

Class 7: Machine Learning 1

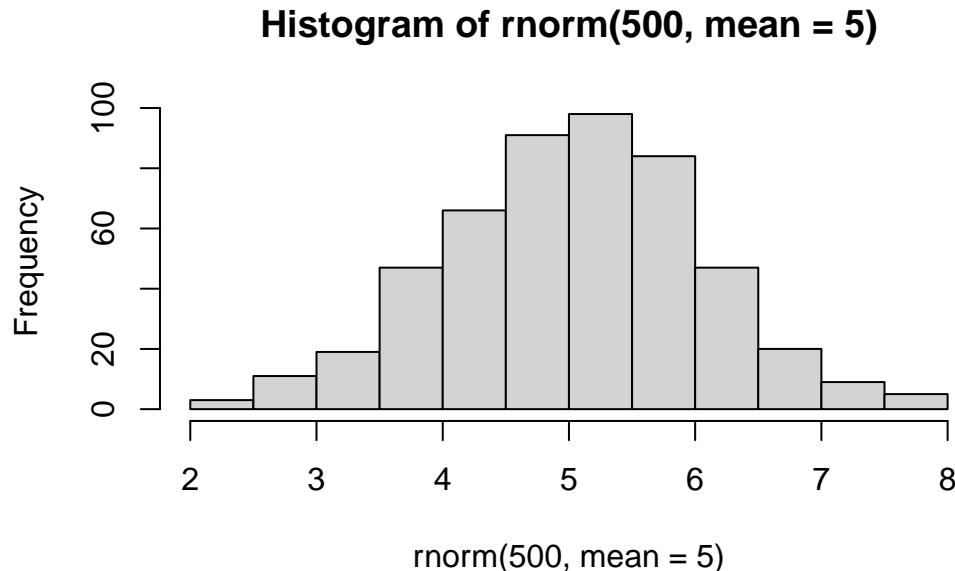
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Today we will explore some fundamental machine learning methods including clustering and dimensionality reduction.

K-means clustering

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

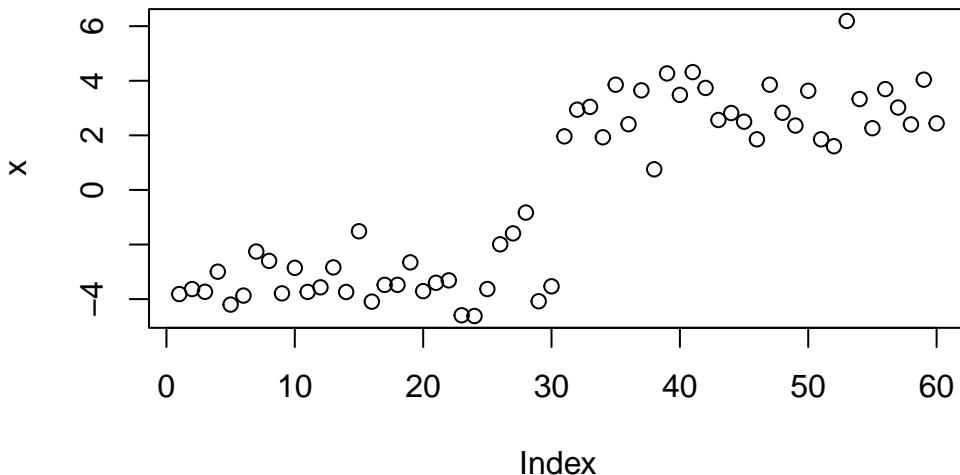
```
hist(rnorm(500, mean = 5))
```



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

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

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



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

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

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

```
Cluster means:
[,1]
1 -3.271442
2  2.986380
```

```
Clustering vector:
```

Within cluster sum of squares by cluster:

```
[1] 23.83912 32.59717  
(between_SS / total_SS =  91.2 %)
```

Available components:

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

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

k\$size

[1] 30 30

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?

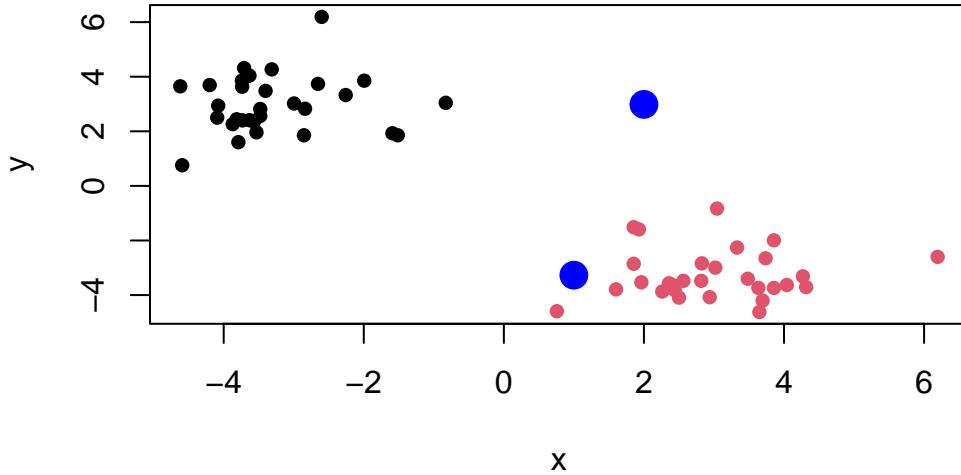
k\$cluster

k\$centers

```
[,1]  
1 -3.271442  
2 2.986380
```

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

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

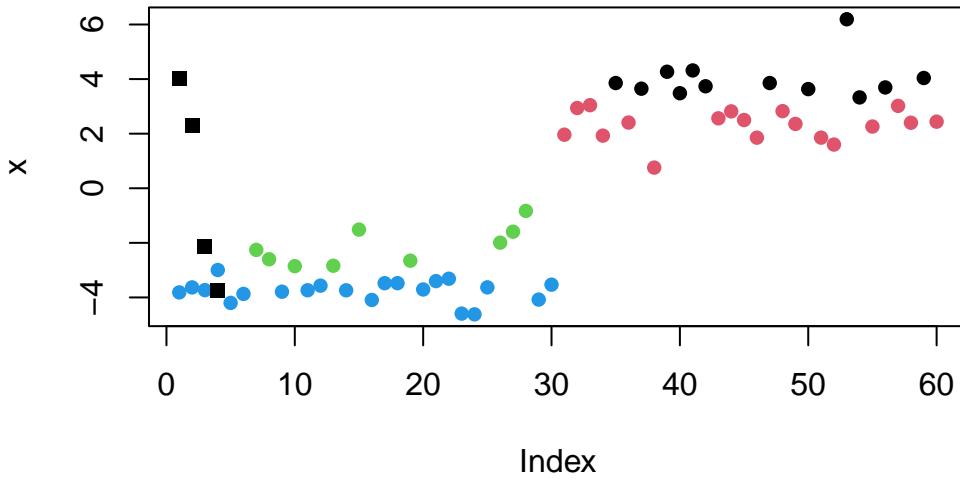


K-means clustering is very popular because it is fast and relatively straightforward: it takes numerical data as input and returns a cluster membership vector, among other results.

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

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

```
k4 <- kmeans(x, centers = 4)
plot(x, col = k4$cluster, pch = 16)
points(k4$centers, pch = 15)
```



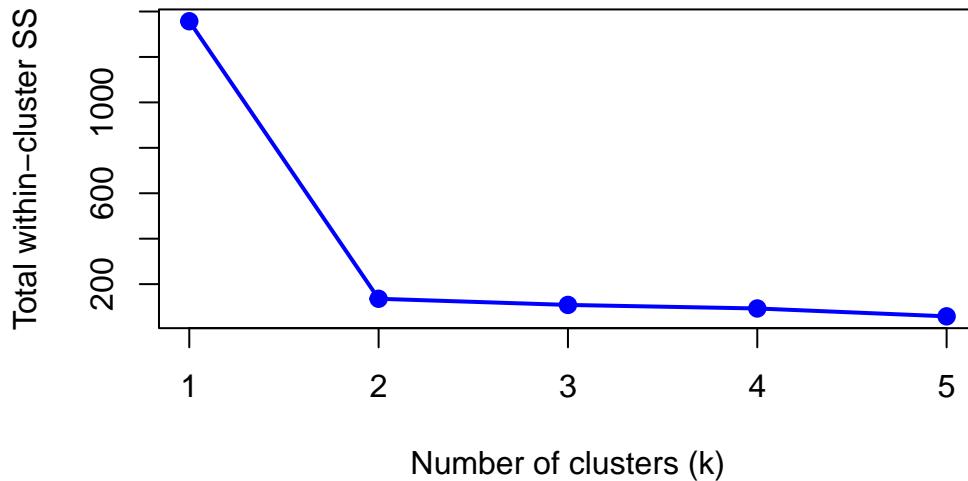
Scree Plot

```
# Example data
x <- c(rnorm(30, mean = -3), rnorm(30, mean = 3))
y <- rev(x)
xy <- cbind(x, y)

# Calculate total within-cluster sum of squares for k = 1 to 5
tot_within <- numeric(5)
for (k in 1:5) {
  km <- kmeans(xy, centers = k)
  tot_within[k] <- km$tot.withinss
}

plot(1:5, tot_within, type = "o",
      pch = 19, col = "blue", lty = 1, lwd = 2,
      xlab = "Number of clusters (k)",
      ylab = "Total within-cluster SS",
      main = "Elbow Plot for k-means Clustering")
```

Elbow Plot for k-means Clustering



A scree plot using K-means shows a line of how “tight” the clusters are for different numbers of clusters, helping you pick the best number.

Hierarchical Clusters

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

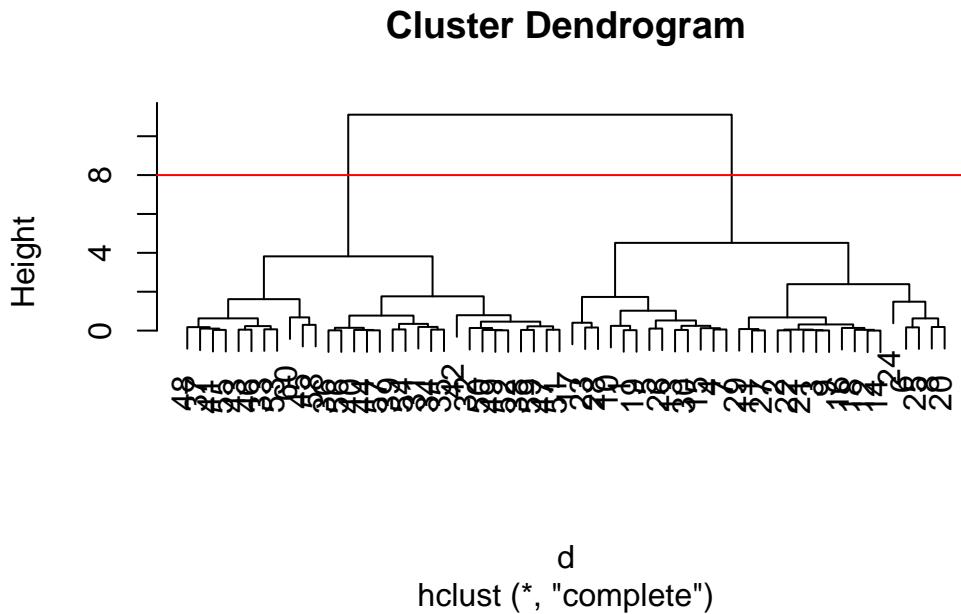
```
d <- dist(x)
hc <- hclust(d)
hc
```

```
Call:
hclust(d = d)
```

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

There is a plot method for `hclust` results lets try it

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



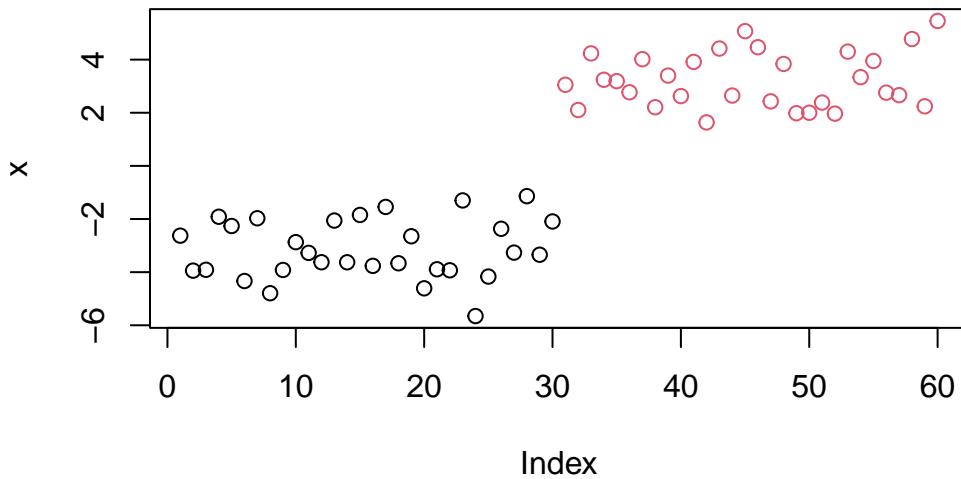
```
clusters <- cutree(hc, h = 8)  
clusters
```

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

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

Q. Plot the data with our hclust result coloring

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



Principal Component Analysis (PCA)

##PCA of UK food data

Import food data from an online CSV file

```
url <- "https://tinyurl.com/UK-foods"  
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

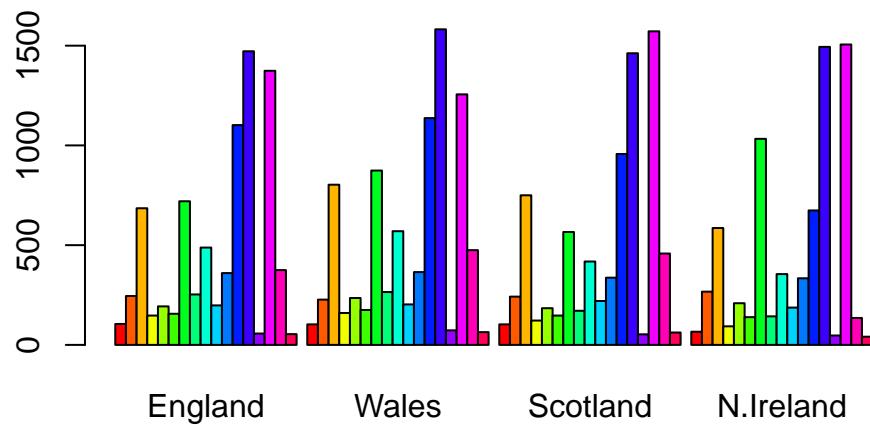
```

	England	Wales	Scotland	N.Ireland
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Carcass_meat	245	227	242	267
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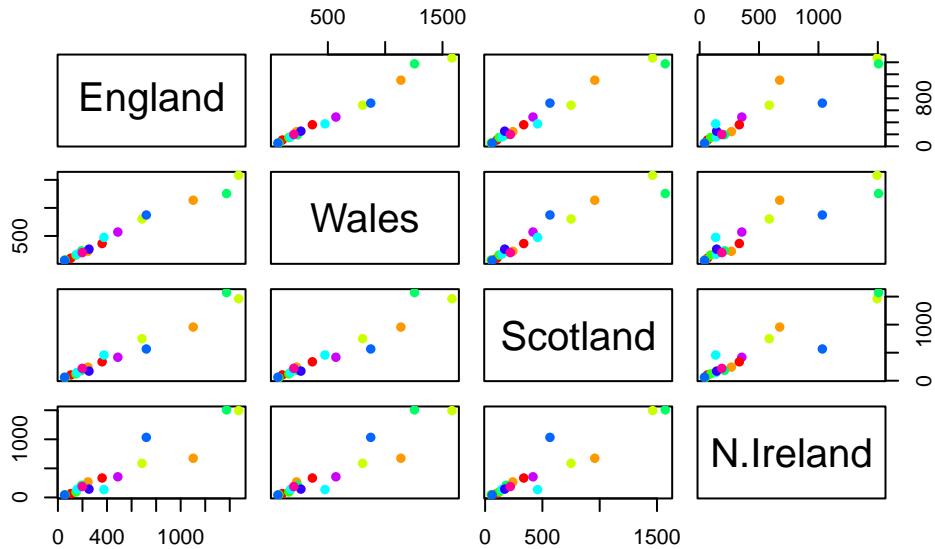
Some base figures

```
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(10), 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). So, let's see if PCA can help!

PCA to the rescue

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

I will take the transpose of our data so the “foods” are in the columns:

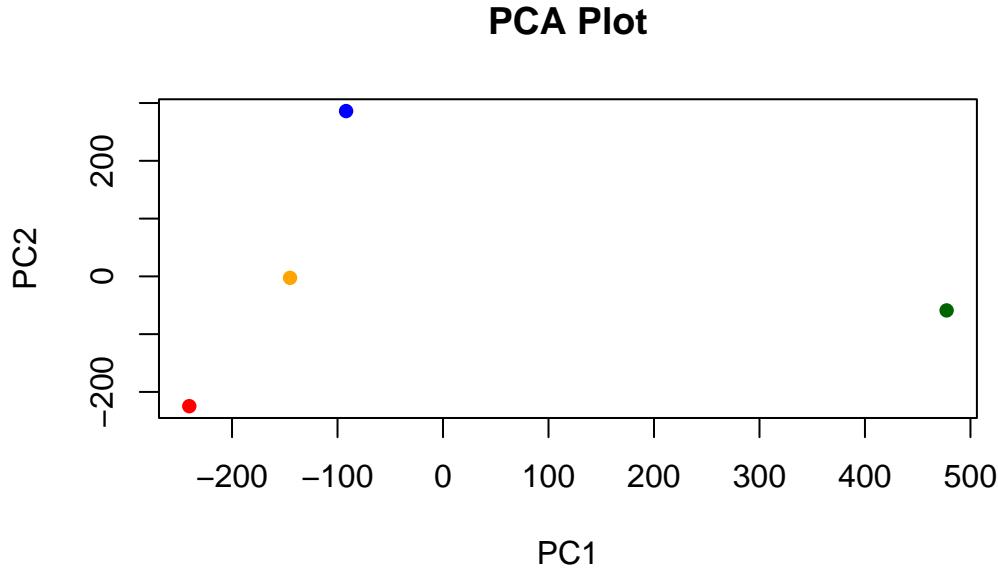
```
pca <- prcomp( t(x) )
summary(pca)
```

Importance of components:

	PC1	PC2	PC3	PC4
Standard deviation	324.1502	212.7478	73.87622	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

Together PC1 and PC2 captures around ~96% variance of the data, good capture of the data

```
# This is what I want to plot
cols <- c("orange", "red", "blue", "darkgreen")
plot(pca$x[,1], pca$x[,2], col = cols, pch = 16,
     xlab = "PC1", ylab = "PC2", main = "PCA Plot")
```

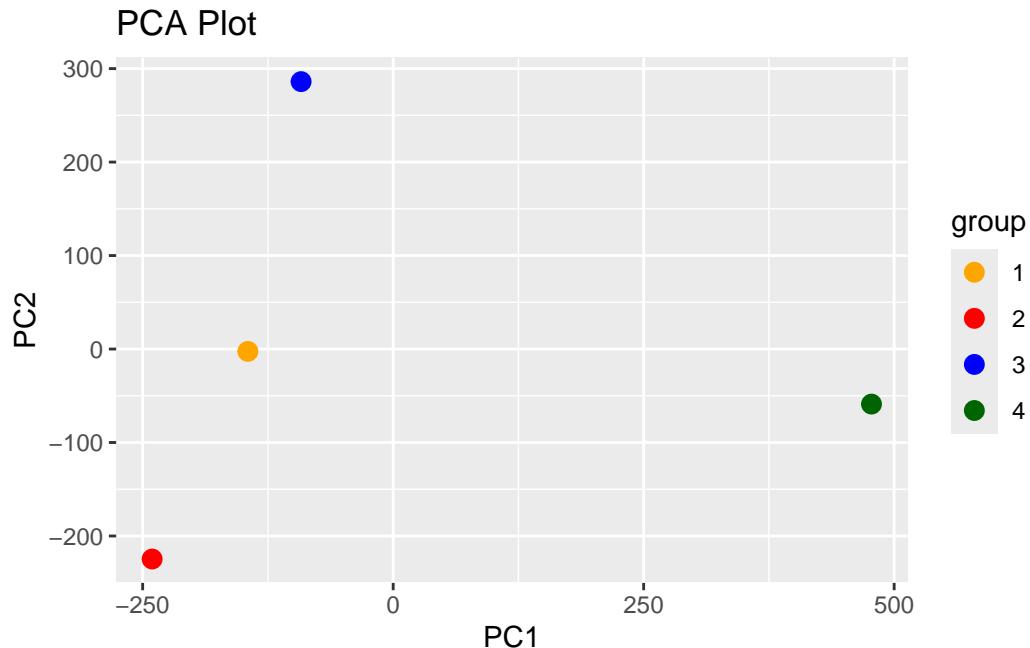


```
library(ggplot2)
```

```
library(ggplot2)

pca_df <- as.data.frame(pca$x)
pca_df$group <- factor(c(1,2,3,4))

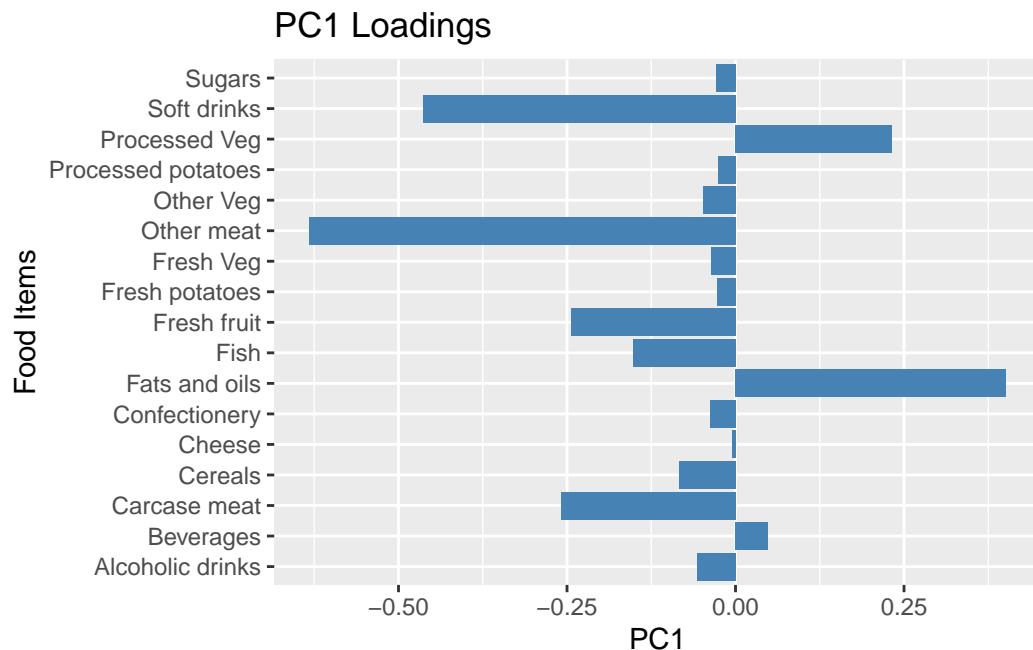
ggplot(pca_df, aes(x = PC1, y = PC2, color = group)) +
  geom_point(size = 3) +
  scale_color_manual(values = c("orange", "red", "blue", "darkgreen")) +
  labs(title = "PCA Plot", x = "PC1", y = "PC2")
```



```
library(ggplot2)
food_items <- c("Alcoholic drinks", "Beverages", "Carcase meat", "Cereals",
                 "Cheese", "Confectionery", "Fats and oils", "Fish",
                 "Fresh fruit", "Fresh potatoes", "Fresh Veg", "Other meat",
                 "Other Veg", "Processed potatoes", "Processed Veg", "Soft drinks", "Sugars")

rotation_df <- as.data.frame(pca$rotation)
rotation_df$Food <- food_items

ggplot(rotation_df, aes(x = PC1, y = Food)) +
  geom_col(fill = "steelblue") +
  labs(title = "PC1 Loadings", x = "PC1", y = "Food Items")
```



PCA looks super useful and we will come back to describe this further next day :)