

Class 7: Machine Learning 1

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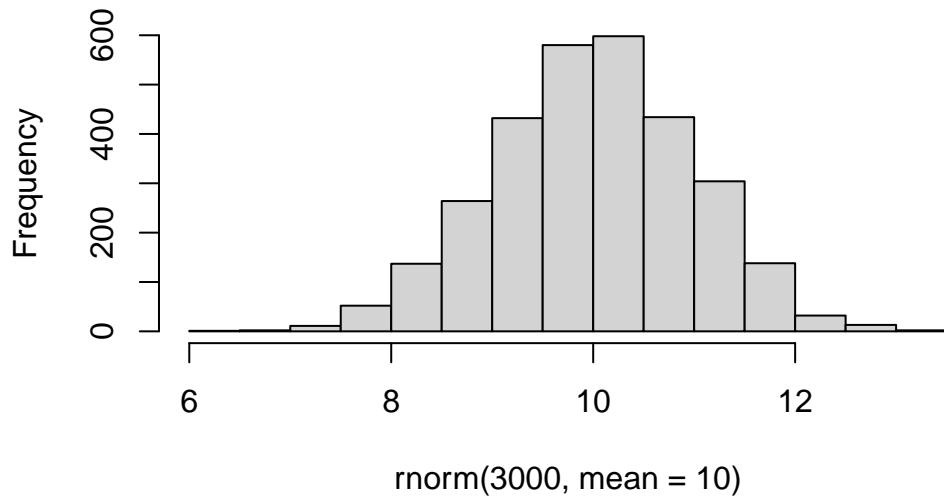
Background

Today we will begin our exploration of important machine learning methods with a focus on **clustering** and **dimensionallity 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))
```

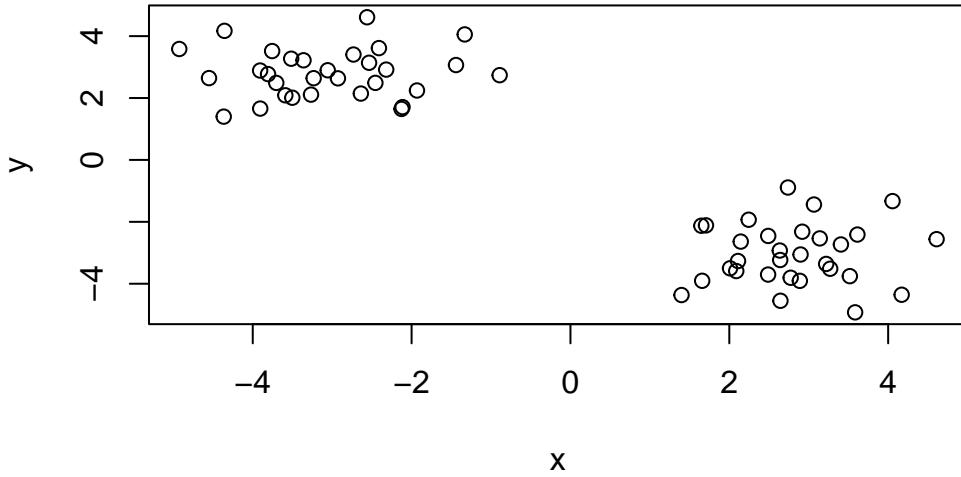
Histogram of rnorm(3000, mean = 10)



Q. Can you generate 30 numbers centered at +3 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	-3.040477	2.792331
2	2.792331	-3.040477

Clustering vector:

Within cluster sum of squares by cluster:

```
[1] 46.23442 46.23442  
(between_SS / total_SS =  91.7 %)
```

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	-3.040477	2.792331
2	2.792331	-3.040477

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

k\$size

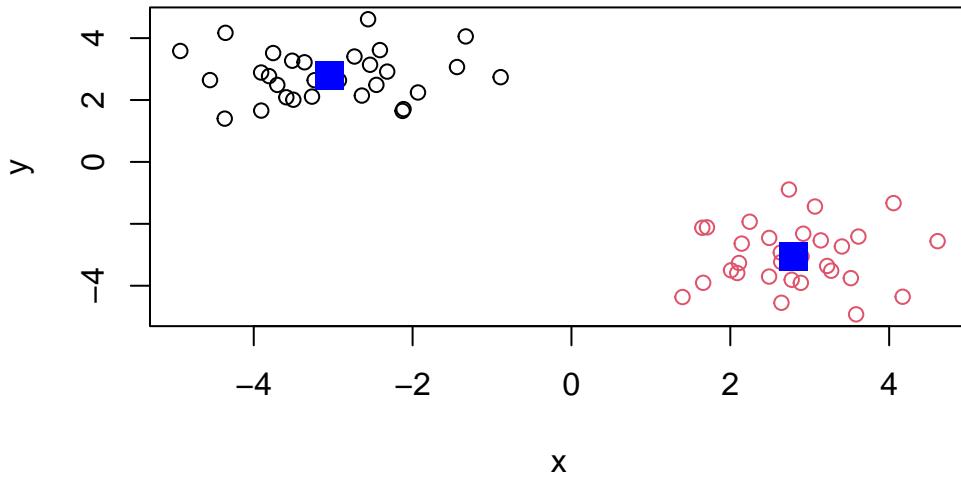
[1] 30 30

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

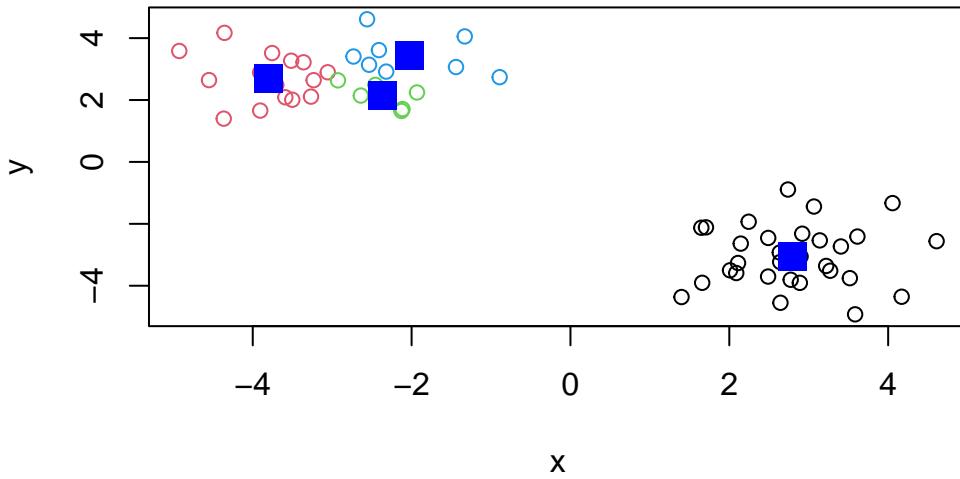
Q. plot the results of clustering (i.e. our data colored by the clustering result) along with the cluster centers.

```
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 clusters and plot the results just like we did above with coloring by cluster and the cluster centers shown in blue?

```
j <- kmeans(x, centers = 4)
plot(x, col=j$cluster)
points(j$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] 92.46883
```

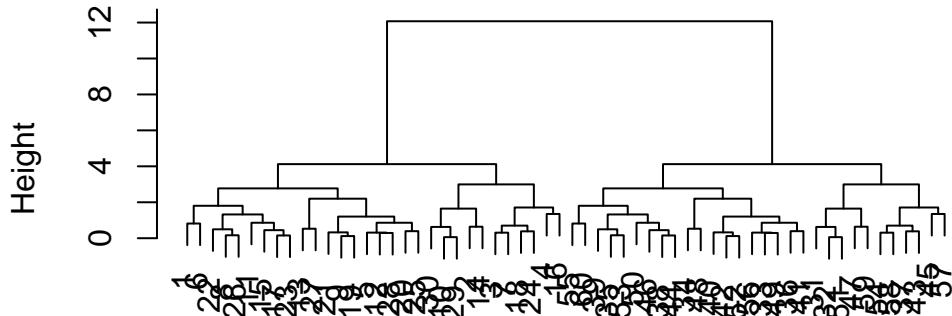
Hierarchical Clustering

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 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

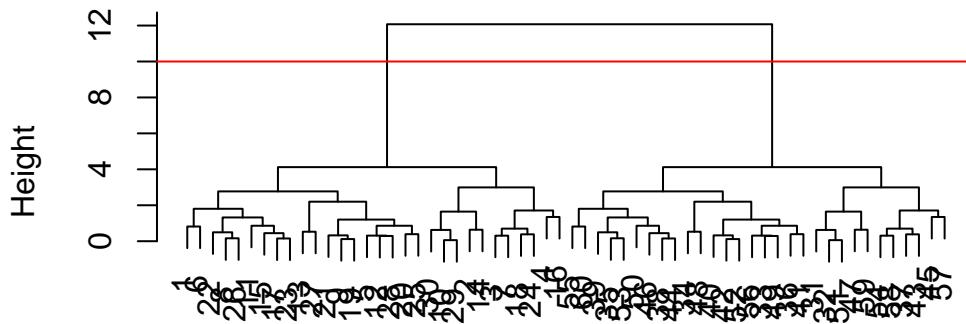


```
d  
hclust (*, "complete")
```

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



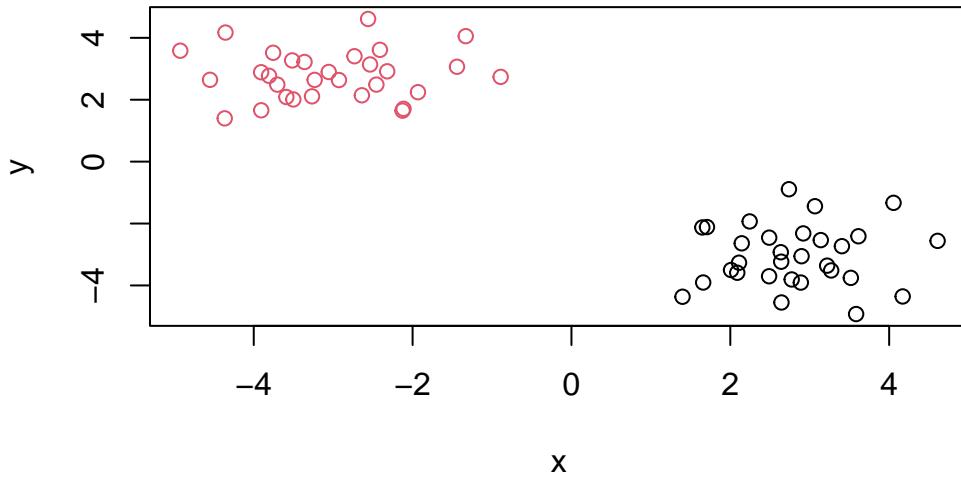
```
d  
hclust (*, "complete")
```

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

grps

Q. Plot our data `x` colored by the 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 names 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
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

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
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
```

```
nrow(x)
```

```
[1] 17
```

```
ncol(x)
```

```
[1] 4
```

17 rows, 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 the method we used that fixed the row names assignment at import time.

Spotting major differences and trends

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

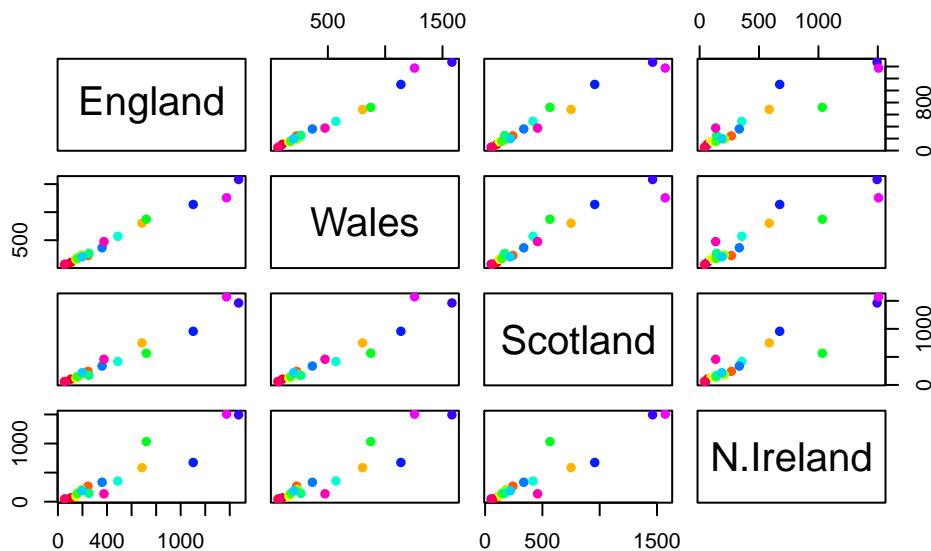
Changing `beside=T` to `beside=F`.

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

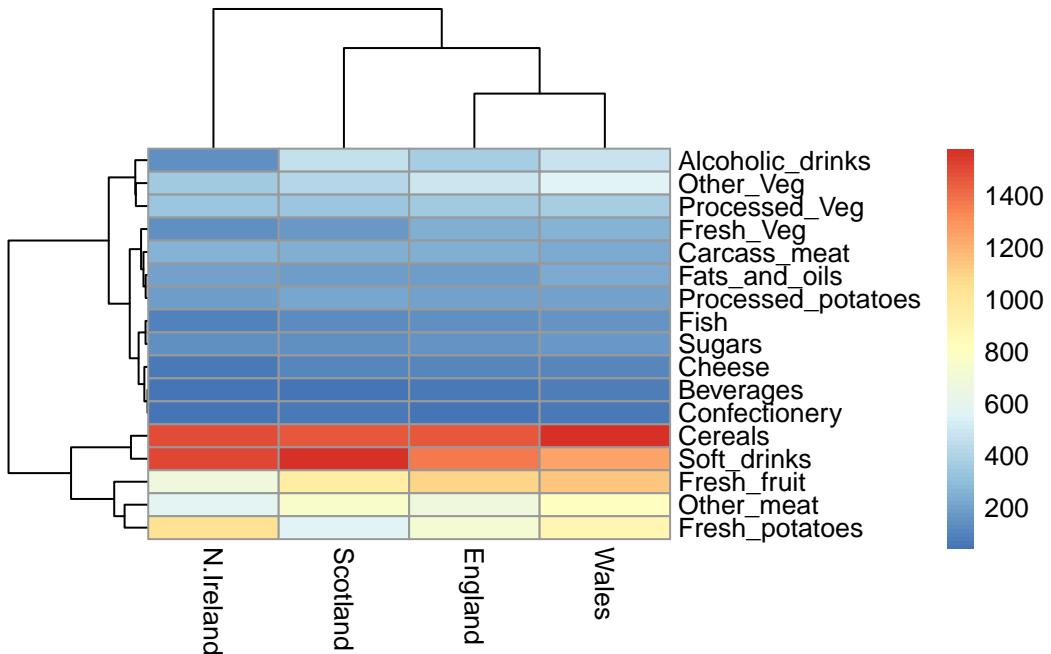
Changing `position = "dodge"` to `position = "stack"`.

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)
```



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



If a given point lies on the diagonal for a given plot, then the two countries match in terms of consumption for a given product. The heatmap shows higher consumption of a product with warmer colors, and lower consumption with cooler colors.

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?

For the most part, each country clusters together except for Northern Ireland reflecting similar food consumption between Scotland, England, and Wales. It's a bit hard to tell, but they mainly differ on consumption of fresh fruit, other meat, and fresh potatoes. It's definitely easier to see a mismatch on the pair plot rather than the heatmap figures, but there is still an observable difference on the heatmap.

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 our quarto document.

Of all these plots really only the `pairs()` plot was useful. This however took a bit of work to interpret and will not scale when I am looking at much bigger datasets.

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	3.176e-14
Proportion of Variance	0.6744	0.2905	0.03503	0.000e+00
Cumulative Proportion	0.6744	0.9650	1.00000	1.000e+00

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

67.4%

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

Two 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”, “ordination plot”, “Score plot”, “PC1 vs PC2 plot”...

```
attributes(pca)
```

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

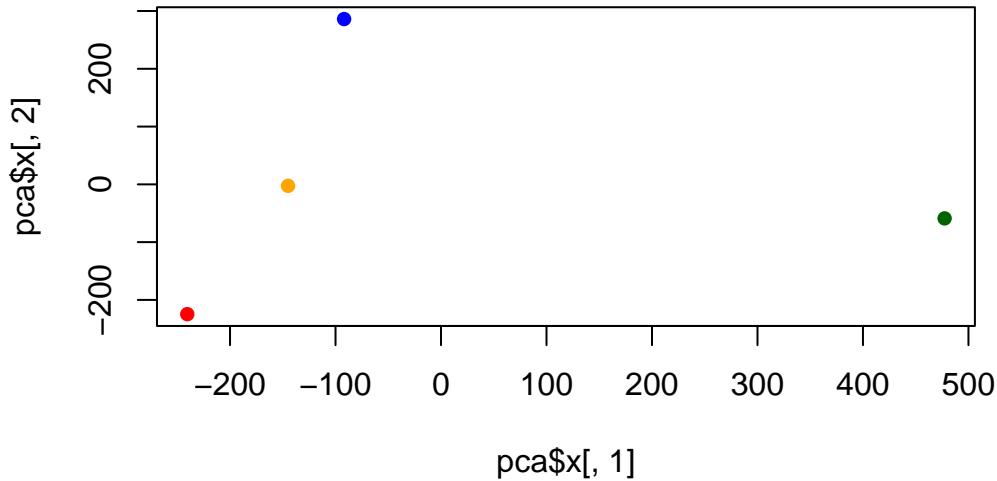
$class
[1] "prcomp"
```

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

```
pca$x
```

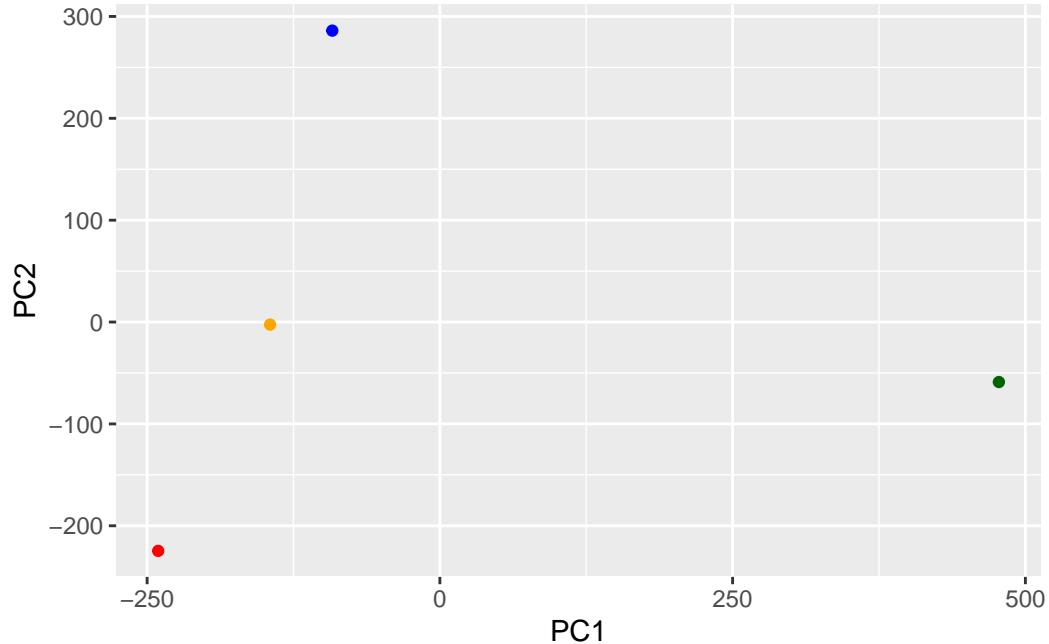
	PC1	PC2	PC3	PC4
England	-144.99315	-2.532999	105.768945	-4.894696e-14
Wales	-240.52915	-224.646925	-56.475555	5.700024e-13
Scotland	-91.86934	286.081786	-44.415495	-7.460785e-13
N.Ireland	477.39164	-58.901862	-4.877895	2.321303e-13

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



```
library(ggplot2)

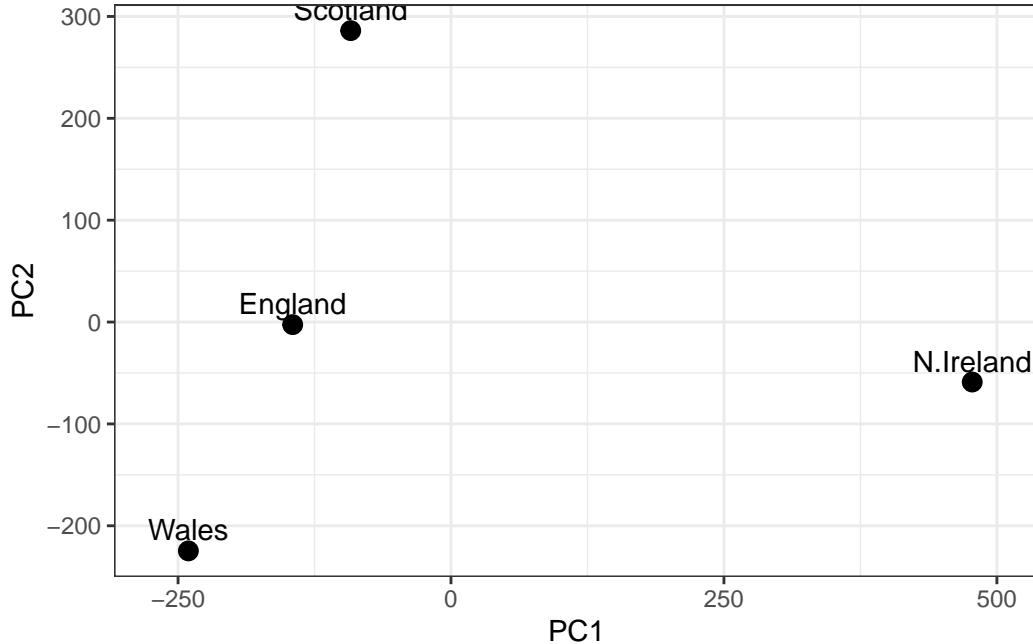
ggplot(pca$x) +
  aes(PC1, PC2) +
  geom_point(col=my_cols)
```



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

```
# Create a data frame for plotting
df <- as.data.frame(pca$x)
df$Country <- rownames(df)

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

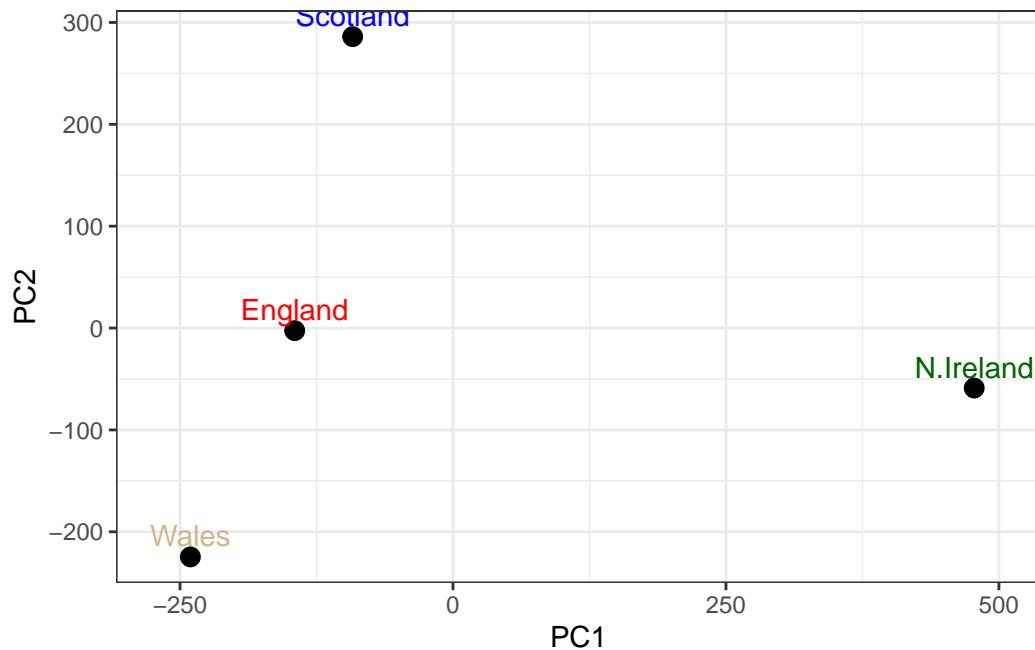


Q8: Customize your plot so that the colors of the country names match the colors in our UK and Ireland map and table at start of this document.

```
# Create a data frame for plotting
df <- as.data.frame(pca$x)
df$Country <- rownames(df)

# Plot PC1 vs PC2 with ggplot
colors <- c(Wales = "red", England = "tan", Scotland = "blue", N.Ireland = "darkgreen")

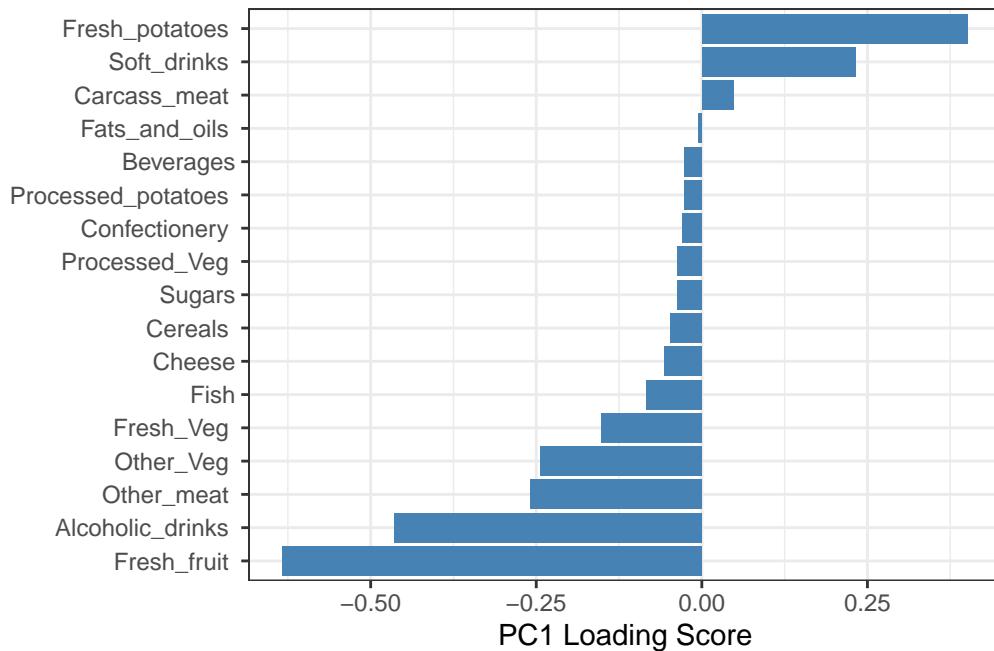
ggplot(pca$x) +
  aes(x = PC1, y = PC2, label = rownames(pca$x)) +
  geom_point(size = 3) +
  geom_text(color = colors, vjust = -0.5) +
  xlim(-270, 500) +
  xlab("PC1") +
  ylab("PC2") +
  theme_bw()
```



Digging deeper (variable loadings)

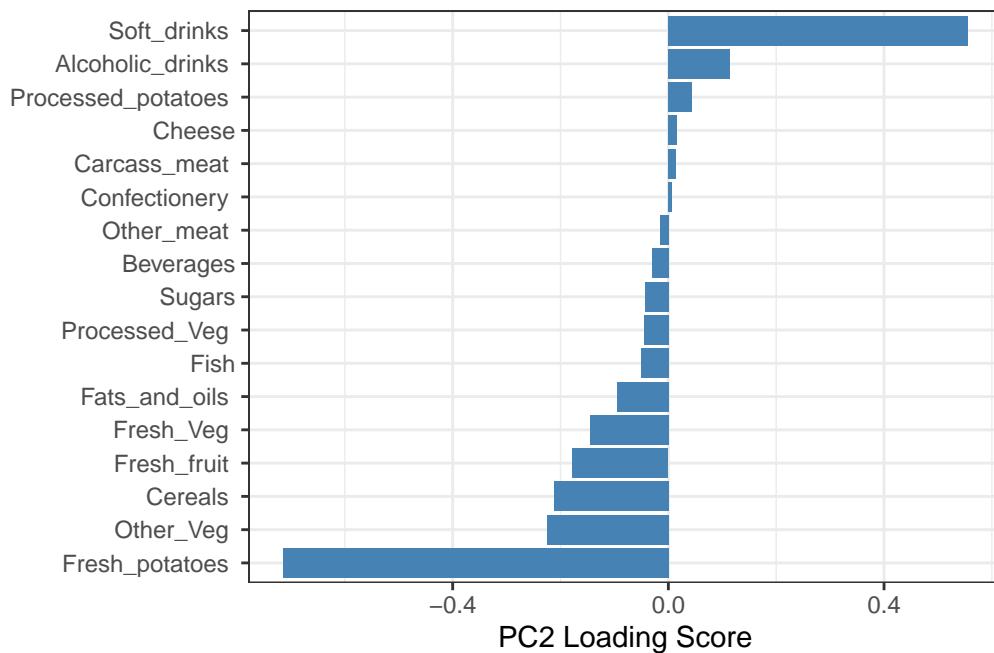
How do the original variables (i.e. the 17 different foods) contribute to our new PCs?

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



The two food groups that are the most prominent are soft drinks and alcoholic drinks. PC2 mainly provides information on the second highest variance in the data, after PC1.