02450: Introduction to Machine Learning and Data Mining

K-means and hierarchical clustering

Jes Frellsen

DTU Compute, Technical University of Denmark (DTU)

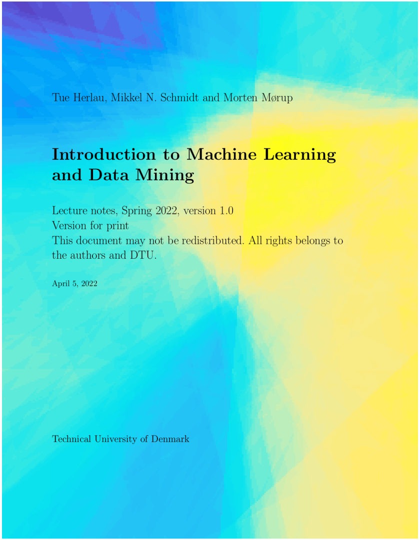
Today

Feedback Groups of the day:

Mikkel Hillebrandt Thorsager, Christian Merithz Uhrenfeldt Nielsen, Mikkel Inti Skærbæk Tabi Espinosa Olsen, Kledi Salla, Anna Melidi, Sebastian Oberg, Baran Öz, Lucian Vrbanc, Mark Waalen Sandberg, Wojciech Stanis¿aw Ponikiewski, Esben Vestergaard Øyan, Emilie Zunda Primdahl Thaulow, Amalie Sommer Thomsen, Magnus Elias Fjellerup Meyer, Ondrej Marvan, Filip Spacek, Jakub Zeman, Jade Jaiyeola Norton, Erikas Mikuzis, Fouad Nara, Dögg Tyril, Sofiya Sayadzade, Thomas Halkier Nicolajsen, Verdande Rani Kim Pedersen, Magnus Leander Ovason, Karítas Ósk Pálmadóttir, Vít Palovský, Anirudh Parakkunnath, Rikke Chrishell Jennifer Dissing Pedersen, Italo Peralta, Mohammad Asim Raja, Viset Raksa, Peter Selzer Rasmussen, Janus Leonard Rasmussen, Eik Lykke Ring

Reading material:

Chapter 18



Lecture Schedule

1. Introduction
   31 January: C1

Data: Feature extraction, and visualization

2. Data, feature extraction and PCA
   7 February: C2, C3
3. Measures of similarity, summary statistics and probabilities
   14 February: C4, C5
4. Probability densities and data visualization
   21 February: C6, C7

Supervised learning: Classification and regression

5. Decision trees and linear regression
   28 February: C8, C9
6. Overfitting, cross-validation and Nearest Neighbor
   7 March: C10, C12 **(Project 1 due before 13:00)**
7. Performance evaluation, Bayes, and Naive Bayes
   14 March: C11, C13
8. Artificial Neural Networks and Bias/Variance
   21 March: C14, C15
9. AUC and ensemble methods
   28 March: C16, C17

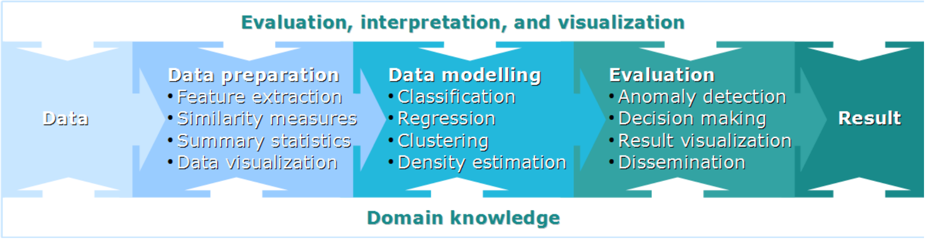
Unsupervised learning: Clustering and density estimation

10. **K-means and hierarchical clustering**
    11 April: C18
11. Mixture models and density estimation
    18 April: C19, C20 **(Project 2 due before 13:00)**
12. Association mining
    25 April: C21

Recap

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

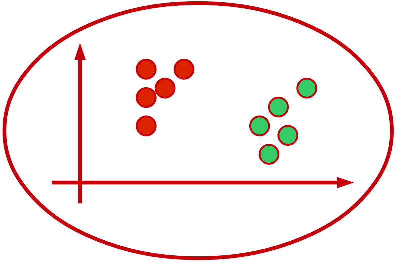
Online 24/7 help: Discussion Forum/Piazza
Streaming & Videos: `https://panopto.dtu.dk/`
Online exercises: MS Teams



Learning Objectives

- Understand the principles behind K-means and hierarchical clustering
- Understand how different linkage functions affects clustering types
- Evaluate clustering quality using class label information

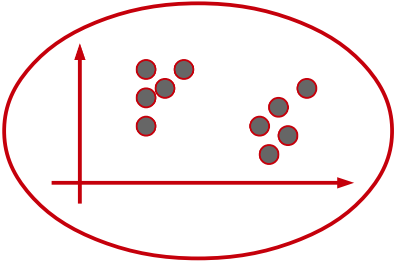
Supervised and Unsupervised learning



Supervised Learning

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

(Classification and Regression)

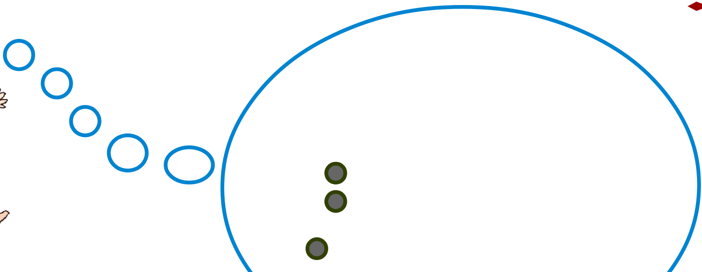


Unsupervised Learning

Input data $\mathbf{x}_n$ alone

(Exploratory analysis)

Imagine you observe the world for the first time!



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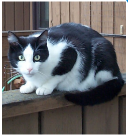

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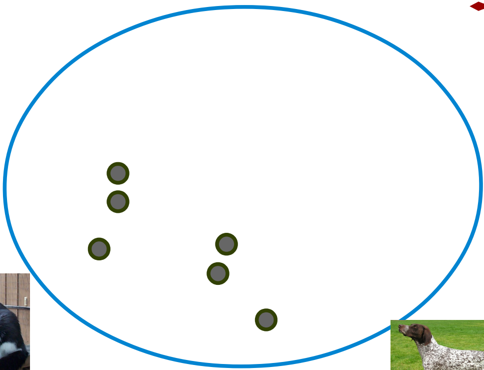

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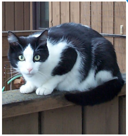

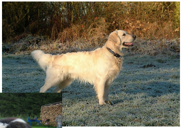


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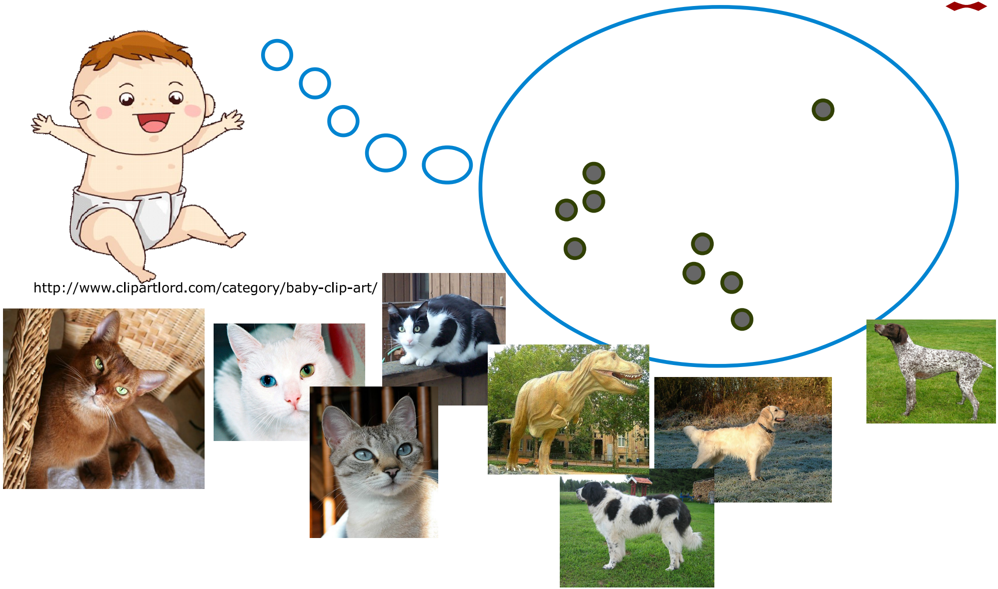

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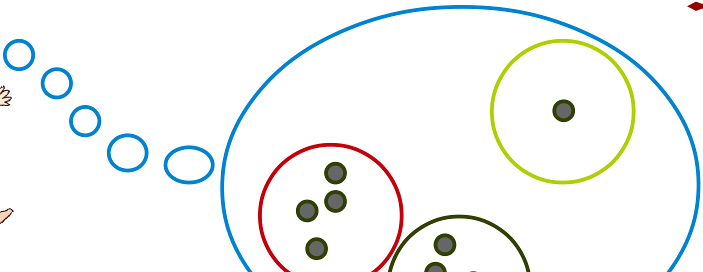

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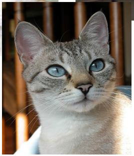

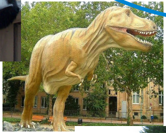

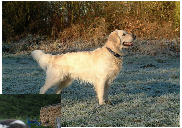

We humans are skilled at dividing objects into groups (clustering), but how do we make computers do the same?

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http://commons.wikimedia.org/wiki/File:Cat_Eyes.jpg
http://commons.wikimedia.org/wiki/File:Black_white_cat_on_fence.jpg
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https://commons.wikimedia.org/wiki/Dog#/media/File:BluetickCoonhound.jpg
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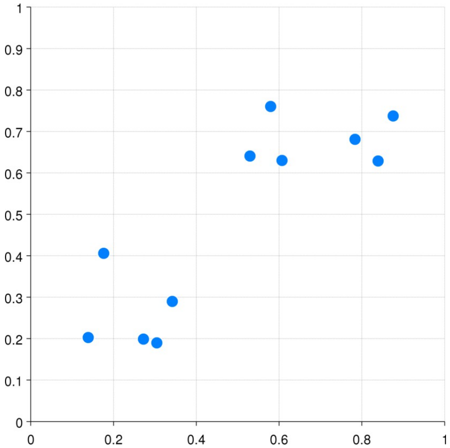
Unsupervised learning

- **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.

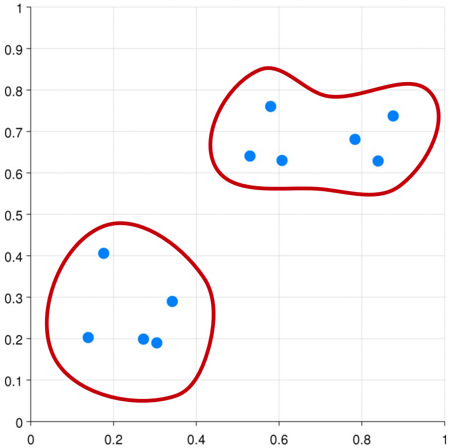
Clustering

- 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



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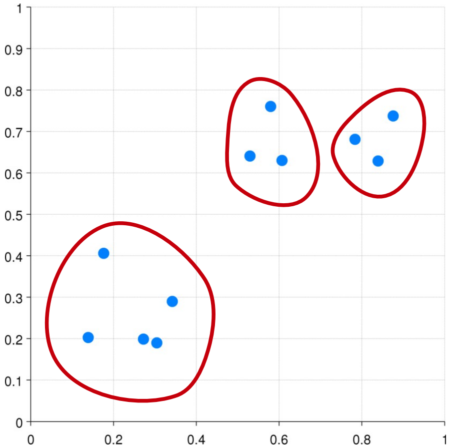

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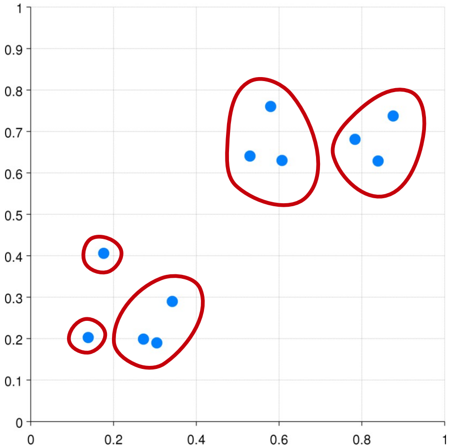
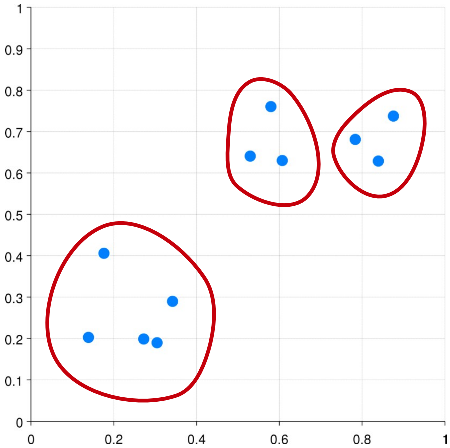
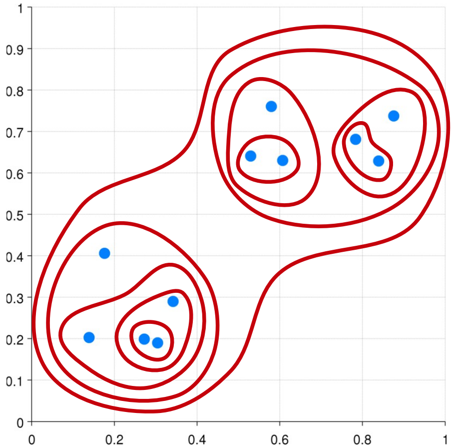


Partitional / hierarchical clustering

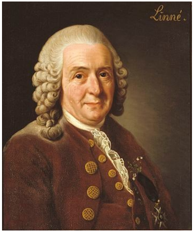
Partitional



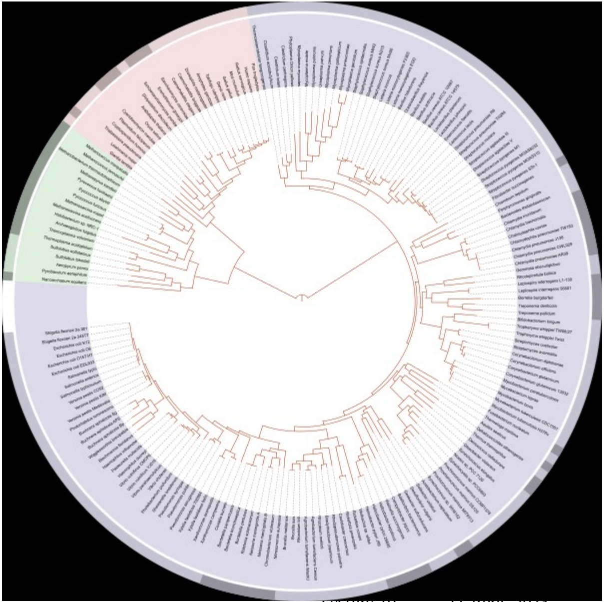
Hierarchical



Phylogenetic trees may be considered a type of hierarchical clustering



Carl Linnaeus
(1707 – 1778)
http://en.wikipedia.org/wiki/Carl_Linnaeus

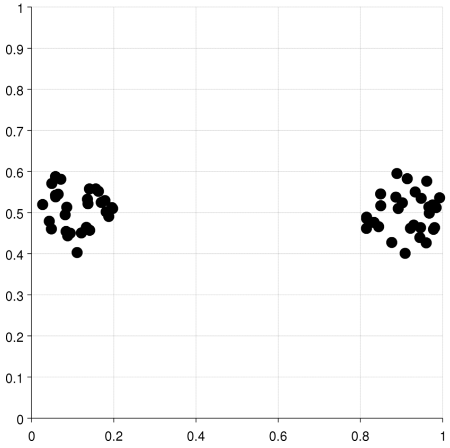


http://en.wikipedia.org/wiki/File:Tree_of_life_SVG.svg

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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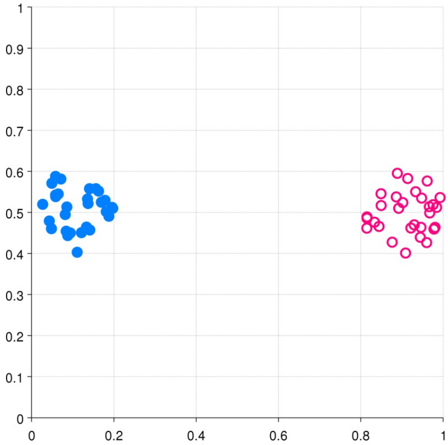
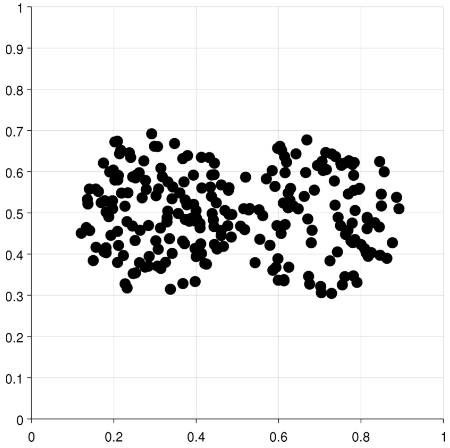


Types of clustering

Center-based

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



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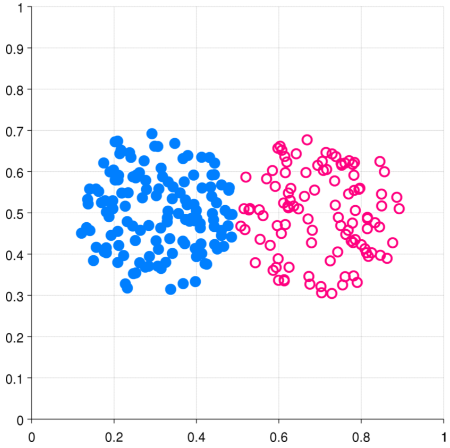
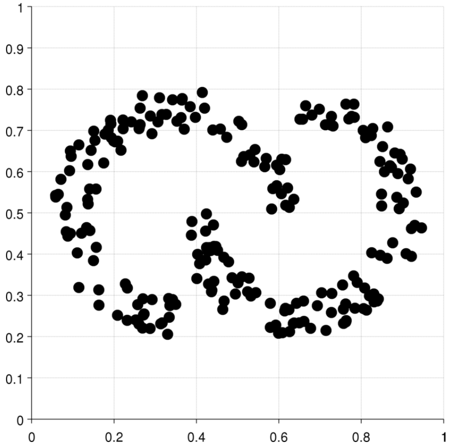


DTU

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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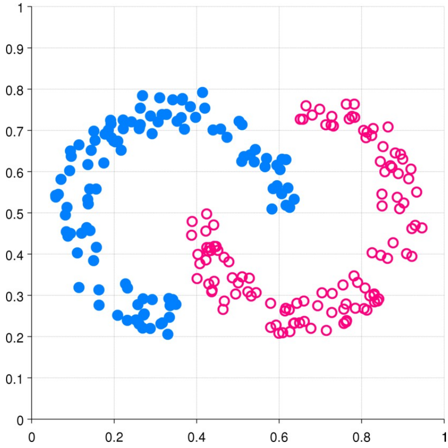
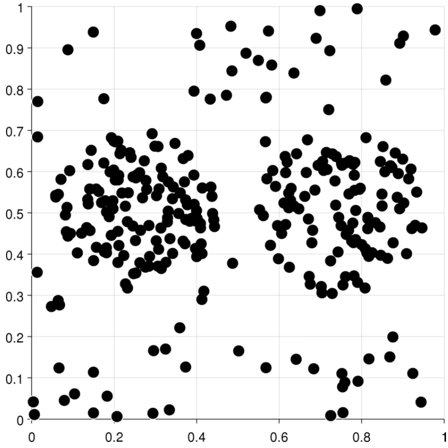


Types of clustering

Density-based

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



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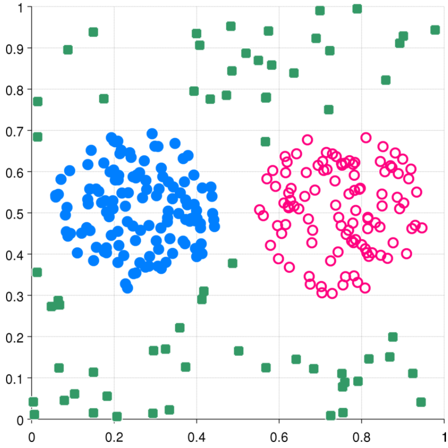
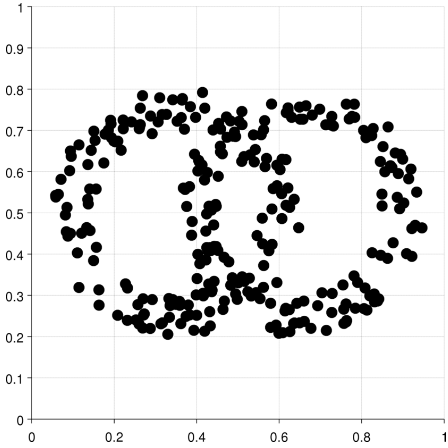


Types of clustering

Conceptual clusters

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



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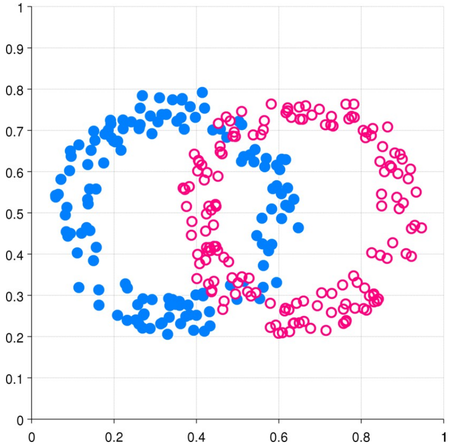

Quiz 01 (please answer on Piazza): Clustering types

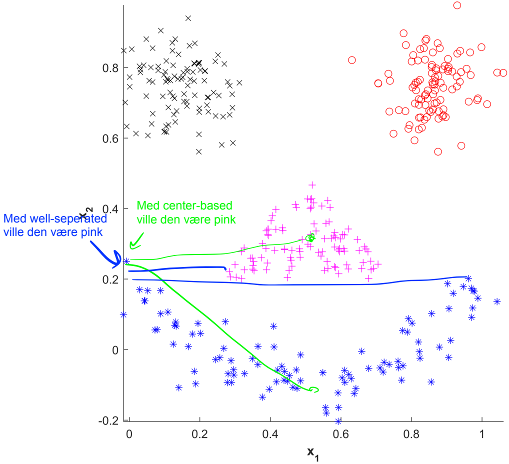

Figure 1: A clustering problem containing four clusters indicated by black crosses, red circles, magenta plusses and blue stars.

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.

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

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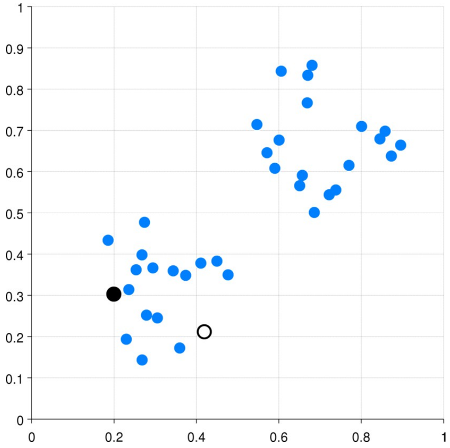

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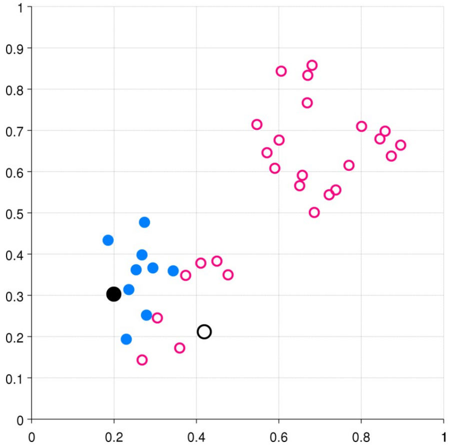

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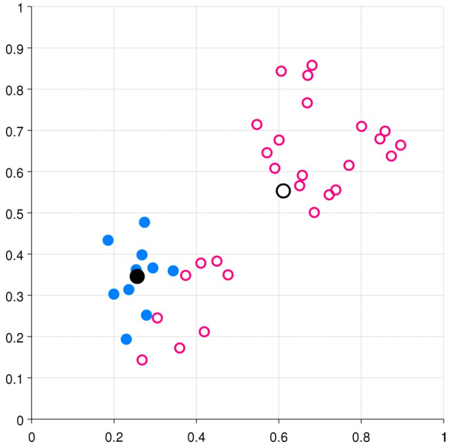

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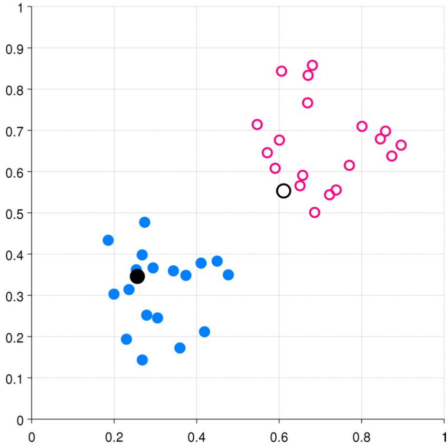

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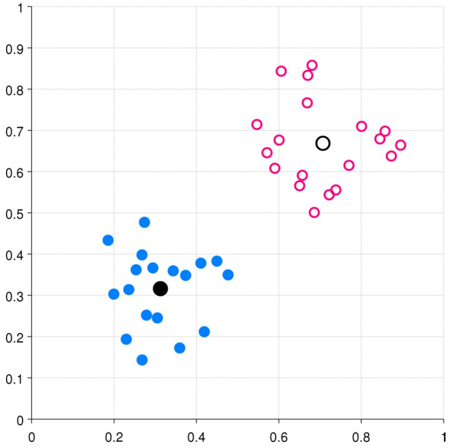


K-means clustering

How do I

- Find the closest centroid?
  - Use a suitable **dissimilarity/similarity measure**
- Compute the cluster centroids
  - Depends on dissimilarity/similarity measure
  - For example, for Euclidean distance the mean is optimal

Quiz 02 (please answer on Piazza): 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. $\{60, 48\}, \{12, 17, 42\}$

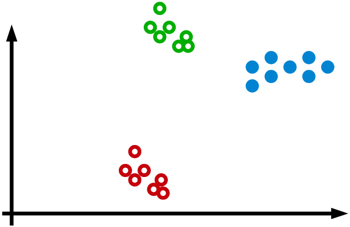
B. $\{42, 60, 48, 17\}, \{12\}$

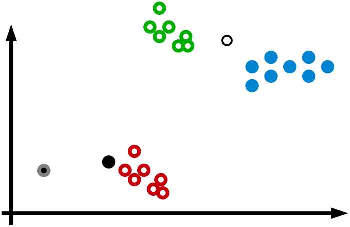
C. $\{60\}, \{12, 17, 42, 48\}$

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

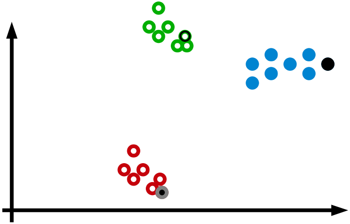
E. Don't know.

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)



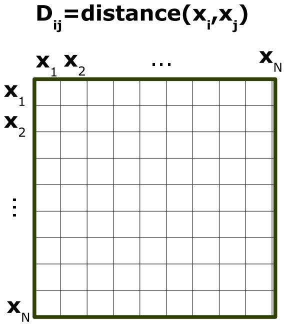
Agglomerative hierarchical clustering

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



Agglomerative hierarchical clustering

Compute the proximity matrix

Repeat

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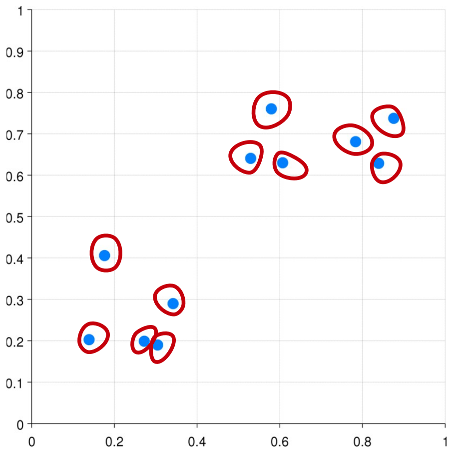

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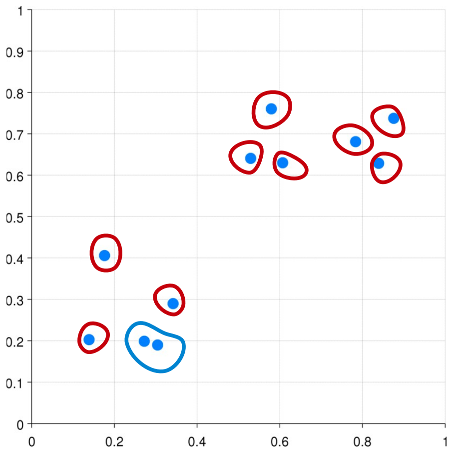

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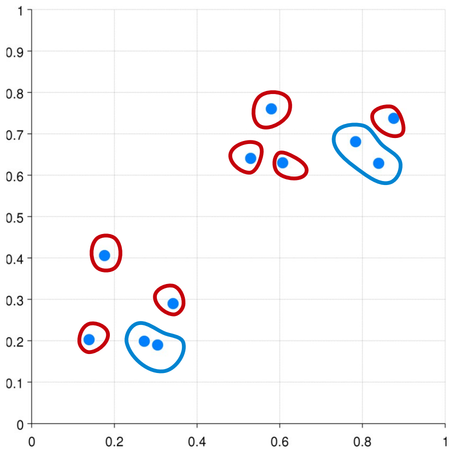

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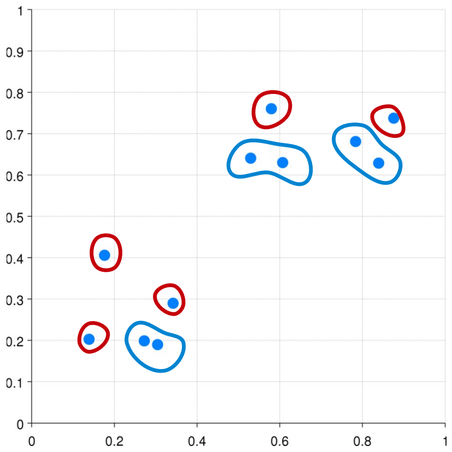

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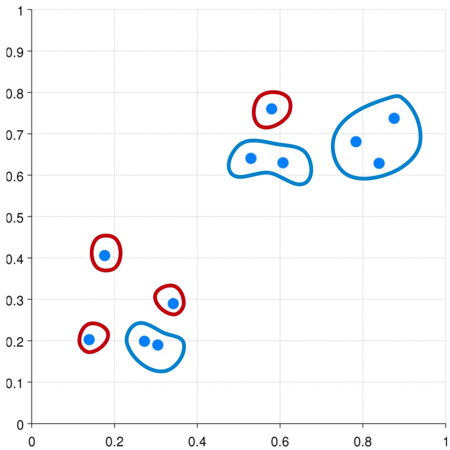

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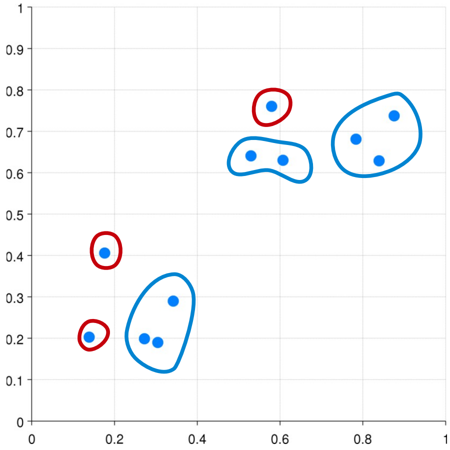

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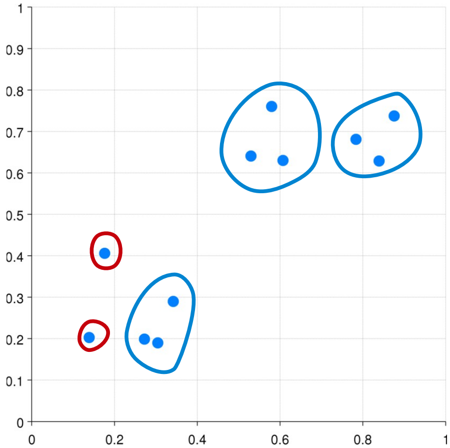

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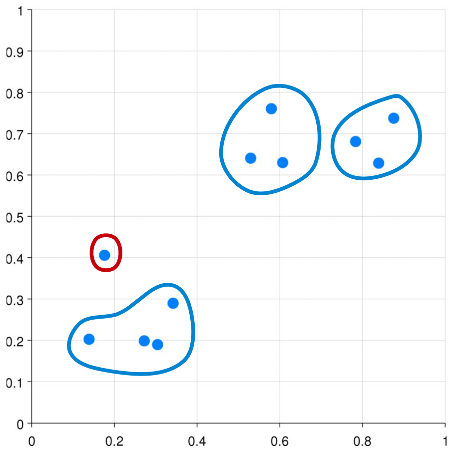
- Update the proximity matrix to reflect the proximity between the new cluster and the original clusters

Until only one cluster remains



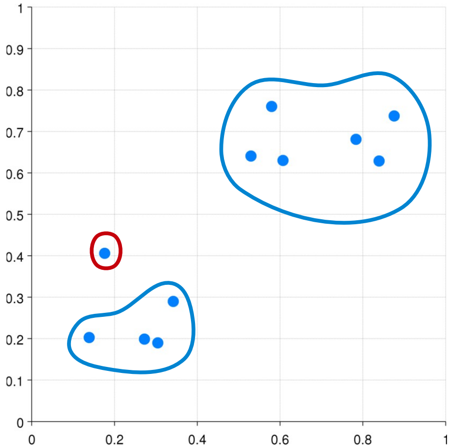
Agglomerative hierarchical clustering

Compute 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



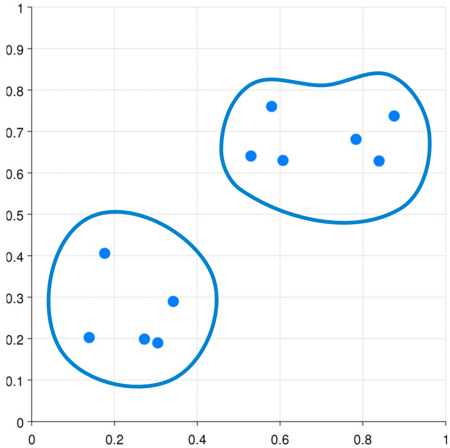
Agglomerative hierarchical clustering

Compute 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



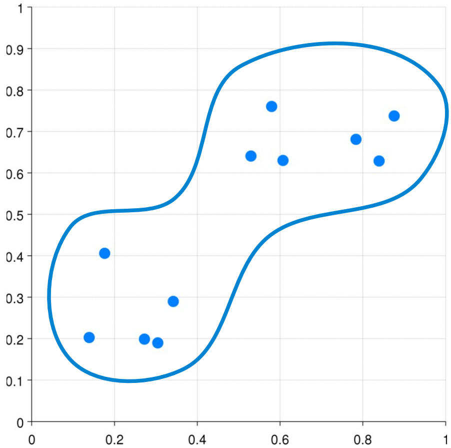
Agglomerative hierarchical clustering

Compute the proximity matrix

Repeat

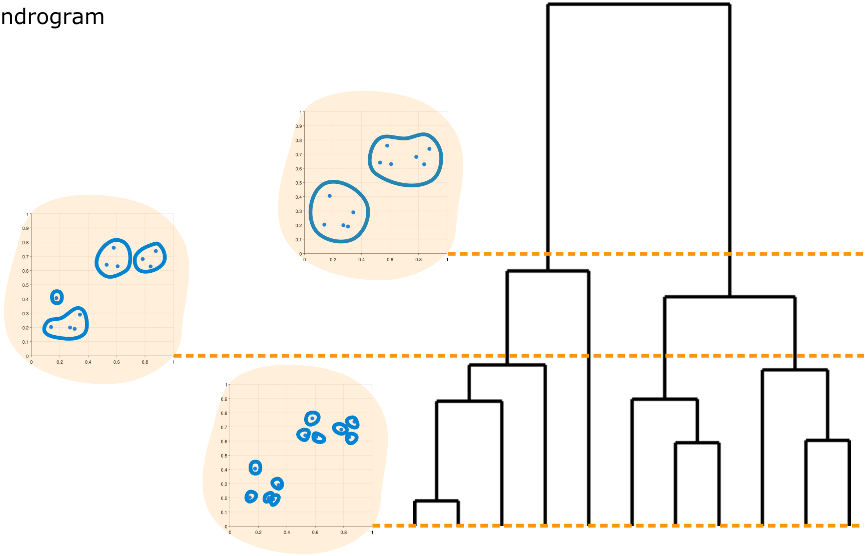
- Merge the two closest clusters
- Update the proximity matrix to reflect the proximity between the new cluster and the original clusters

Until only one cluster remains



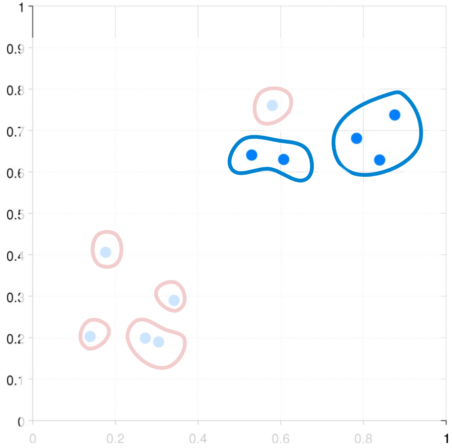
Agglomerative hierarchical clustering

- Dendrogram



Similarity between clusters

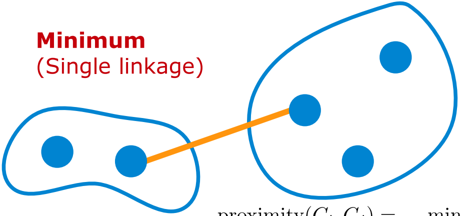
- The **key operation** in agglomerative hierarchical clustering is measuring **distance (dissimilarity) between clusters**



Proximity between clusters

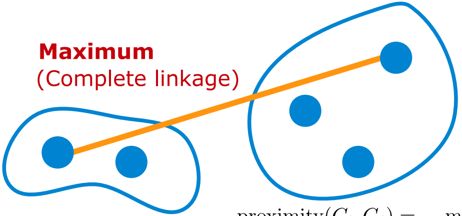
- Can be computed using **proximity between objects**
- In our example before we used Euclidian distance as proximity measure

Minimum
(Single linkage)



$$\text{proximity}(C_i, C_j) = \min_{\boldsymbol{x} \in C_i, \boldsymbol{y} \in C_j} d(\boldsymbol{x}, \boldsymbol{y})$$

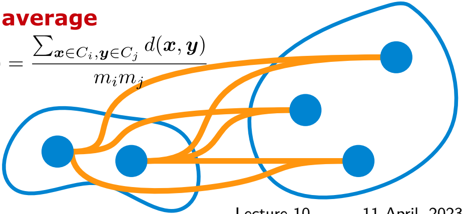
Maximum
(Complete linkage)



$$\text{proximity}(C_i, C_j) = \max_{\boldsymbol{x} \in C_i, \boldsymbol{y} \in C_j} d(\boldsymbol{x}, \boldsymbol{y})$$

Group average

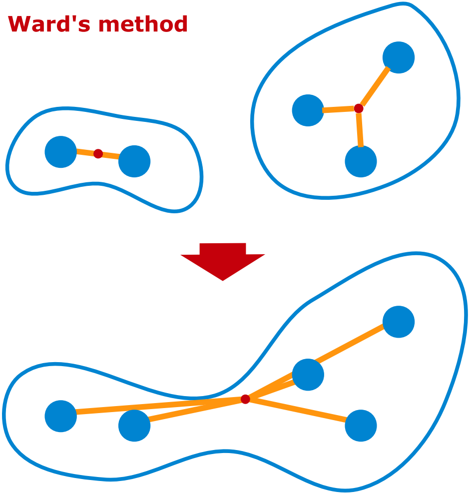
$$\text{proximity}(C_i, C_j) = \frac{\sum_{\boldsymbol{x} \in C_i, \boldsymbol{y} \in C_j} d(\boldsymbol{x}, \boldsymbol{y})}{m_i m_j}$$



C_i: Observations in cluster i
C_j: Observations in cluster j
m_i: Number of observations in cluster i
m_j: Number of observations in cluster j

Similarity between clusters

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

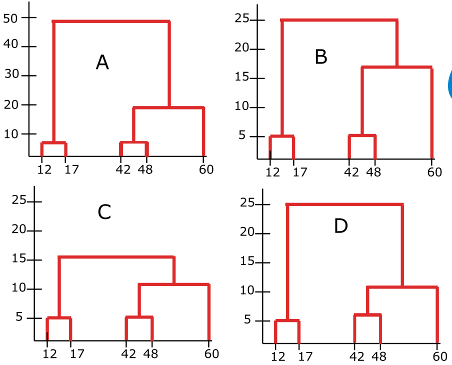


Quiz 03 (please answer on Piazza): Dendrograms

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

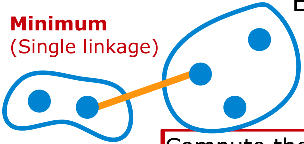
B. Dendrogram B

C. Dendrogram C

D. Dendrogram D

E. Don't know.

Minimum
(Single linkage)



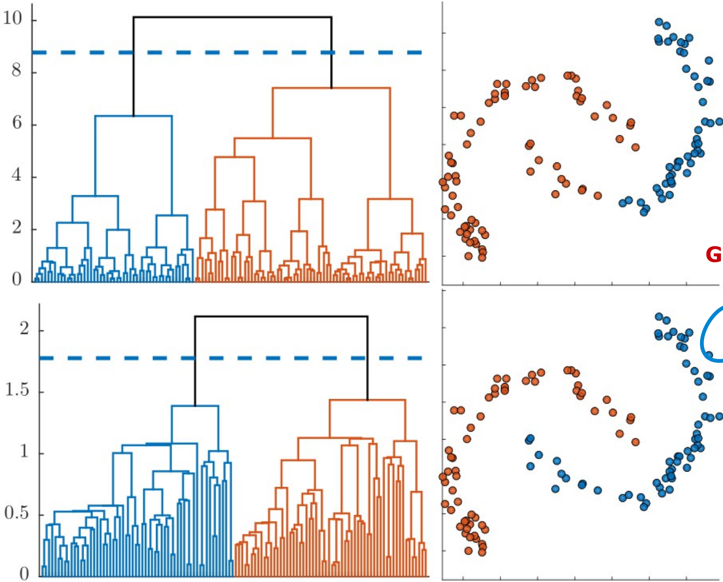
Compute the proximity matrix

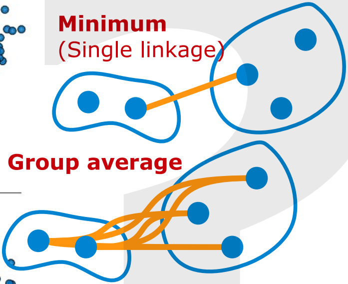
Repeat

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

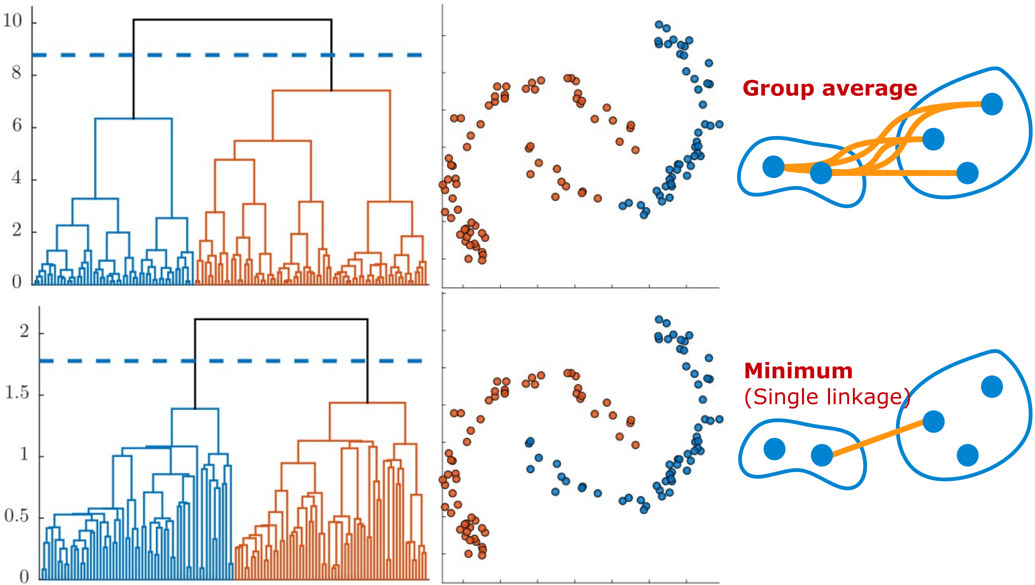
Until only one cluster remains

Clusterings and linkage function

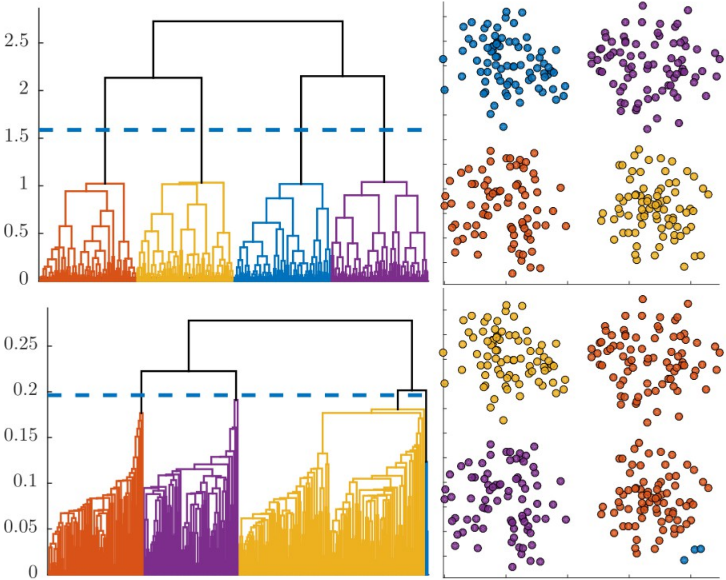


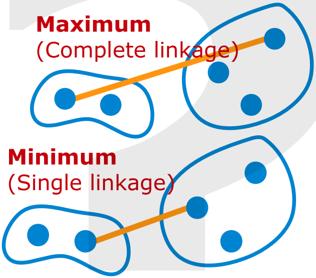


Clusterings and linkage function

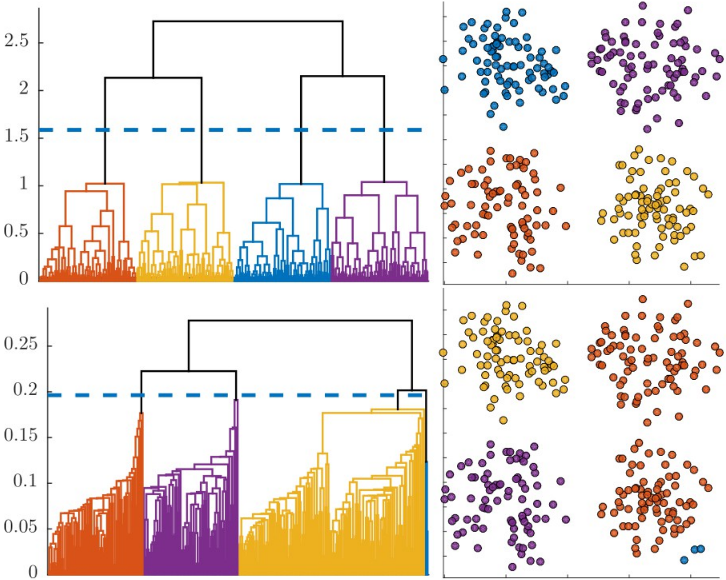


Clusterings and linkage function

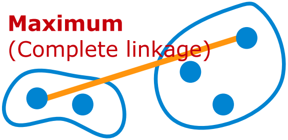




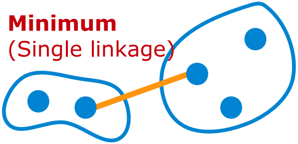
Clusterings and linkage function



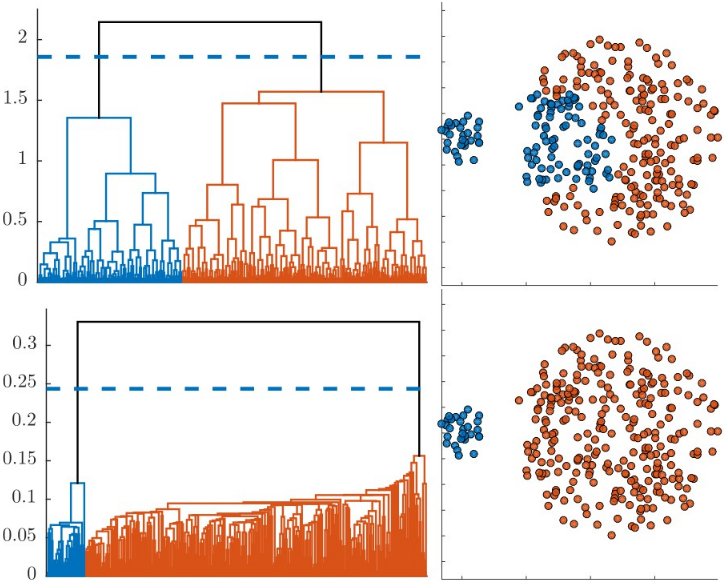
Maximum
(Complete linkage)

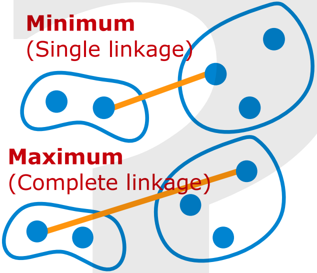


Minimum
(Single linkage)

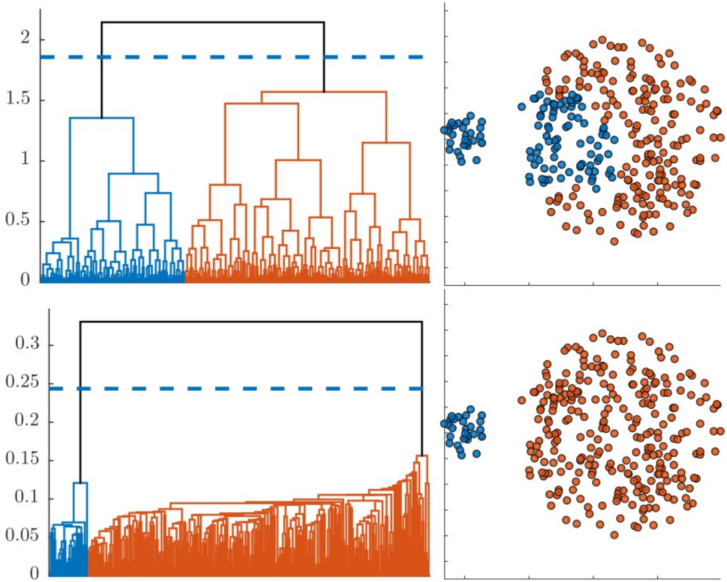


Clusterings and linkage function

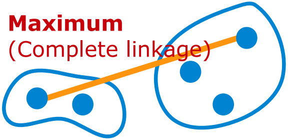




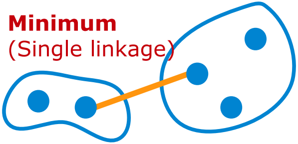
Clusterings and linkage function



Maximum
(Complete linkage)

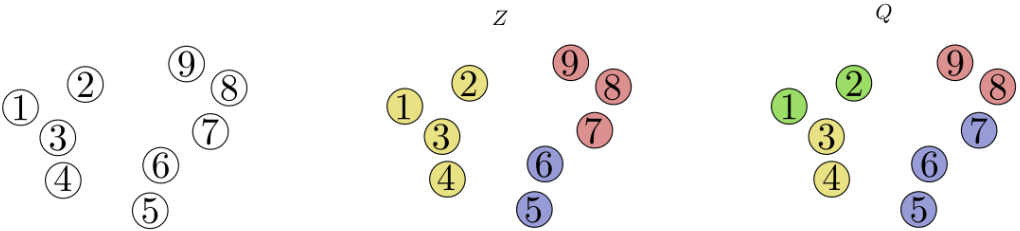


Minimum
(Single linkage)



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

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

Encoding

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

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

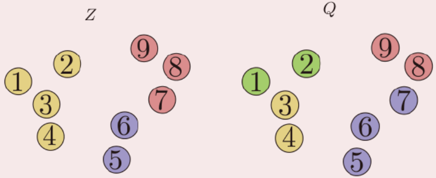
$$\boldsymbol{n}^Q = \{\text{Number of observations assigned to cluster } m \text{ in } Q\} = \sum_{k=1}^{K} n_{km}$$

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

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

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

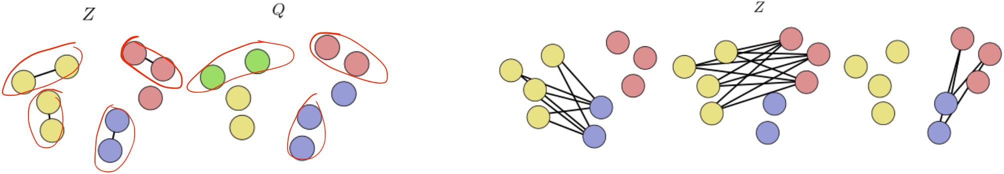
$$Z = \begin{bmatrix} 1 & 1 & 1 & 1 & 2 & 2 & 3 & 3 & 3 \end{bmatrix}$$
$$Q = \begin{bmatrix} 4 & 4 & 1 & 1 & 2 & 2 & 2 & 3 & 3 \end{bmatrix}$$



Jaccard and SMC

- Any two observations i, j can either be in the same cluster, or in different clusters
- There are $\frac{1}{2}N(N-1)$ pairs total
- We get two $\frac{1}{2}N(N-1)$-long binary vectors corresponding to each pair i, j

$$S = \{\text{ Number of pairs } i, j \text{ in the same cluster in } Z, Q\}$$
$$D = \{\text{ Number of pairs } i, j \text{ in different clusters in } Z, Q\}$$



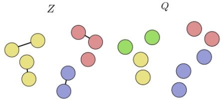
$$\text{Rand index: } R(Z,Q) = \frac{S+D}{\frac{1}{2}N(N-1)} = \frac{4+24}{\frac{1}{2}9\cdot 8} = \frac{7}{9},$$

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

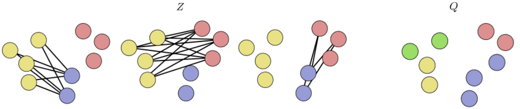
Jaccard and rand index in general

Recall

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



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



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

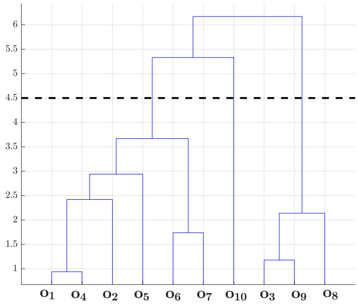


Figure 1: Dendrogram with a cutoff generating 3 clusters.

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

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

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

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

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

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

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

E. Don't know.

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

$$I = -\log p_i$$

- 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:

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

- **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**:

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