Data Mining

HIERARCHICAL CLUSTERING

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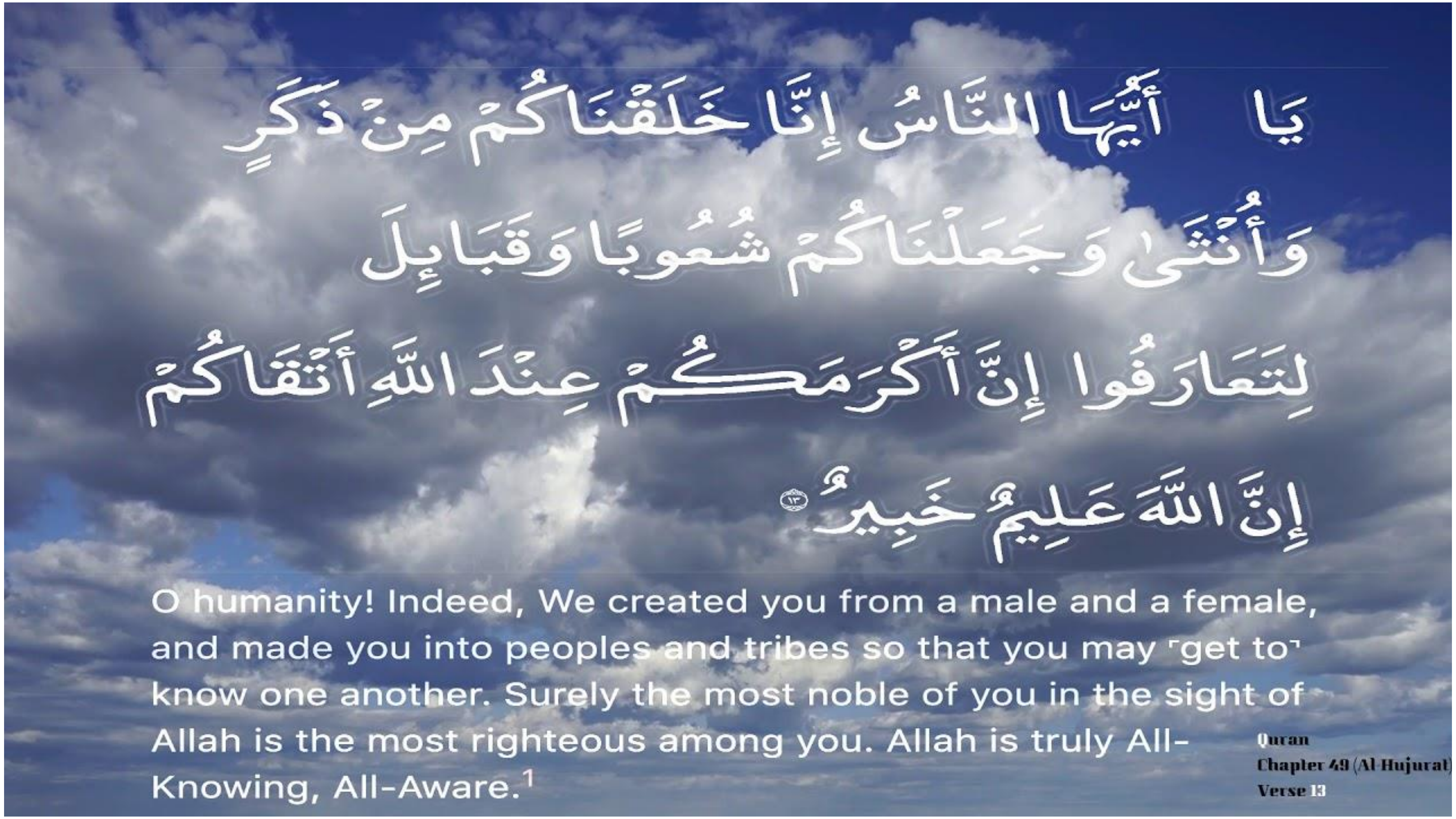
Lesson from Holy Quran



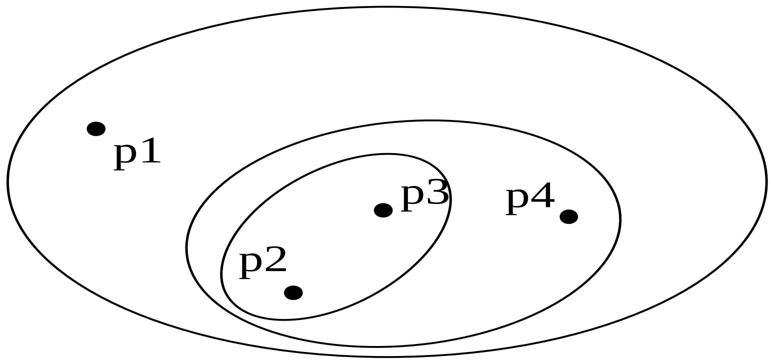
Types of Clusterings

- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

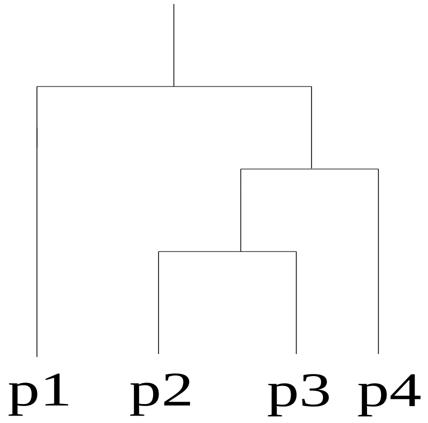
Hierarchical Clustering

- Two main types of hierarchical clustering
  - Agglomerative:
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive:
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

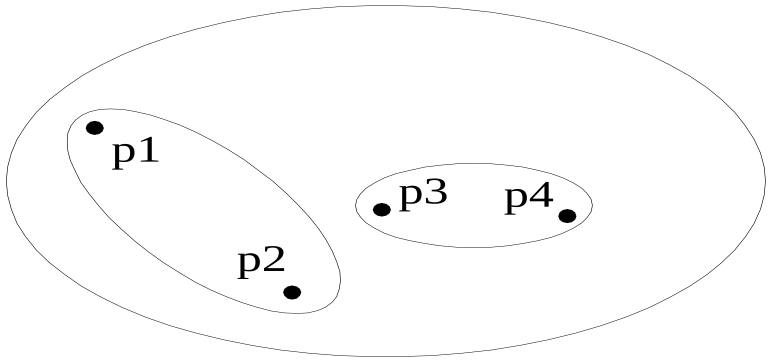
Hierarchical Clustering



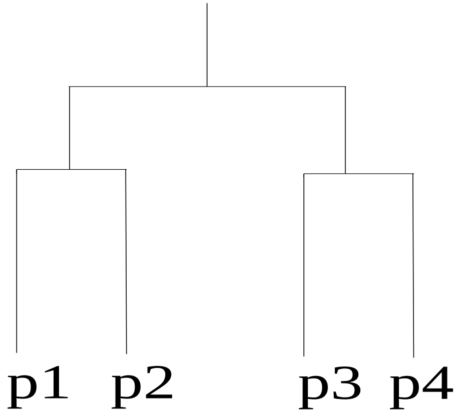
Traditional Hierarchical Clustering



Traditional Dendrogram



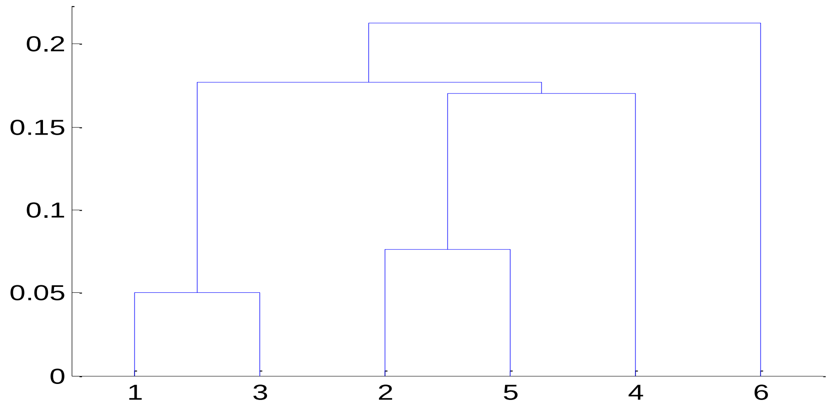
Non-traditional Hierarchical Clustering

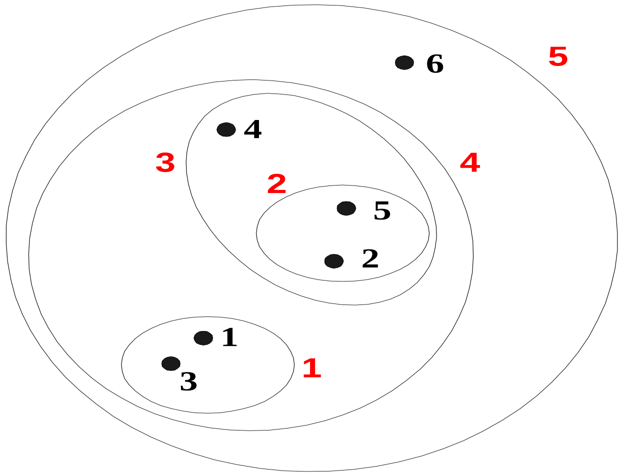


Non-traditional Dendrogram

Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - A tree like diagram that records the sequences of merges or splits





Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by ‘cutting’ the dendogram at the proper level
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, …)

Agglomerative Clustering Algorithm

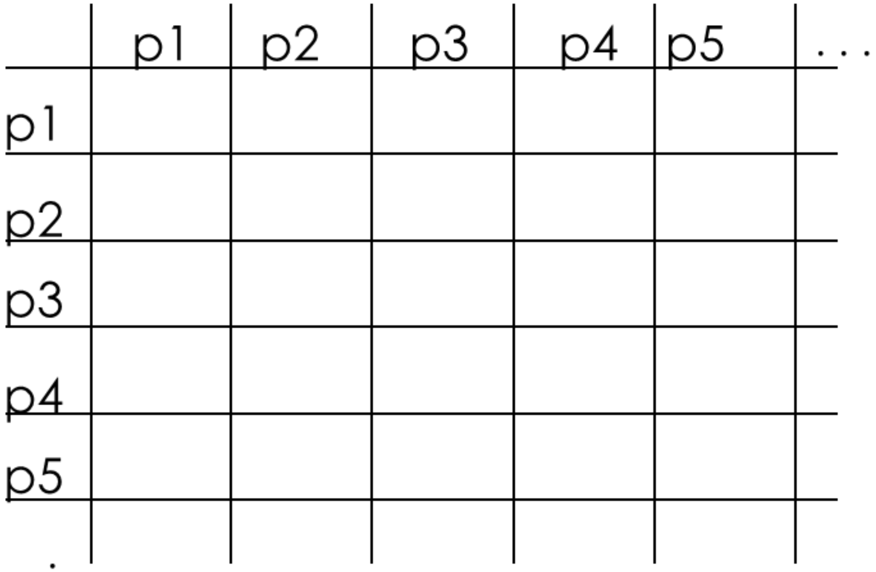
- More popular hierarchical clustering technique

- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. **Repeat**
  4. Merge the two closest clusters
  5. Update the proximity matrix
  6. **Until** only a single cluster remains

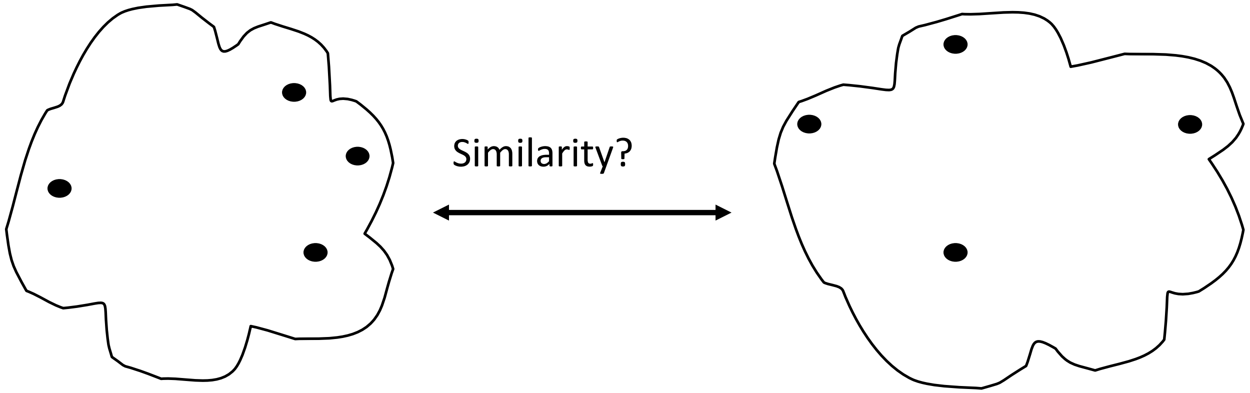
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance between clusters distinguish the different algorithms

How to Define Inter-Cluster Similarity

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  - Ward's Method uses squared error



Proximity Matrix



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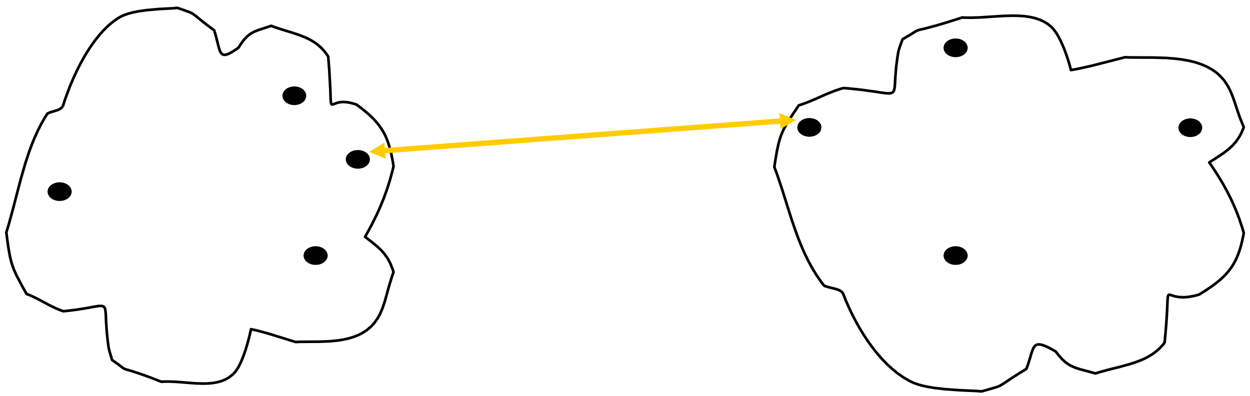

	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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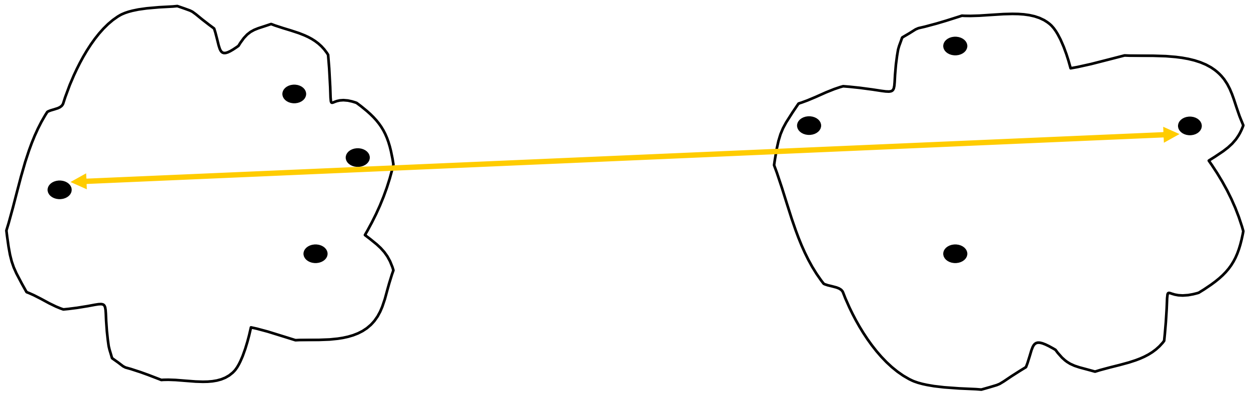

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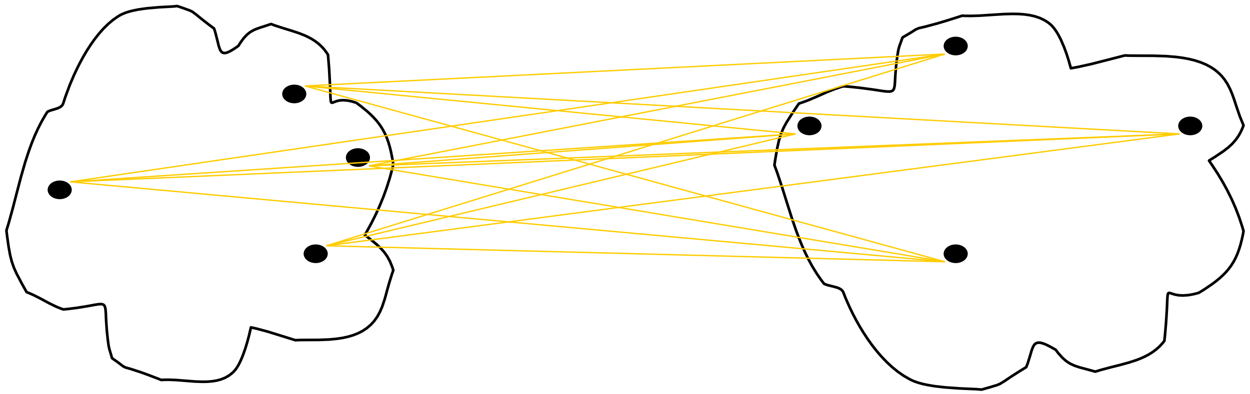

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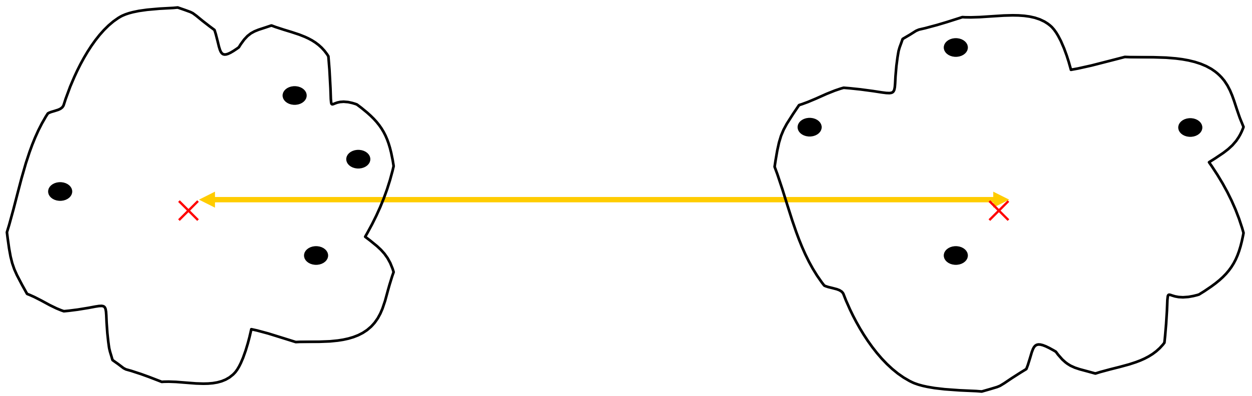

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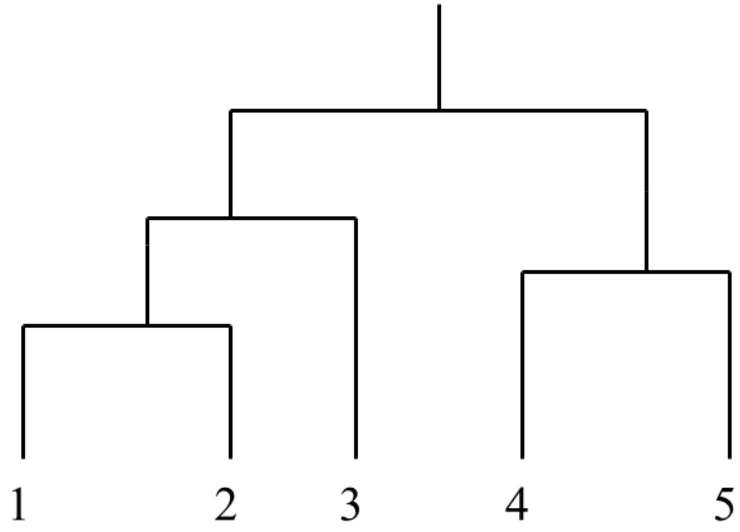
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

Cluster Similarity: MIN

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



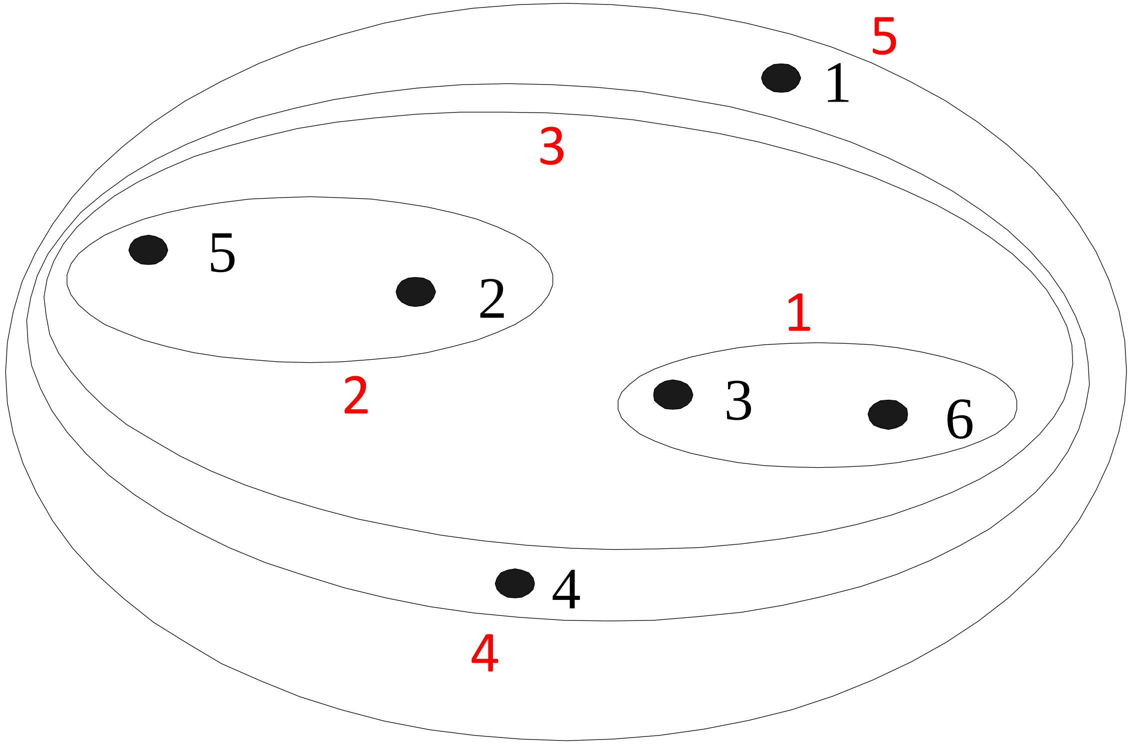
example to create Hierarchical Clustering using MIN

Point	X coordinate	Y coordinate
P1	0.40	0.53
P2	0.22	0.38
P3	0.35	0.32
P4	0.26	0.19
P5	0.08	0.41
P6	0.45	0.30

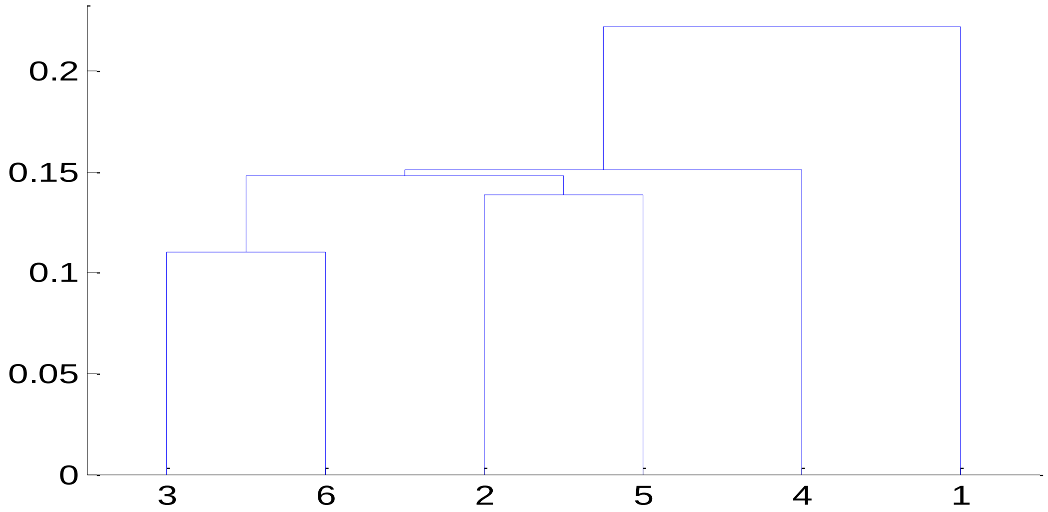
Proximity matrix (Euclidean Distance)

	P1	P2	P3	P4	P5	p6
P1	0.00	0.24	0.22	0.37	0.34	0.23
P2	0.24	0.00	0.15	0.20	0.14	0.25
P3	0.22	0.15	0.00	0.15	0.28	**0.11**
P4	0.37	0.14	0.28	0.00	0.29	0.39
P5	0.34	**0.14**	0.28	0.29	0.00	0.39
P6	0.23	0.25	0.11	0.22	0.39	0.00

Hierarchical Clustering: MIN



Nested Clusters



Dendrogram

1) Min distance of individual in matrix
2) For Grouped values, compute combined min
3) For instance

$$\begin{aligned}\text{Dist}(\{3,6\},\{2,5\}) &= \min(\text{dist}(3,2),\ \text{dist}(6,2),\ \text{dist}(3,5),\ \text{dist}(6,5)) \\ &= \min(0.15,\ 0.25,\ 0.28,\ 0.39) \\ &= 0.15\end{aligned}$$

Finding Distance of [3,6] from 1 and 4 as well:

Dist ({3,6},4}) = min(dist(3,4), dist(6,4))

= min(0.15, 0.22)

= 0.15

Dist ({3,6},1}) = min(dist(3,1), dist(6,1))

= min(0.22, 0.23)

= 0.22

Cluster Validity

- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall
- For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters?
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

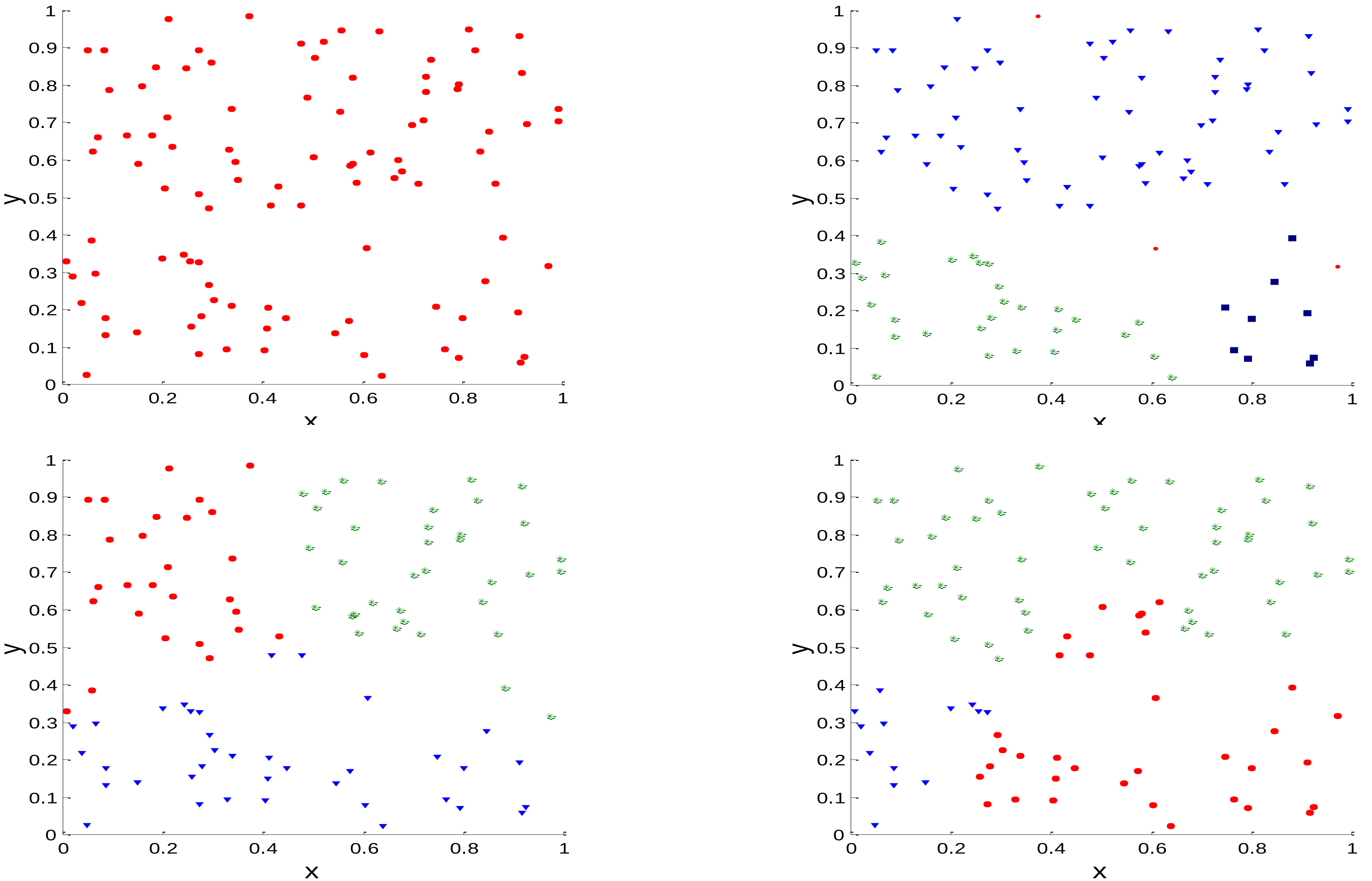
Clusters found in Random Data

Random Points

DBSCAN

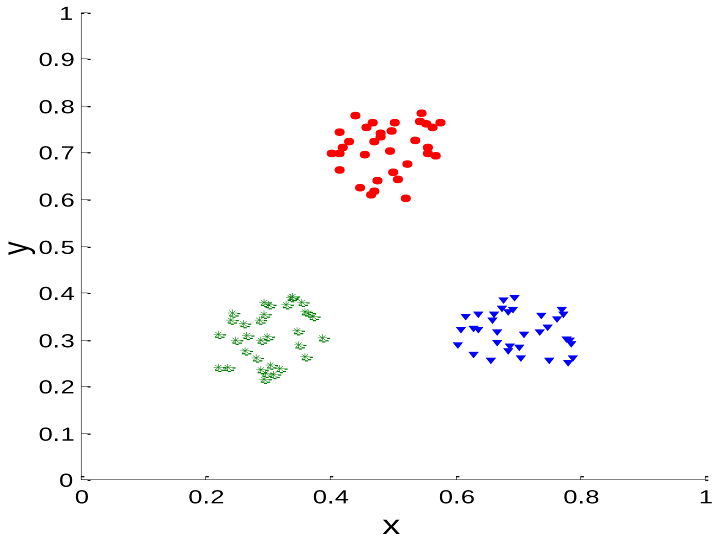
K-means

Complete Link

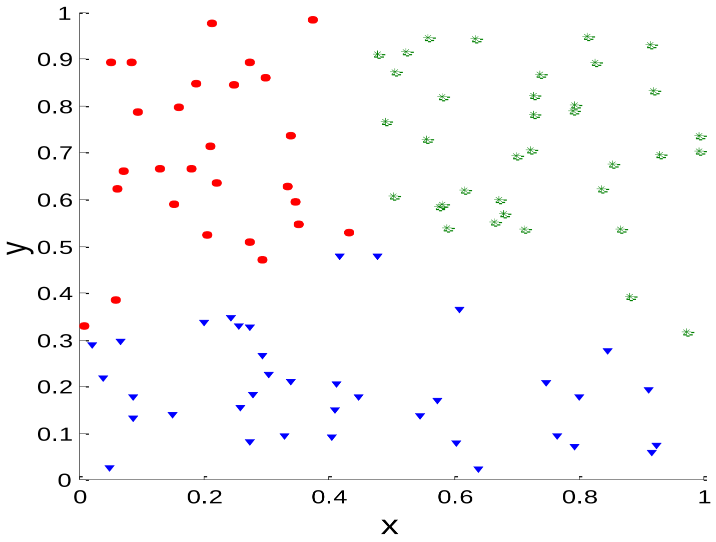


Measuring Cluster Validity Via Correlation

- Correlation of incidence and proximity matrices for the K-means clustering of the following two data sets.

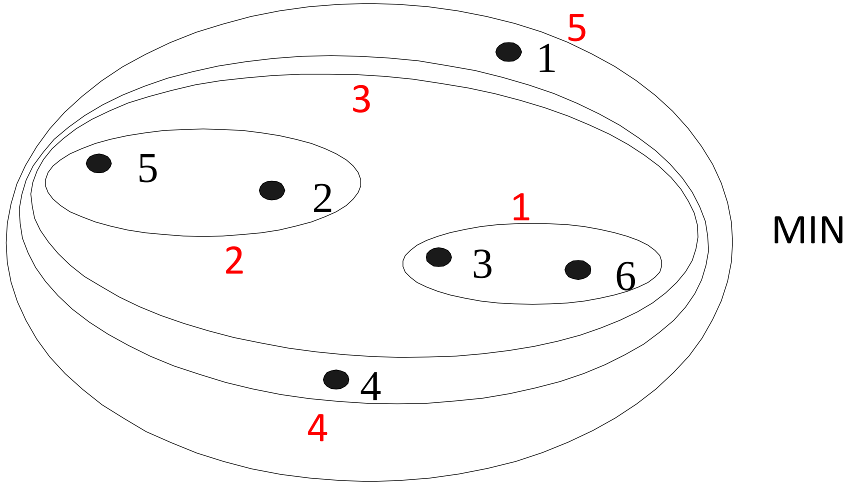


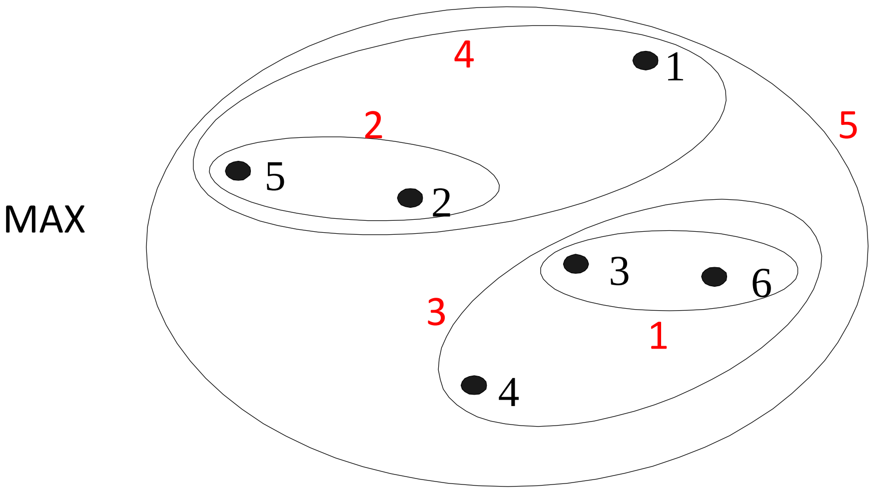
Corr = -0.9235

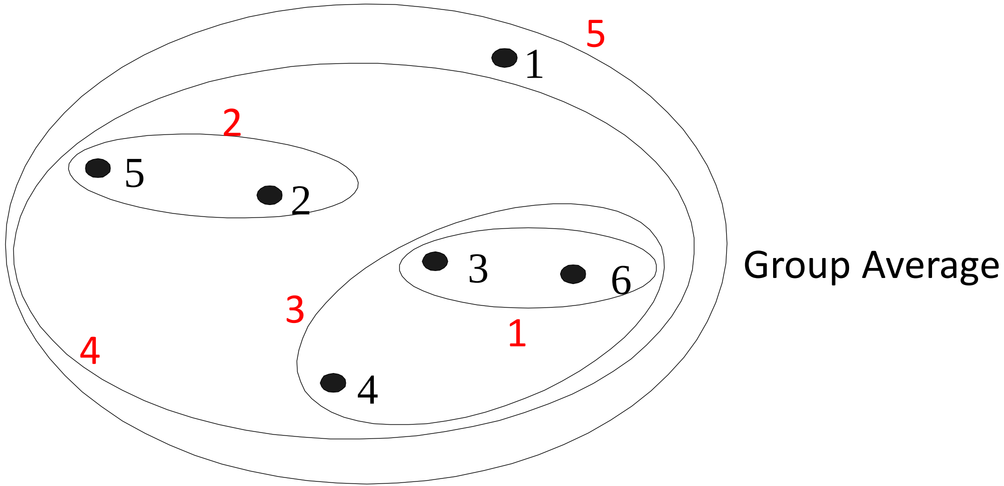


Corr = -0.5810

Hierarchical Clustering: Comparison







Internal Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
  - Example: Sum of Square Error (SSE)
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)

$$WSS = \sum_{i} \sum_{x \in C_i} (x - m_i)^2$$

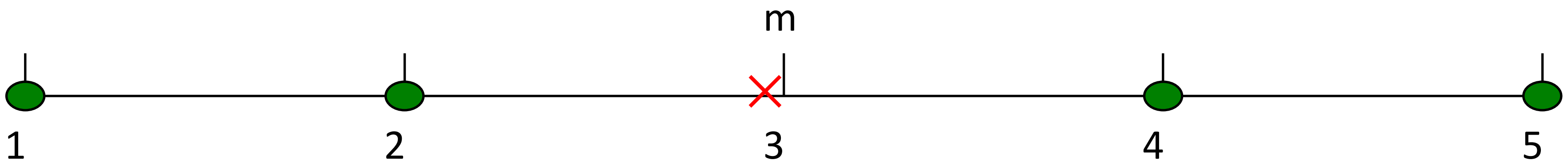
  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_{i} |C_i| (m - m_i)^2$$

    - Where $|C_i|$ is the size of cluster i

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

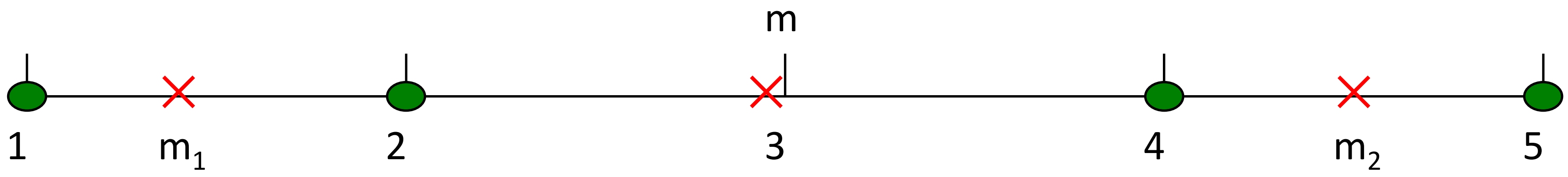
$$WSS = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$BSS = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

$$BSS = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

$$Total = 1 + 9 = 10$$

K=2 clusters:

$$WSS = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$BSS = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$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