DTU

02450 Introduction to Machine Learning and Data Mining

Week 10: K-means and hierarchical clustering

Bjørn Sand Jensen

8 April 2025

DTU Compute, Technical University of Denmark

Today

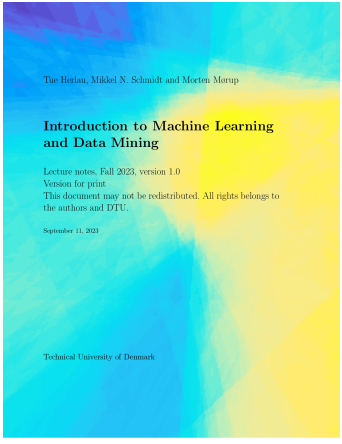
Feedback Groups of the day:

Emiliano Carrara, August Rendtorff, Joschka Eckert-Boulet, Rikke Hertz Thomsen, Samuele Dilengite, Kazi Sazzad Hossen, Seddiga Mahmoud, Hagai Ofer, Pablo Zorrilla Medina Luna, Nicola Stefani, Agnes Lund Olsen, Wojciech Kudla, Anders Helmuth Rame, Martin Agger Nexø, Aliakbar Roozshenas, Mateo de Assas, Gustav Walker Petersen, Truls Straumøy, Ari Nathan Visesa Lie, Sebastian Mariegaard, Daniel Heiðar Qasemiani, Amin Amajjan, Mathias Lindeloff, Jack Smith, Kasper Buchbjerg Friis-Jensen, Patrick Heide Rosquist, Alexander Christian Hougaard, Pedro Francisco Martínez Bulacio, Marius Drachmann Niss, Mathilde Melgaard Larsen, Elias Haynie-Gay, Gloria Stucchi, Fabian Schiøler Würtz, Özge Can Özel, Álvaro Quintana López, Alberte Grostøl Bonde, Md Rasel Mahmud, Julie Dolinger Petersen, Fiona Vivian Wennberg, Srivishnu Piratla, Christian Alexander Halberg, Sebastian Friis Kongsbak

Reading/homework material:

Chapter 18

P18.1, P18.2, P18.3



Lecture Schedule

1. Introduction
   4 February: C1,C2

Data: Feature extraction, and visualization

2. Summary statistics, similarity and visualization
   11 February: C4,C7
3. Computational linear algebra and PCA
   18 February: C3
4. Probability and probability densities
   25 February: C5, C6

Supervised learning: Classification and regression

5. Decision trees and linear regression
   4 March: C8, C9 **(Project 1 due 6 March at 17:00)**
6. Overfitting, cross-validation and Nearest Neighbor
   11 March: C10, C12
7. Performance evaluation, Bayes, and Naive Bayes
   18 March: C11, C13
8. Artificial Neural Networks and Bias/Variance
   25 March: C14, C15
9. AUC and ensemble methods
   1 April: C16, C17

Unsupervised learning: Clustering and density estimation

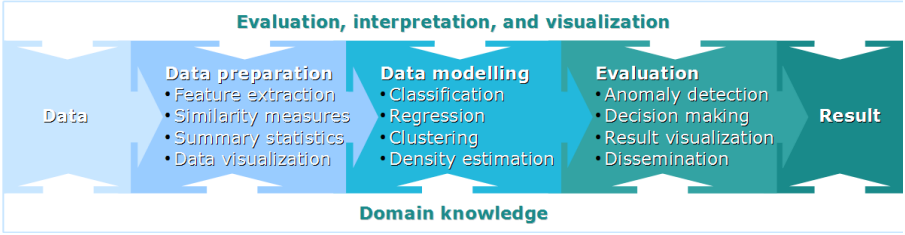
10. **K-means and hierarchical clustering**
    8 April: C18 **(Project 2 due 10 April at 17:00)**
11. Mixture models and density estimation
    22 April: C19, C20
12. Association mining
    29 April: C21

Recap

13. Recap and discussion of the exam
    6 May: C1-C21

Online help: Piazza
Videos of lectures: `https://panopto.dtu.dk`
Streaming of lectures: Zoom (link on DTU Learn)

Learning Objectives



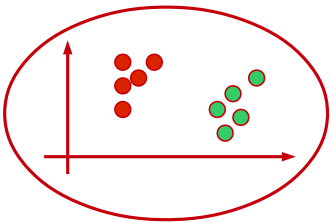
Learning Objectives

- Understand the principles behind K-means and hierarchical clustering
- Understand how different linkage functions affects clustering types
- Compare clustering solutions using Rand index, Jaccard and NMI
- Evaluate clustering quality using class labels

Practicalities and announcements

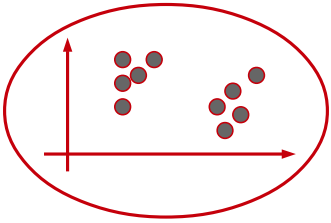
- Project 2 due 10th April @ 17:00

Supervised and Unsupervised learning



Supervised Learning
Input data $\mathbf{x}_n$ and output y_n

(Classification and Regression)



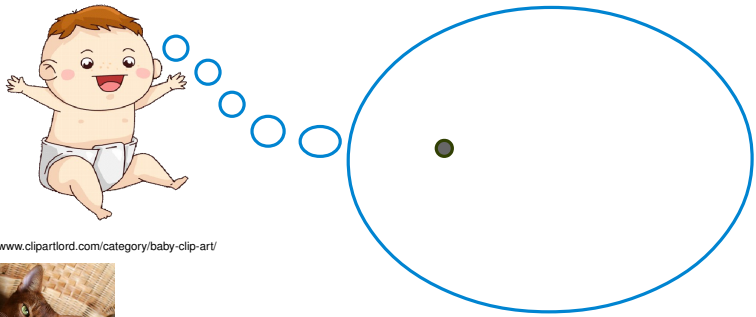
Unsupervised Learning
Input data $\mathbf{x}_n$ alone

(Exploratory analysis)

Imagine you observe the world for the first time!

http://www.clipartlord.com/category/baby-clip-art/

Imagine you observe the world for the first time!



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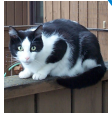

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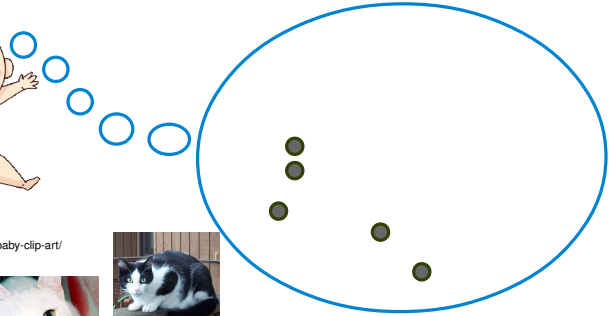

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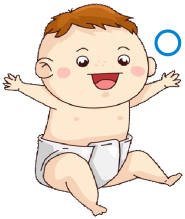

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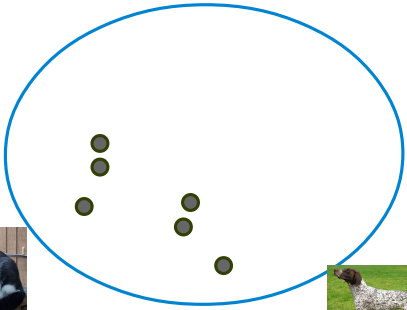

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We humans are skilled at dividing objects into groups (clustering), but how do we make computers do the same?

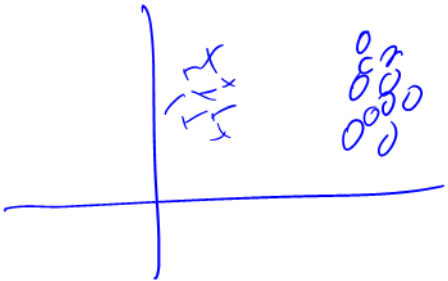
Source (animal images): commons.wikimedia.org

Unsupervised learning

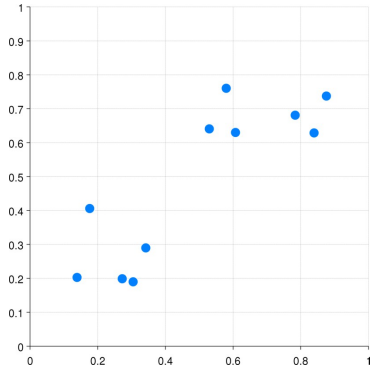
- Supervised learning
  - Use the data to learn the output values
- Unsupervised learning
  - No output variables available
  - Sometimes called exploratory analysis
  - What to learn from the data?
    - Structure
    - Regularities
    - Hidden information
    - Etc.

Clustering

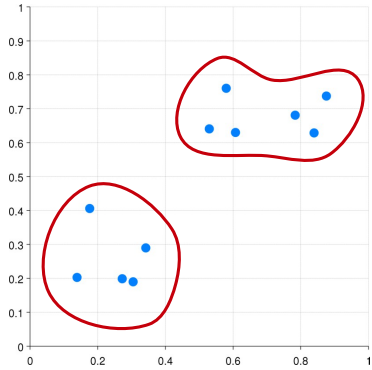
- Divide data into groups (subsets/clusters) that are
  - **Meaningful:** Capture the natural structure of the data
  - **Useful:** Depends on purpose
- Observations in the same cluster are **similar in some sense**
- Unsupervised classification



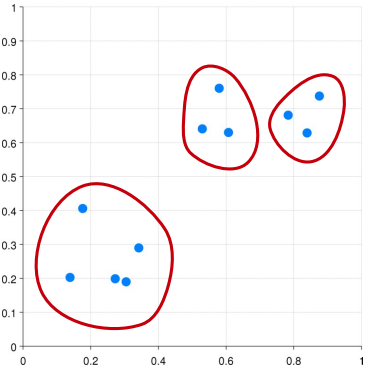
Clustering



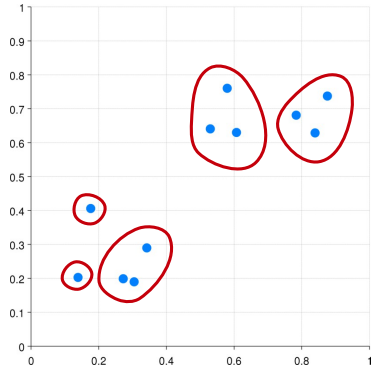
Clustering



Clustering

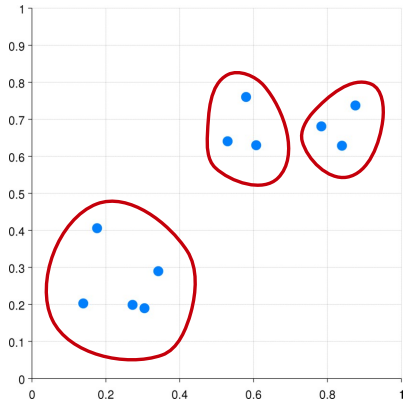


Clustering

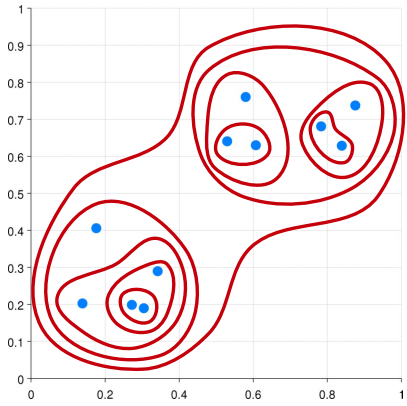


Partitional / hierarchical clustering

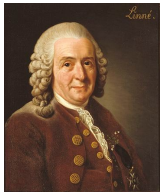
Partitional



Hierarchical



Phylogenetic trees



Carl Linnaeus
(1707 – 1778)

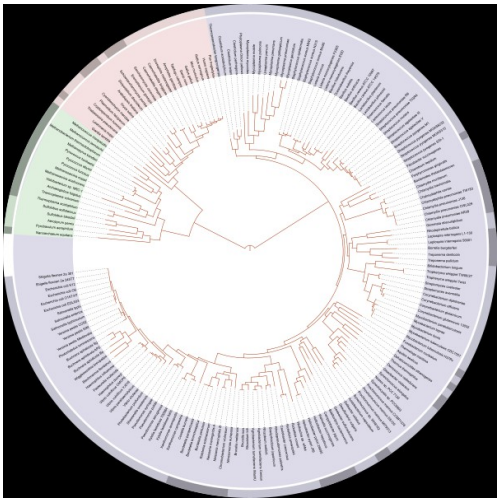
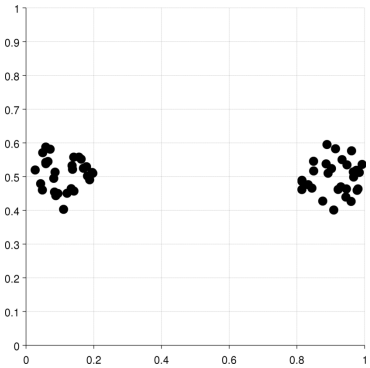


Image source:
http://en.wikipedia.org/wiki/Carl_Linnaeus
http://en.wikipedia.org/wiki/File:Tree_of_life_SVG.svg

Types of clustering

Well-separated

- Each point is closer to all points in its cluster than any point in another cluster.



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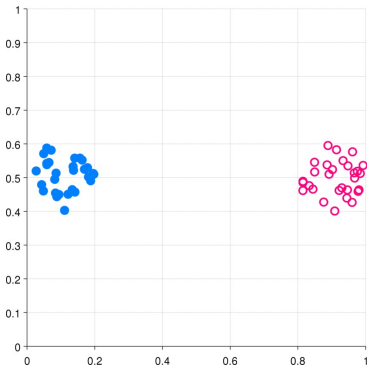
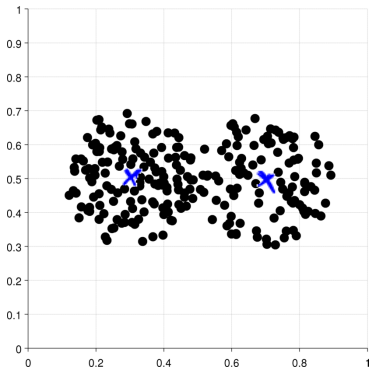


Types of clustering

Center-based

- Each point is closer to the center of its cluster than to the center of any other cluster



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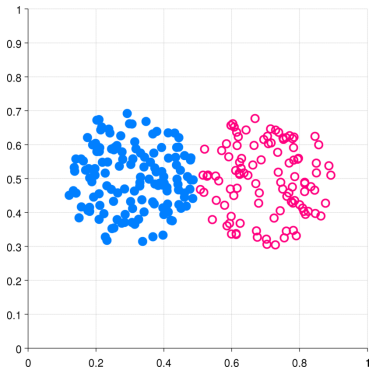
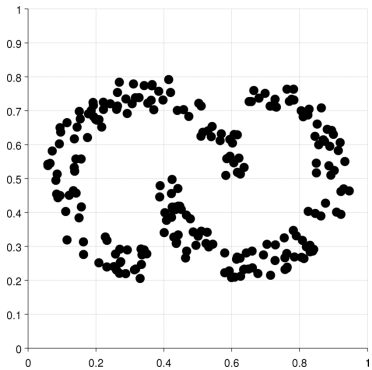


Types of clustering

Contiguity-based

- Each point is closer to at least one point in its cluster than to any point in another cluster



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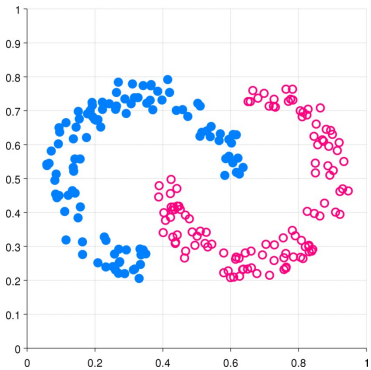
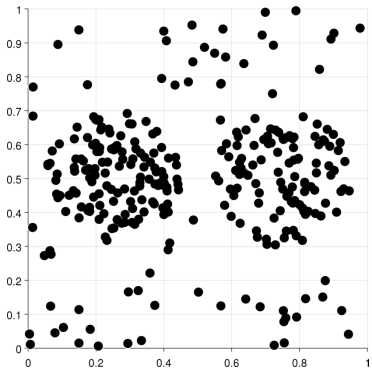


Types of clustering

Density-based

- Clusters are regions of high density separated by regions of low density



Types of clustering

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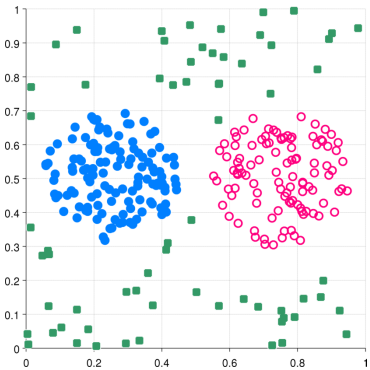
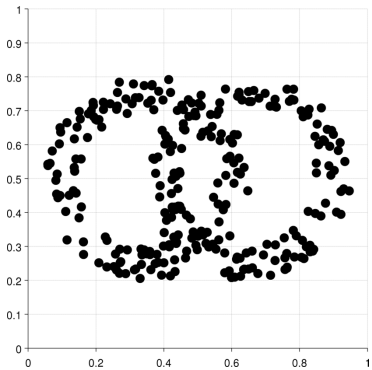


Types of clustering

Conceptual clusters

- Points in a cluster share some general property that derives from the entire set of points



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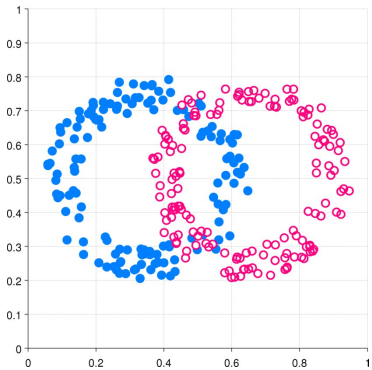


Quiz 01: Clustering types

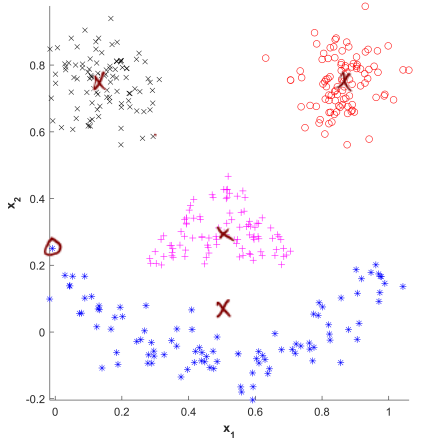


Figure 1: A clustering problem containing four clusters indicated by black crosses, red circles, magenta plusses and blue stars.

Consider the clustering problem given in Figure 1. Which clustering approach is *most* suited for correctly separating the data into the four groups indicated by black crosses, red circles, magenta plusses, and blue asterics?

A. A well-separated clustering approach.

B. A contiguity-based clustering approach.

C. A center-based clustering approach.

D. A conceptual clustering approach.

E. Don't know.

Solution:

As the observation in each cluster is at least closest to one other observation in its cluster than to an observation in another cluster a contiguity based approach is most suited.

K-means clustering

Select K points as initial centroids
Repeat

- Form K clusters by assigning each point to its closest centroid
- Recompute the centroids of each cluster

Until centroids do not change

Default distance function: The basic/classical K-means algorithm uses the sqaured Euclidian distance.

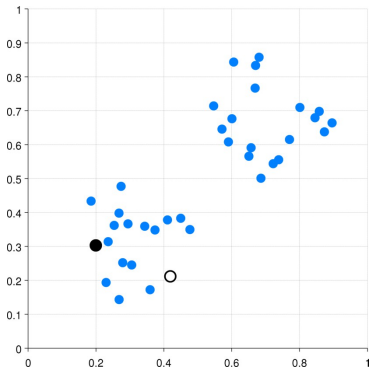
K-means clustering

Select K points as initial centroids, $\mu_1, \mu_2 \in \mathbb{R}^2$

Repeat

- Form K clusters by assigning each point to its closest centroid
- Recompute the centroids of each cluster

Until centroids do not change



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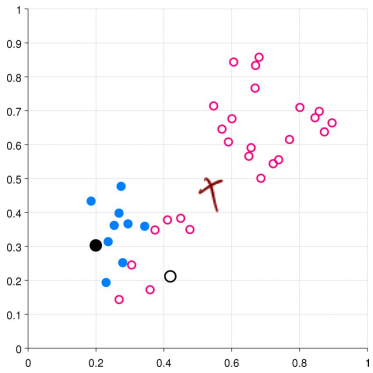

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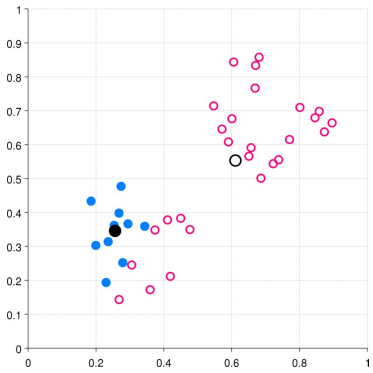

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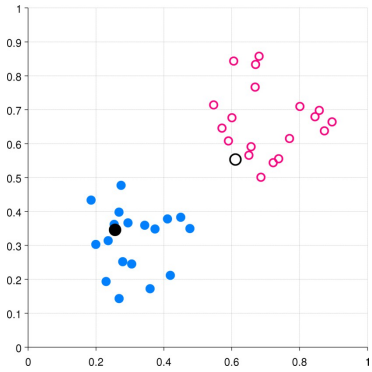

K-means clustering

Select K points as initial centroids
Repeat

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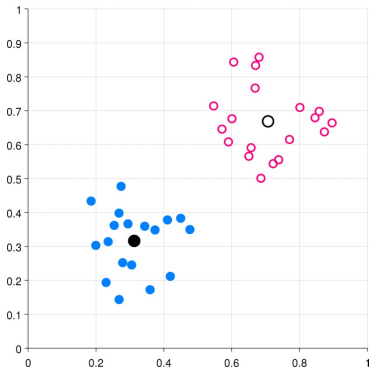
Until centroids do not change



Quiz 02: K-means

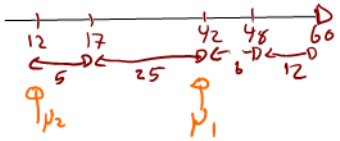
Consider the following dataset

$$\boldsymbol{X} = \{42, 60, 17, 48, 12\}$$

Select K points as initial centroids
Repeat

- Form K clusters by assigning each point to its closest centroid
- Recompute the centroids of each cluster

Until centroids do not change



We wish to apply the K-means algorithm with $K = 2$ clusters to this dataset and we initialize with cluster centroids at $\mu_1 = 17$ and $\mu_2 = 12$. Carefully, using pen and paper, go through each step of the K-means algorithm until it converge. What is the final clustering?

A. $\{60, 48\}, \{12, 17, 42\}$

B. $\{42, 60, 48, 17\}, \{12\}$

C. $\{60\}, \{12, 17, 42, 48\}$

D. $\{42, 60, 48\}, \{12, 17\}$

E. Don't know.

① [1 1 1 1 2]

$\mu_1 = \frac{17+42+48+60}{4} \approx 41.75$

$\mu_2 = \frac{12}{1} = 12$

② [1 1 2 1 2]

$\mu_2 = \frac{12+17}{2} = 14.5$

$\mu_1 = \frac{42+48+60}{3} = 50$

Solution:

The correct answer is D. We will verify this by listing the intermediate steps of the K-means algorithm:

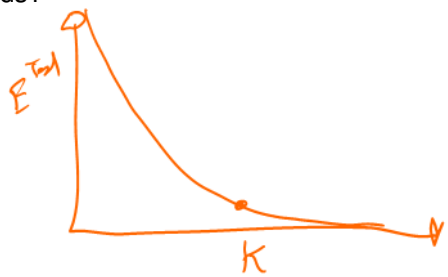
1. The initial clustering will be
$$\{42, 60, 48, 17\}, \quad \{12\}.$$
2. The new centroids will be
$$\mu_1 = \frac{42 + 60 + 48 + 17}{4} = 41.75, \mu_2 = \frac{12}{1} = 12.$$
3. The new clusters will then be
$$\{42, 60, 48\}, \quad \{12, 17\}.$$
4. The centroids then become:
$$\mu_1 = \frac{42 + 60 + 48}{3} = 50, \mu_2 = \frac{12 + 17}{2} = 14.5.$$

It is easy to verify the cluster assignment/centroids will no longer be updated and the method therefore stops.

K-means clustering

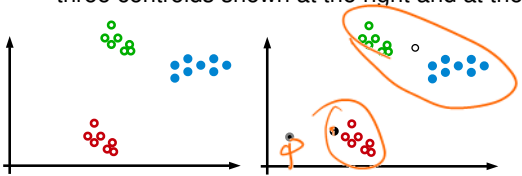
How do I

- Find the clostest centroid?
  - Use a suitable **dissimilarity/similarity measure**
- Compute the cluster centroids?
  - Depends on dissimilarity/similarity measure
  - For example, for sqaured Euclidean distance the mean is optimal
- Decide on K - the number of centroids?
- Initialize the K centroids?

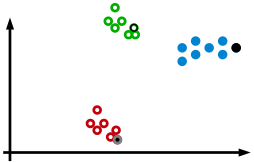


K-means clustering - initializaiton

- How will the data (top-left diagram) be clustered given the initialization of the three centroids shown at the right and at the bottom?



- What could we do if we have an empty cluster?
- What could be a good initialization procedure? (Farthest First)



The K-means solution depends on the initialization!

Agglomerative hierarchical clustering

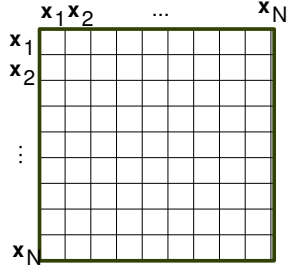
14:00

Initialize the proximity matrix
Repeat

- Merge the two closest clusters
- Update the proximity matrix to reflect the proximity between the new cluster and the original clusters

Until only one cluster remains

$$D_{ij} = distance(x_i, x_j)$$



Agglomerative hierarchical clustering

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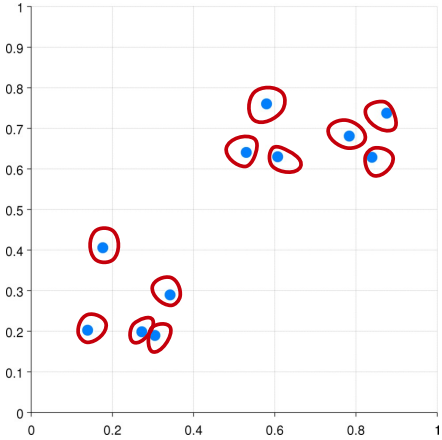
Until only one cluster remains



Agglomerative hierarchical clustering

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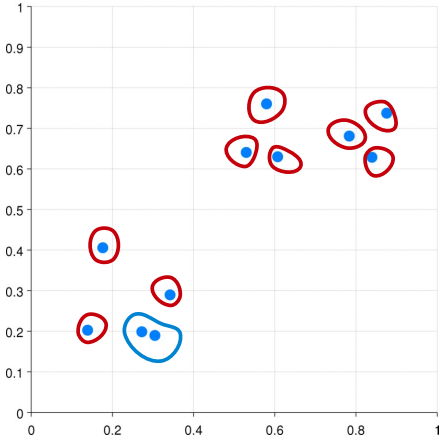

Agglomerative hierarchical clustering

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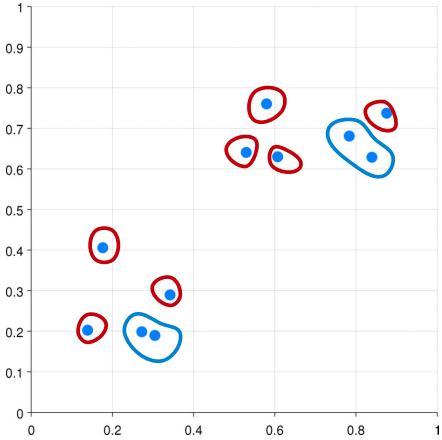

Agglomerative hierarchical clustering

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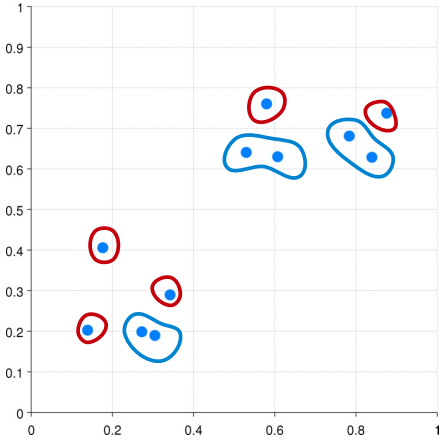

Agglomerative hierarchical clustering

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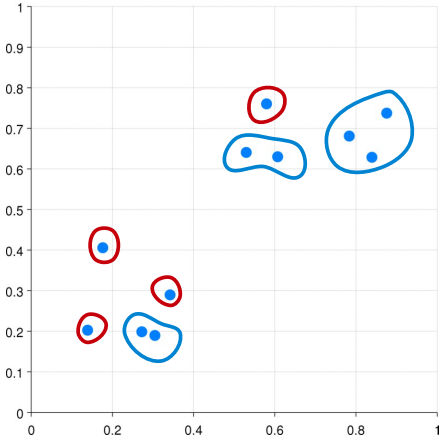

Agglomerative hierarchical clustering

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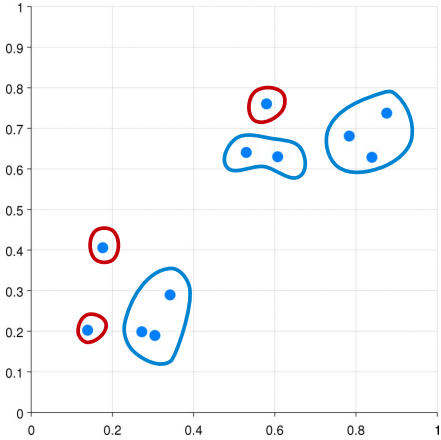
Until only one cluster remains



Agglomerative hierarchical clustering

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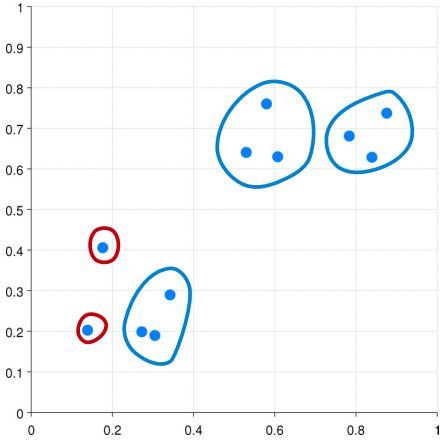

Agglomerative hierarchical clustering

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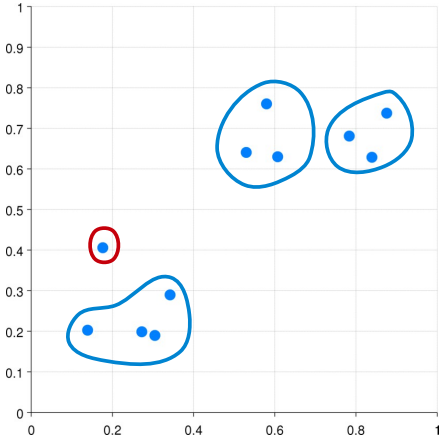
Until only one cluster remains



Agglomerative hierarchical clustering

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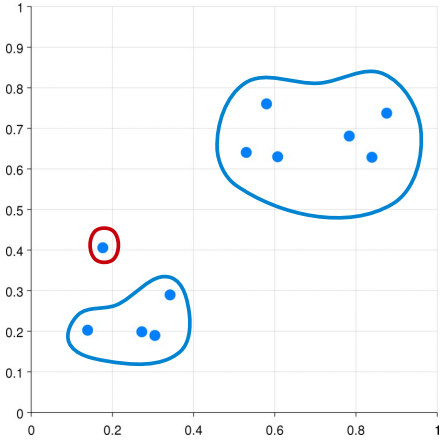

Agglomerative hierarchical clustering

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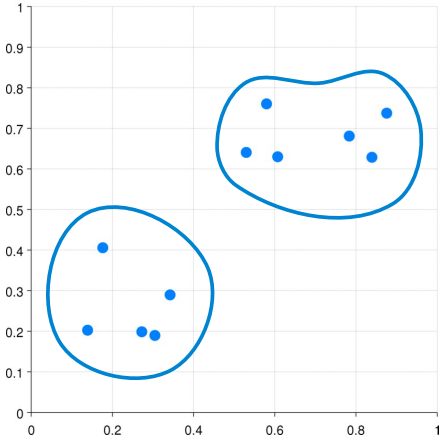

Agglomerative hierarchical clustering

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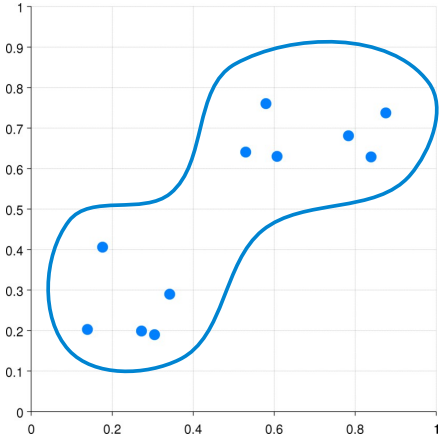
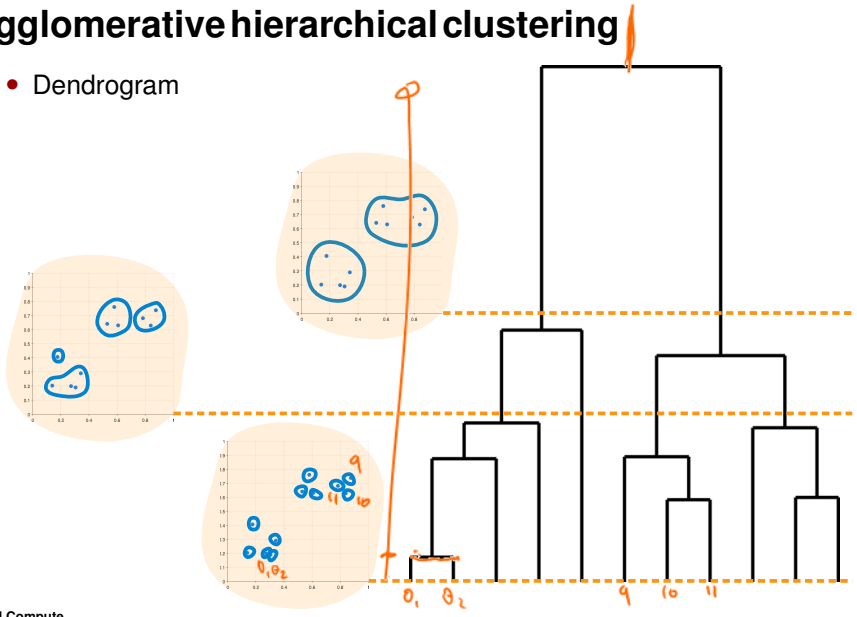


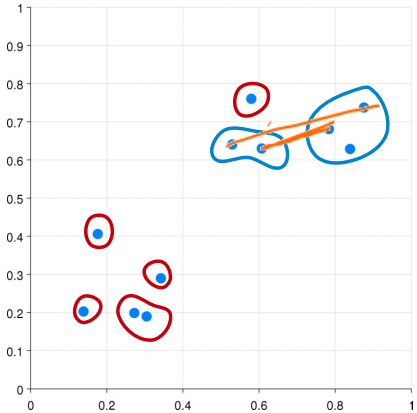
Agglomerative hierarchical clustering

- Dendrogram



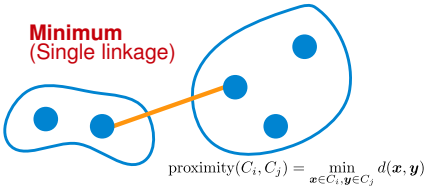
Similarity between clusters

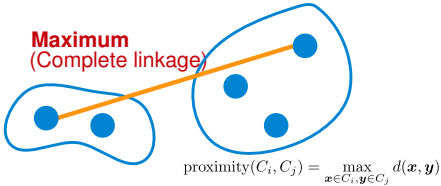
- The **key operation** in in agglomerative hierarchical clustering is measuring distance (dissimilarity) between clusters

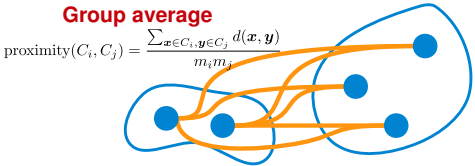


Proximity between clusters

- Can be computed using **proximity between objects**
- In our example before we used Euclidian distance as proximity measure







C_i: Observations in cluster i

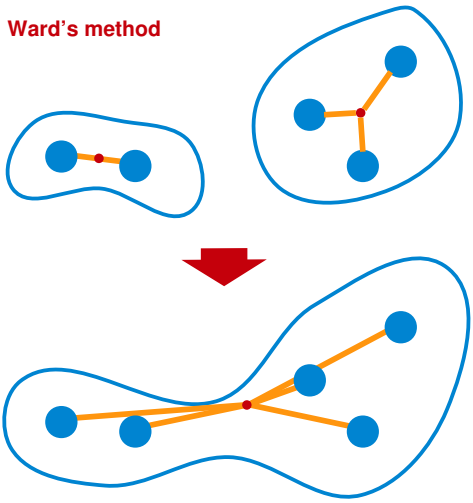
C_j: Observations in cluster j

m_i: Number of observations in cluster i

m_i: Number of observations in cluster j

Proximity between clusters

- Increase in sum of squared error after merging the two clusters should be as small as possible

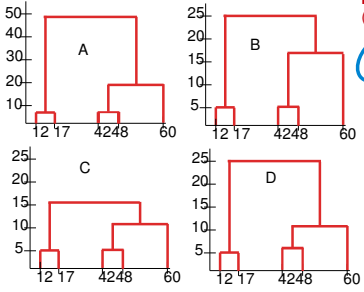


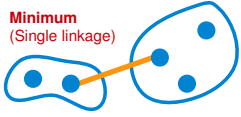
Quiz 03: Dendrograms

Consider once more the dataset:

$$\boldsymbol{X} = \{42, 60, 17, 48, 12\}$$

Using pen-and-paper, carefully build a dendrogram from X one step at a time using Euclidean distance and *minimum* (single) linkage. What will the dendrogram look like?





A. Dendrogram A

B. Dendrogram B

C. Dendrogram C

D. Dendrogram D

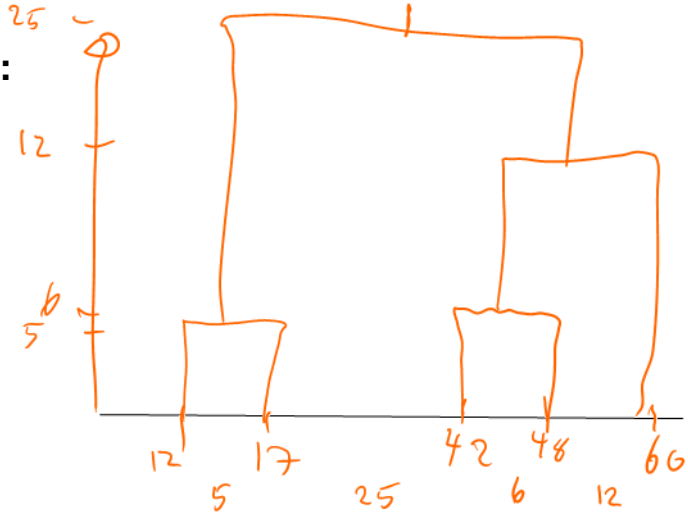
E. Don't know.

Initialize the proximity matrix
Repeat

- Merge the two closest clusters
- Update the proximity matrix to reflect the proximity between the new cluster and the original clusters

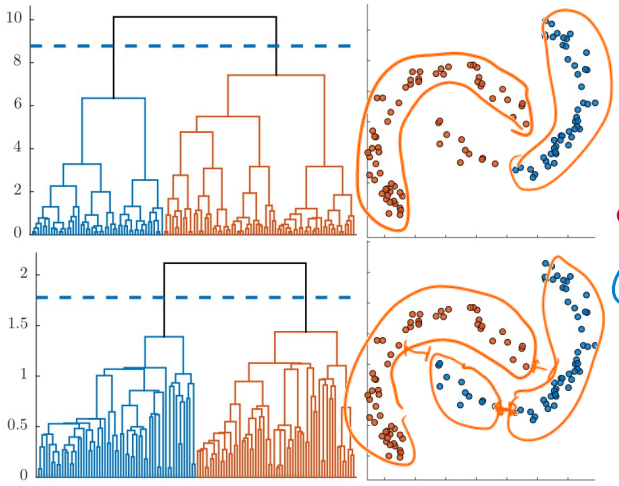
Until only one cluster remains

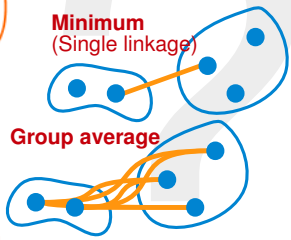
Solution:



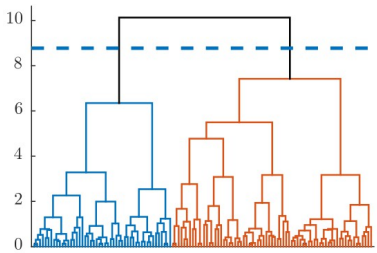
The correct answer is D. The clusters will merge at height 5, 6, 12 and 25.

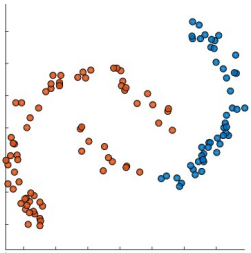
Clusterings and linkage functions



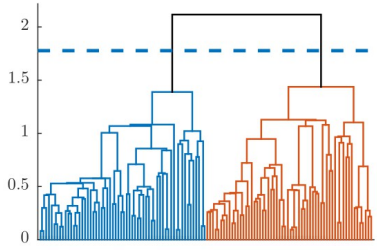


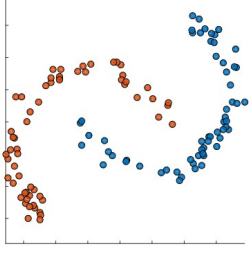
Clusterings and linkage functions





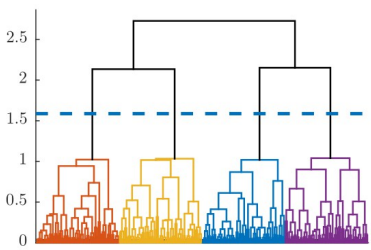
Group average

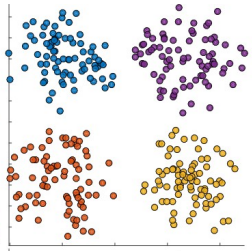


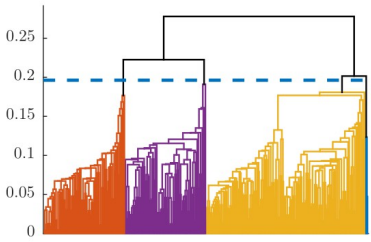


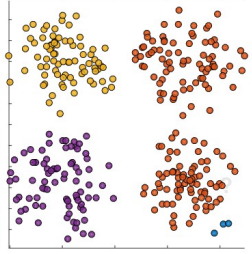
Minimum
(Single linkage)

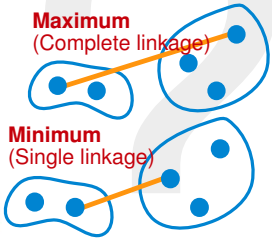
Clusterings and linkage functions



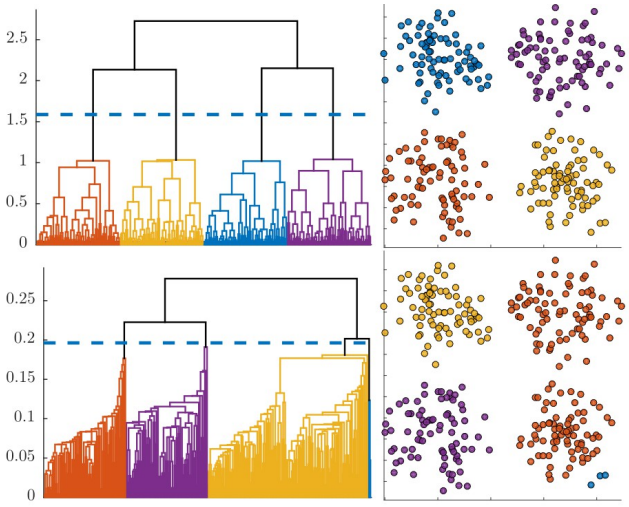








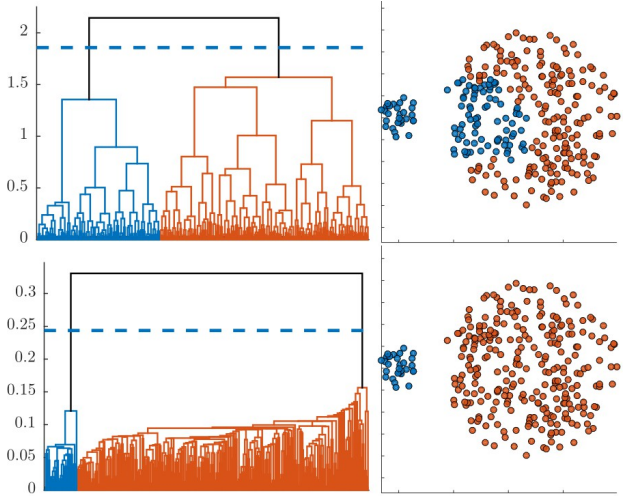
Clusterings and linkage functions

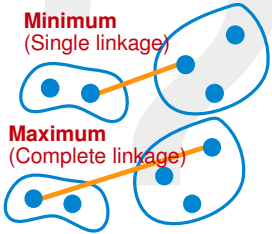


Maximum
(Complete linkage)

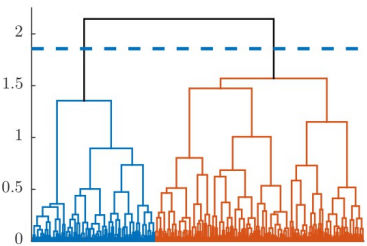
Minimum
(Single linkage)

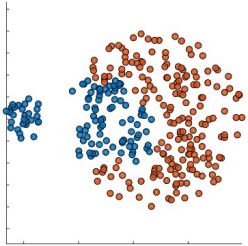
Clusterings and linkage functions



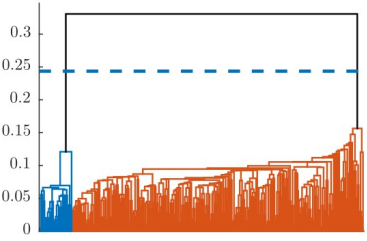


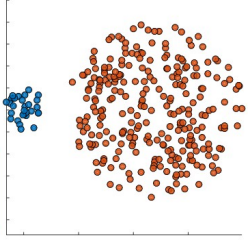
Clusterings and linkage functions





Maximum
(Complete linkage)

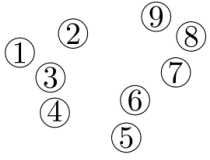


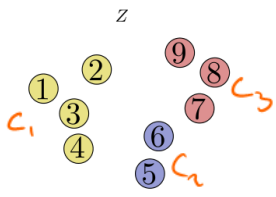


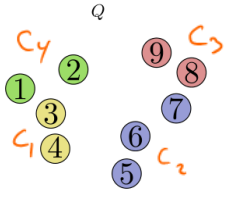
Minimum
(Single linkage)

Comparing partitions

- How similar are Q and Z





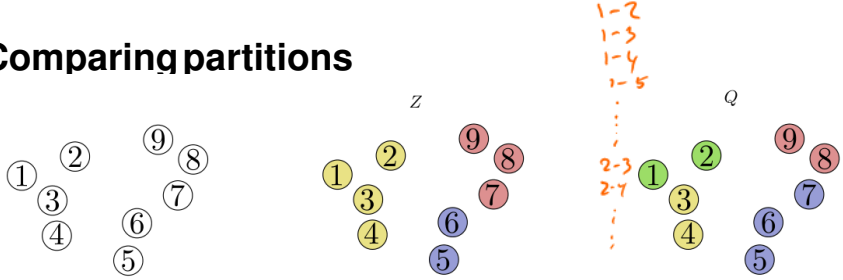


$$Z = \begin{bmatrix} 1 & 1 & 1 & 1 & 2 & 2 & 3 & 3 & 3 \end{bmatrix}$$
$$Q = \begin{bmatrix} 4 & 4 & 1 & 1 & 2 & 2 & 2 & 3 & 3 \end{bmatrix}$$

- Note encoding is (and should be!) arbitrary

$$Q' = \begin{bmatrix} 10 & 10 & 3 & 3 & 8 & 8 & 8 & 1 & 1 \end{bmatrix}$$

Comparing partitions



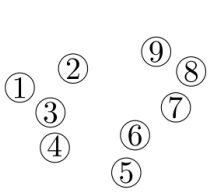
- For a given partition, any two observations i, j can either be in the same cluster, or in different clusters

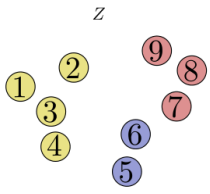
$$\delta_{i,j} = \begin{cases} 0 \text{ if } o_i \text{ and } o_j \text{ are in different clusters} \\ 1 \text{ if } o_i \text{ and } o_j \text{ are in the same cluster} \end{cases}$$

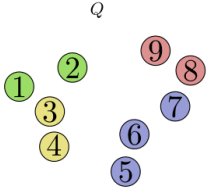
- There are $\frac{1}{2}N(N-1)$ unique pairs in total
- We get two $\frac{1}{2}N(N-1)$-long binary vectors corresponding to each pair (i, j)

$$\begin{aligned} \mathbf{b}^Z &= [\ \delta_{1,2}\ \ \delta_{1,3}\ \ \delta_{1,4}\ \ \delta_{1,5}\ \ \cdots\ \ \delta_{2,3}\ \ \delta_{2,4}\ \ \cdots\ \ \delta_{3,5}\ \ \cdots\ \ \delta_{N,N-1}\ ] \\ &= [\ 1\ \ 1\ \ 1\ \ 0\ \ \cdots\ \ 1\ \ 1\ \ \cdots\ \ 0\ \ \cdots\ \ 1\ ] \\ \mathbf{b}^Q &= [\ 1\ \ 0\ \ 0\ \ 0\ \ \cdots\ \ 0\ \ 0\ \ \cdots\ \ 0\ \ \cdots\ \ 1\ ] \end{aligned}$$

Comparing partitions - Jaccard and SMC/Rand index







$$\begin{aligned}\mathbf{b}^Z &= [\ 1\ \ 1\ \ 1\ \ 0\ \ \cdots\ \ 1\ \ 1\ \ \cdots\ \ 0\ \ \cdots\ \ 1\ ]\\ \mathbf{b}^Q &= [\ 1\ \ 0\ \ 0\ \ 0\ \ \cdots\ \ 0\ \ 0\ \ \cdots\ \ 0\ \ \cdots\ \ 1\ ]\end{aligned}$$

$S = \{$ Number of pairs in the same cluster in Z **and** $Q\}$ f_{11}

$D = \{$ Number of pairs in different clusters in Z **and** $Q\}$ f_{00}

Rand index: $R(Z,Q) = \dfrac{S+D}{\frac{1}{2}N(N-1)} = \dfrac{4+24}{\frac{1}{2}9\cdot 8} = \dfrac{7}{9},$ (SMC)

Jaccard similarity: $J(Z,Q) = \dfrac{S}{\frac{1}{2}N(N-1)-D} = \dfrac{4}{\frac{1}{2}9\cdot 8-24} = \dfrac{1}{3}$

An effecient encoding

$$n_{km} = \{\text{Observations assigned to cluster } k \text{ in } Z \text{ and } m \text{ in } Q\} = \sum_{i=1}^{N}\sum_{j=1}^{N} \delta_{z_i,k}\delta_{z_j,m}$$

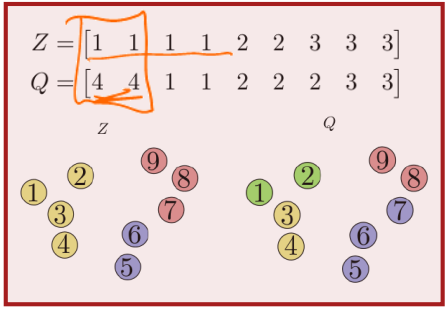
$$\boldsymbol{n}^Z = \{\text{Number of observations assigned to cluster } k \text{ in } Z\} = \sum_{m=1}^{M} n_{km}$$

$$\boldsymbol{n}^Q = \{\text{Number of observations assigned to cluster } m \text{ in } Q\} = \sum_{k=1}^{K} n_{km}$$

$$\boldsymbol{n} = \begin{bmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 0 & 0 \\ 0 & 1 & 2 & 0 \end{bmatrix}$$

Note the horizontal/vertical sums of $\boldsymbol{n}$:

$$\boldsymbol{n}^Z = \begin{bmatrix} 4 \\ 2 \\ 3 \end{bmatrix}, \quad \boldsymbol{n}^Q = \begin{bmatrix} 2 & 3 & 2 & 2 \end{bmatrix}$$



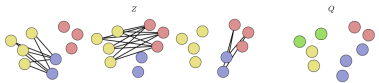
Jaccard and rand index in general

Recall

$$\boldsymbol{n} = \begin{bmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 0 & 0 \\ 0 & 1 & 2 & 0 \end{bmatrix}, \quad \boldsymbol{n}^Z = \begin{bmatrix} 4 \\ 2 \\ 3 \end{bmatrix}, \quad \boldsymbol{n}^Q = \begin{bmatrix} 2 & 3 & 2 & 2 \end{bmatrix}$$

$$\begin{aligned} S &= \{ \text{ Number of pairs } i, j \text{ in the same cluster in } Z, Q \} \\ &= \sum_{k=1}^{K} \sum_{m=1}^{M} \frac{n_{km}(n_{km}-1)}{2} \\ &= \frac{2(2-1)}{2} + \frac{2(2-1)}{2} + \frac{2(2-1)}{2} + \frac{1(1-1)}{2} + \frac{2(2-1)}{2} = 4 \end{aligned}$$

$$\begin{aligned} D &= \{ \text{ Number of pairs } i, j \text{ in different clusters in } Z, Q \} \\ &= \frac{N(N-1)}{2} - \sum_{k=1}^{K} \frac{n_k^Z(n_k^Z-1)}{2} - \sum_{m=1}^{M} \frac{n_m^Q(n_m^Q-1)}{2} + S \\ &= 36 - 10 - 6 + 4 = 24 \end{aligned}$$



Quiz 04: Cluster overlap

	o_1	o_2	o_3	o_4	o_5	o_6	o_7	o_8	o_9	o_{10}
o_1	0.0	2.0	5.7	0.9	2.9	1.8	2.7	3.7	5.3	5.1
o_2	2.0	0.0	5.6	2.4	2.5	3.0	3.5	4.3	6.0	6.2
o_3	5.7	5.6	0.0	5.0	5.1	4.0	3.3	5.4	1.2	1.8
o_4	0.9	2.4	5.0	0.0	2.7	2.1	2.2	3.5	4.6	4.4
o_5	2.9	2.5	5.1	2.7	0.0	3.5	3.7	4.0	5.8	5.7
o_6	1.8	3.0	4.0	2.1	3.5	0.0	1.7	5.3	3.8	3.7
o_7	2.7	3.5	3.3	2.2	3.7	1.7	0.0	4.2	3.1	3.2
o_8	3.7	4.3	5.4	3.5	4.0	5.3	4.2	0.0	5.5	6.0
o_9	5.3	6.0	1.2	4.6	5.8	3.8	3.1	5.5	0.0	2.1
o_{10}	5.1	6.2	1.8	4.4	5.7	3.7	3.2	6.0	2.1	0.0

Table 1: The pairwise distances between $N = 10$ observations from the travel review dataset. the colors indicate classes

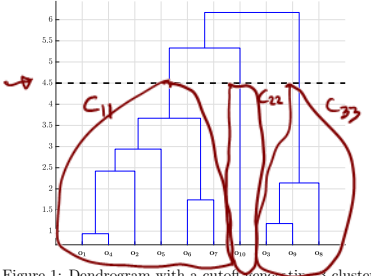


Figure 1: Dendrogram with a cutoff generating 3 clusters.

Consider the dendrogram in Figure 1. Suppose we apply a cutoff (indicated by the black line) thereby generating three clusters. We wish to compare the quality of this clustering, Q, to the ground-truth clustering, Z, indicated by the colors in Table 1. Recall the *Jaccard similarity* of the two clusters is

$$\mathrm{J}[Z, Q] = \frac{S}{\frac{1}{2}N(N-1) - D}$$

in the notation of the lecture notes. What is the Jaccard similarity of the two clusterings?

A. $\mathrm{J}[Z, Q] \approx 0.104$

B. $\mathrm{J}[Z, Q] \approx 0.143$

C. $\mathrm{J}[Z, Q] \approx 0.174$

D. $\mathrm{J}[Z, Q] \approx 0.153$

E. Don't know.

Solution:

$$S = \sum_k \sum_m \frac{n_{km}(n_{km}-1)}{2} = 4$$

$$D = \frac{N(N-1)}{2} - \sum_k \frac{n_k^2(n_k^2-1)}{2} - \sum_m \frac{n_m^2(n_m^2-1)}{2} + S$$

$$= \frac{10 \cdot 9}{2} - \left(\frac{2 \cdot 1}{2} + \frac{3 \cdot 2}{2} + \frac{5 \cdot 4}{2}\right) - \left(\frac{6 \cdot 5}{2} + 0 + \frac{3 \cdot 2}{2}\right) + 4$$

$$= 17$$

To compute J[Z, Q], note Z is the clustering corresponding to the colors in **??** and Q the clustering obtained by cutting the dendrogram in **??** given as:

$$\{10\}, \{1, 2, 4, 5, 6, 7\}, \{3, 8, 9\}$$

From this information we can define the counting matrix $\boldsymbol{n}$ as

$$\boldsymbol{n} = \begin{bmatrix} 0 & 2 & 0 \\ 0 & 2 & 1 \\ 1 & 2 & 2 \end{bmatrix}$$

Note: This result is different (but not incorrect) from ours because the naming/ordering is different.... J[Z,Q] is going to be the same

It is then a simple matter of using the definitions in the lecture notes (see chapter 17.4) to compute

$$S = 4, D = 17$$

From this the answer by simply plugging the values into the formula given in the text and answer B is correct.

Entropy and mutual information recap

- Consider a probability distribution $P(X = x_i) = p_i$, $i = 1, \ldots, n$
- **Information** obtained from observing x_i is

$$I = -\log p_i = \log \frac{1}{p_i}$$

- Average information obtained is called the **entropy**

$$H[p_X] = \mathbb{E}[I] = -\sum_{i=1}^{n} p_i \log p_i$$

- Entropy is defined for general densities $P(X = x_i, Y = y_j) = p_{ij}$

$$H[p_{XY}] = -\sum_{i=1}^{n}\sum_{j=1}^{m} p_{ij} \log p_{ij}$$

- The **Mutual information** is defined as

$$\mathrm{MI}[X, Y] = H[P_X] + H[P_Y] - H[P_{XY}]$$

- The **Normalized mutual information** is defined as

$$\mathrm{NMI}[X, Y] = \frac{\mathrm{MI}[X, Y]}{\sqrt{H[P_X]}\sqrt{H[P_Y]}}$$

Comparing using mutual information

We define $P_{ZQ}(i,j) = \frac{1}{N} n_{ij}$, $P_Z(i) = \frac{n_i^Z}{N}$ and $P_Q(j) = \frac{n_j^Q}{N}$. Example:

$$P_{ZQ} = \frac{1}{9}\begin{bmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 0 & 0 \\ 0 & 1 & 2 & 0 \end{bmatrix},\ P_Z = \frac{1}{9}\begin{bmatrix} 4 \\ 2 \\ 3 \end{bmatrix},\ P_Q = \frac{1}{9}\begin{bmatrix} 2 & 3 & 2 & 2 \end{bmatrix}$$

- **Entropy** computed as $H[p_X] = -\sum_{i=1}^{n} p_i \log p_i$:

$$\text{Entropy of } Z: \quad H[Z] = -\frac{4}{9}\log\frac{4}{9} - \frac{1}{3}\log\frac{1}{3} - \frac{2}{9}\log\frac{2}{9} \approx 1.06$$

$$\text{Entropy of } Q: \quad H[Q] = -\frac{2}{9}\log\frac{2}{9} - \frac{2}{9}\log\frac{2}{9} - \frac{2}{9}\log\frac{2}{9} - \frac{1}{3}\log\frac{1}{3} \approx 1.37$$

$$\text{Entropy of } Z \text{ and } Q: \quad H[ZQ] = -4 \times \frac{2}{9}\log\frac{2}{9} - \frac{1}{9}\log\frac{1}{9} = 1.58.$$

- **Mutual information**:

$$\mathrm{MI}[Z,Q] = H[Z] + H[Q] - H[Z,Q] \approx 1.06 + 1.37 - 1.58 \approx 0.85.$$

- **Normalized mutual information**:

$$\mathrm{NMI}[Z,Q] = \frac{\mathrm{MI}[Z,Q]}{\sqrt{H[Z]}\sqrt{H[Q]}} \approx \frac{0.85}{\sqrt{1.06}\sqrt{1.37}} \approx 0.70.$$

Summary

- **Clustering**
  Idea: *Group observations that a similar in some way*
  - K-means

    Key aspects: K, initialization, distance function and method for recomputing centroids
  - Hierachical clustering and linkage functions

    Key aspects: distance function, linkage function (minimum/signal, maximum/complete, average and Ward), and K/cutoff threshold
- **Comparison of clustering solutions**
  Idea: *Consider which observations are clustered together (or not) in the two solutions*
  - Rand index
  - Jaccard
  - NMI

Resources