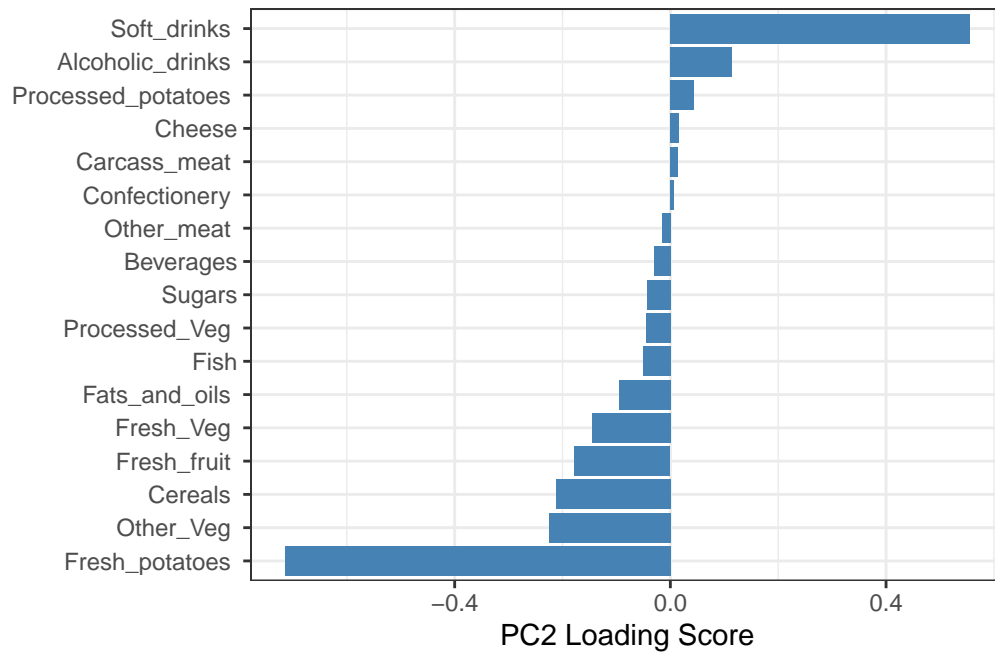
How do the original variables (i.e. the 17 different foods) contribute to our new PCs?

```
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))
```



Q9: Generate a similar 'loadings plot' for PC2. What two food groups feature prominently and what does PC2 mainly tell us about?

```
ggplot(pca$rotation)+
  aes(PC2, reorder(rownames(pca$rotation),PC2))+
  geom_col(fill='steelblue')+
  xlab("PC2 Loading Score") +
  ylab("") +
  theme_bw()+
  theme(axis.text.y = element_text(size = 9))
```



Soft_drinks and Fresh_potatoes feature prominently.