

Class 7: Machine Learning 1

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Today we will begin our exploration of some “classical” machine learning approaches. We will start with clustering:

First we'll make up some data to cluster with a known answer.

```
hist(rnorm(1000))
```

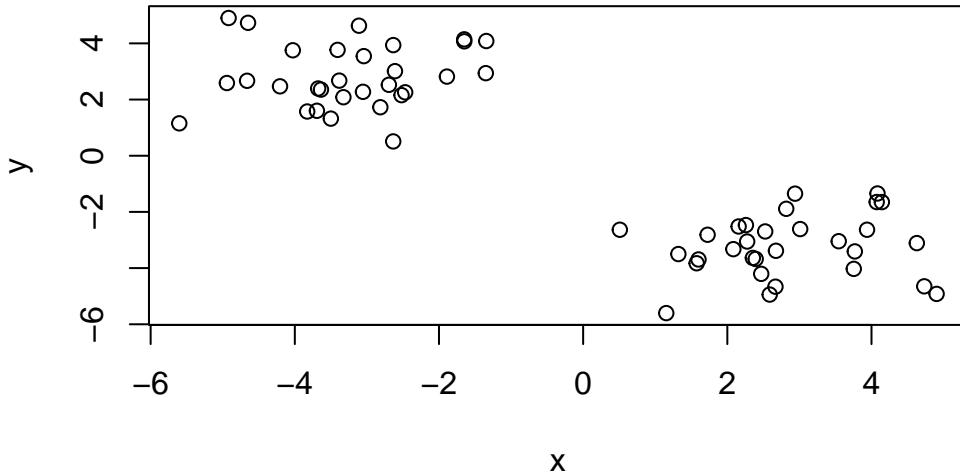


```
x <- c(rnorm(30, mean = -3), rnorm(30, mean = 3))
y <- rev(x)

z <- cbind(x,y)
```

Lets plot our data:

```
plot(z)
```



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

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

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

Cluster means:

	x	y
1	-3.230984	2.822229
2	2.822229	-3.230984

Clustering vector:

Within cluster sum of squares by cluster:

```
[1] 71.42634 71.42634  
(between_SS / total_SS = 88.5 %)
```

Available components:

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

Q. How big are the clusters (i.e their size)?

k\$size

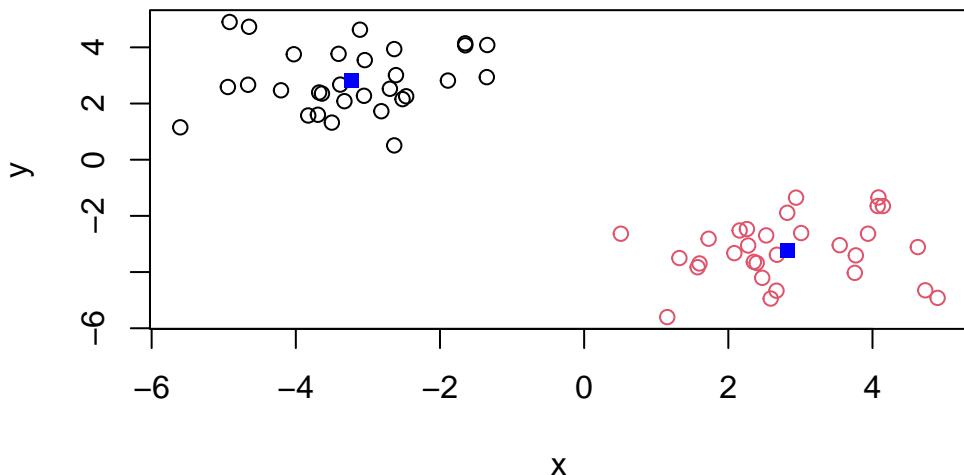
[1] 30 30

Q. What clusters do my data points reside in?

k\$cluster

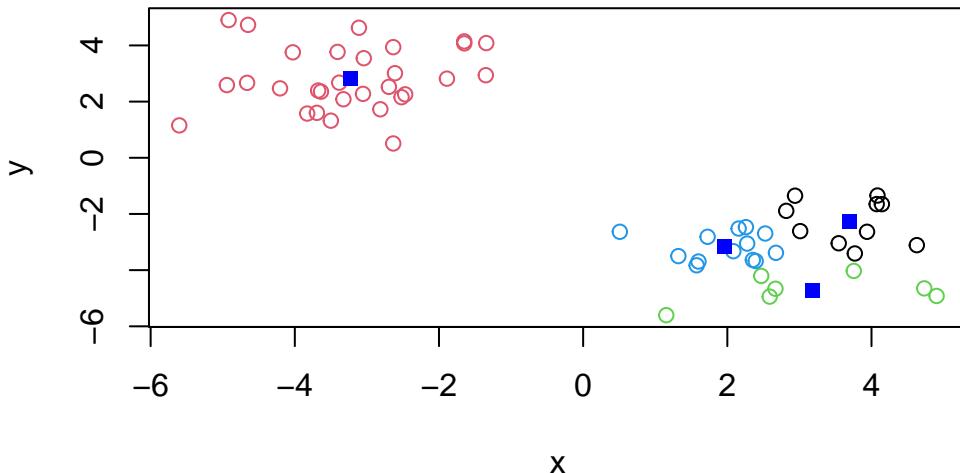
Q. Make a plot of our data colored by cluster assignment - i.e. Make a result figure...

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



Q. Cluster with k-means into 4 clusters and plot your results as above

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



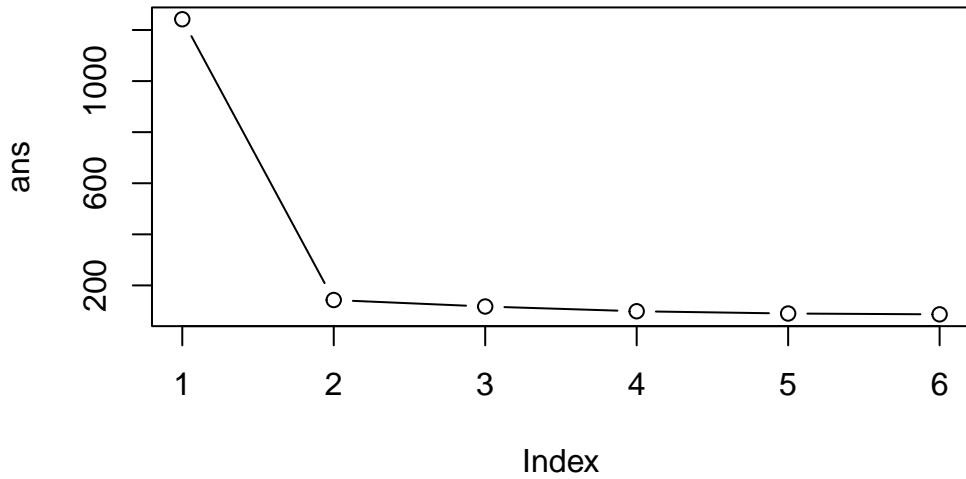
Q. Run kmeans with centers (i.e. values of k) equal 1 to 6, using a for loop

```
ans <- NULL
for(i in 1:6){
  ans <- c(ans, kmeans(z, centers = i)$tot.withinss)
}
ans
```

```
[1] 1242.09413 142.85268 117.46022 98.89684 90.03766 86.73170
```

Plot this “scree-plot”

```
plot(ans, typ="b")
```



Hierarchical Clustering

The main function in “base” R for this is called `hclust()`.

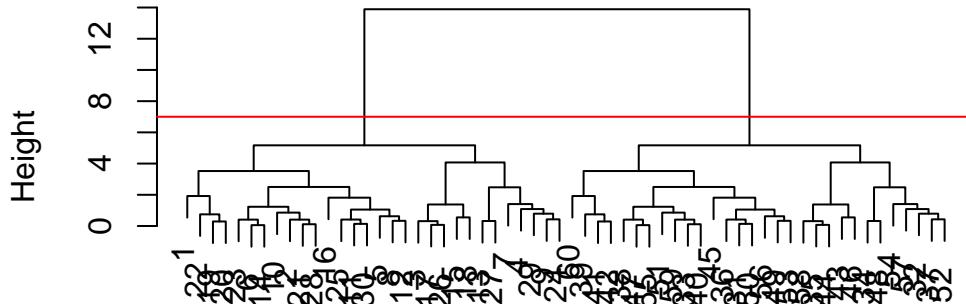
```
d <- dist(z)
hc <- hclust(d)
hc
```

Call:
`hclust(d = d)`

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

```
plot(hc)
abline(h=7, col="red")
```

Cluster Dendrogram



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

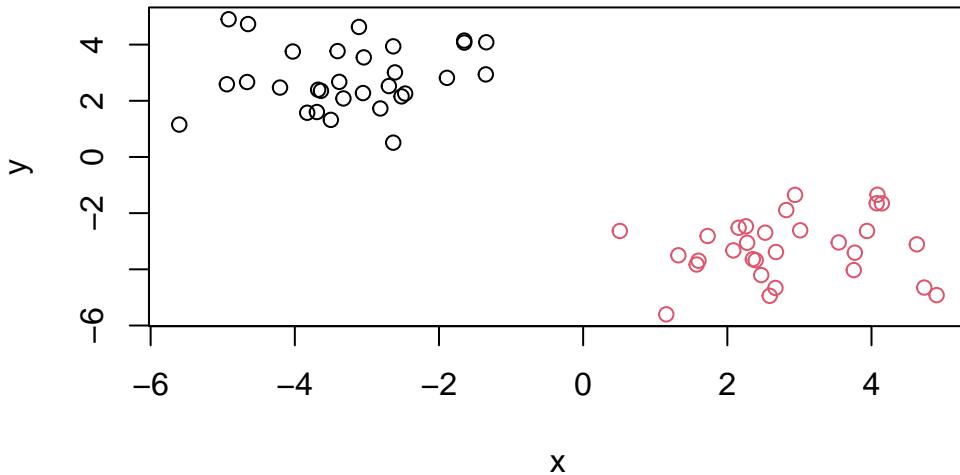
To obtain clusters from our `hclust` object `hc` we “cut” the tree to yield different sub branches. For this we use the `cutree()` function.

```
grps <- cutree(hc, h=7)  
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 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 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 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 2 2 2 2 2 2 2 2
```

Results Figure

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



PCA's!!!! (Principal Component Analysis)

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

Q1. How many rows and columns are in your new data frame named x? What R functions could you use to answer this question?

```
dim(data)
```

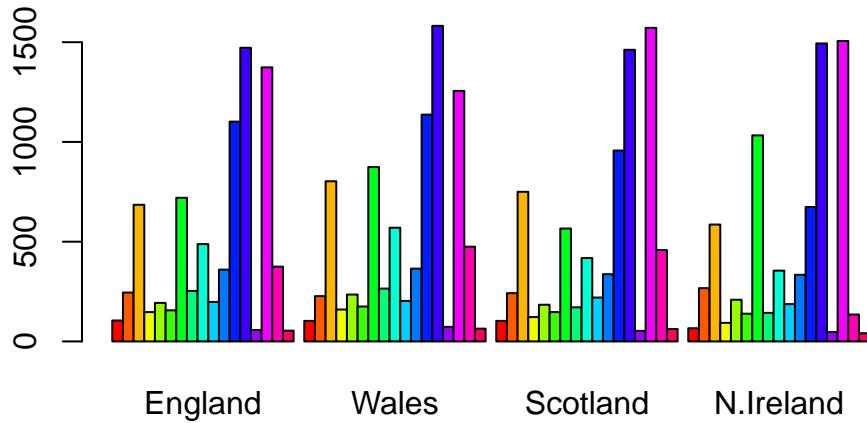
```
[1] 17 4
```

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 prefer the second method (`read.csv(url, row.names=1)`) so that my row names are not lost with no danger to losing data (like calling `x <- x[,-1]` multiple times)

Spotting major differences and trends

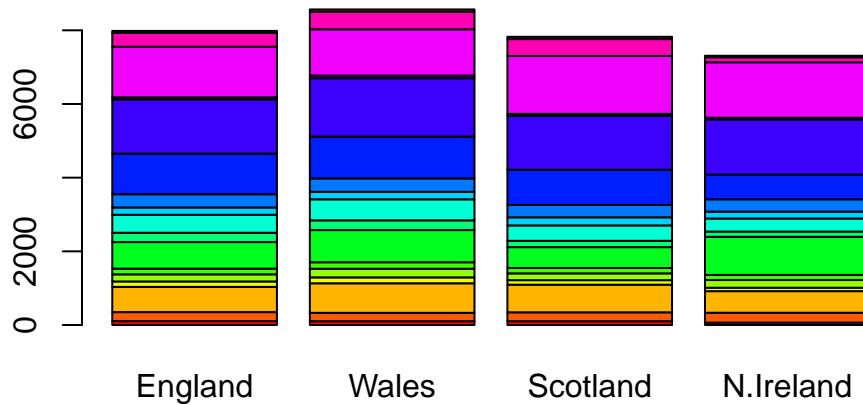
```
barplot(as.matrix(data), beside=T, col=rainbow(nrow(data)))
```



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

Changing the besides arugment to false will result in the following plot

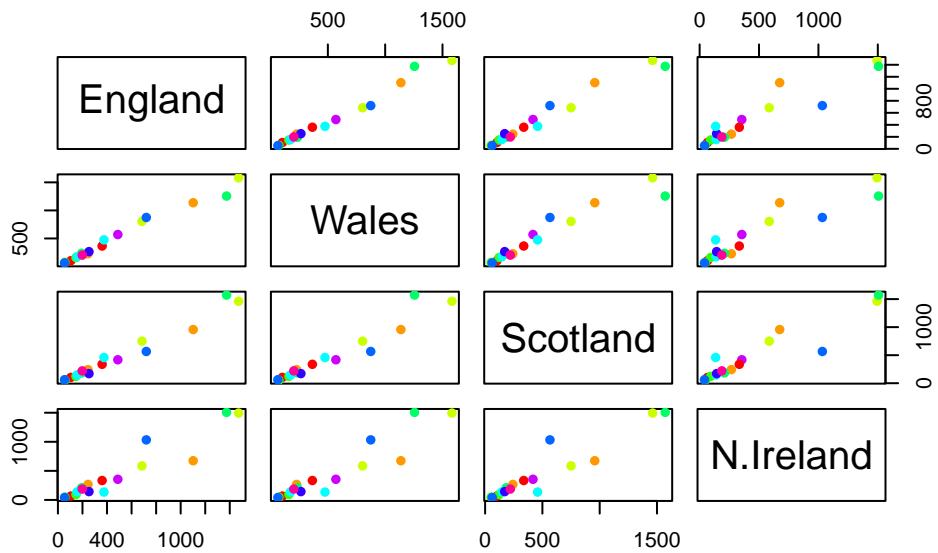
```
barplot(as.matrix(data), beside=F, col=rainbow(nrow(data)))
```



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?

If a given point lies on the diagonal, it is the same (or very similar) for both datasets (countries) being compared.

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



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

It's hard to tell, it seems like N. Ireland consumes more dark blue food group. Wales and England look very similar.

PCA to the rescue

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

But first we must transpose our dataset so the foods (dependent var) are in the columns and the countries (independent var) are in the rows using the `t()` function.

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

Importance of components:

	PC1	PC2	PC3	PC4
Standard deviation	324.1502	212.7478	73.87622	2.921e-14
Proportion of Variance	0.6744	0.2905	0.03503	0.000e+00
Cumulative Proportion	0.6744	0.9650	1.00000	1.000e+00

Our result object is called `pca` and it has a `$x` component that we will look at first

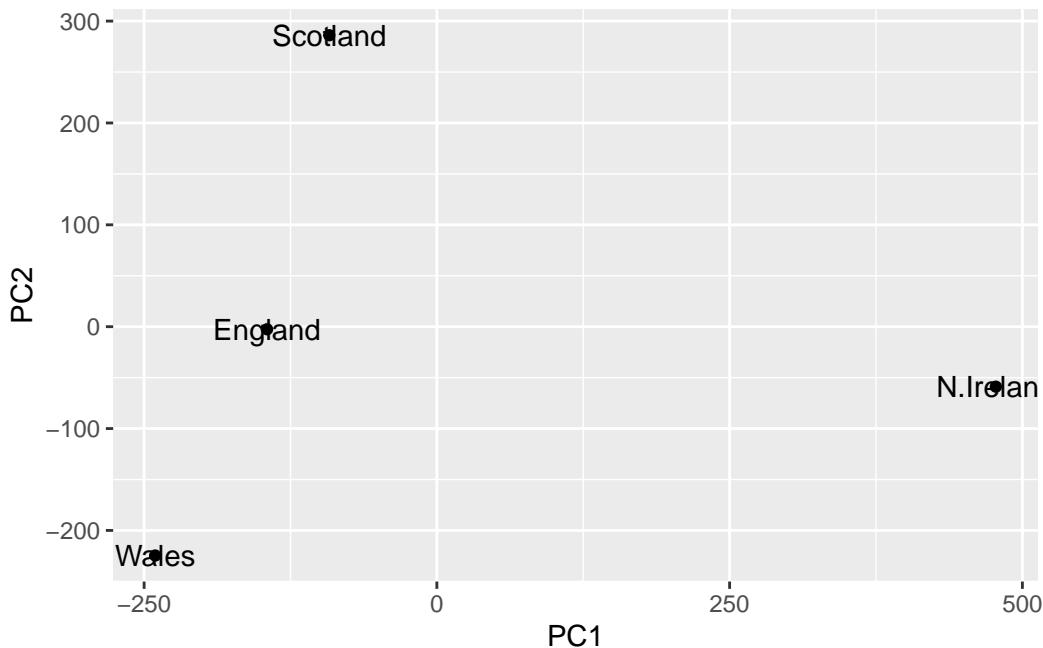
```
pca$x
```

	PC1	PC2	PC3	PC4
England	-144.99315	-2.532999	105.768945	-9.152022e-15
Wales	-240.52915	-224.646925	-56.475555	5.560040e-13
Scotland	-91.86934	286.081786	-44.415495	-6.638419e-13
N.Ireland	477.39164	-58.901862	-4.877895	1.329771e-13

Making a ordination plot

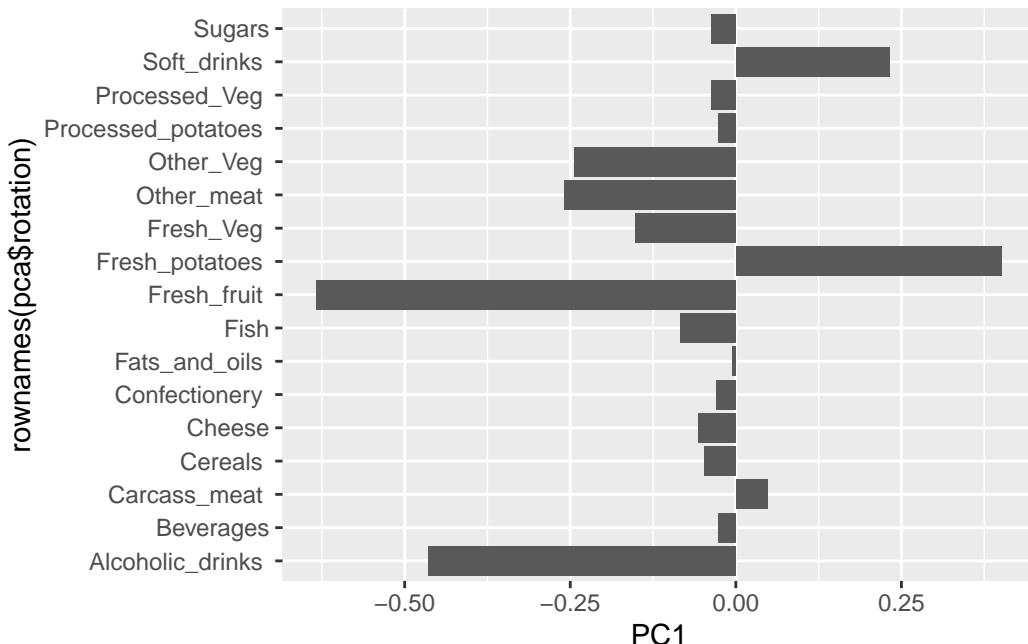
```
library(ggplot2)

ggplot(pca$x, aes(PC1, PC2, label=rownames(pca$x))) +
  geom_point() +
  geom_text()
```



Another major result out of PCA is the so-called “variable loadings” or `$rotation` that tells us how the original variables (foods) contribute to PCs (i.e. our new axis).

```
ggplot(pca$rotation) +
  aes(PC1, rownames(pca$rotation)) +
  geom_col()
```



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()
```

