浙江大学爱丁堡大学联合学院

ZJU-UoE Institute

Unsupervised learning methods

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Learning objectives

At the end of this lecture you should be able to:

- Explain the difference between supervised and unsupervised learning
- Give examples of when these methods can be used
- Explain the k-means and hierarchical clustering methods and discuss their advantages and disadvantages

Machine learning in biology

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How do we solve these problems?

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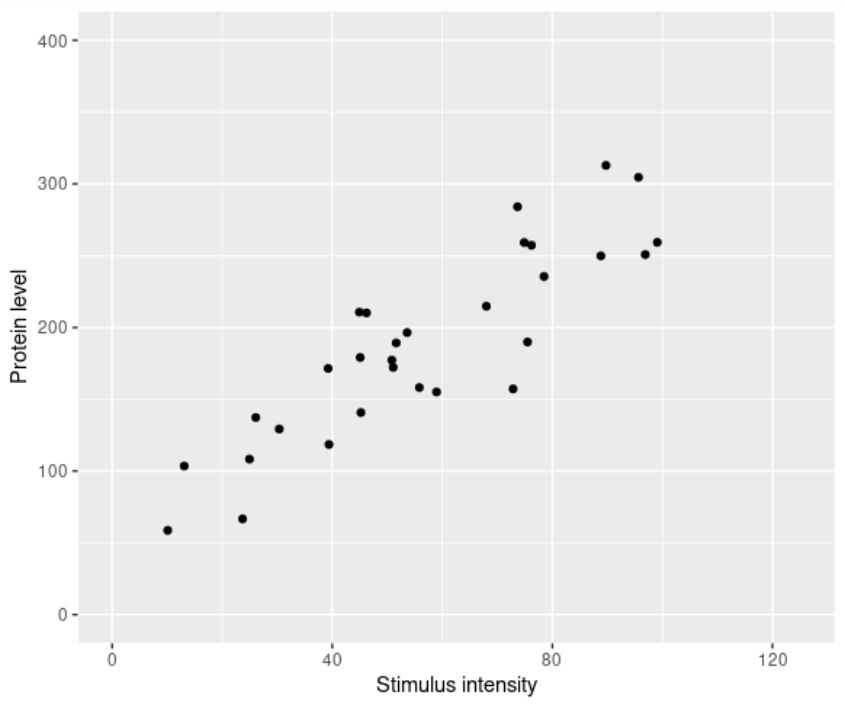

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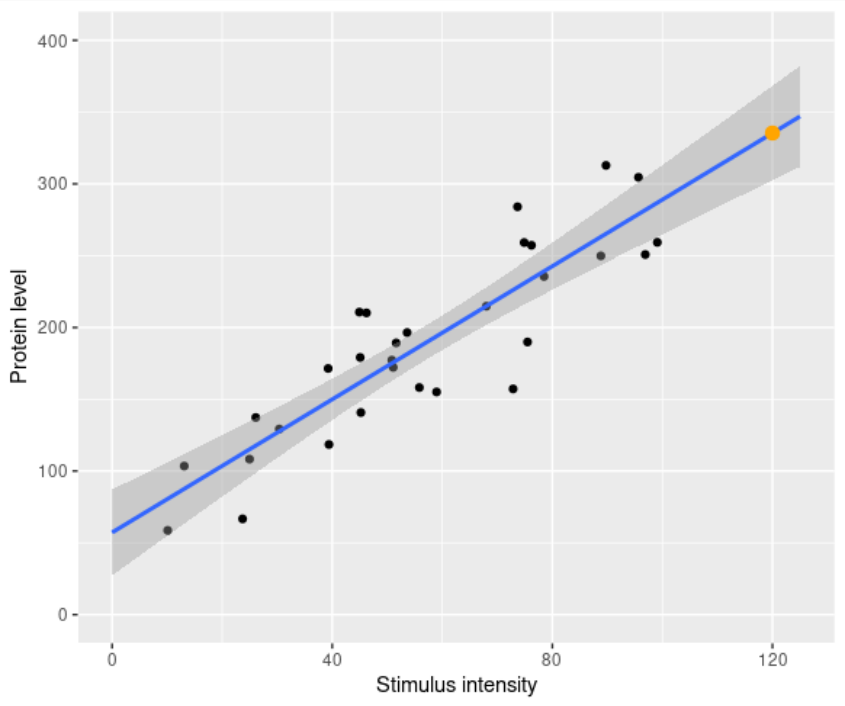
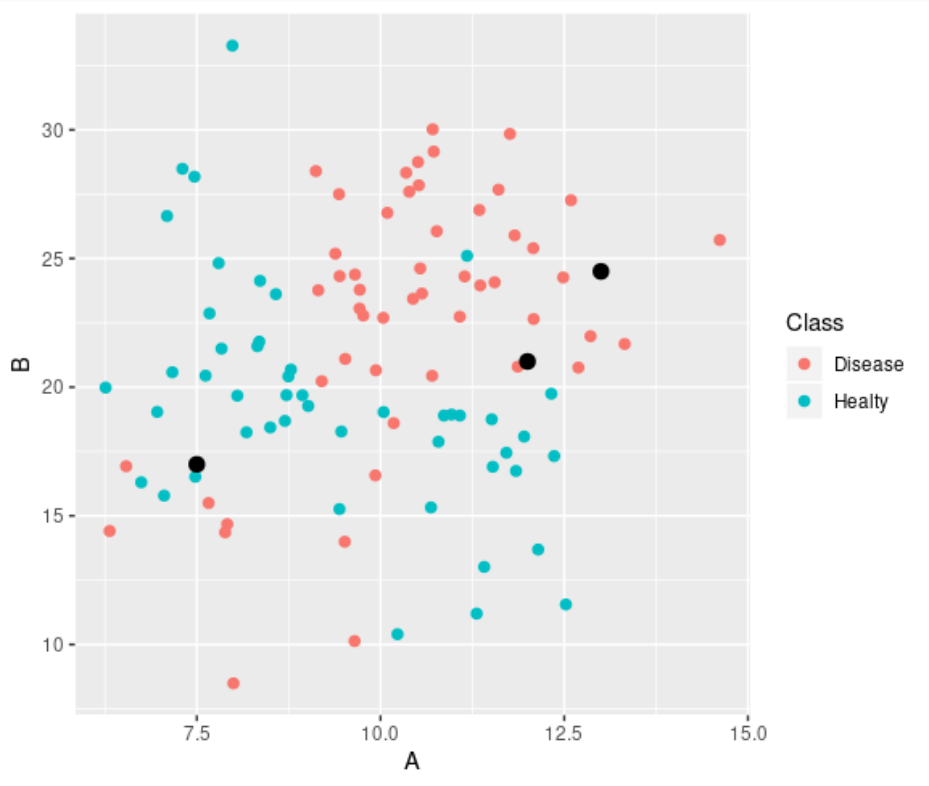


Regression

```
lm(protein ~ stimulus)
```

Problem 2

We measure hormonal levels in healthy controls or patients with an illness. Given measures from a new individual, can we predict whether they are healthy or ill?



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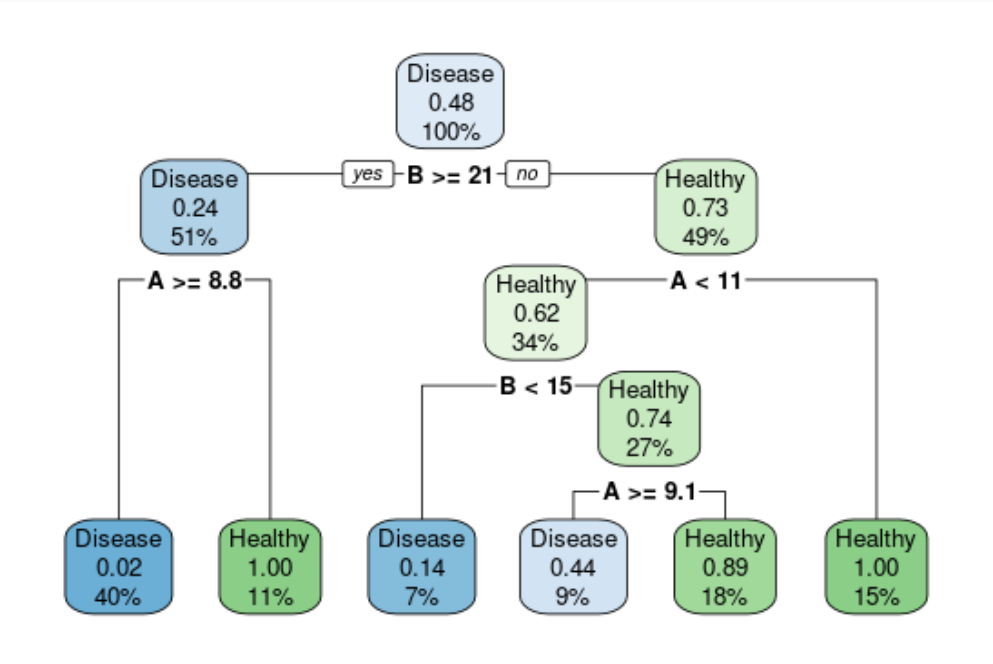
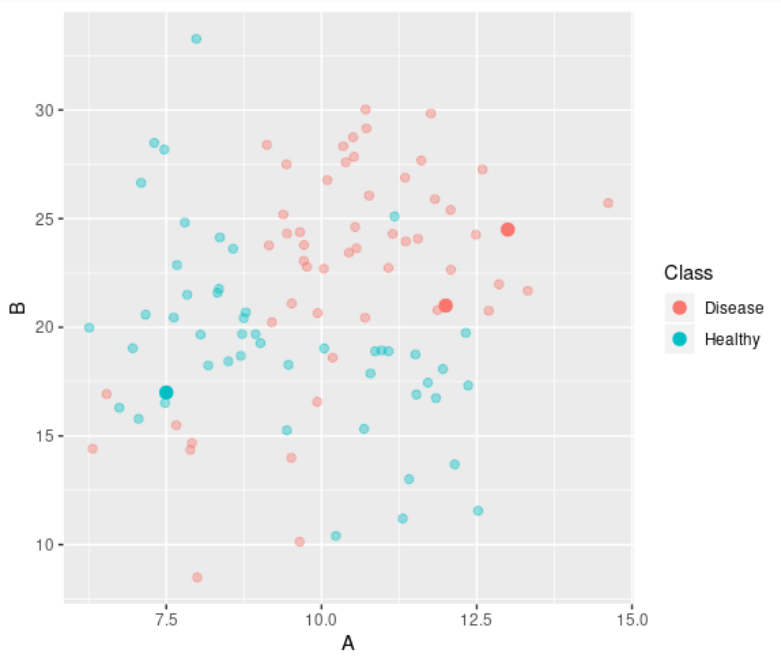


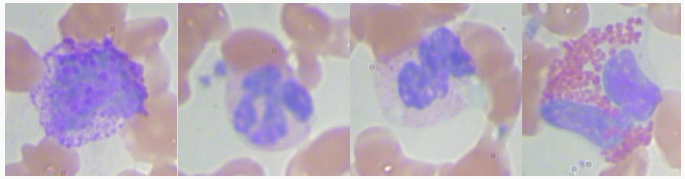


Classification

```
rpart(Class ~ A + B)
```

Problem 3 and 4

- Given a set of photos of cells we want to divide depending on their shape.



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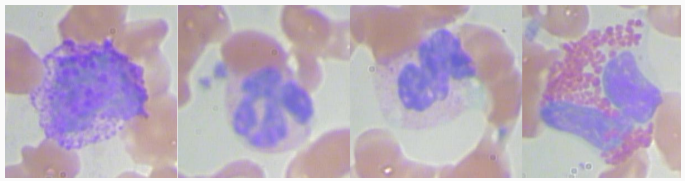

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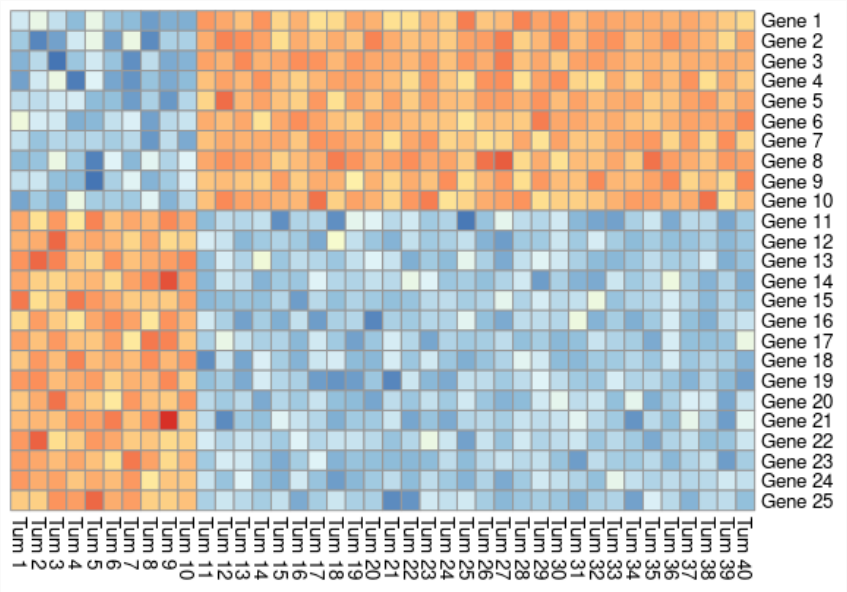

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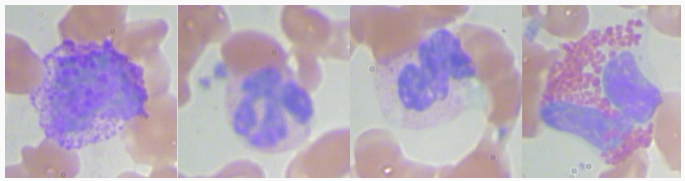

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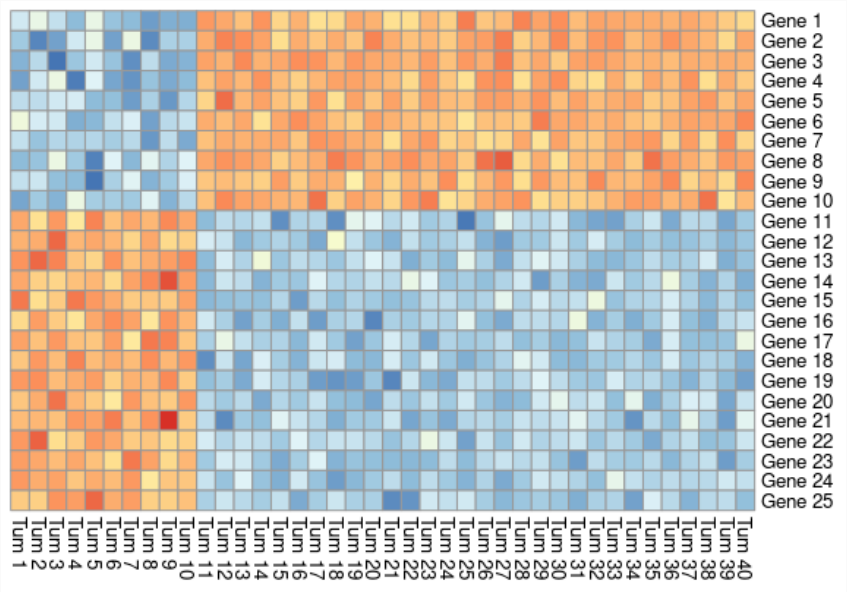

How to do this? We don't have information to train a model.

Supervised vs unsupervised learning

Machine learning methods can be broadly divided into supervised and unsupervised.

Supervised methods

- We train a model using a training set with known labels
- We test the accuracy of the model on a test set with known labels, but that we did not use for training.
- We can use the model for prediction/classification.
- Examples: binary trees, RandomForest, SVM, Neural Networks, ...

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Unsupervised methods

- We have an unlabelled dataset.
- We use a model to find data patterns/groupings (**clustering**).
- Examples: k-means, hierarchical clustering (this lecture), dimensionality reduction (next lecture)...

Clustering

Cluster analysis or **clustering** is the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar (in some sense) to each other than to those in other groups (clusters). (*Wikipedia*)

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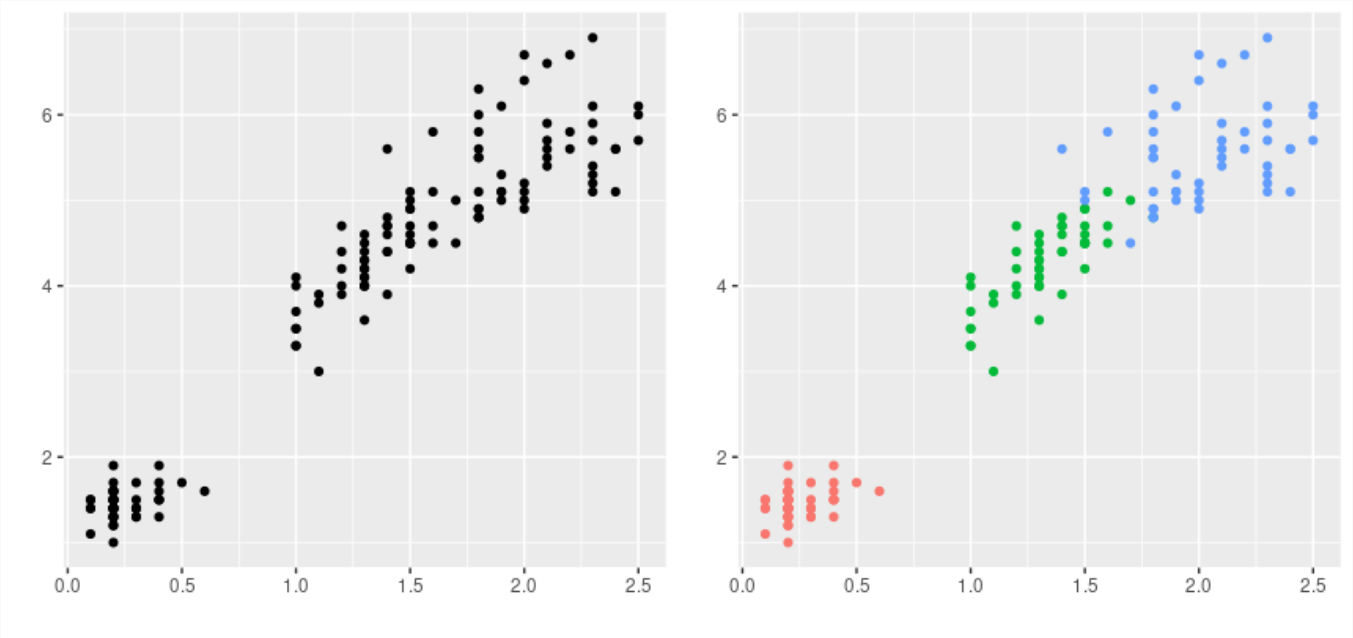

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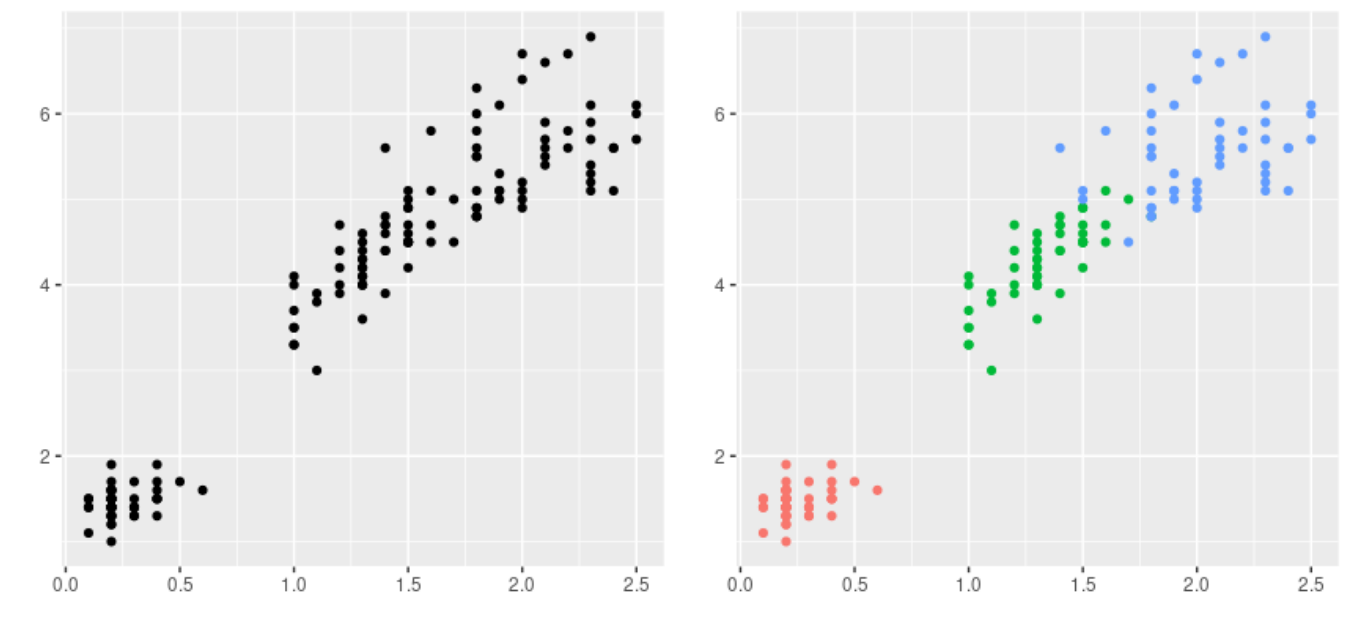


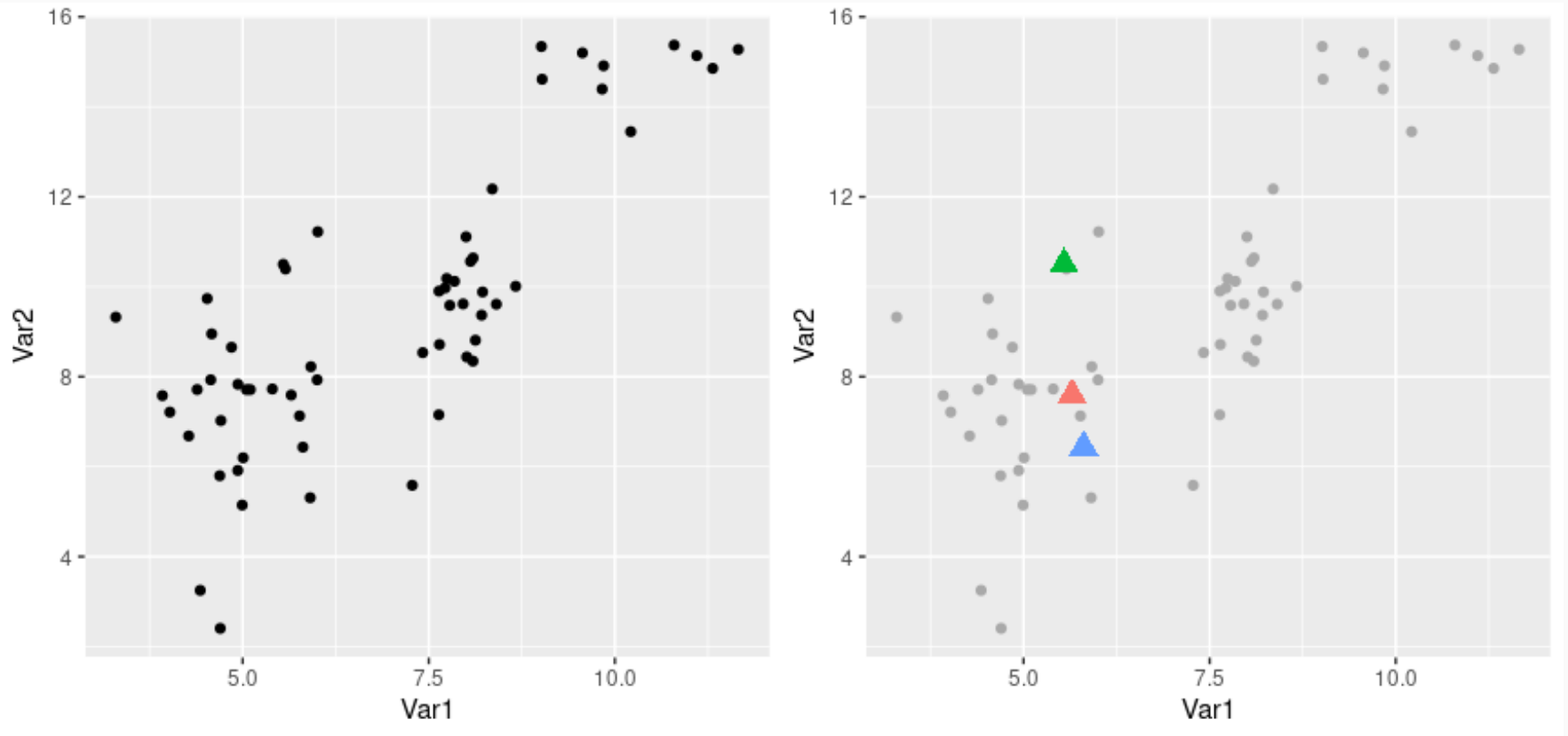
The number of clusters in an unknown data set is not trivial to determine.

The k-means algorithm

- One of the simplest approaches to clustering
- It's an iterative algorithm that divides the dataset in k clusters

k-means - Step 1

- We select k random points as starting centers (called *centroids*)
- We assign each point in the dataset to the closest centroid, thus defining k clusters



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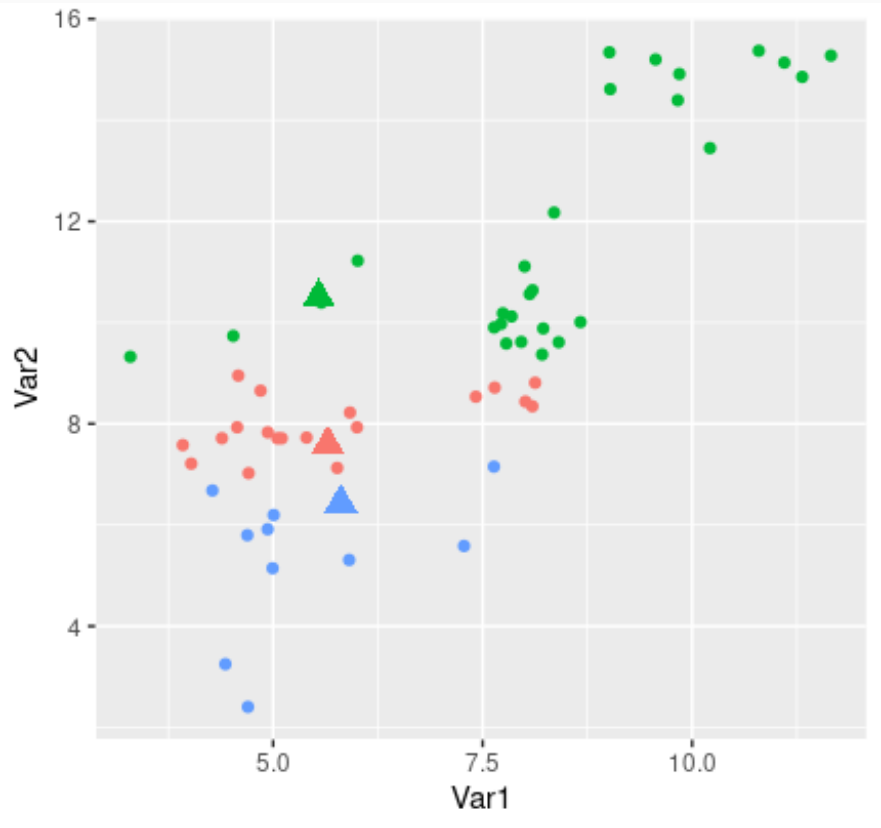
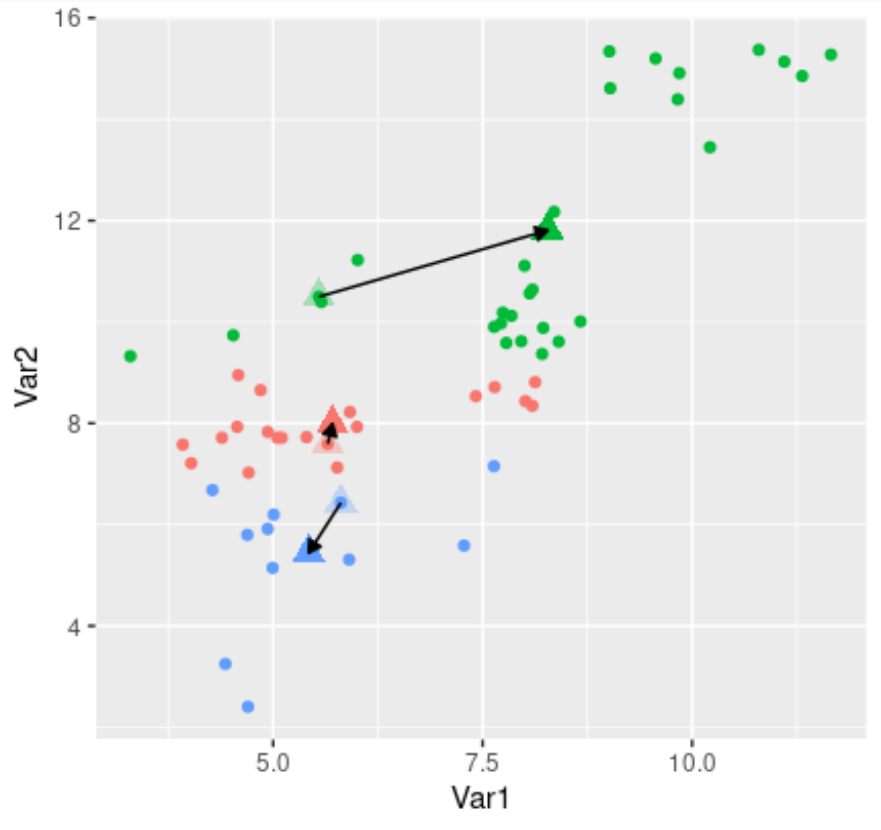


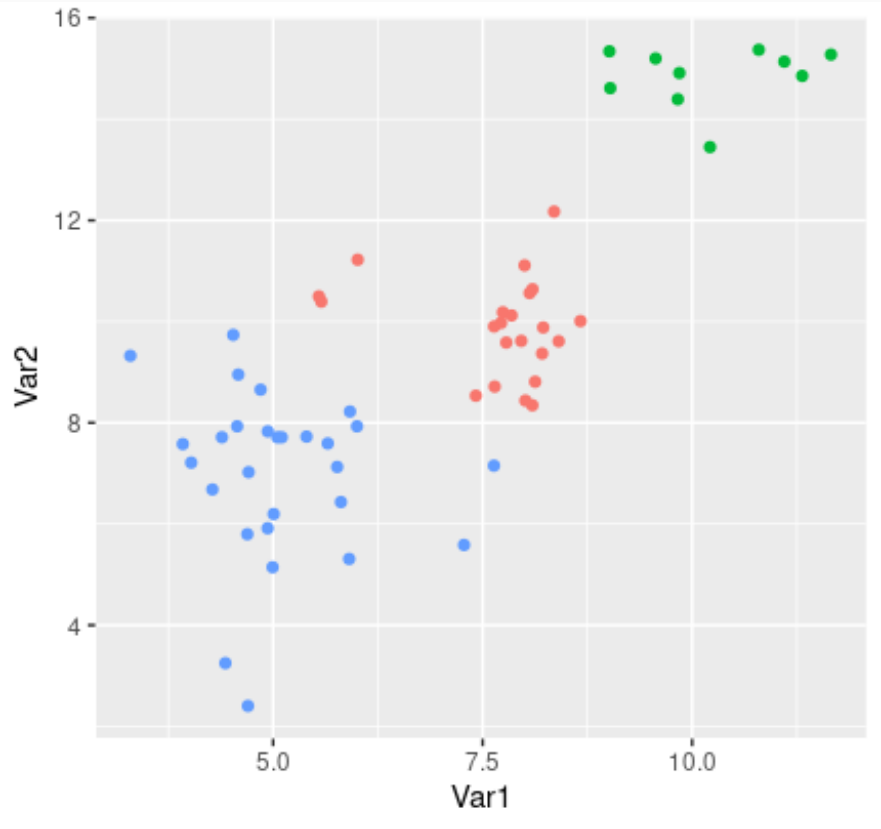
k-means - Step 2

- We move the centroids to the center of each cluster
- We reassign cluster memberships and continue repeating until clusters don't change anymore or until we reach a certain number of iterations
- Most often k-means converges after 10-20 iterations



k-means final clustering

Our final result



How to do k-means in R?

It's really simple!

```
km <- kmeans(mydata, centers=3)
# We can choose multiple sets of starting centroids
km <- kmeans(mydata, centers=3, nstart=50)
# Clusters can be found in km$cluster
```

We will see some use of this in Workshop 7!

k-means pros and cons

Advantages

- Generally fast
- Computationally easy to implement

Disadvantages

- Results are heavily dependent on the random choice of centroids at the start
- Need to specify the number of clusters in advance
- Works better with equally sized clusters
- Sensible to outliers

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- Determining the number of clusters is difficult.
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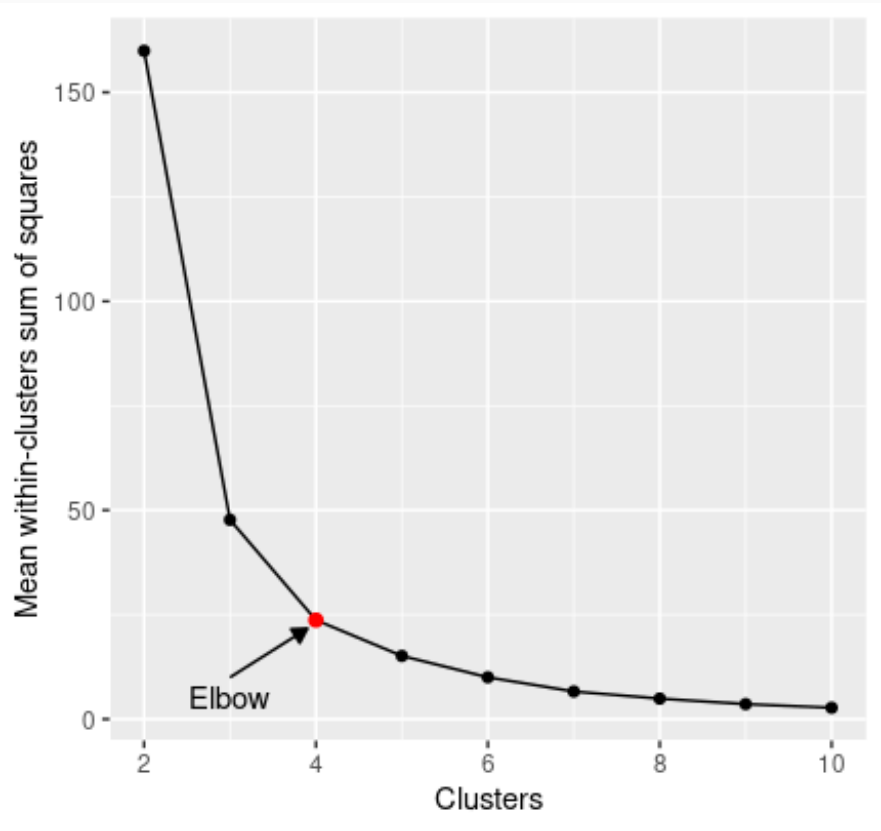
- Empirical method - **elbow plot**

```
km$tot.withinss / n.cluster
```



Alternative strategy - hierarchical clustering

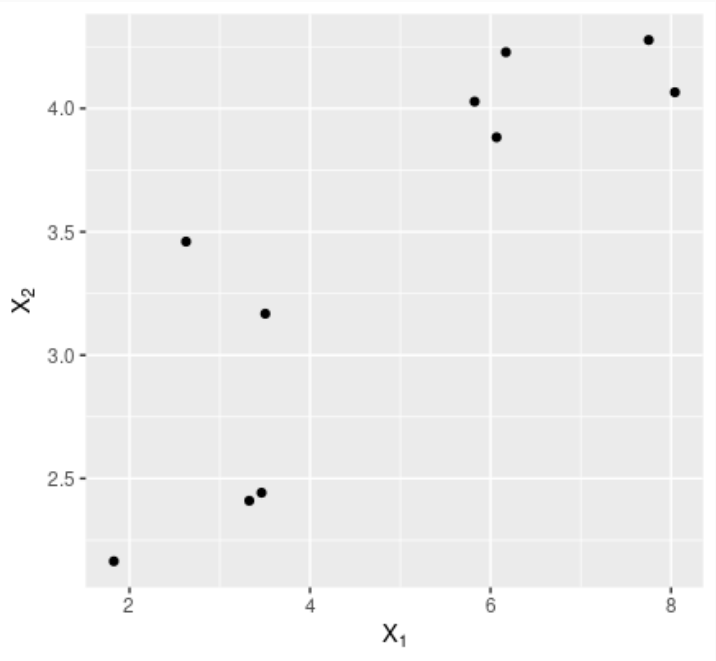
Hierarchical clustering is a method of cluster analysis which seeks to build a hierarchy of clusters. (*Wikipedia*)

Two main strategies:

- Agglomerative or "bottom-up" hierarchical clustering initially creates one cluster per observation and then merge them depending on their similarity
- Divisive or "top-down" hierarchical clustering puts all observations in one cluster then recursively splits the cluster.
- Generates a *dendrogram* (tree like plot)

Agglomerative hierarchical clustering

- We start from n data points, each in a clusters
- We define some distance metrics (see later)
- We find the pair of points with the smaller distance
- We start building our dendrogram



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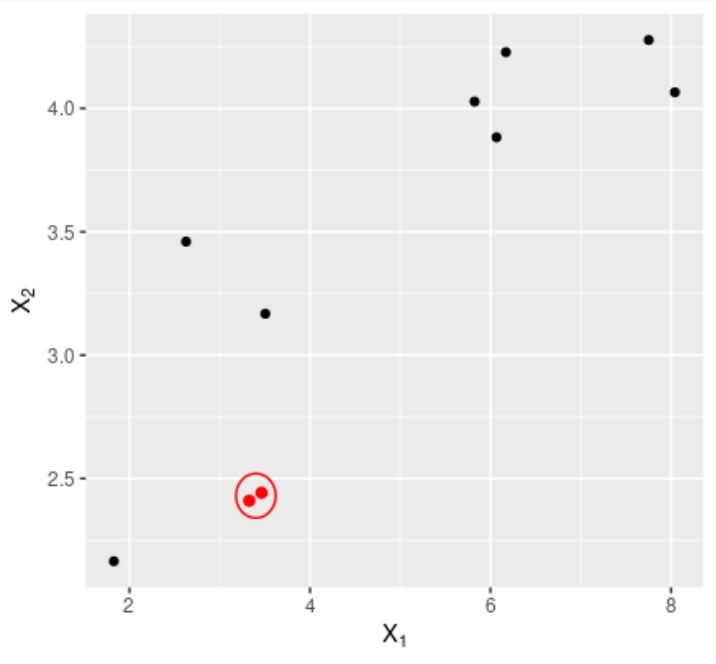

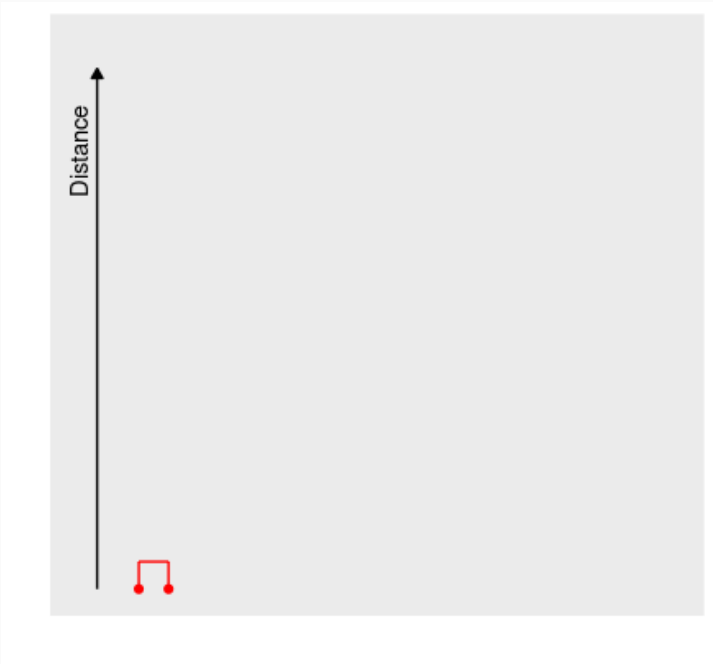

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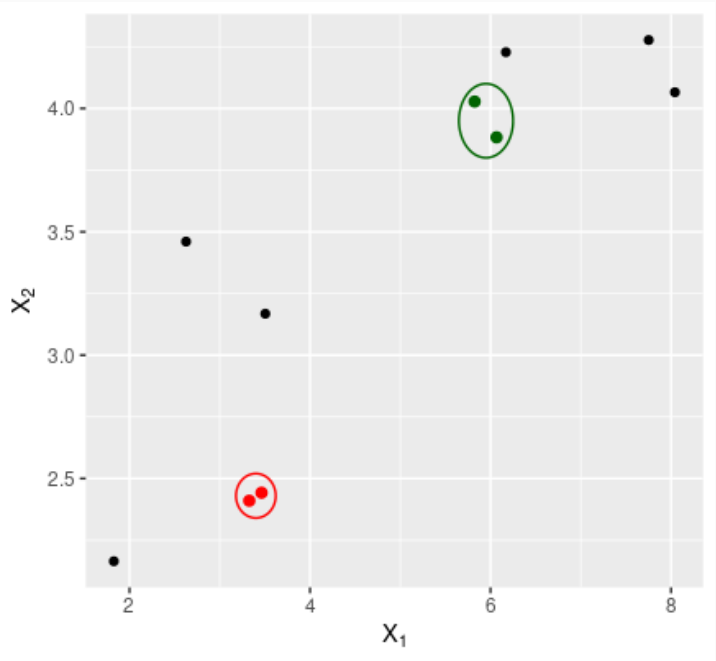

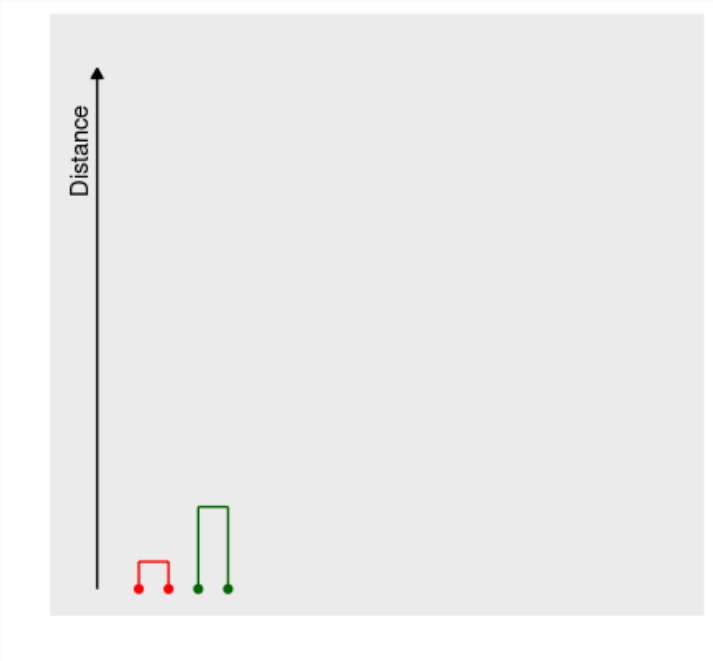

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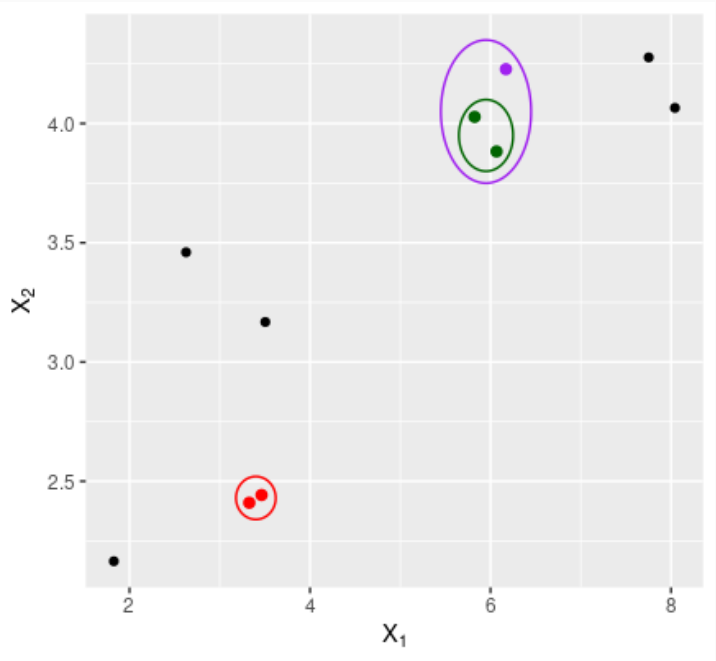
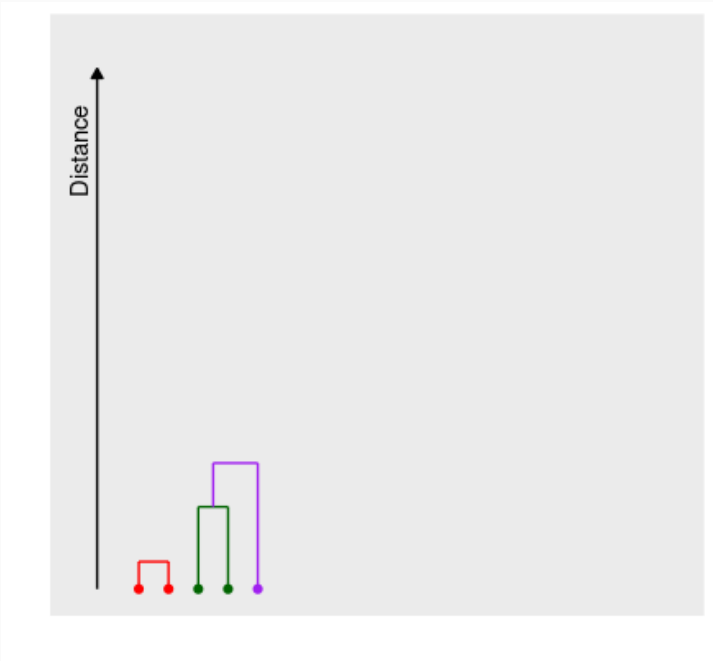
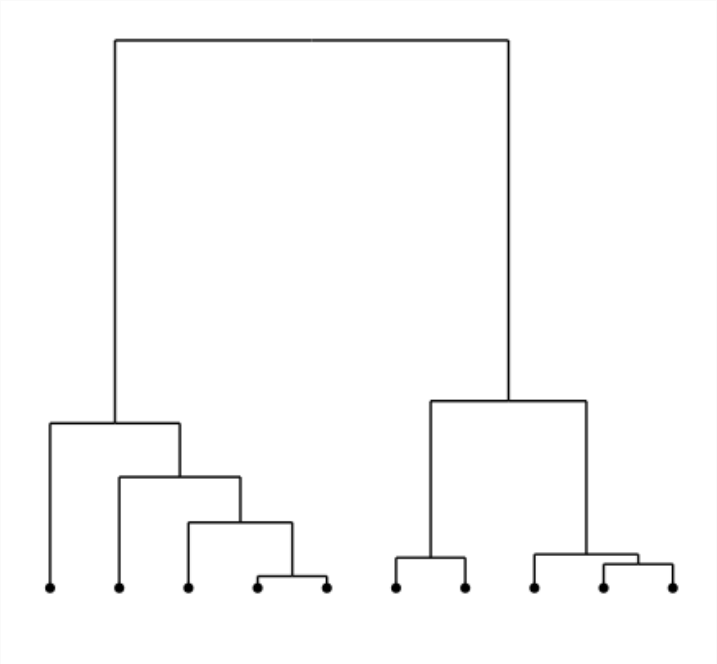




Agglomerative hierarchical clustering

... and so on until every point has been clustered!



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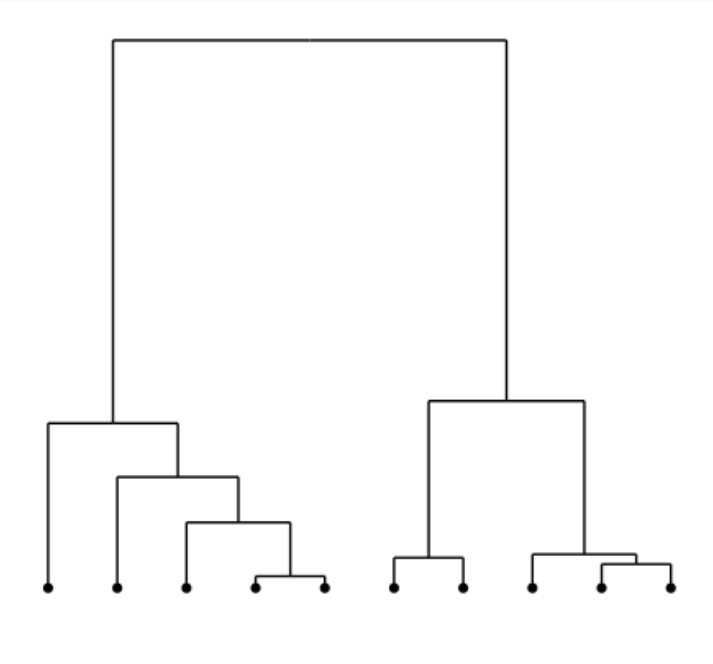
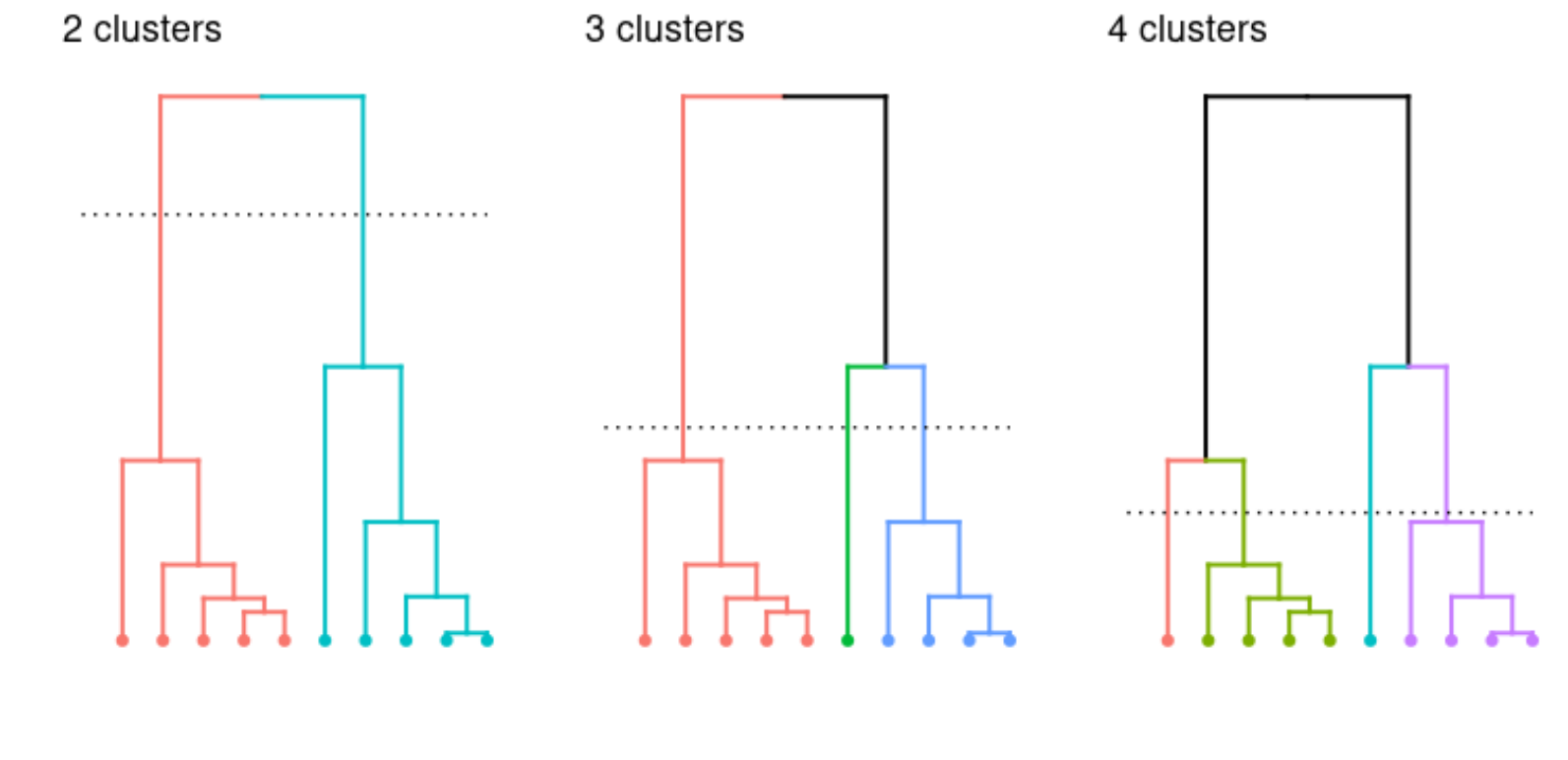


```
pt.dist <- dist(hc, method = "euclidean")
hc <- hclust(pt.dist, method = "complete")
```

How many clusters do we have?



Distance methods

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  $d = \sqrt{(X1_A - X1_B)^2 + (X2_A - X2_B)^2 + ... + (Xn_A - Xn_B)^2}$

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- Maximum distance $d = max\{|X1_A - X1_B|, |X2_A - X2_B|, ..., |Xn_A - Xn_B|\}$
- See `?dist` for full list and details

Linkages

```
hc <- hclust(pt.dist, method = "complete")
```

- Similarly, the `method` parameter defines how the dendrogram is built
- Common values are: `complete`, `average`, `ward.D2`
- See `?hclust` for details

Summary

- Statistical models and machine learning algorithms allow us to answer many biological questions
- Choosing the right method to answer the right question is not easy
- Clustering methods are becoming very important, especially when dealing with large dataset and/or data with high dimensionality (more on that in the next two data analysis lectures)
- Many other approaches apart from those we saw today!