Lab7: Introduction to machine learning for Bioinformatics

Duy An Le (PID: A16400411)

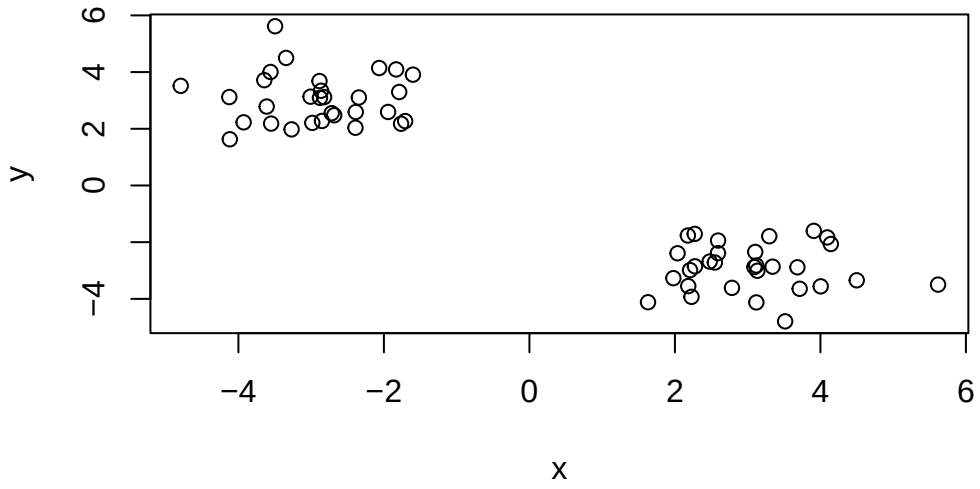
Today we will start our multi-part exploration of some key machine learning methods. We will begin with clustering- finding groupings in data, and then dimensionality reduction.

Clustering

K-means Clustering

Let's start with "k-means" clustering. The main function in base R for this is `kmeans()`.

```
# Make up some data
temp <- c(rnorm(30, -3), rnorm(30, +3))
data <- cbind(x=temp, y=rev(temp))
plot(data)
```



Now let's try out `kmeans()`

```
km <- kmeans(data, centers=2)
km
```

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

Cluster means:
          x         y
1 -2.898597  3.045677
2  3.045677 -2.898597

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 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

Within cluster sum of squares by cluster:
[1] 42.76429 42.76429
 (between_SS / total_SS =  92.5 %)

Available components:
```

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

Q. How many points in each cluster?

```
km$size
```

```
[1] 30 30
```

Q. What component of your result object details cluster assignment/membership?

```
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 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
```

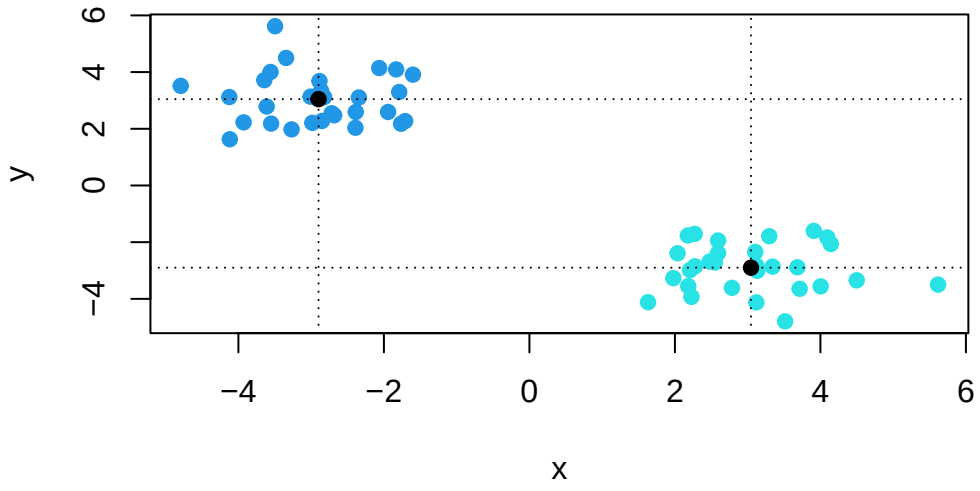
Q. What are centers/mean values of each cluster?

```
km$centers
```

```
          x         y
1 -2.898597  3.045677
2  3.045677 -2.898597
```

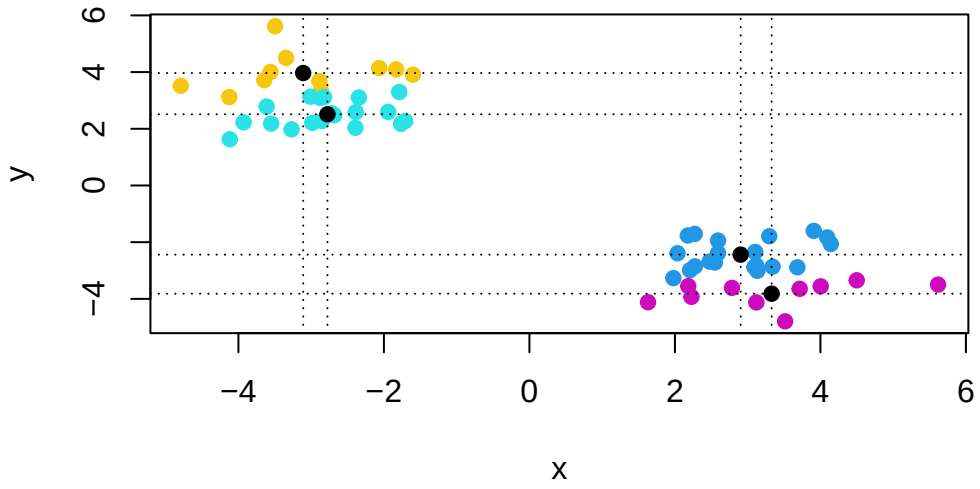
Q. Make a plot of your data showing your clustering results (groupings/clusters and cluster centers).

```
plot(data, col=km$cluster+3, pch=19)
points(km$centers, pch=19)
abline(v=km$centers[,1], h=km$centers[,2], lty=3)
```



Q. Run `kmeans()` again and cluster in 4 groups and plot the results.

```
km2 <- kmeans(data, centers=4)
plot(data, col=km2$cluster+3, pch=19)
points(km2$centers, pch=19)
abline(v=km2$centers[,1], h=km2$centers[,2], lty=3)
```



Hierarchical Clustering

This "bottom-up" form of clustering aims to reveal the structure in your data by progressively grouping points into an ever smaller number of clusters.

The main function in base R for this called `hclust()`. This function does not take our input data directly, but wants a "distance matrix" that details how (dis)similar all our input points are to each other.

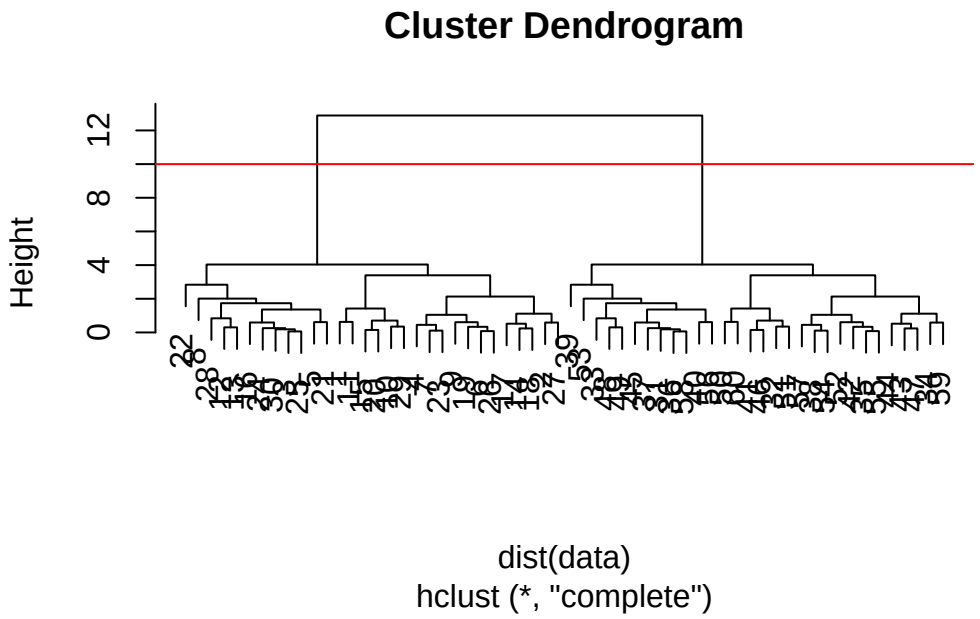
```
hc <- hclust(dist(data))
hc
```

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

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

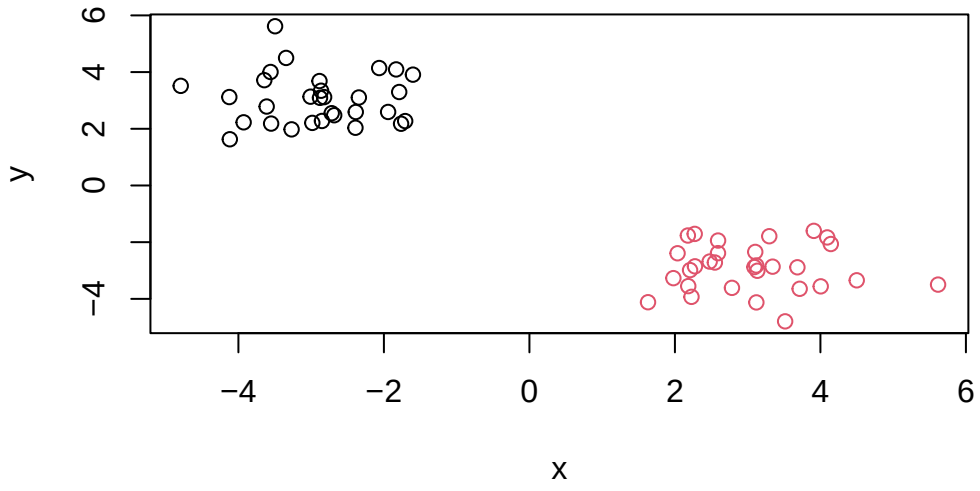
The print out above is not very useful (unlike with `kmeans()`) but there is a useful `plot()` method.

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



To get my main result (my cluster membership vector) I need to "cut" my tree using the function `cutree()`.

```r
grps <- cutree(hc, h=10)
plot(data, col=grps)
```



Principal Component Analysis

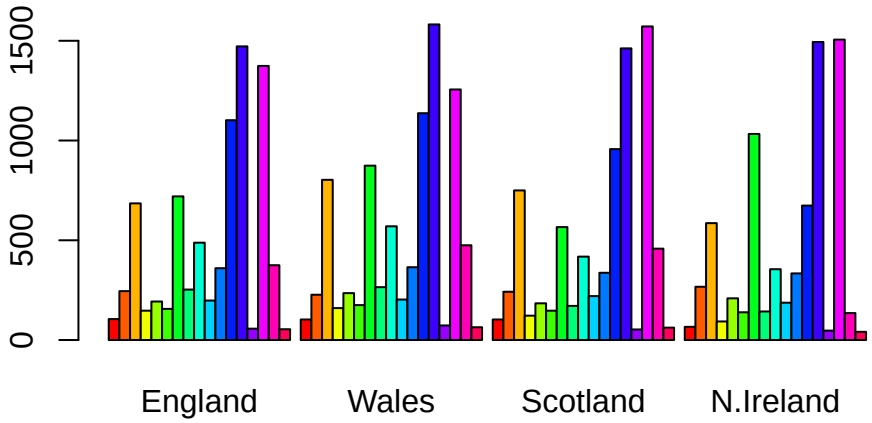
Importing and inspecting data:

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

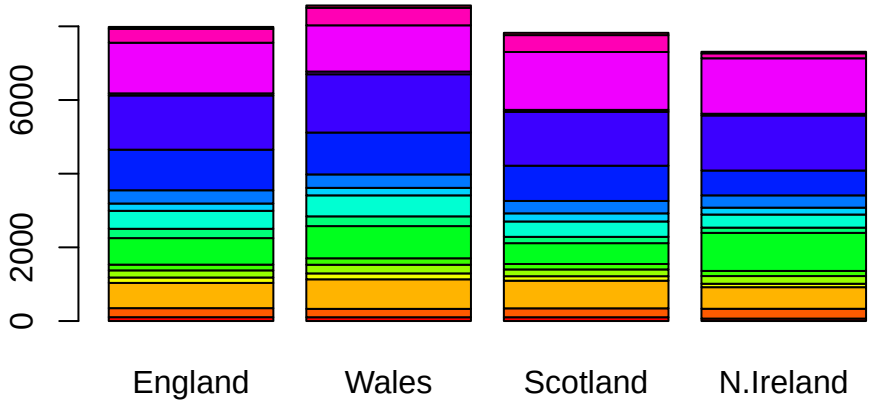
```
               England Wales Scotland N.Ireland
Cheese             105   103      103        66
Carcass_meat       245   227      242       267
Other_meat         685   803      750       586
Fish               147   160      122        93
Fats_and_oils      193   235      184       209
Sugars             156   175      147       139
```

Initial plots, spotting any differences:

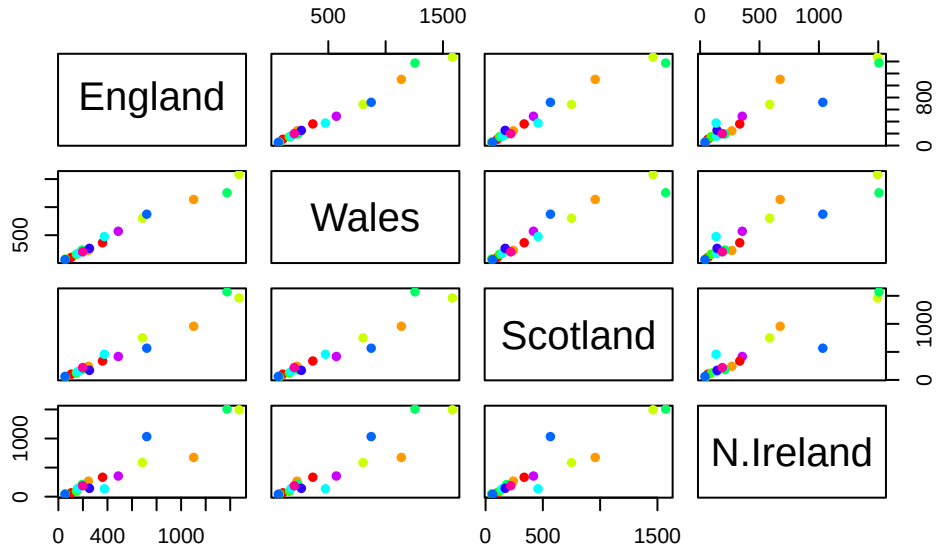
```
barplot(as.matrix(ukFoods_df), beside=T, col=rainbow(nrow(ukFoods_df)))
```




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



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



In general, these plots are unhelpful for analyzing datasets with multiple dimensions. PCA is a better way of finding these differences and trends among data points.

Use `prcomp()` to perform PCA.

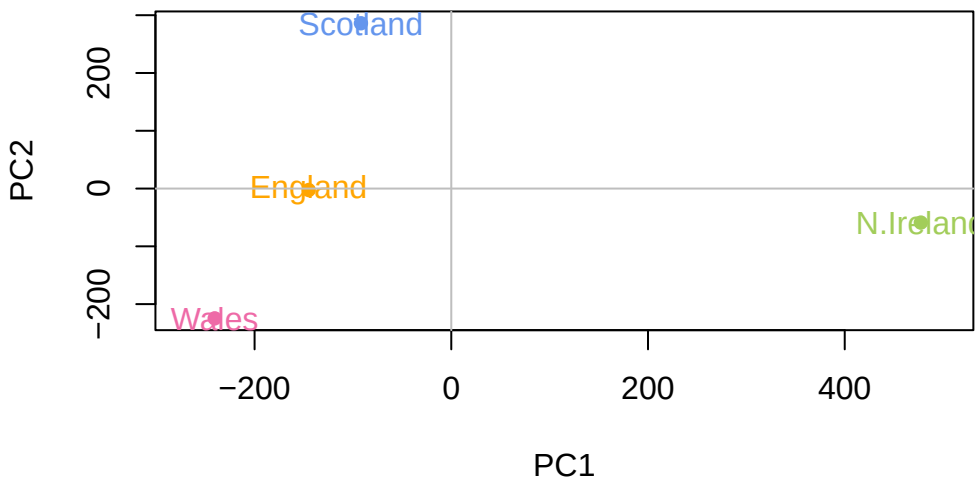
```
pca <- prcomp(t(ukFoods_df))
summary(pca)
```

```
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
```

PC1 and PC2 account for ~96.5% of the variance in the data, useful to plot these two against each other to see differences in data. This is called an ordination plot.

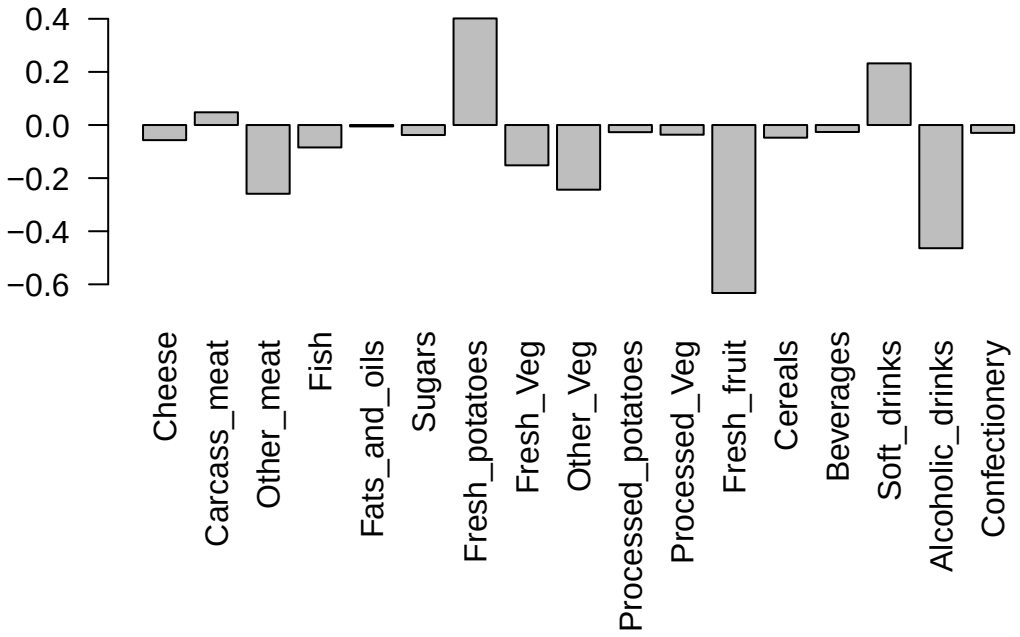
```
# Plot PC1 vs PC2
color=c("orange", "hotpink2", "cornflowerblue", "darkolivegreen3")
```

```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500), pch=16, col=color)
text(pca$x[,1], pca$x[,2], colnames(ukFoods_df), col=color)
abline(v=0, h=0, col="gray")
```



Another inportant output from pCA is called the "loadings" vector or the "rotation" component - this tells us how much the original variables (the foods in this case) contribute to the new PCs.

```
## Lets focus on PC1 as it accounts for > 67% of variance
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



PCA looks to be a super useful method for gaining some insight into high dimensional data that is difficult to examine in other ways.