Master Degree in Artificial Intelligence for Science and Technology

Cluster Analysis: Hierarchical Clustering

UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA

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OUTLOOK

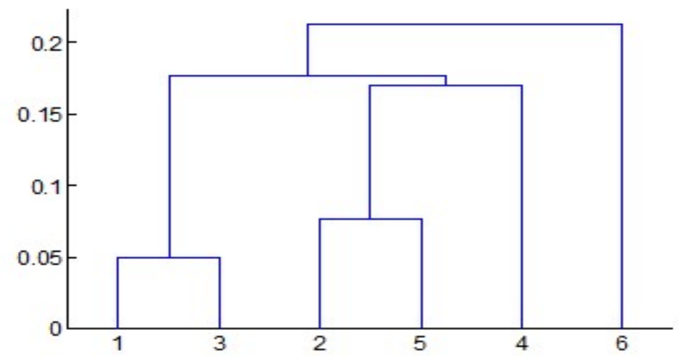
- Concept
- Strengths
- Types
  - ➢ Agglomerative
    - – single linkage
    - – complete linkage
    - – average linkage
    - – Ward's method
  - ➢ Divisive
- Complexity
- Limitations

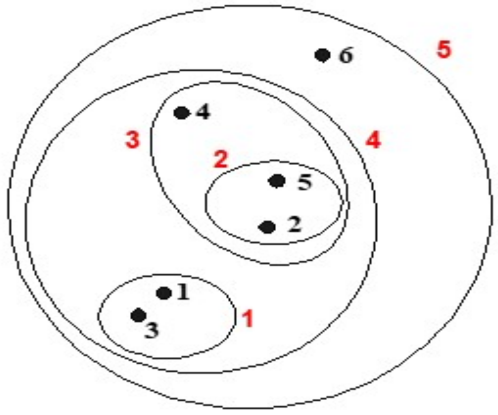
CONCEPT

— produces a set of **NESTED CLUSTERS** organized as a **HIERARCHICAL TREE**

— can be visualized as a **DENDROGRAM**

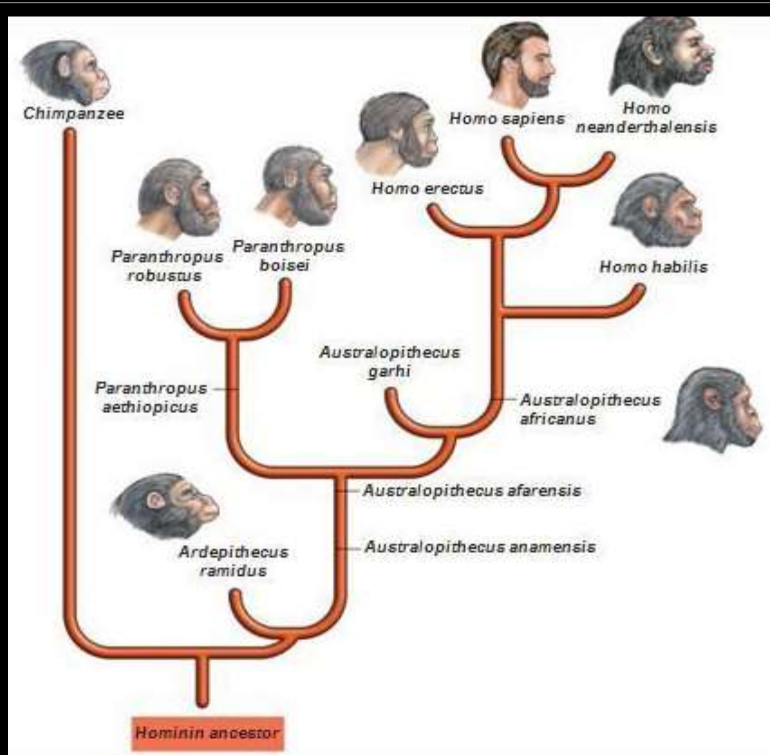
- a tree like diagram that records the sequences of merges or splits





STRENGTHS

- — do not have to assume any particular number of clusters
  - any desired number of clusters can be obtained by 'cutting' the dendrogram at the proper level
- — they may correspond to meaningful taxonomies
  - example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)



TYPES OF 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 an individual point (or there are k clusters)

- Traditional hierarchical algorithms use a similarity or distance matrix
  - merge or split one cluster at a time

AGGLOMERATIVE CLUSTERING

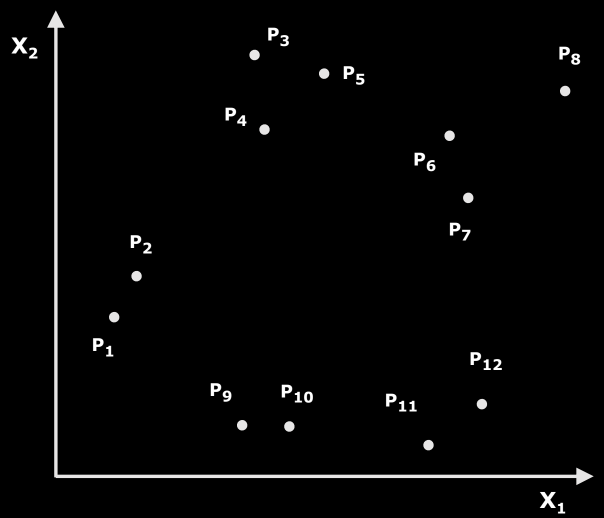
— **KEY IDEA**: successively merge closest clusters

BASIC ALGORITHM

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

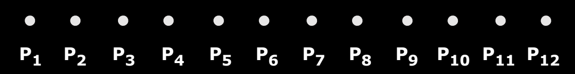
- Key operation is the computation of the proximity of two clusters
- Different approaches to defining the distance between clusters distinguish the different algorithms

AGGLOMERATIVE CLUSTERING



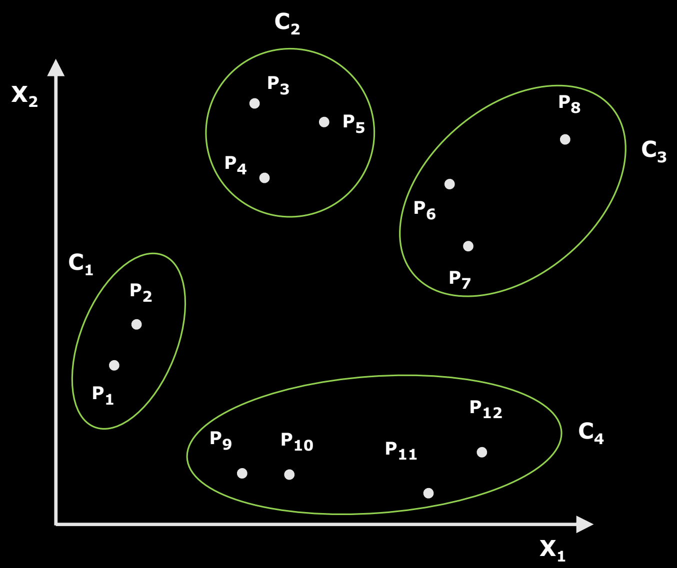
- **STEP 1:** compute the proximity matrix

	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12
p1												
p2												
p3												
p4												
p5												
p6												
p7												
p8												
p9												
p10												
p11												
p12												



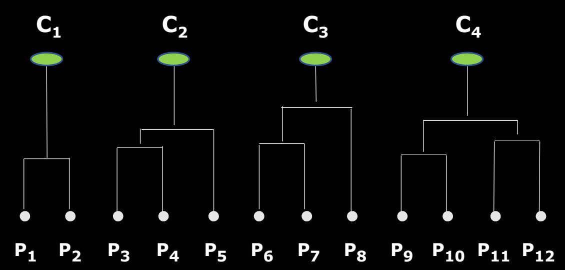
- **STEP 2:** each point is a cluster

AGGLOMERATIVE CLUSTERING



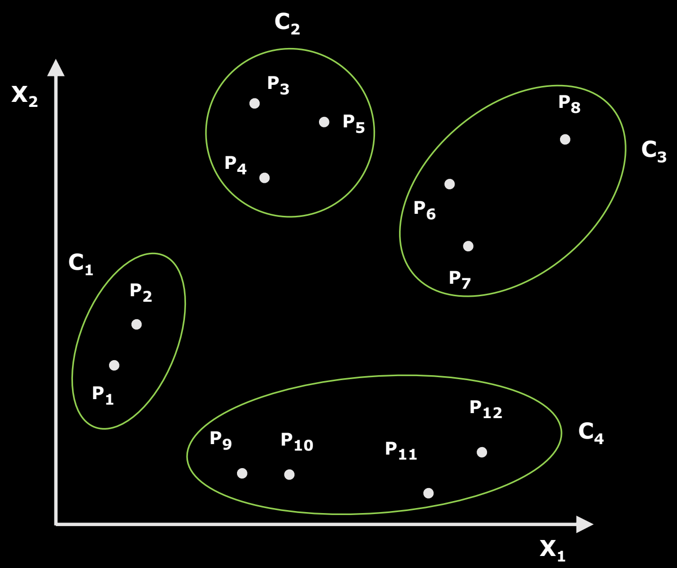
	C1	C2	C3	C4
C1				
C2				
C3				
C4				

PROXIMITY MATRIX



After some merging steps we have some clusters

AGGLOMERATIVE CLUSTERING



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C1				
C2				
C3				
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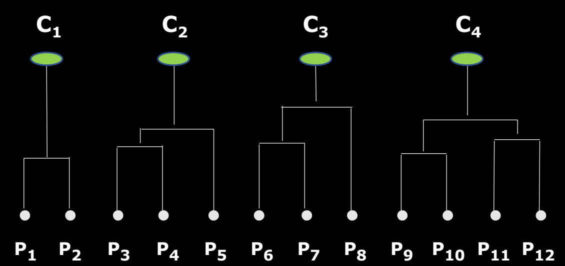
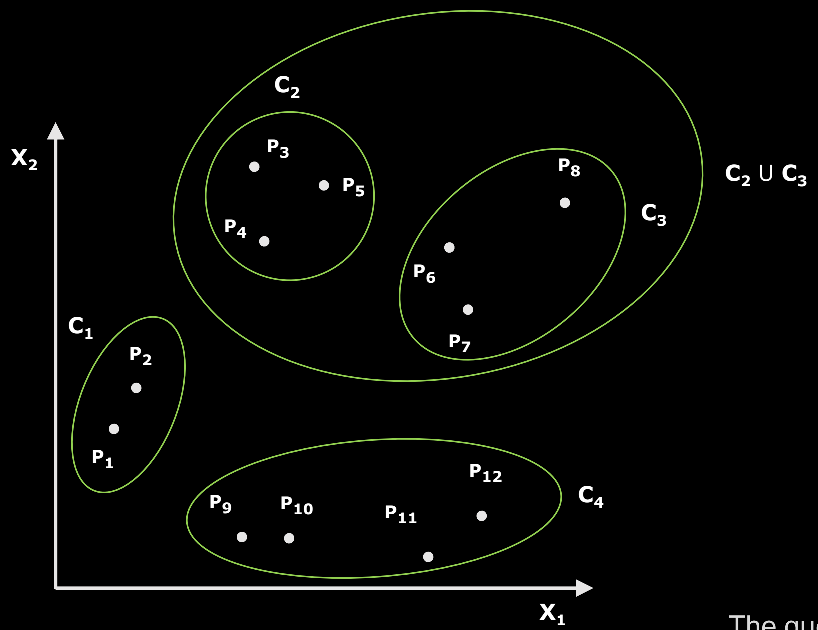


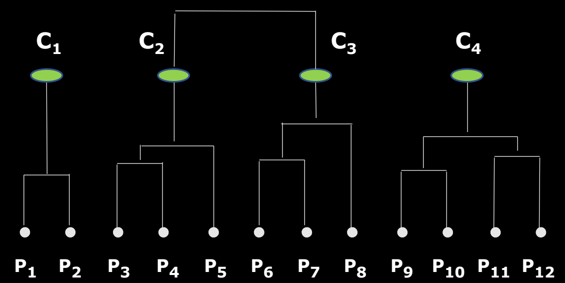
We want to merge the two closest clusters (C_2 and C_3) and update the proximity matrix.

AGGLOMERATIVE CLUSTERING



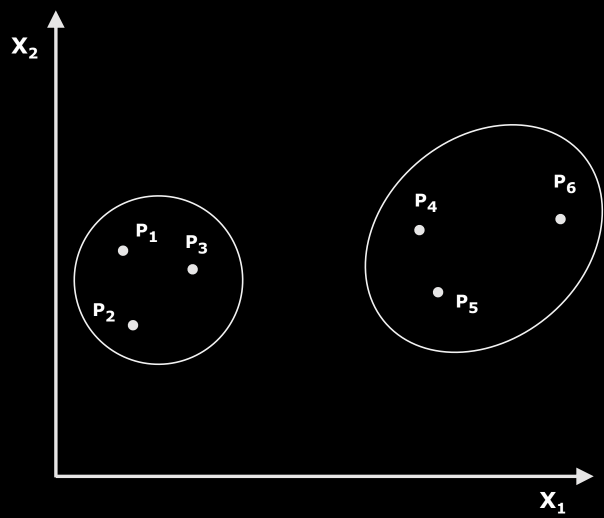
	C1	C2 C3	C4
C1		?	
C2 C3	?	?	?
C4		?	

PROXIMITY MATRIX



The question is "How do we update the proximity matrix?"

HOW TO DEFINE INTER-CLUSTER PROXIMITY?

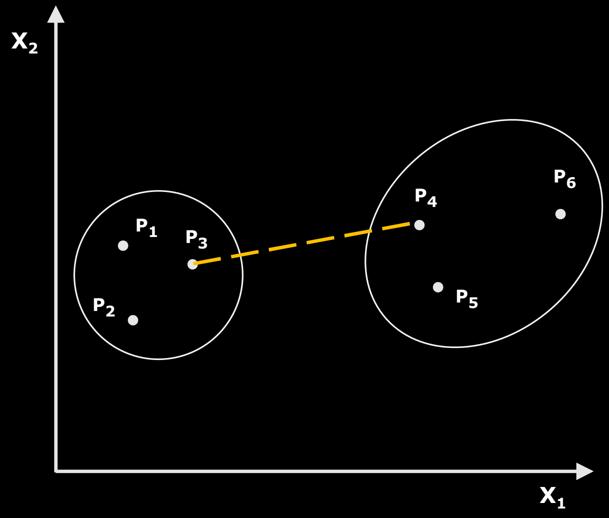


	C1	C2	C3	C4
C1				
C2				
C3				
C4				

PROXIMITY MATRIX

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

HOW TO DEFINE INTER-CLUSTER PROXIMITY?



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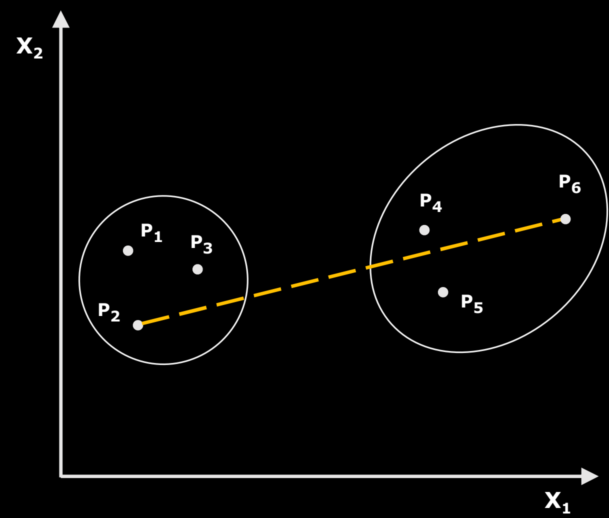

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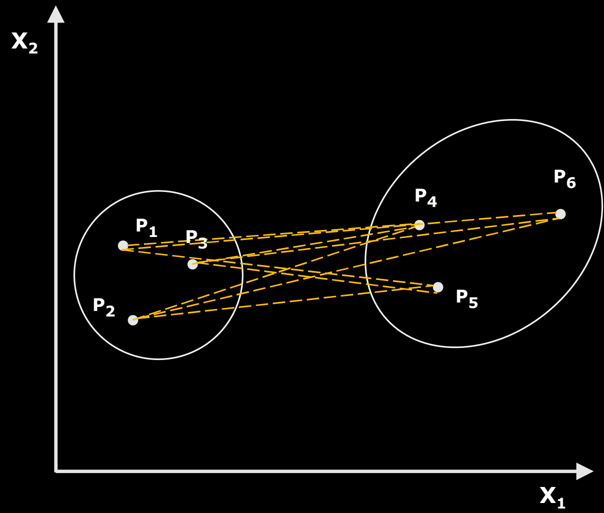

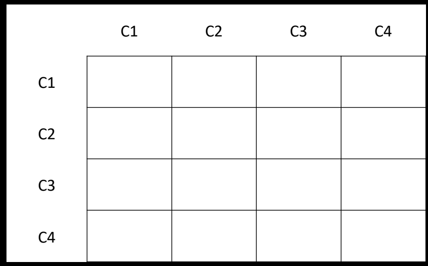

PROXIMITY MATRIX

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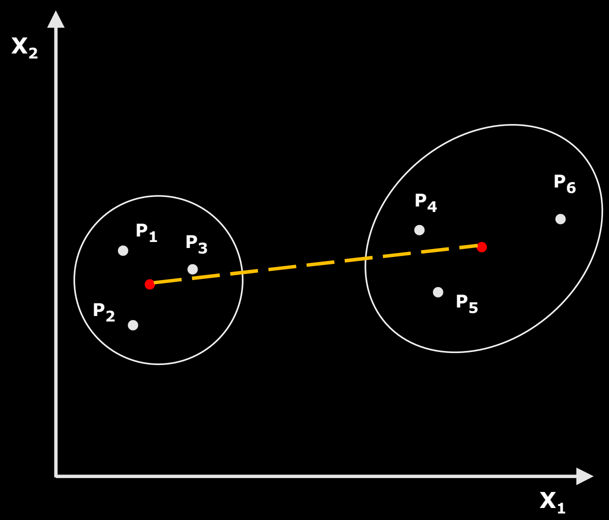

	C1	C2	C3	C4
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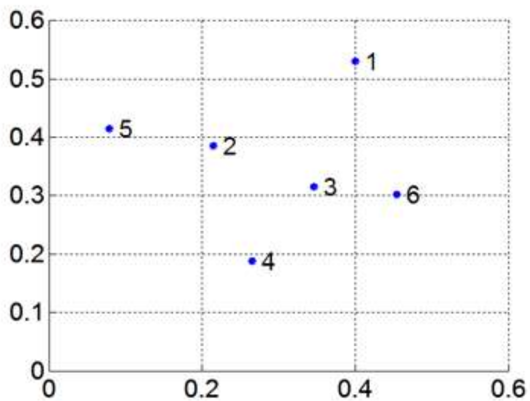
C2				
C3				
C4				

PROXIMITY MATRIX

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

MIN OR SINGLE LINKAGE

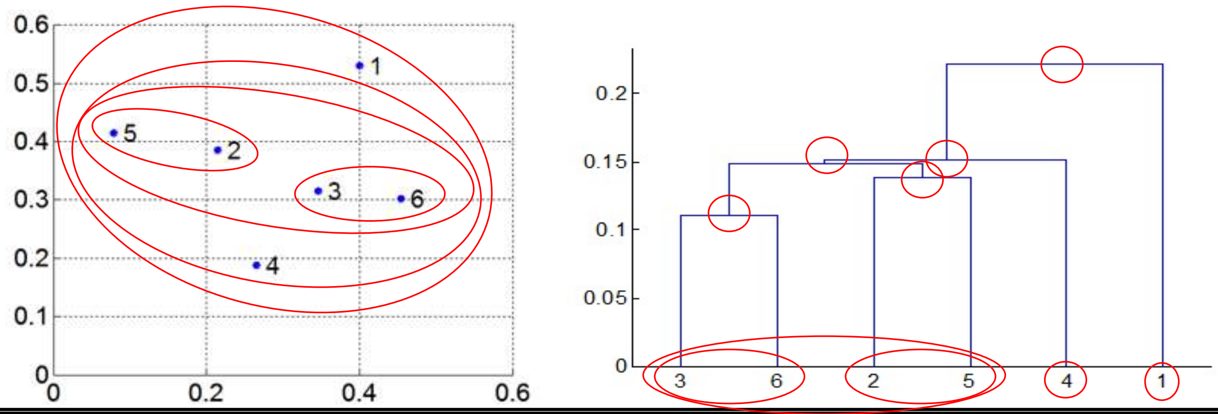
- Proximity of two clusters is based on the two closest points in the different clusters
  - determined by one pair of points, i.e., by one link in the proximity graph



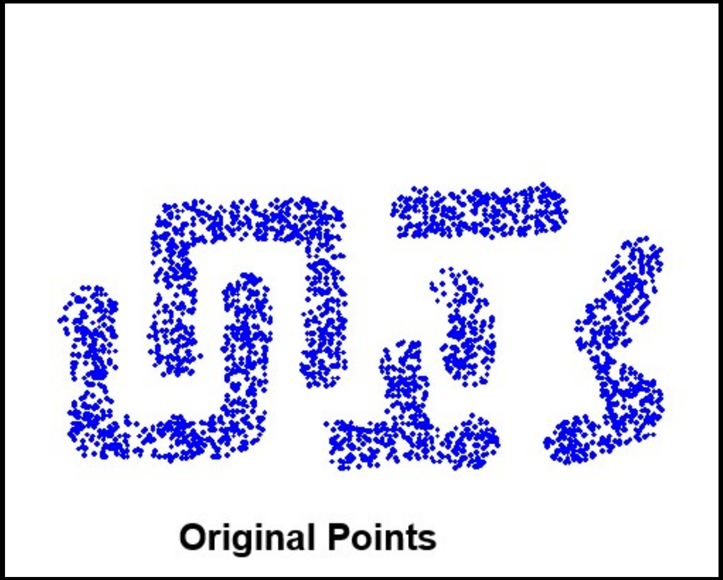
Distance Matrix:

	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	0.20	0.15	0.00	0.29	0.22
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

MIN OR SINGLE LINKAGE



MIN OR SINGLE LINKAGE (STRENGTHS)



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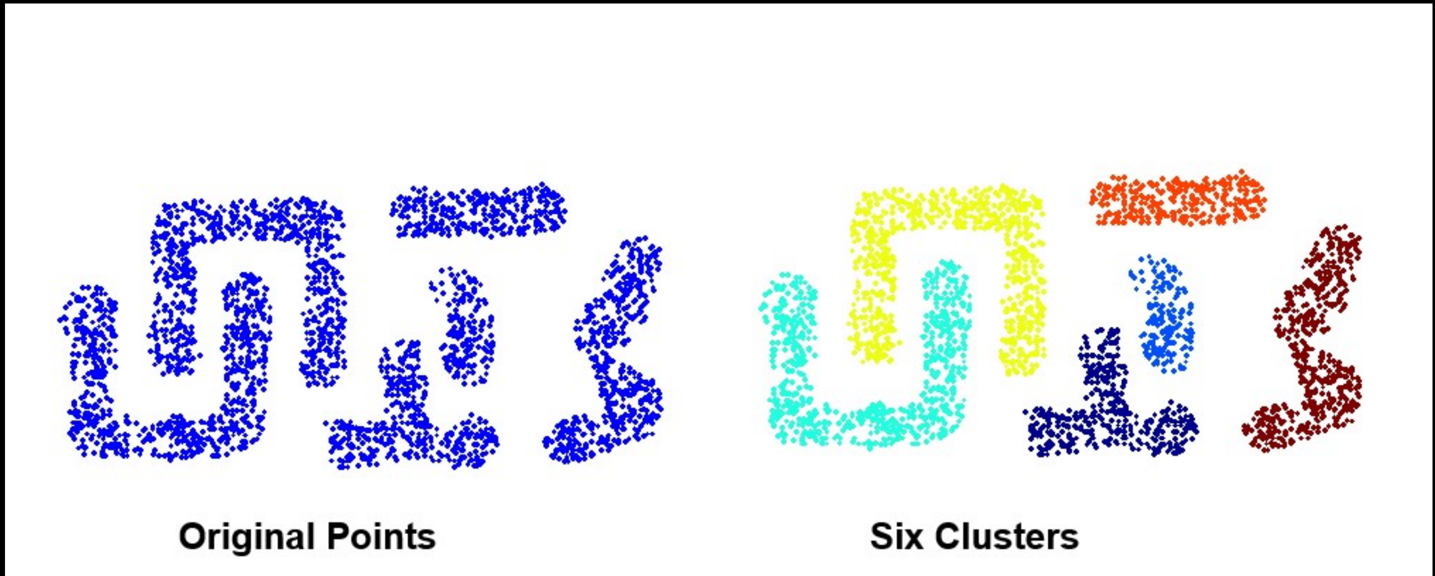
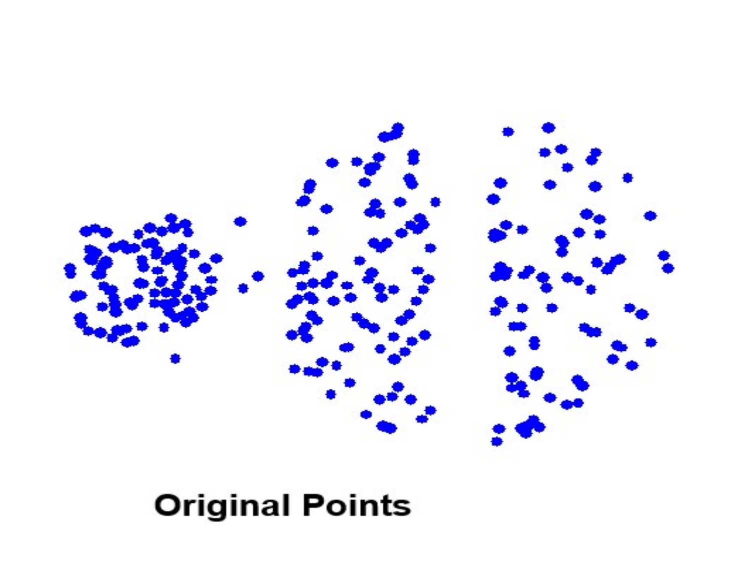


Can handle non-elliptical shapes

MIN OR SINGLE LINKAGE (LIMITATIONS)



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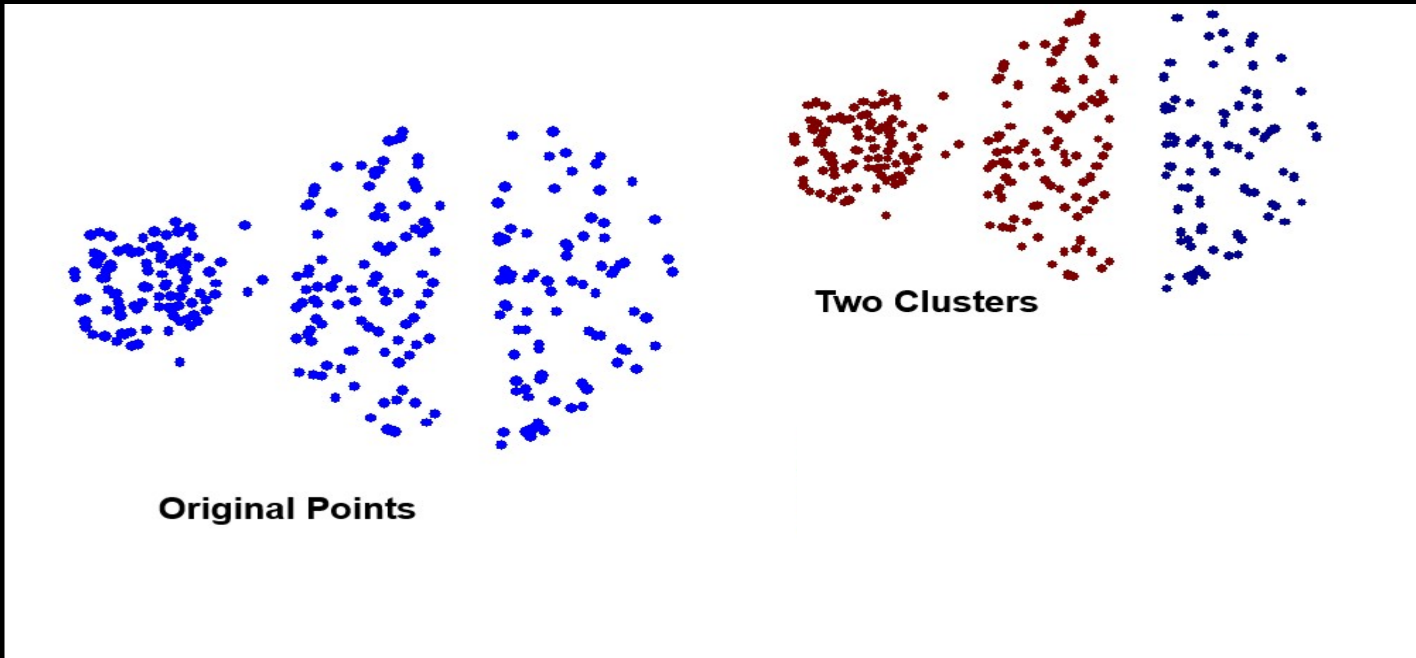

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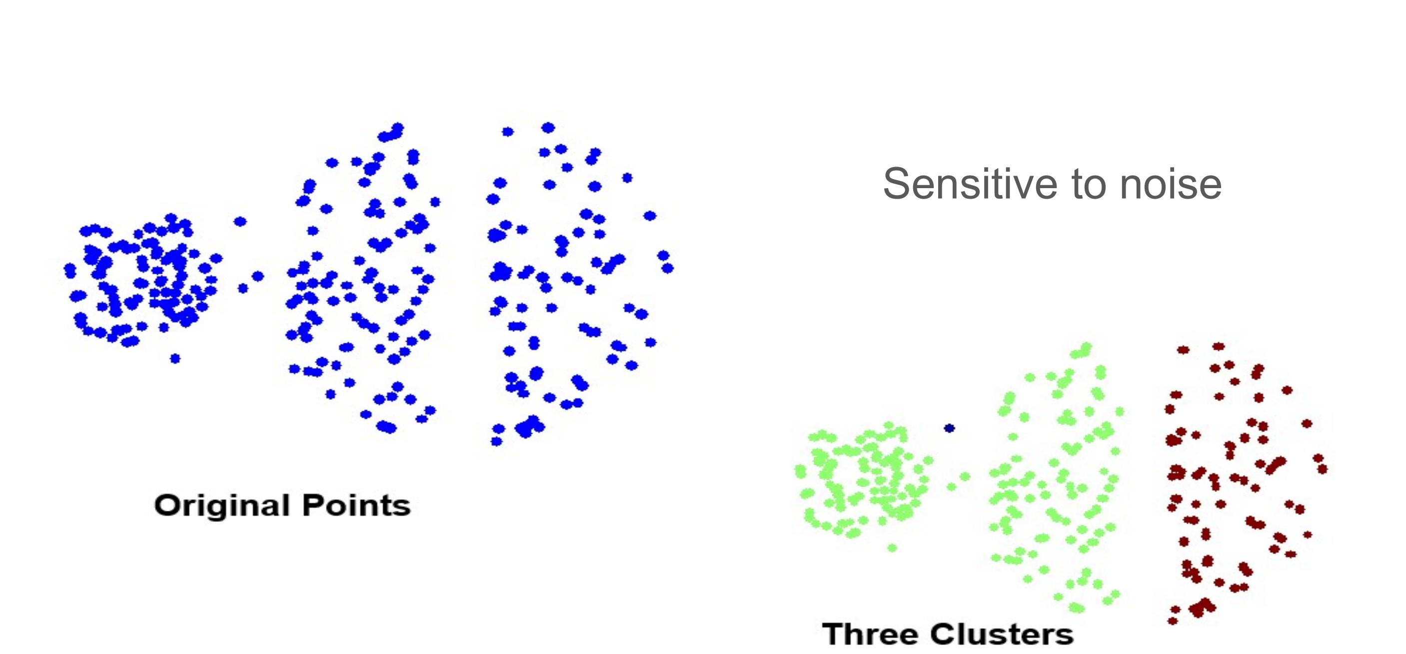
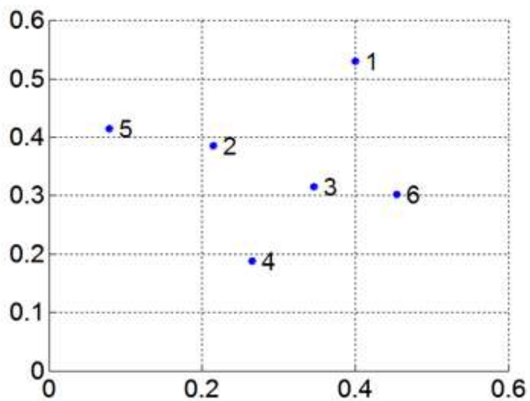


MAX OR COMPLETE LINKAGE

- Proximity of two clusters is based on the two most distant points in the different clusters
  - determined by all pairs of points in the two clusters



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p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
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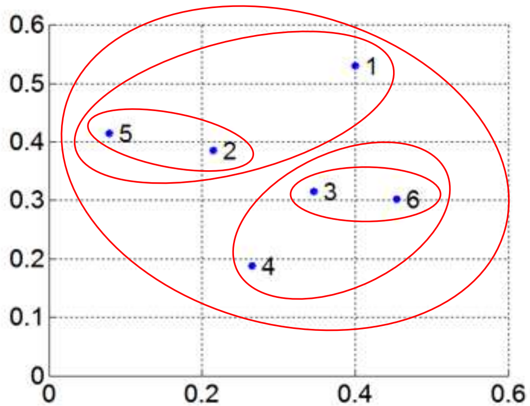
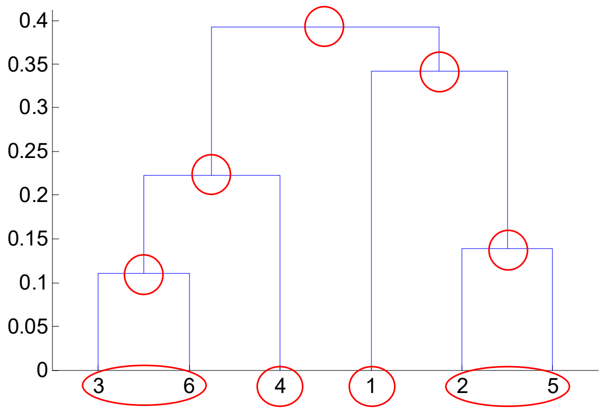
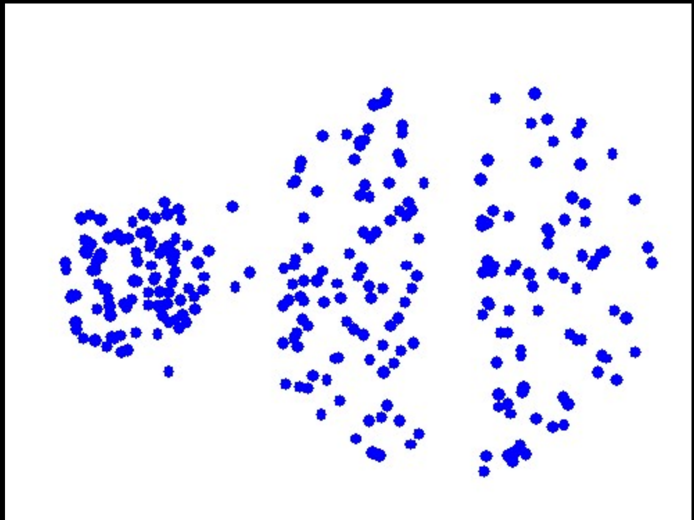
MAX OR COMPLETE LINKAGE

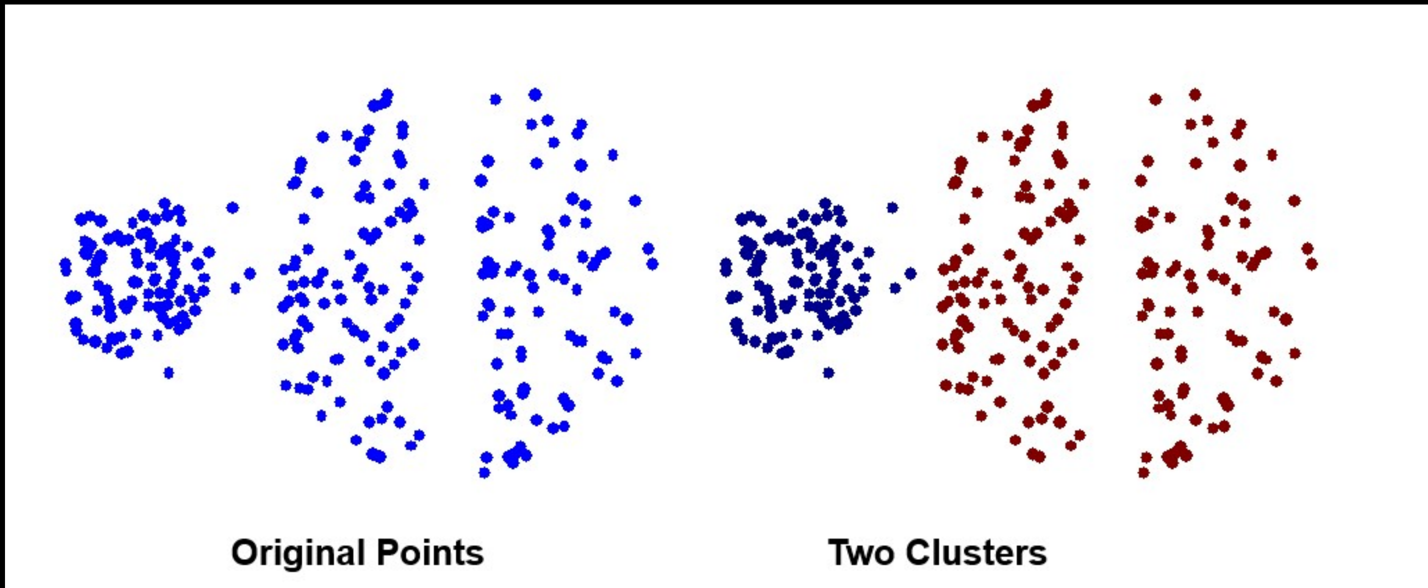




MAX OR COMPLETE LINKAGE (STRENGHTS)

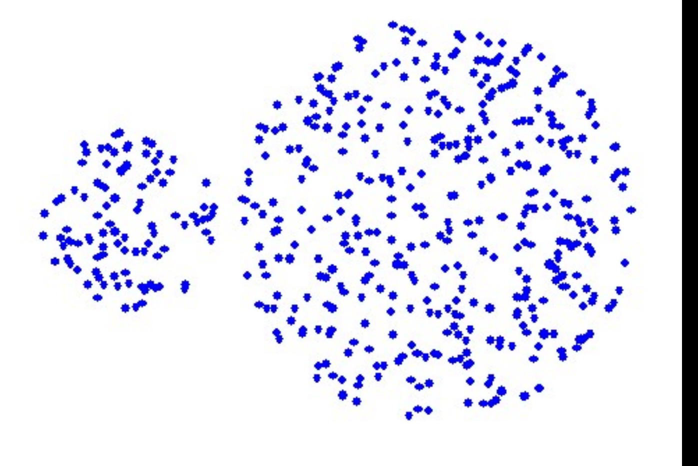

Original Points

MAX OR COMPLETE LINKAGE (STRENGHTS)



Less susceptible to noise

MAX OR COMPLETE LINKAGE (LIMITATIONS)



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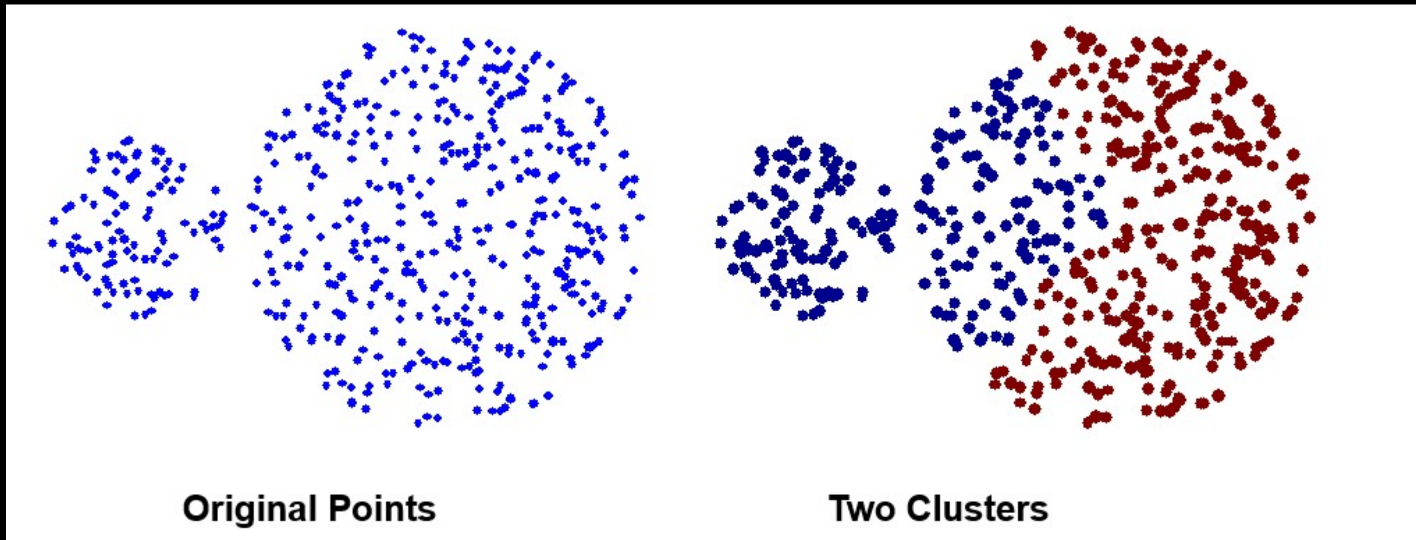
MAX OR COMPLETE LINKAGE (LIMITATIONS)

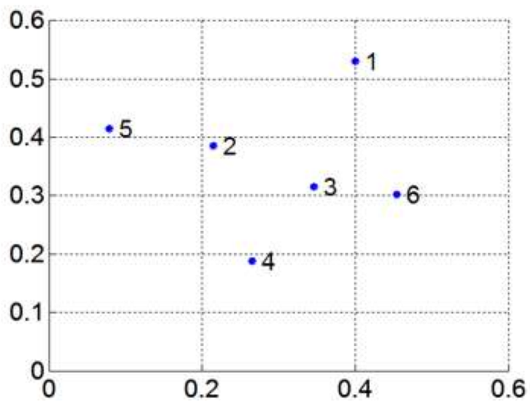


- Tends to break large clusters
- Biased towards globular clusters

GROUP AVERAGE

- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

$$\text{proximity}(C_i, C_j) = \frac{\sum_{p_k \in C_i, p_m \in C_j} \text{proximity}(p_k, p_m)}{|C_i||C_j|}$$



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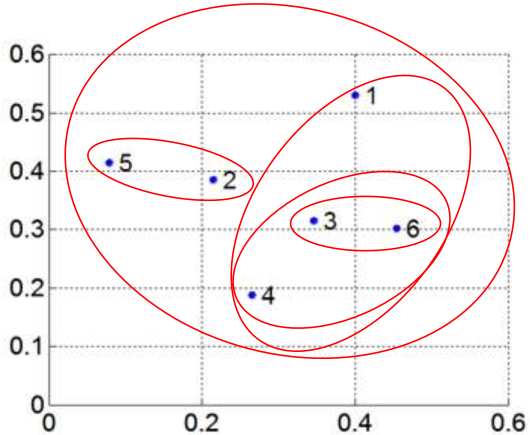
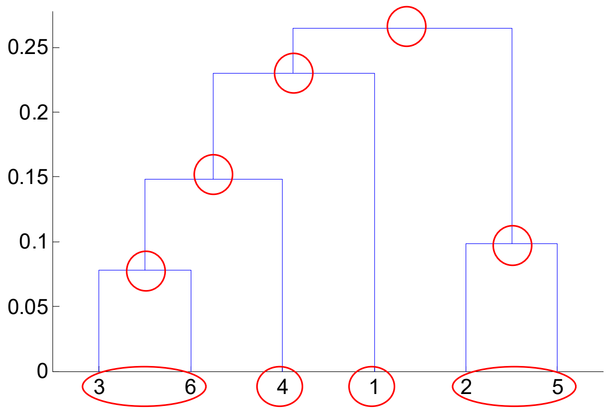
GROUP AVERAGE





GROUP AVERAGE

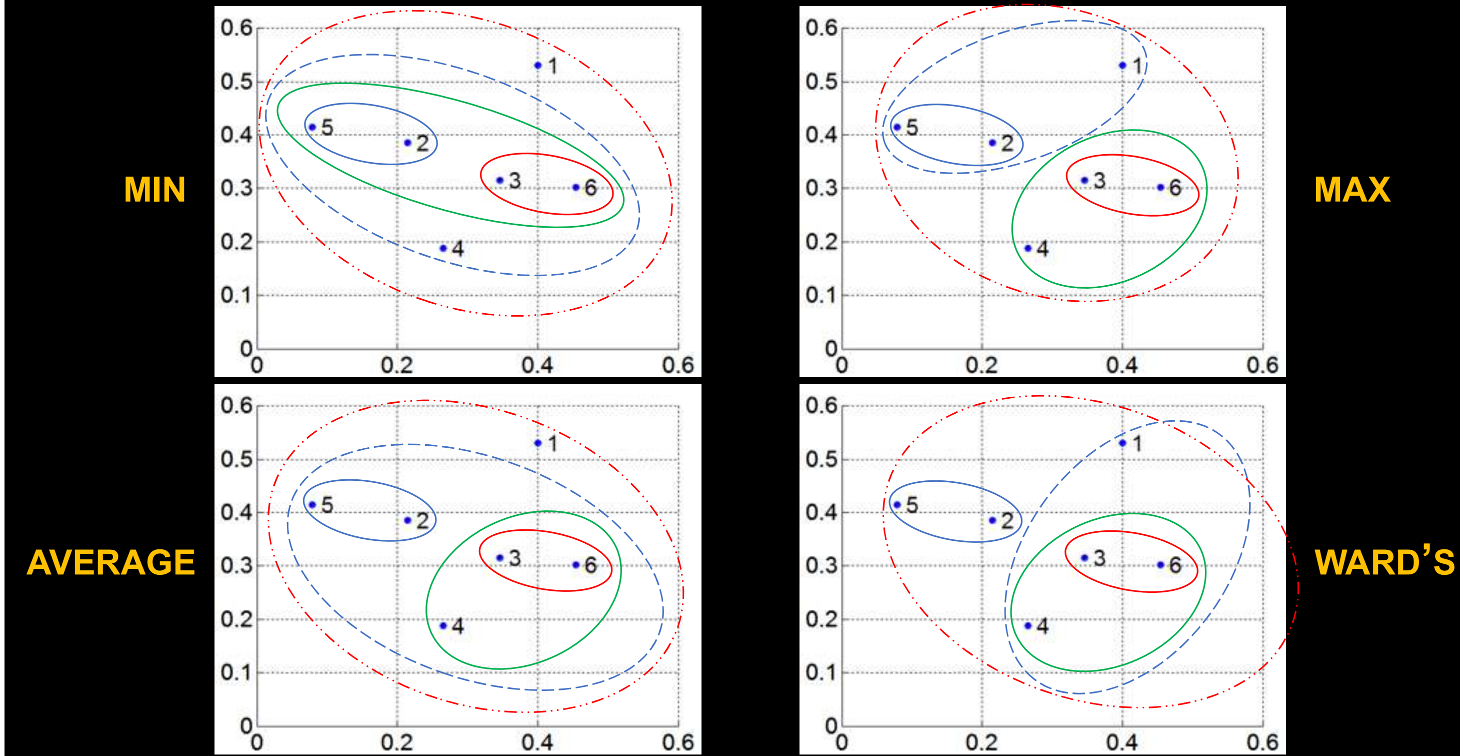
- Compromise between single and complete link

- Strengths
  - less susceptible to noise

- Limitations
  - biased towards globular clusters

WARD'S METHOD

- Similarity of two clusters is based on the increase in squared error when two clusters are merged
  - similar to group average if distance between points is distance squared
- Less susceptible to noise
- Biased towards globular clusters
- Hierarchical analogue of K-means
  - can be used to initialize K-means


MIN
MAX
AVERAGE
WARD'S
0.6
0.5
0.4
0.3
0.2
0.1
0
0.2
0.4
1
2
3
4
5
6

HIERARCHICAL CLUSTERING: TIME AND SPACE REQUIREMENTS

- $O(N^2)$ space since it uses the proximity matrix.
  - N is the number of points.
- $O(N^3)$ time in many cases
  - there are N steps and at each step the size, N^2 proximity matrix must be updated and searched
  - complexity can be reduced to $O(N^2 \log(N))$ time with some cleverness

HIERARCHICAL CLUSTERING: PROBLEMS AND LIMITATIONS

- Once a decision is made to combine two clusters, it cannot be undone
- No global objective function is directly minimized
- Different schemes have problems with one or more of the following:
  - sensitivity to noise
  - difficulty handling clusters of different sizes and non-globular shapes
  - breaking large clusters

RECAP

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