Chapter 5

Clustering

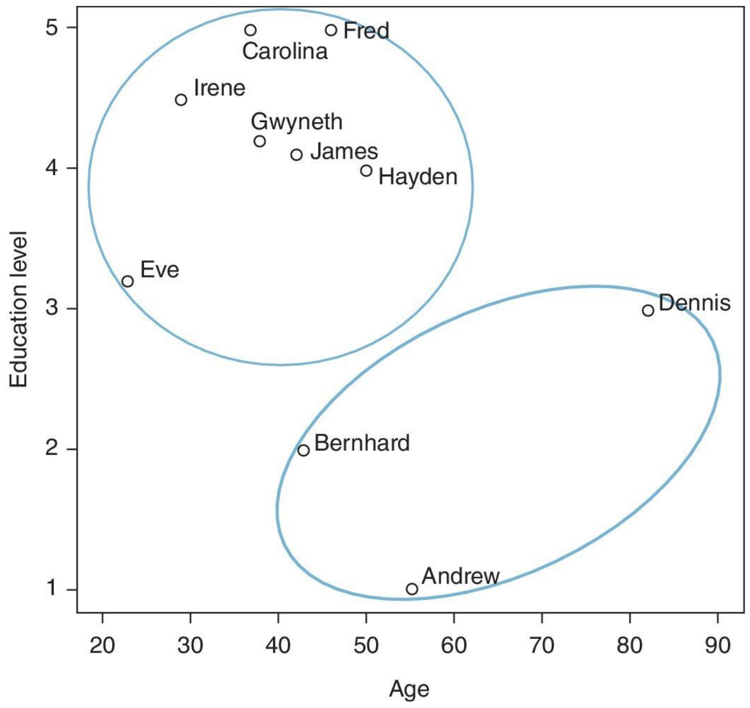
Problem definition

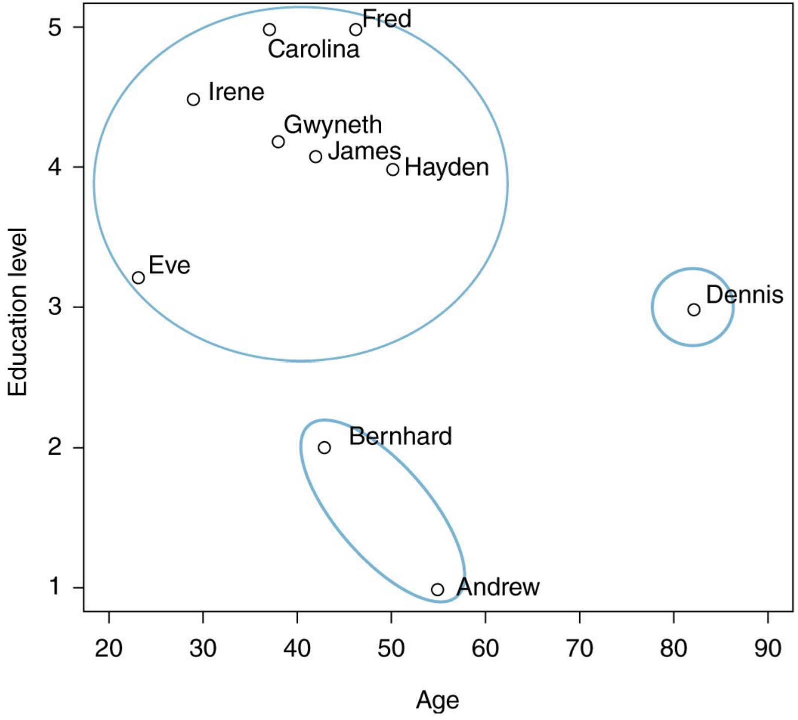
Partitioning the data

- Such that objects belonging to the same group (cluster) are more similar to each other than objects belonging to different groups
- Similarity of objects and groups is a key concept in clustering
- The number of clusters has to be set up by a human expert, in general

Name	Age	Educational level
Andrew	55	1
Bernhard	43	2
Carolina	37	5
Dennis	82	3
Eve	23	3.2
Fred	46	5
Gwyneth	38	4.2
Hayden	50	4
Irene	29	4.5
James	42	4.1

Example of clusters





Similarity Measurement

- Quantitative attributes

$$d(a,b) = |a-b|$$

- Qualitative attributes (ordinal)

$$d(a,b) = \frac{|pos_a - pos_b|}{n-1}$$

  - Where n is the number of different values, and pos_a and pos_b are the positions of the values a and b, respectively, in a ranking of possible values.

- Qualitative attributes (nominal)

$$d(a,b) = \begin{cases} 1 & \text{if } a \neq b \\ 0 & \text{if } a = b \end{cases}$$

Example

Difference between the attributes of Andrew (a) and Carolina (b) are

- Age (Quantitative)
  - `d(a,b) = d(55,37) = |55-37| = 18`
- Education level (Ordinal)
  - `d(a,b) = d(1,5) =` $|pos_1 - pos_5|$ `/ 4 = |1-5| / 4 = 1`
- Name (Nominal)
  - `d(a,b) = d("Andrew","Carolina") = 1`

Difference between sequences

Hamming distance

- Applicable for sequences of characters
- Calculates the number of positions at which the corresponding characters in the two strings are different
- Only applicable for strings of the same length

- **Example:**
  $d_{Hamming}$(“James”, “Jimmy”) = 3,
  $d_{Hamming}$(“Tom”, “Tim”) = 1

Difference between sequences

Levenshtein or edit distance

- Calculates the minimum number of operations necessary to transform one sequence into another
  - Insertion
  - Removal
  - Substitution
- Can be calculated for arbitrary strings
- Example

  d_{edit}("Johnny", "Jonston") = 5
  - 4 substitutions (h→n, n→s, n→t, y→o)
  - 1 insertion (adding "n" to the end)

Difference between sequences

Bag-of-words vector similarity

- Long texts converted to a quantitative vector where each position is associated with one of the words found and its value is the number of times this word appeared in the text
- Difference of two texts is calculated as the distance between their bag-of-word vectors
- **Example:**
  text A = "I will go to the party. But first, I will have to work."
  text B = "They have to go to the work by bus."

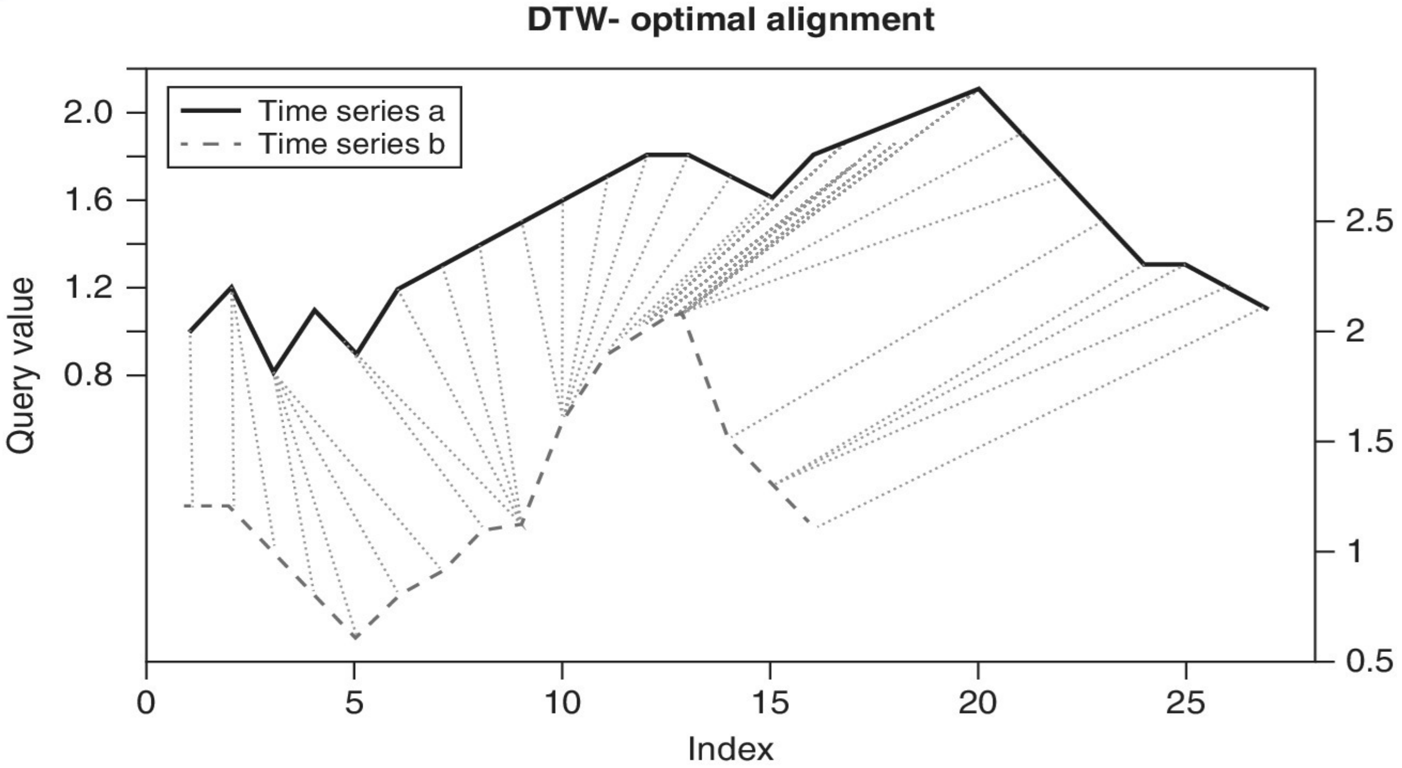
	I	will	go	to	the	party	but	first	have	work	they	by	bus
A	2	2	1	2	1	1	1	1	1	1	0	0	0
B	0	0	1	2	1	0	0	0	1	1	1	1	1

Difference between sequences

Dynamic Time Warping

- Calculates distance between time series data
- Returns the value of the best match between the two series, considering variations and shifts in time and speed
- The most optimal matching is calculated such that:
  - Each index from series a is matched with 1 or more index from series b
  - First and last index from series a is matched with the first and last index of series b
  - Monotonically increasing matches;
    if `i, j` are indices of `series a` such that `i < j`, and `k, l` are indices of `series b` such that `k < l` then they **must not** be matched `i <-> l` and `k <-> j` (No crosses can occur in matching)
- Optimality is based on the pairwise similarity cost calculation
- Computationally heavy

Difference between sequences



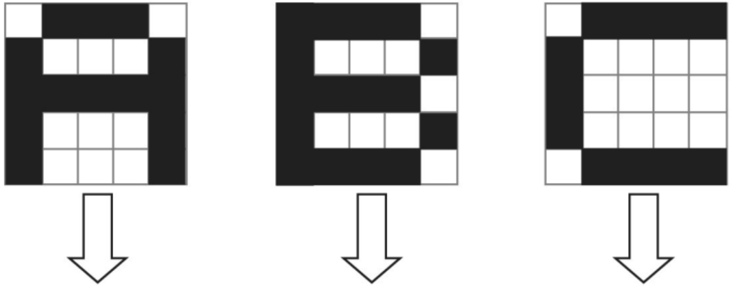
Distance between images

Features representation

- Features associated with the application are be extracted from the images
  - e.g. the distance between the eyes, number of hot pixels, image brightness etc.
- An image is represented by a vector of real numbers, where each element corresponds to one particular feature

Matrix/vector of pixels

- Each pixel or some area of pixels is converted into an integer value
- The size of the area is associated with the granularity required for the image



0	1	1	1	0
1	0	0	0	1
1	1	1	1	1
1	0	0	0	1
1	0	0	0	1

1	1	1	1	0
1	0	0	0	1
1	1	1	1	0
1	0	0	0	1
1	1	1	1	0

0	1	1	1	1
1	0	0	0	0
1	0	0	0	0
1	0	0	0	0
0	1	1	1	1

	1st row					2nd row					3rd row					4th row					5th row				
A	0	1	1	1	0	1	0	0	0	1	1	1	1	1	1	1	0	0	0	1	1	0	0	0	1
B	1	1	1	1	0	1	0	0	0	1	1	1	1	1	0	1	0	0	0	1	1	1	1	1	0
C	0	1	1	1	1	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	1	1	1	1

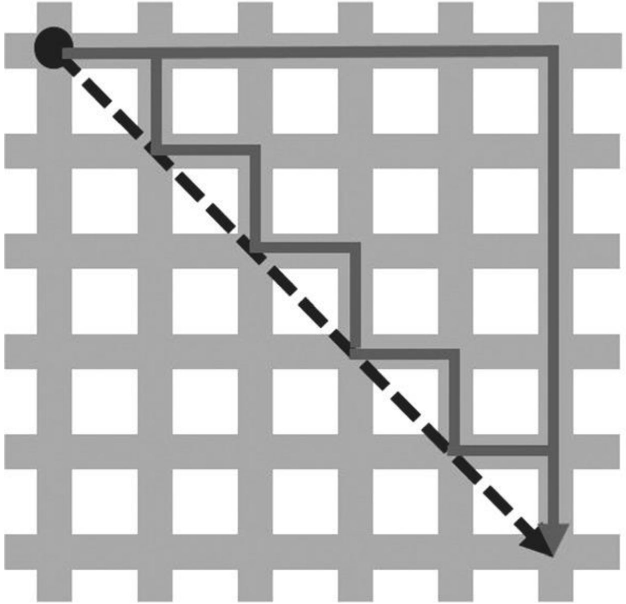
Multi-dimension distance measures

Minkowski distance

$$d(p,q) = \sqrt[r]{\sum_{k=1}^{m} |p_k - q_k|^r}$$

- Manhattan distance (r=1)
- Euclidean distance (r=2)

Usually, objects with mixed attribute types can be transformed to objects with only quantitative attributes.



Clustering techniques

Centroid Based

- Each object in the cluster is closer to a centroid representing the cluster than to a centroid representing any other cluster

Prototype-based

- Each object in the cluster is closer to a prototype representing the cluster than to a prototype representing any other cluster

Graph-based

- Represents the data set by a graph structure associating each node with an object and connecting objects that belong to the same cluster with an edge

Density-based

- A cluster is a region with high density of objects surrounded by a region of low density

K-means

- The most popular clustering algorithm
- Centroid/Partitional method
- Simple, good for convex clusters

DBSCAN

- Density-based method
- Excels in case of non-convex clusters

Agglomerative hierarchical clustering

- Easy-to-understand and interpret
- Graph-based method

K-means clustering

Input:

The dataset *D*,

the distance measure *d*,

the number *K* of clusters

Initialize the *K* centroids (cluster centers) randomly

repeat

  associate each instance in *D* with the

  closest centroid according to *d*

    recalculate each centroid using all

  instances from *D* associated with it

until no instance from *D* implies the change of its associated centroid

Centroid

- a prototype or profile of all the objects in a cluster, for example the average of all the objects in the cluster

Medoid

- the instance with the shortest sum of distances to the other instances of the cluster

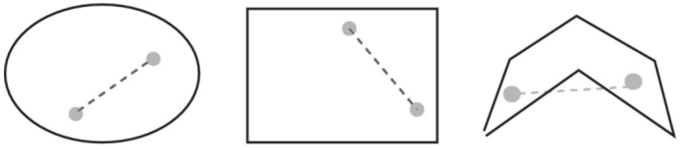
K-means clustering

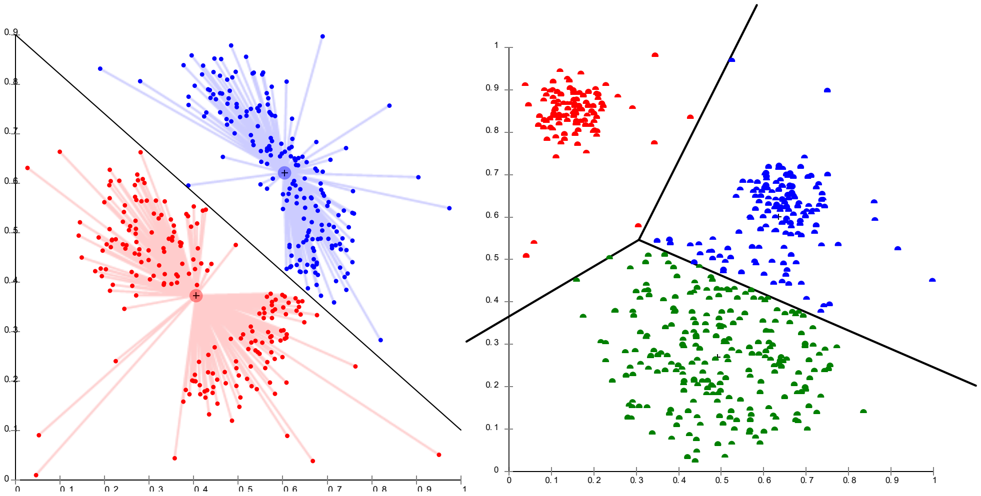
Pros

- Computationally efficient
- Often finds good results

Cons

- It might get stuck in local optima
  - Multiple runs with re-initializations
- Need to define *K* in the beginning
- Not good in case of noisy data and outliers
- Can find only convex shaped clusters





source: https://en.wikipedia.org/wiki/Cluster_analysis#Centroid-based_clustering

Optimal number of clusters

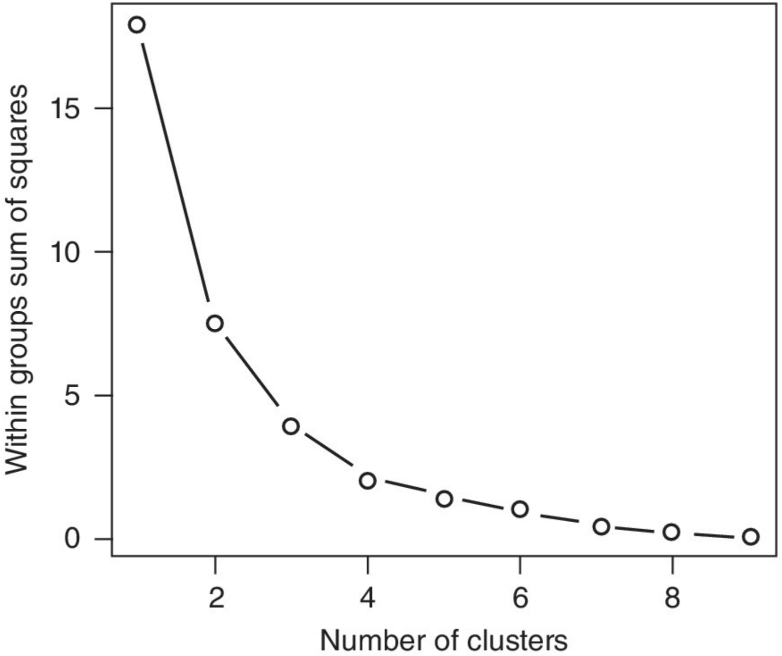
Within-groups sum of squares

- Sums up the squared Euclidean distance (sed) between each instance and the centroid of its cluster

$$s = \sum_{i=1}^{K} \sum_{j=1}^{J_i} sed(p_j, C_i)$$

  - where K is the number of clusters and J_i is the number of instances in cluster i, and C_i is the centroid of the cluster i.

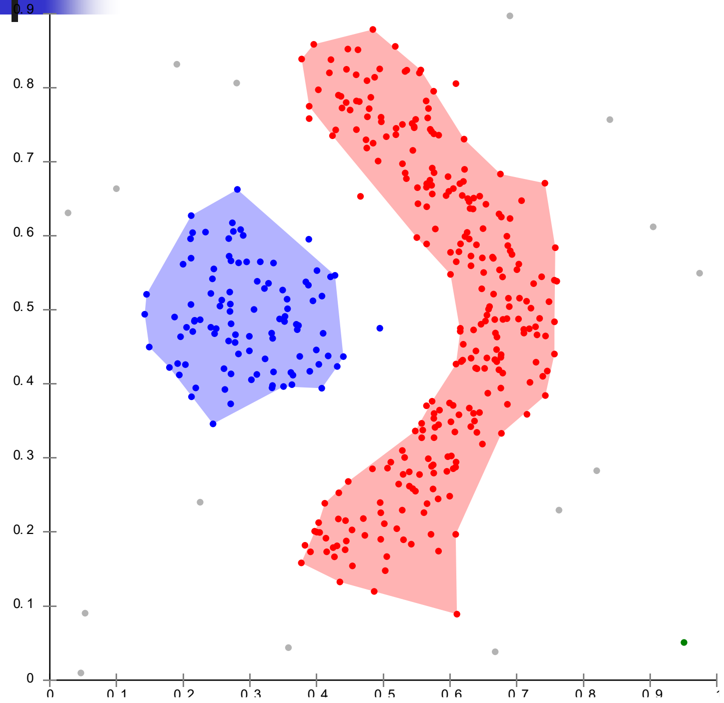
- Elbow curve
  - Optimal K is at the elbow



DBSCAN

- Density-based spatial clustering of applications with noise (DBSCAN)
- Input: $minPts$, ε
- A point p is a *core point* if at least $minPts$ points are within distance ε of it (including p).
- A point q is *directly reachable* from p if point q is within distance ε from core point p. Points are only said to be directly reachable from core points.
- A point q is *reachable* from p if there is a path $p_1, \ldots, p_n$ with $p_1 = p$ and $p_n = q$, where each p_{i+1} is directly reachable from p_i.
- All points not reachable from any other point are *outliers* or *noise points*.
- Core points form a cluster with the reachable points
- Algorithm stops when no more clusters can be formed

DBSCAN



Pros

- Automatically defines the number of clusters
- Can detect clusters of arbitrary shape
- Robust to outliers

Cons

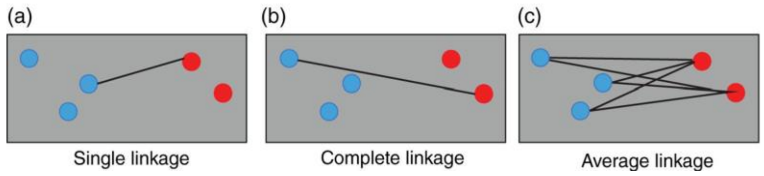
- Computationally more complex than K-means
- Difficulty in setting the hyper-parameter values ($minPts,\ \varepsilon$)

Agglomerative Hierarchical Clustering

Input:

The dataset *D*,

the linkage criterion



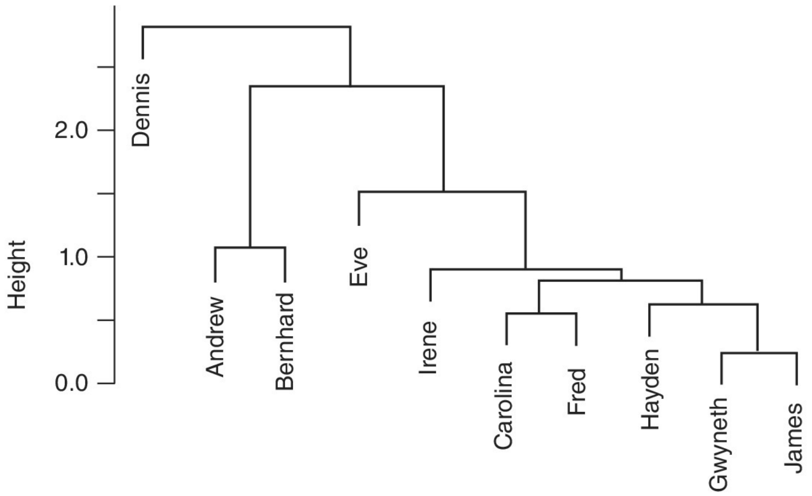
Initialize the clusters such that each object belongs to a separate cluster (Each object is its own cluster)

repeat

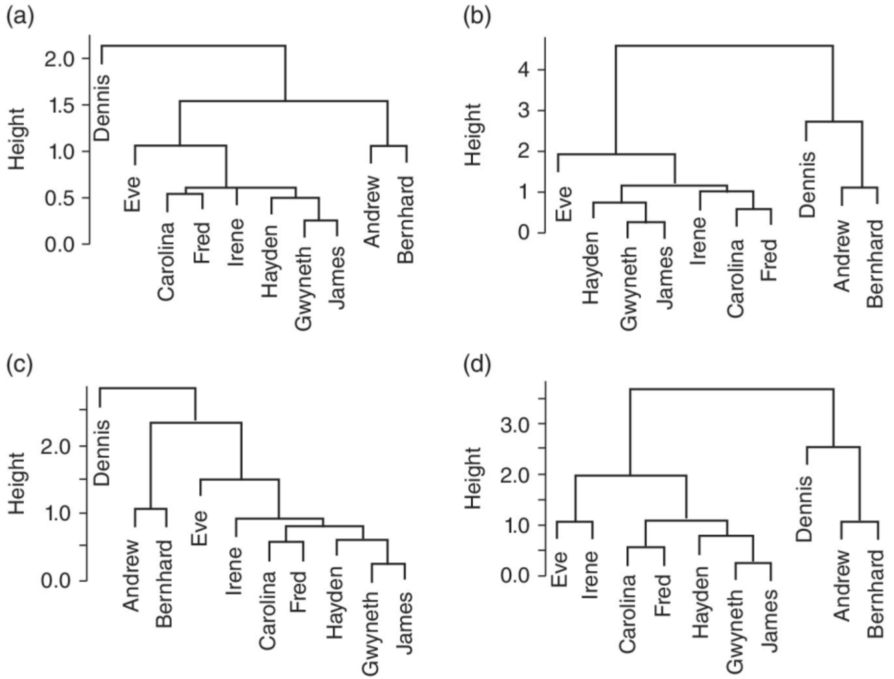
> **join** the two most closest clusters according to the chosen linkage criterion

until the number of desired clusters is reached

Dendrograms



Agglomerative Hierarchical Clustering



Pros

- Easily interpretable, but more confusing for large datasets
- Setting of hyper-parameter values is easy

Cons

- Computationally more complex than K-means
- Interpretation of dendrograms can be, in several domains, quite subjective
- Often gets stuck in local optima

Evaluation of clusters

Silhouette

- Evaluates compactness inside clusters
  - How close to each other the objects inside a cluster are
  - How far the objects in each cluster are to the closest object from another cluster
- Meaning:
  - Silhouette value close to 1 means that x is in the centre of its cluster and far away from the neighboring clusters
  - Silhouette value close to -1 means that x is probably assigned to a wrong cluster
  - Silhouette value close to 0 means that x is on the boundary of two neighboring clusters
- The average over all objects is returned as the silhouette value for the whole clustering

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i, i \neq j} d(i,j)$$

$$b(i) = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} d(i,j)$$

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}, \text{ if } |C_i| > 1$$

Within-groups sum of squares

- Explained before

Final remarks and Literature

- Similarity measures have to be chosen carefully.
- Various techniques and even various launches of the same technique might end up with different results.
- Presence of correlated, irrelevant or redundant attributes can increase the computational cost and reduce the quality of the solutions found.
  - The lack of knowledge regarding class labels makes the identification of the relevant features in the feature selection process harder.

Literature

- Tan, P., Steinbach, M., and Kumar, V. (2014).Introduction to Data Mining, Pearson Education.

Questions?