Class 7: Machine Learning 1

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In this class we will explore clustering and dimensionality reduction methods.

K-means

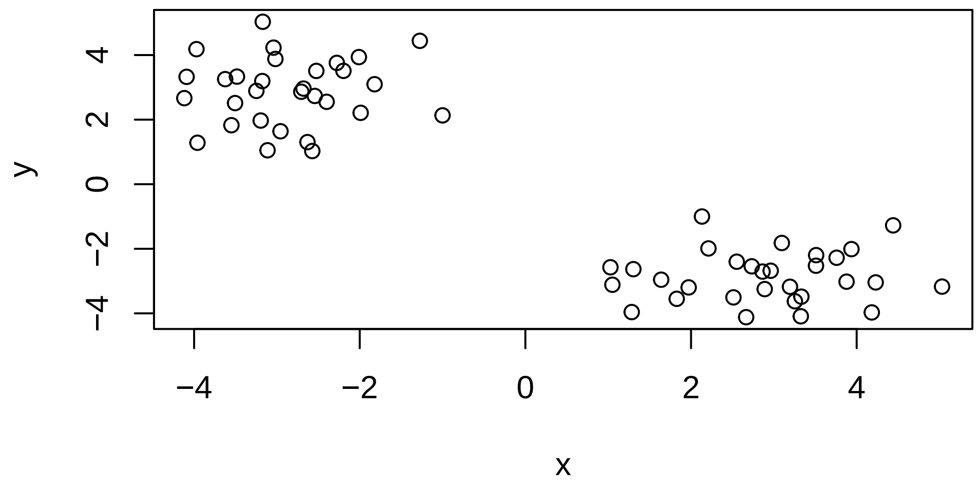
Make up some input data where we know what the answer should be.

```
tmp <- c(rnorm(30, -3),rnorm(30,+3))
x <- cbind(x=tmp,y=rev(tmp))
head(x)
```

```
             x        y
[1,] -2.399717 2.551936
[2,] -3.248220 2.889529
[3,] -3.625024 3.253826
[4,] -3.195864 1.971380
[5,] -3.549455 1.827113
[6,] -2.631174 1.303893
```

Quick plot of x to see the two groups at -3,+3 and +3,-3.

```
plot(x)
```



Use the `kmeans()` function, setting k to 2 and nstart=20.

```
km <- kmeans(x,centers=2,nstart=20)
km
```

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

Cluster means:
          x         y
1 -2.861686  2.876645
2  2.876645 -2.861686

Clustering vector:
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2

Within cluster sum of squares by cluster:
[1] 49.47816 49.47816
 (between_SS / total_SS =  90.9 %)

Available components:
```

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

> Q. How many points are in each cluster?

```r
km$size
```

```
[1] 30 30
```

> Q. What 'component' of your result object details cluster assignment/membership and cluster center?

```r
km$cluster
```

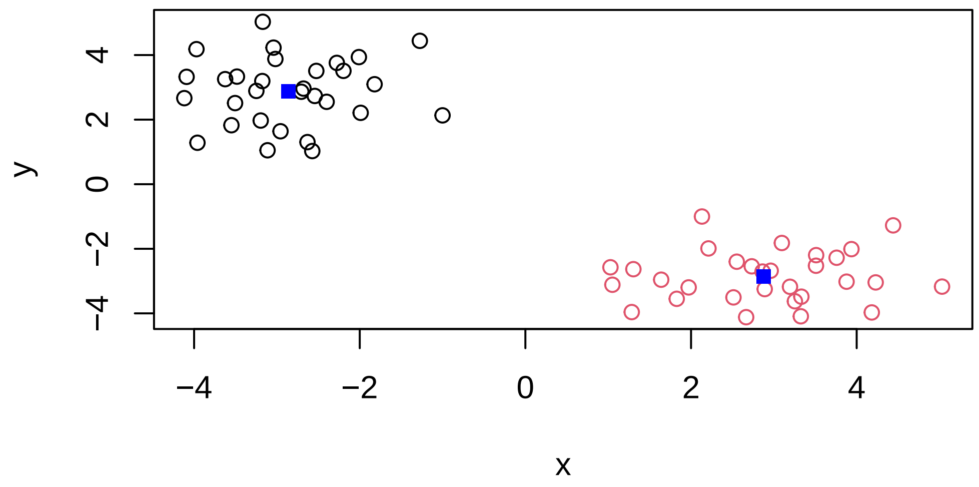
```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

```r
km$centers
```

```
          x         y
1 -2.861686  2.876645
2  2.876645 -2.861686
```

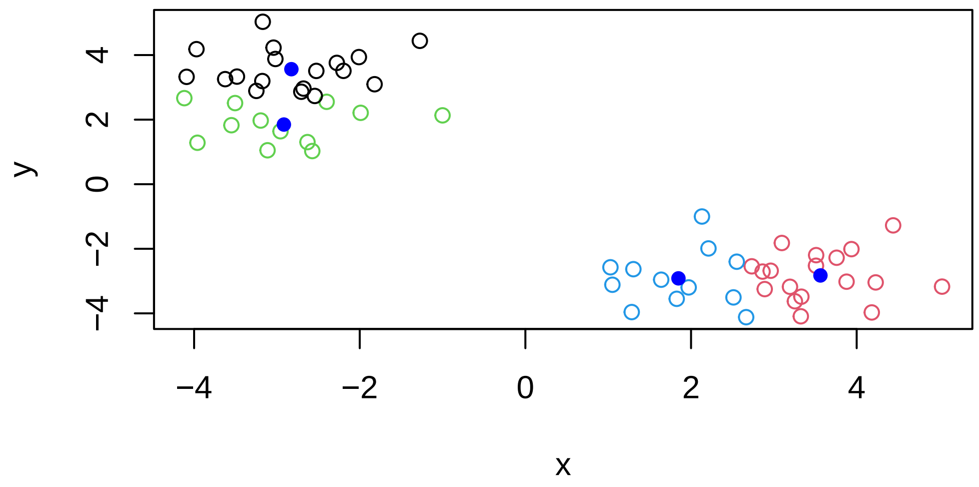
> Q. Plot x colored by the kmeans cluster assignment and add cluster centers as blue points.

```r
plot(x, col=km$cluster)
points(km$centers,col="blue", pch=15)
```



Play with kmeans and ask for different number of clusters.

```
km <- kmeans(x,centers=4,nstart=20)
plot(x, col=km$cluster)
points(km$centers,col="blue", pch=16)
```



Hierarchical Clustering

This is another very useful and widely employed clustering method which has the advantage over k-means in that is can help reveal something about the true grouping in your data set.

The `hclust()` function wants a distance matrix as input. We can get this from the `dist()` function.

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

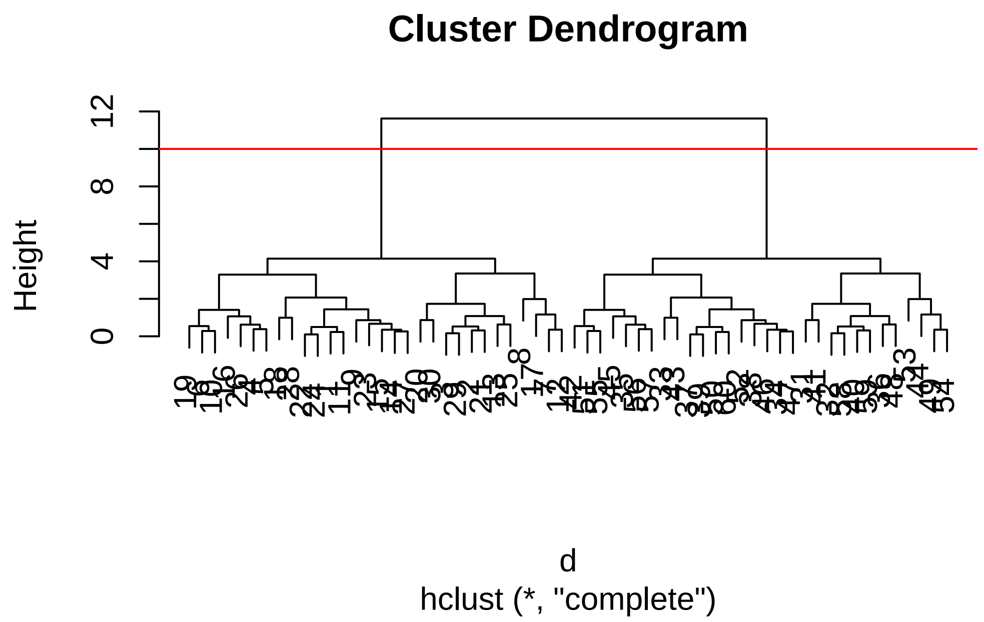
```

Call:
hclust(d = d)

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

There is a plot method for `hclust()` results:

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

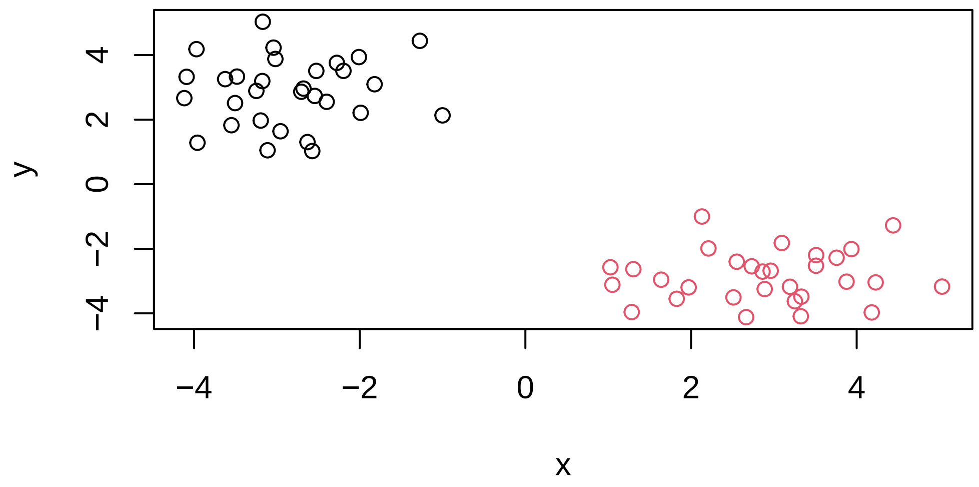


To get my cluster membership vector I need to "cut" my tree to yield sub-trees or branches with all the members of a given cluster. The function to do this is called `cutree()`.

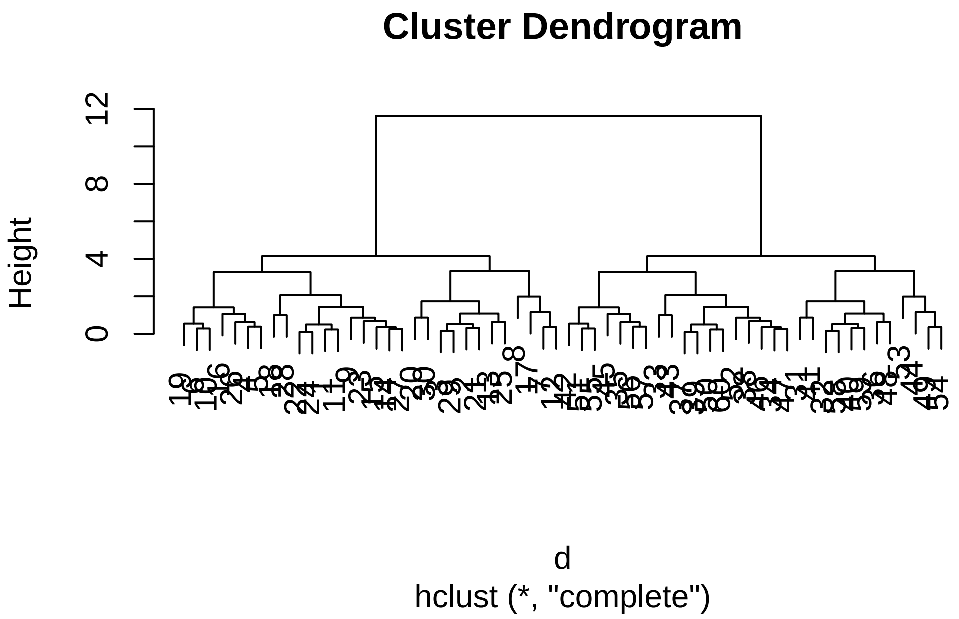
```
grps <- cutree(hc,h=10)
grps
```

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

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


y
4
2
0
−2
−4
−4
−2
0
2
4
x

```
plot(hc)
```


Cluster Dendrogram
Height
12
8
4
0
d
hclust (*, "complete")

It is often helpful to use the `k=` argument to `cutree()` rather than the `h=` height of cutting with `cutree()`. This will cut the tree to yield the number of clusters you want.

```
cutree(hc,k=4)
```

```
 [1] 1 2 2 1 1 1 2 2 1 1 1 2 2 1 1 1 2 1 1 2 2 1 1 1 2 1 1 1 2 2 3 3 4 4 4 3 4 4
[39] 4 3 3 4 4 3 4 4 4 3 3 4 4 4 3 3 4 4 4 3 3 4
```

Principal Component Analysis (PCA)

The base R function for PCA is called `prcomp()`. Let's play with some 17D data (a very small dataset) and see how PCA can help.

PCA of UK Food Data

Import the data

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
head(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
```

> 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
```

I used the `dim()` function to find the number of columns and rows.

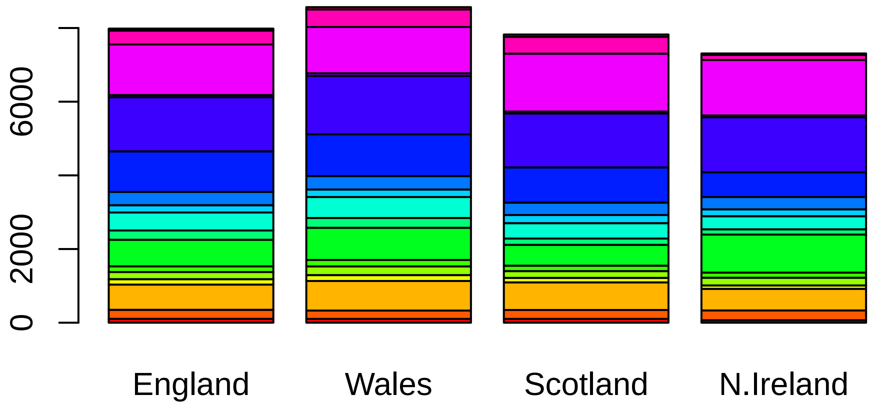
```
# Note how the minus indexing works
#rownames(x) <- x[,1]
#x <- x[,-1]
#head(x)
```

There are 17 rows and 4 columns once I adjusted it so that row-names was not the first column.

> 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?

The second approach (fixing the problem when importing the data) is probably ideal since running the `x <- x[-1]` multiple times will remove a column each time. I have commented out these lines for subsequent runs of code.

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

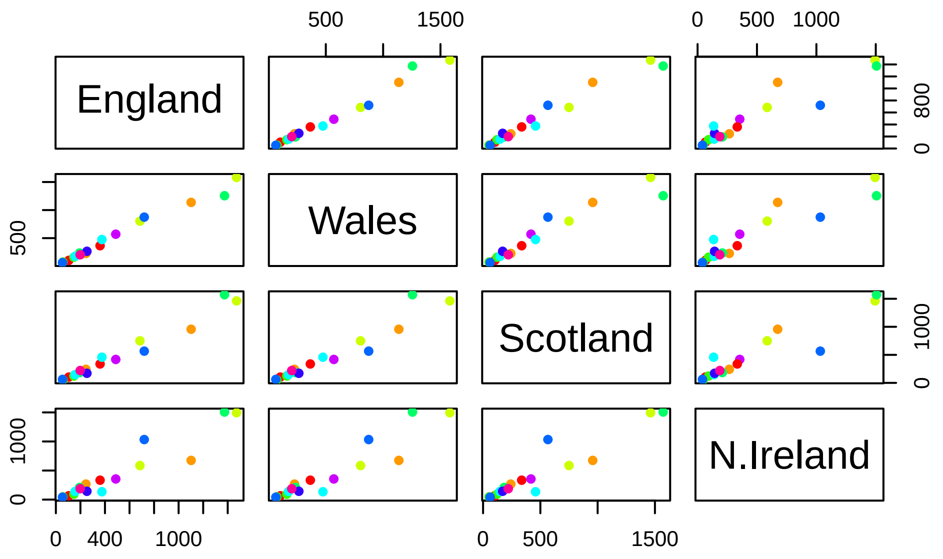


> Q3: Changing what optional argument in the above barplot() function results in the following plot?

Changing the "beside" argument to be "FALSE" or "F" changes the `barplot()`. Leaving this argument out would have the same effect since the default value for this argument is

"FALSE".

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



> 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?

In this case, the pair-wise plots show comparisons between all countries vs. all other countries in different food categories (i.e there is a plot where each country is on the x-axis and another plot where it is on the y-axis vs. all other countries). If a point lies on the diagonal of a given plot, the two countries have the same value for that food category.

> Q6. What is the main differences between N. Ireland and the other countries of the UK in terms of this data-set?

N. Ireland's data is least similar to other countries in the dataset (i.e values for respective food categories are not very often the same between N. Ireland vs. England, Wales, or Scotland).

```
# Use the prcomp() PCA function
pca <- prcomp( t(x) )
summary(pca)
```

```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 4.189e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

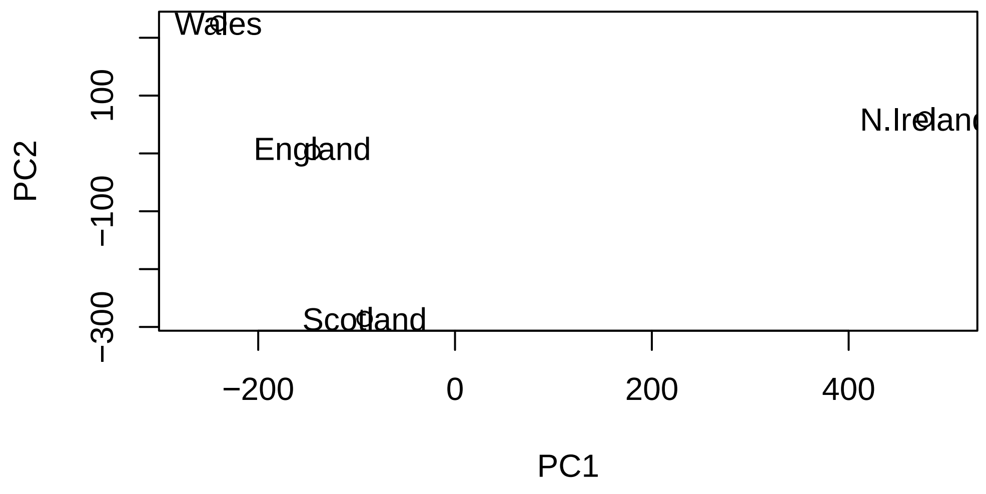
A "PCA plot": PC1 vs. PC2

```
pca$x
```

```
                PC1         PC2         PC3           PC4
England   -144.99315    2.532999 -105.768945  2.842865e-14
Wales     -240.52915  224.646925   56.475555  7.804382e-13
Scotland   -91.86934 -286.081786   44.415495 -9.614462e-13
N.Ireland  477.39164   58.901862    4.877895  1.448078e-13
```

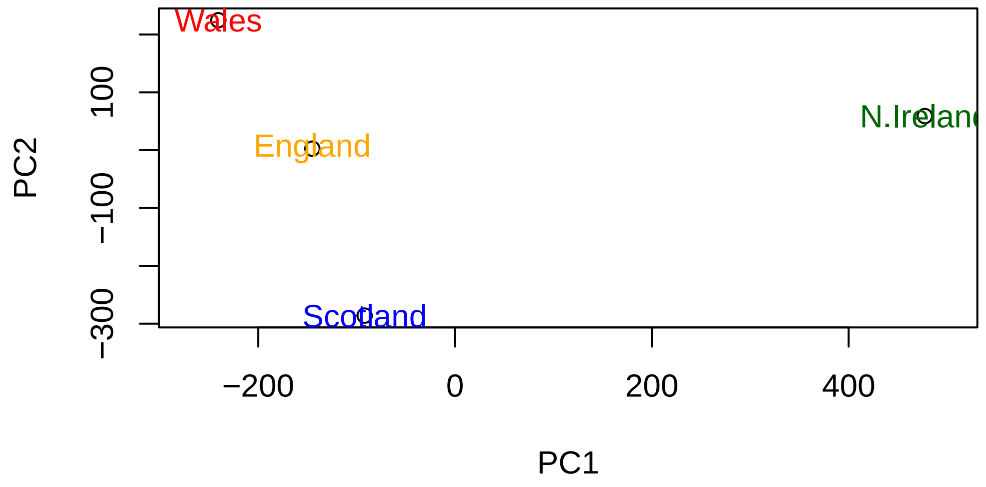
> Q7. Complete the code below to generate a plot of PC1 vs PC2. The second line adds text labels over the data points.

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x))
```



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.

```
# Plot PC1 vs PC2 with country names colored
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col=c("orange", "red", "blue", "darkgreen"))
```



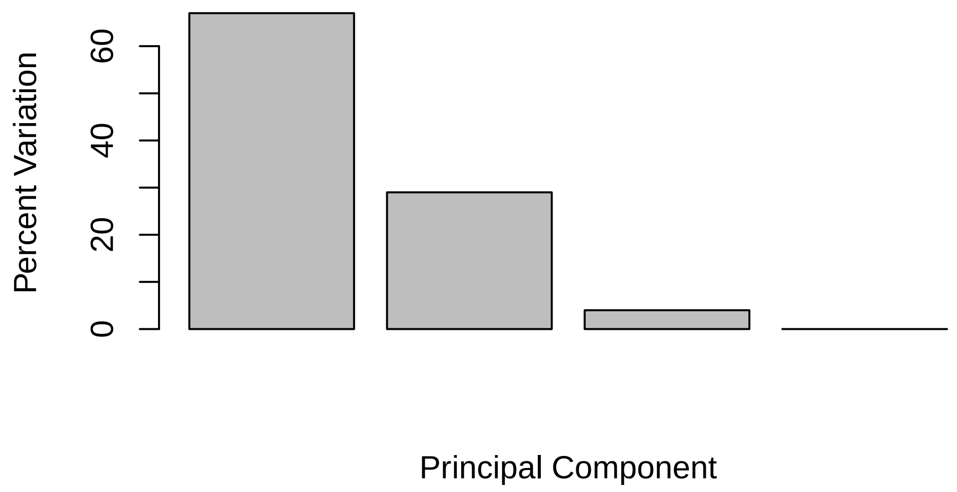
```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

```
[1] 67 29  4  0
```

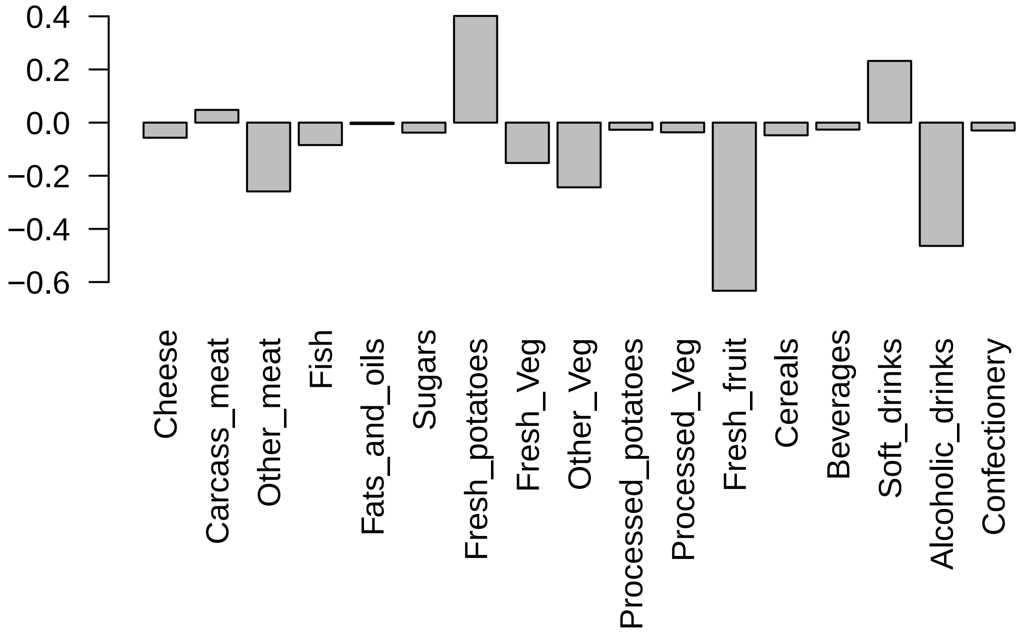
```
z <- summary(pca)
z$importance
```

```
                             PC1       PC2      PC3          PC4
Standard deviation     324.15019 212.74780 73.87622 4.188568e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

```r
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```



```r
## 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 )
```


0.4
0.2
0.0
−0.2
−0.4
−0.6
Cheese
Carcass_meat
Other_meat
Fish
Fats_and_oils
Sugars
Fresh_potatoes
Fresh_Veg
Other_Veg
Processed_potatoes
Processed_Veg
Fresh_fruit
Cereals
Beverages
Soft_drinks
Alcoholic_drinks
Confectionery