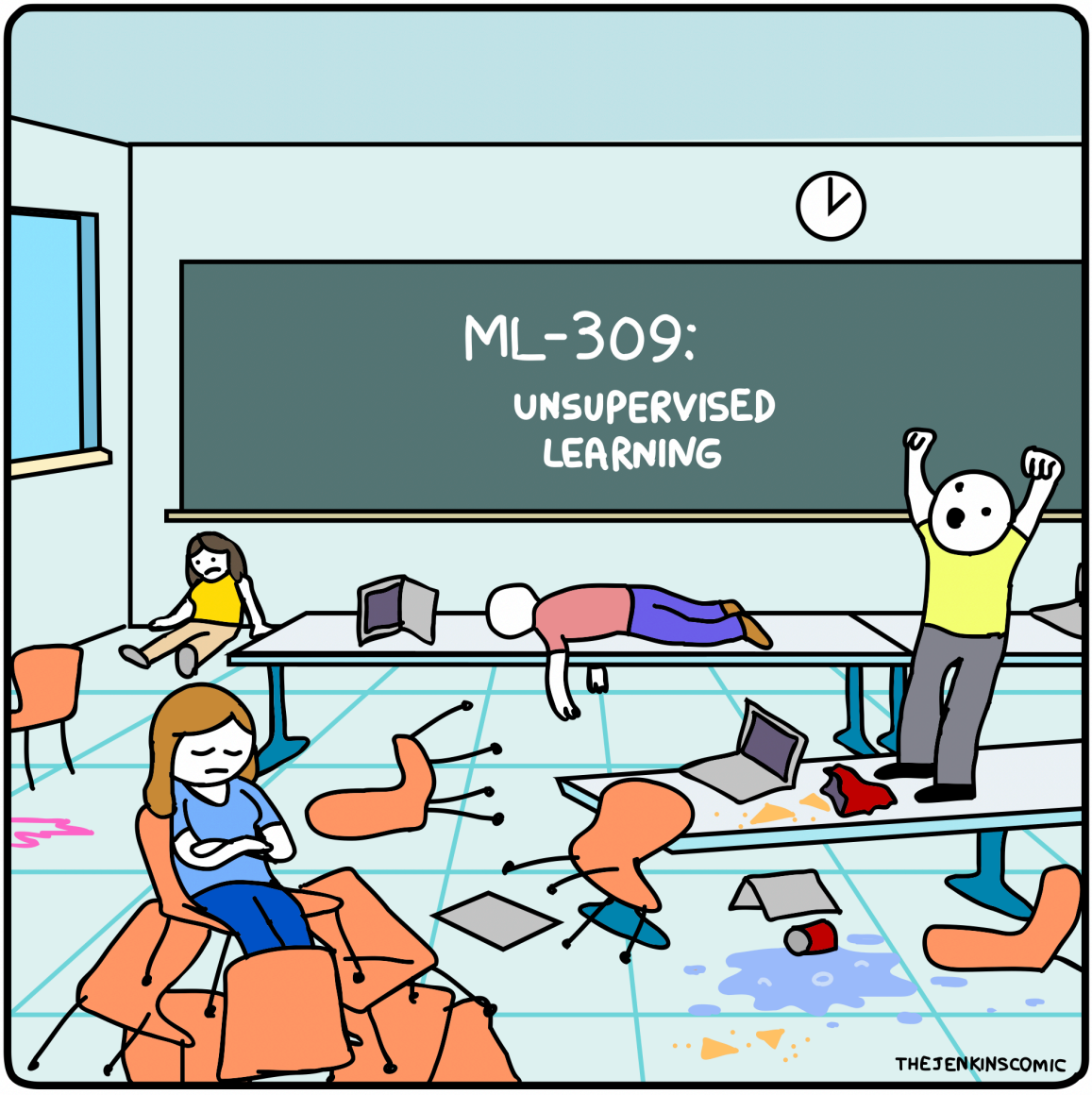
Chapter 10: Unsupervised Learning



Credit: https://thejenkinscomic.net/?id=366

This chapter will focus on methods intended for the setting in which we only have a set of features $X_1, \ldots, X_p$ measured on n observations.

We are not interested in prediction because we have no associated response Y.

Goal: discover interesting things about the measurements $X_1, \ldots, X_p$

- Is there an informative way to plot the data?
- Can we discover subgroups among the variables or the observations?

1 The Challenge of Unsupervised Learning

Supervised learning is a well-understood area.

You have a good grasp of supervised learning.

If you were given a task in which you need to predict a binary response you could use:

logistic regression, LDA, QDA, classification trees, RF, boosting, SVM, etc.

and a clear understanding of how to assess the quality of your results:

estimate test error using CV!

In contrast, unsupervised learning is often much more challenging.

more subjective, no simple goal for the analysis, e.g. prediction.

Unsupervised learning is often performed as part of an *exploratory data analysis*.

1st part of analysis, before fitting any models

It can be hard to assess the results obtained from unsupervised learning methods.

No universally accepted way to assess approach → no validation or CV

Because there is no way to "check our work" w/ response

↳ we don't know the true answers.

Techniques for unsupervised learning are of growing importance in a number of fields.

Cancer research: assay gene expression levels in 100 patients and look for subgroups among cancer samples to better understand the disease.

online shopping: identify similar groups of shoppers and show prefer. ed items.

(my research) Entity resolution: many noisy databases without unique identifying information → can we find duplicates?

2 Principal Components Analysis

We have already seen principal components as a method for dimension reduction.

Principal Components Analysis (PCA) refers to the process by which principal components are computed and the subsequent use of these components to understand the data.

Apart from producing derived variables forr use in supervised learning, PCA also serves as a tool for data visualization.

2.1 What are Principal Components?

Suppose we wish to visualize n observations with measurements on a set of p features as part of an exploratory data analysis.

Goal: We would like to find a low-dimensional representation of the data that captures as much of the information as possible.

PCA provides us a tool to do just this.

Idea: Each of the n observations lives in p dimensional space, but not all of these dimensions are equally interesting.

The *first principal component* of a set of features $X_1, \ldots, X_p$ is the normalized linear combination of the features

that has the largest variance.

Given a $n \times p$ data set $\boldsymbol{X}$, how do we compute the first principal component?

There is a nice geometric interpretation for the first principal component.

After the first principal component Z_1 of the features has been determined, we can find the second principal component, Z_2. The second principal component is the linear combination of $X_1, \ldots, X_p$ that has maximal variance out of all linear combinations that are uncorrelated with Z_1.

Once we have computed the principal components, we can plot them against each other to produce low-dimensional views of the data.

```
str(USArrests)
```

```
## 'data.frame':    50 obs. of  4 variables:
##  $ Murder  : num  13.2 10 8.1 8.8 9 7.9 3.3 5.9 15.4 17.4 ...
##  $ Assault : int  236 263 294 190 276 204 110 238 335 211 ...
##  $ UrbanPop: int  58 48 80 50 91 78 77 72 80 60 ...
##  $ Rape    : num  21.2 44.5 31 19.5 40.6 38.7 11.1 15.8 31.9 25.8
...
```

```
USArrests_pca <- USArrests |>
  prcomp(scale = TRUE, center = TRUE)

summary(USArrests_pca) # summary
```

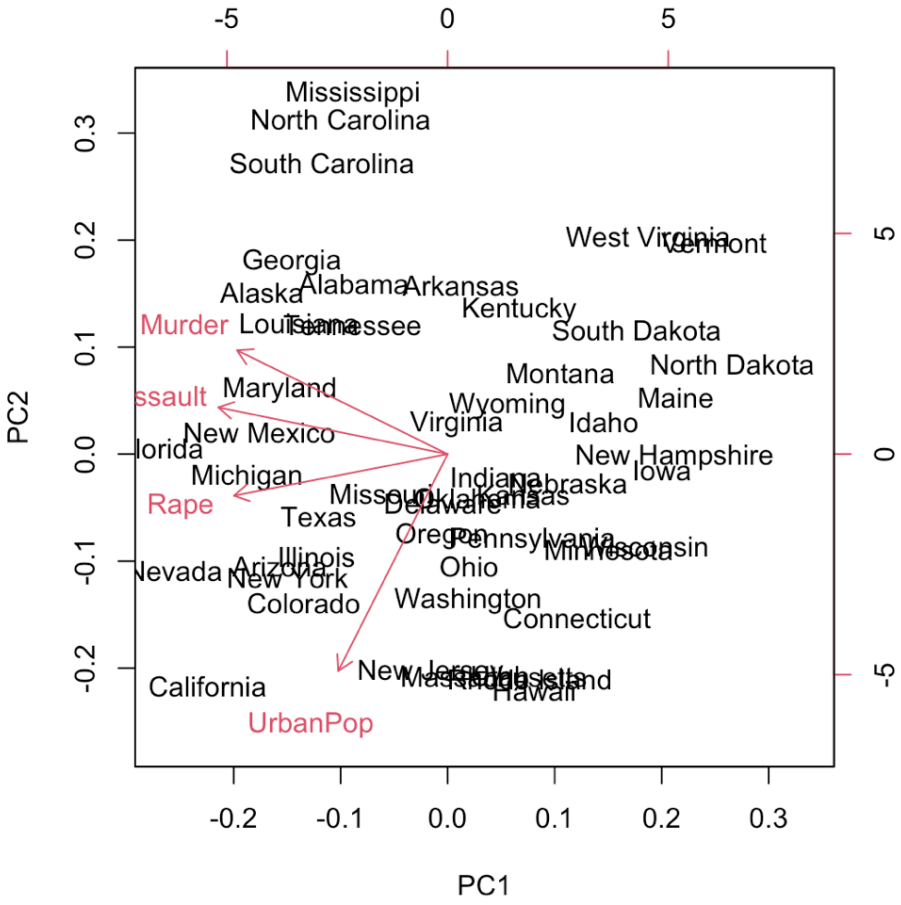
```
## Importance of components:
##                           PC1    PC2     PC3     PC4
## Standard deviation     1.5749 0.9949 0.59713 0.41645
## Proportion of Variance 0.6201 0.2474 0.08914 0.04336
## Cumulative Proportion  0.6201 0.8675 0.95664 1.00000
```

```
tidy(USArrests_pca, matrix = "loadings") |> # principal components
        loading matrix
  pivot_wider(names_from = PC, values_from = value)
```

```
## # A tibble: 4 × 5
##   column      `1`    `2`    `3`     `4`
##   <chr>     <dbl>  <dbl>  <dbl>   <dbl>
## 1 Murder   -0.536  0.418 -0.341  0.649
## 2 Assault  -0.583  0.188 -0.268 -0.743
## 3 UrbanPop -0.278 -0.873 -0.378  0.134
## 4 Rape     -0.543 -0.167  0.818  0.0890
```

```
## plot scores + directions
```

```
biplot(USArrests_pca)
```



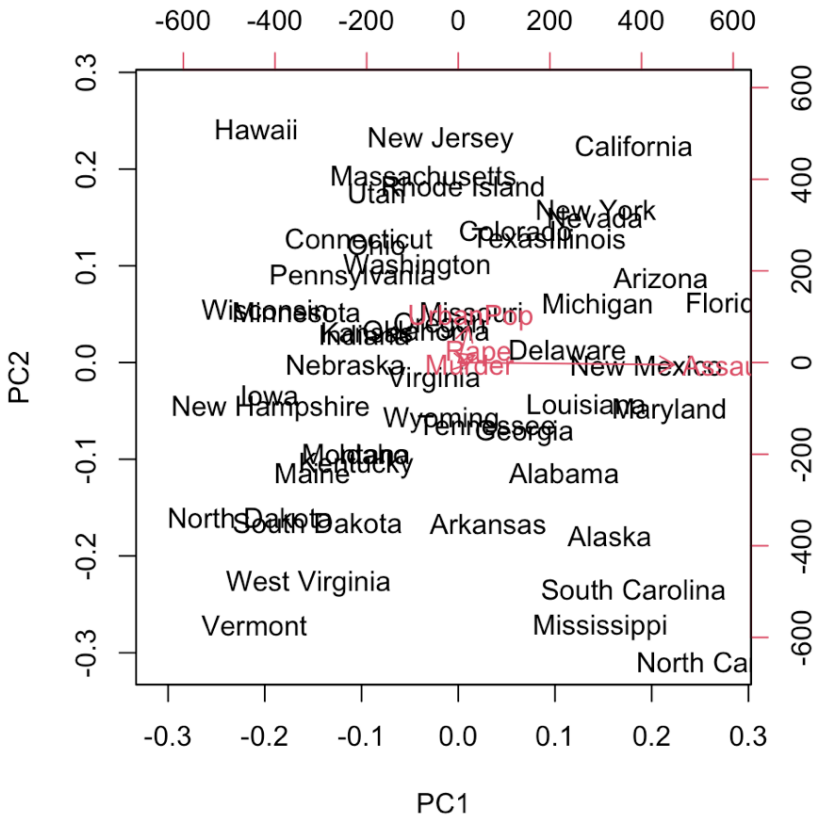
2.2 Scaling Variables

probably.

to have same variance.

We've already talked about how when PCA is performed, the varriables should be centered to have mean zero.

This is in contrast to other methods we've seen before.



2.3 Uniqueness

Each principal component loading vector is unique, up to a sign flip.

Similarly, the score vectors are unique up to a sign flip.

2.4 Proportion of Variance Explained

We have seen using the `USArrests` data that e can summarize 50 observations in 4 dimensions using just the first two principal component score vectors and the first two principal component vectors.

Question:

More generally, we are interested in knowing the *proportion of vriance explained (PVE)* by each principal component.

2.5 How Many Principal Components to Use

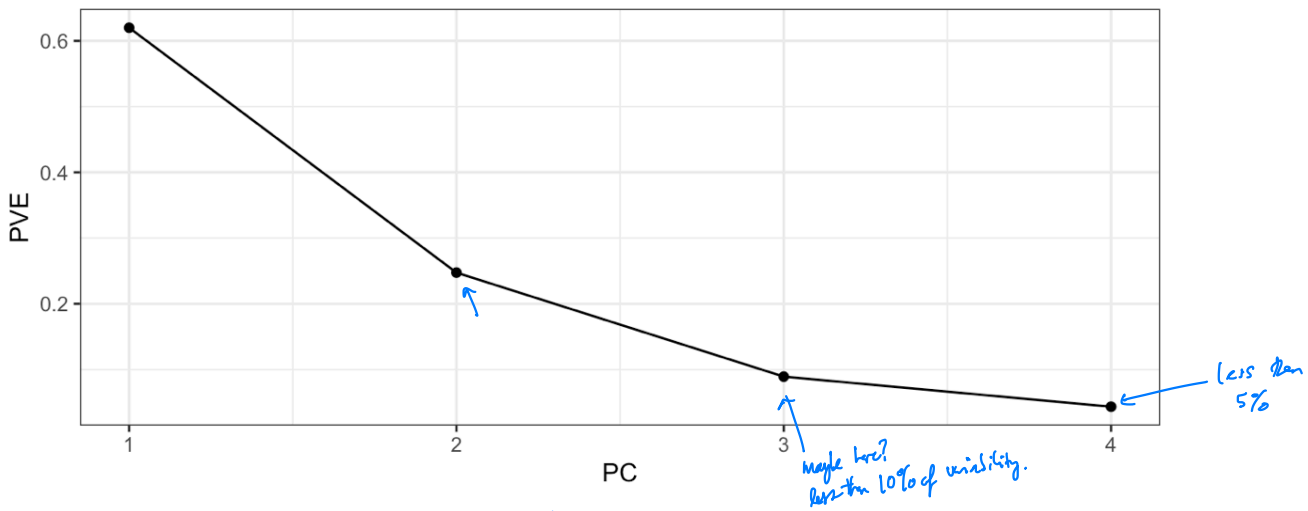
In general, a $n \times p$ matrix $\boldsymbol{X}$ has $\min(n-1, p)$ distinct principal components.

Rather, we would like to just use the first few principal components in order to visualize or interpret the data.

Want to use the smallest # to get a good understanding of the data.

We typically decide on the number of principal components required by examining a *scree plot*.

Scree plot.



look for a point that has an "elbow", where plot stops dropping sharply.

2.6 Other Uses for Principal Components

We've seen previously that we can perform regression using the principal component score vectors as features for dimension reduction.

Many statistical techniques can be easily adapted to use the $n \times M$ matrix whose columns are the first $M << p$ principal components.

e.g. regression, classification, clustering.

This can lead to *less noisy* results.

3 Clustering

Clustering refers to a broad set of techniques for finding *subgroups* in a data set.

We seek to partition observations into distinct groups so that
- observations within a group are similar
- observations in different groups are dissimilar

need to define, can depend on domain.

For instance, suppose we have a set of n observations, each with p features. The n observations could correspond to tissue samples for patients with breast cancer and the p features could correspond to measurements collected for each tissue sample

- clinical measurements, e.g. tumor stage or grade.
- gene expression measurements.

diversity in character

We may have reason to believe there is heterogeneity among the n observations.

e.g. unknown subtype of cancer.

This is *unsupervised* because

We are trying to discover structure (distinct clusters)
This is different from supervised problems because we are not "predicting"

Both clustering and PCA seek to simplify the data via a small number of summaries.

- PCA – find a low-dimensional representation of observations that explain most of the variability.

- Clustering – find homogeneous subgroups among observations.

Since clustering is popular in many fields, there are many ways to cluster.

2 best known:

- K-means clustering

  partition the observations into a pre-specified # of clusters

- Hierarchical clustering

  we don't know how many clusters we want.
  we obtain clusterings for $1, \ldots, n$ clusters and plot as a dendrogram.

In general, we can cluster observations on the basis of features (1) or we can cluster features on the basis of observations (2).

(1) identify subgroups among observations
(2) identify subgroups among features.

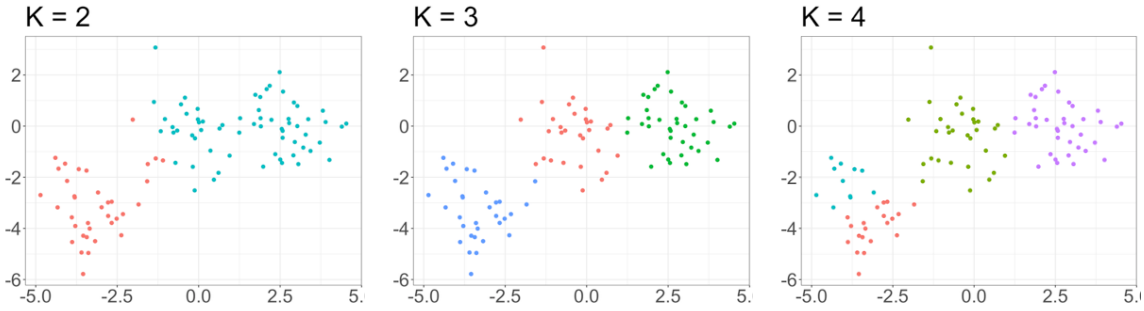
We will focus on (1), but can perform (2) by just transposing data matrix X.

3.1 K-Means Clustering

Simple and elegant approach to parition a data set into K distinct, non-overlapping clusters.

First specify how many clusters K,
K-means assigns each observation to one of the clusters.

eg. clustering n=100 observations into K clusters using p=2 features.



The K-means clustering procedure results from a simple and intuitive mathematical problem. Let $C_1, \ldots, C_K$ denote sets containing the indices of observations in each cluster. These satisfy two properties:

e.g. if obs i is in cluster k, $i \in C_k$

1. $C_1 \cup C_2 \cup \cdots \cup C_K = \{1, \ldots, n\}$
   each obs. belongs to a cluster

2. $C_k \cap C_{k'} = \emptyset \quad \forall\, k \neq k'$
   the clusters are non overlapping.

Idea: good clustering is one for which the within-cluster variation is small.

The *within-cluster variation* for cluster C_k is a measure of the amount by which the observations within a cluster differ from each other.

Call this $W(C_k)$.

We want to

$$\underset{C_1,\dots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} W(C_k) \right\}$$

To solve this, we need to define within-cluster variation.

Many ways to do this.

Most common way: squared euclidean distance

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

This results in the following optimization problem that defines K-means clustering:

"objective function"

$$\underset{C_1,\dots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

This is very difficult to solve exactly $\approx K^n$ ways to partition n obs. into K clusters.

A very simple algorithm has been shown to find a local optimum ("pretty good solution") to this problem:

1. randomly assign a number from 1 to K to each observation. initial cluster assignment.
2. Iterate until cluster assignments stop changing:
   (a) for each of the K clusters, compute the cluster centroid. vector in p dim. representing the "center" of the cluster
   ⇒ p feature means in each cluster.
   (b) assign each observation to closest cluster centroid.
   ↳ euclidean distance.

Algorithm is guaranteed to decrease value of objective function at each step.

When assignments stop changing this is a local minimum

↳ not global ⇒ clustering depends on the initialization (step 1).

⇒ run algorithm multiple times and choose clustering w/ smallest objective function.

⇒ Need to choose K! ← no 1 answer

within cluster variation to be small compared to between cluster variation.
e.g. "Dunn index"

3.2 Hierarchical Clustering

ahead of time.

One potential disadvantage of K-means clustering is that it requires us to specify the number of clusters K. *Hierarchical clustering* is an alternative that does not require we commit to a particular K.

also get tree representation.

clusters getting larger.

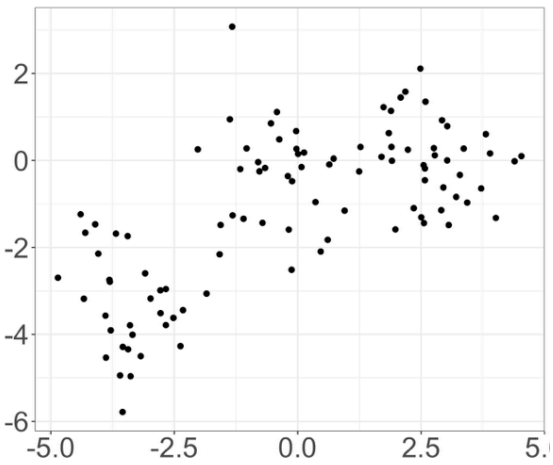
We will discuss *bottom-up* or "*agglomerative*" clustering.

start w/ every obs in its own cluster and merge clusters until all observations are in a single cluster.

n clusters → 1 cluster

3.2.1 Dendrograms

same simulated data w/ n=100, p=2.

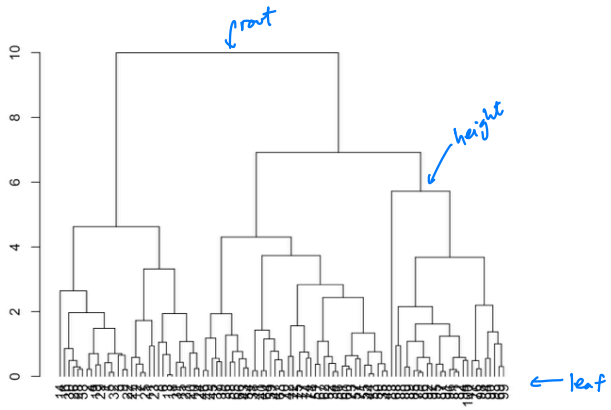


dendrogram

root

height

leaf

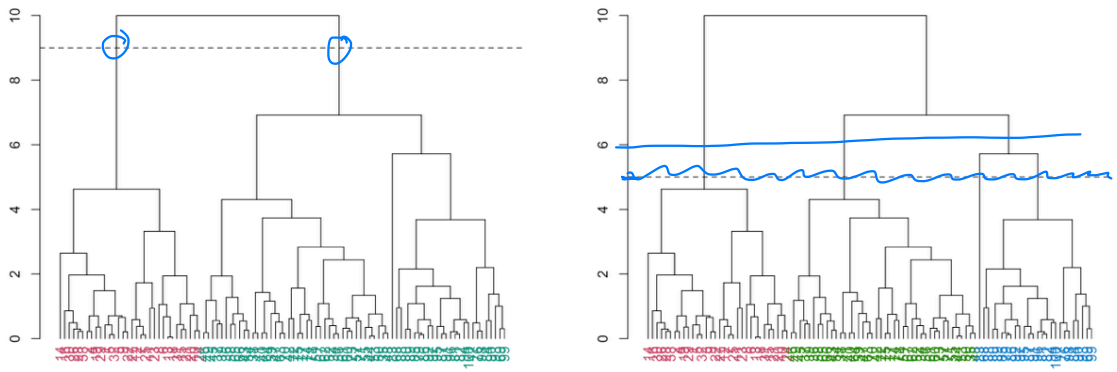


Each *leaf* of the dendrogram represents one of the 100 simulated data points.

As we move up the tree, leaves begin to fuse into branches, which correspond to observations that are similar to each other.

For any two observations, we can look for the point in the tree where branches containing those two observations are first fused.

How do we get clusters from the dendrogram?

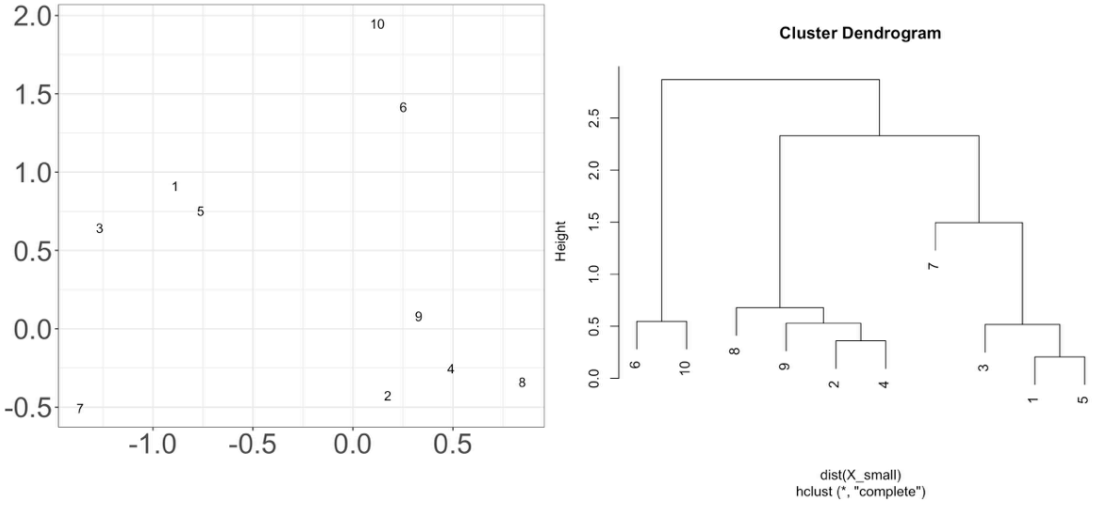


The term *hierarchical* refers to the fact that clusters obtained by cutting the dendrogram at a given height are necessarily nested within the clusters obtained by cutting the dendrogram at a greater height.

3.2.2 Algorithm

First, we need to define some sort of *dissimilarity* metric between pairs of observations.

Then the algorithm proceeds iteratively.



More formally,

One issue has not yet been addressed.

How do we determine the dissimilarity between two clusters if one or both of them contains multiple observations?

1.

2.

3.

4.

3.2.3 Choice of Dissimilarity Metric

3.3 Practical Considerations in Clustering

In order to perform clustering, some decisions should be made.

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-
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Each of these decisions can have a strong impact on the results obtained. What to do?