Master Degree in Artificial Intelligence for Science and Technology

# Cluster Analysis: Hierarchical Clustering

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# OUTLOOK

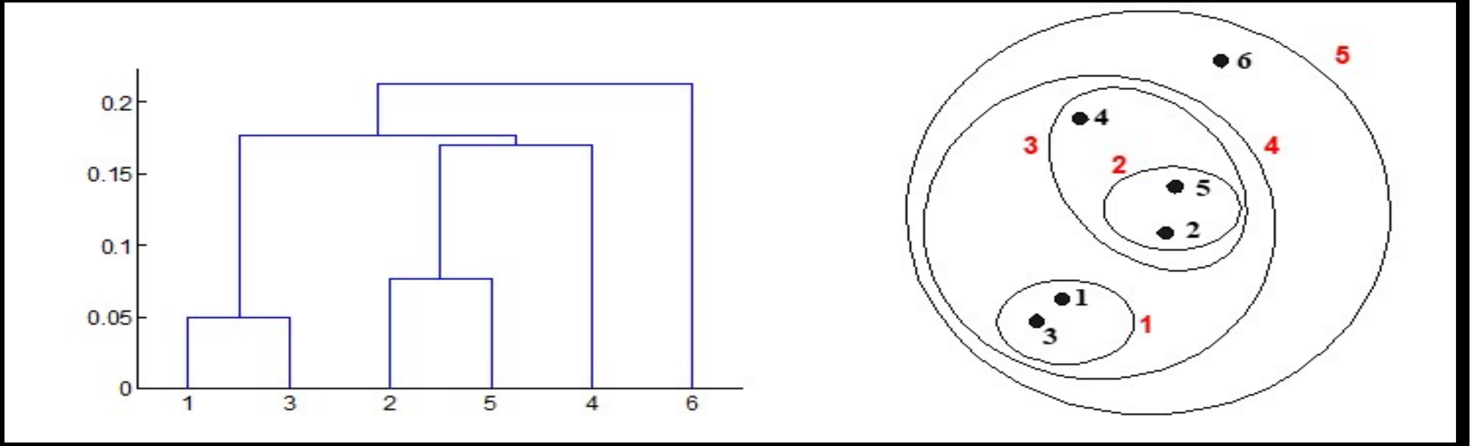
- Concept
- Strengths
- Types
  - Agglomerative
    - single linkage
    - complete linkage
    - average linkage
    - Ward's method
  - Divisive
- Complexity
- Limitations

## CONCEPT

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

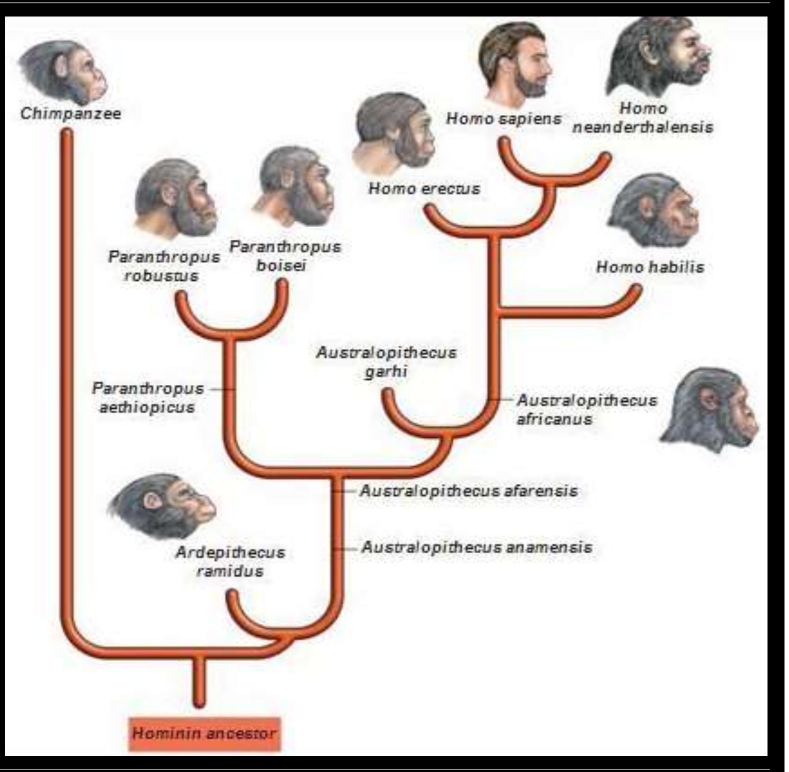
— can be visualized as a **DENDROGRAM**

- 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

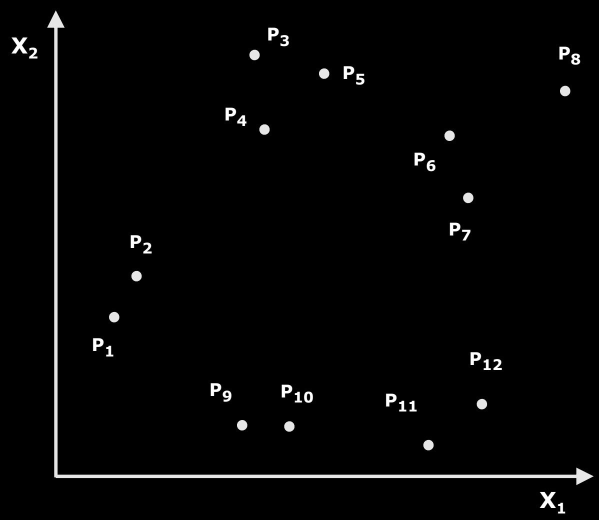
— **KEY IDEA**: successively merge closest clusters

**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

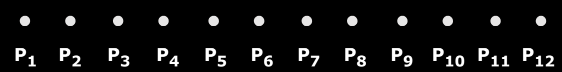
- Key operation is the computation of the proximity of two clusters
- Different approaches to defining the distance between clusters distinguish the different algorithms

## 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 | | | | | | | | | | | | |

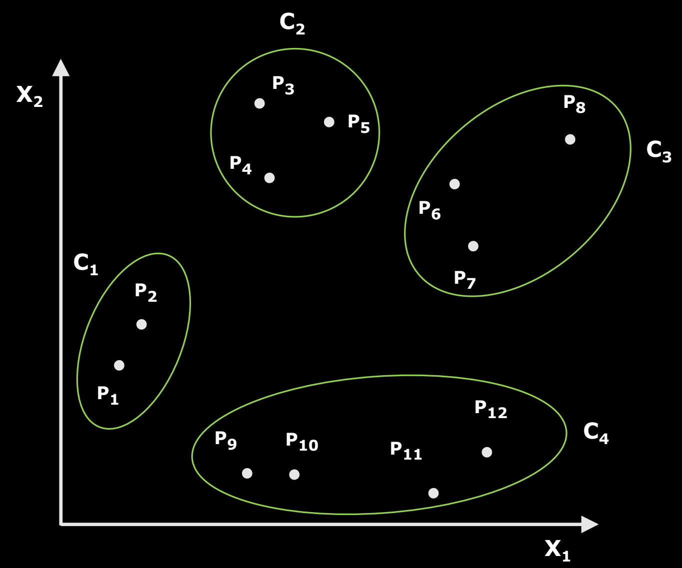


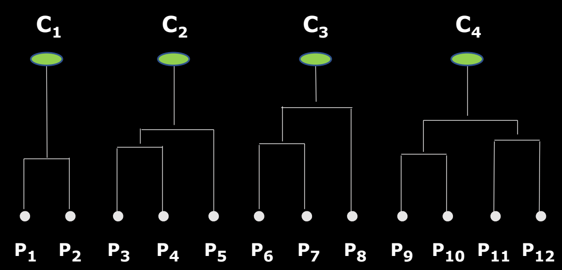

- **STEP 2:** each point is a cluster

## AGGLOMERATIVE CLUSTERING

| | C1 | C2 | C3 | C4 |
|---|---|---|---|---|
| C1 | | | | |
| C2 | | | | |
| C3 | | | | |
| C4 | | | | |

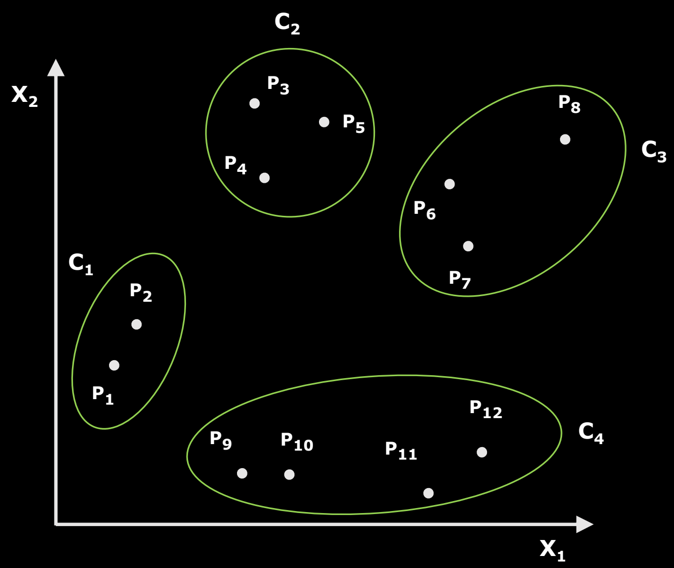
**PROXIMITY MATRIX**




After some merging steps we have some clusters

## AGGLOMERATIVE CLUSTERING




| | C1 | C2 | C3 | C4 |
|---|---|---|---|---|
| C1 | | | | |
| C2 | | | | |
| C3 | | | | |
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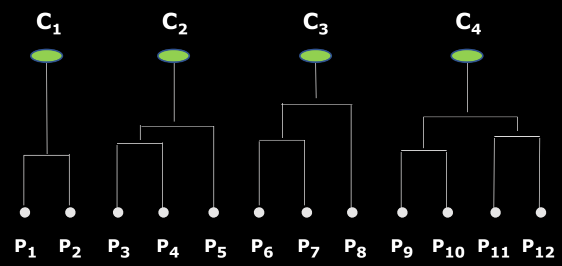
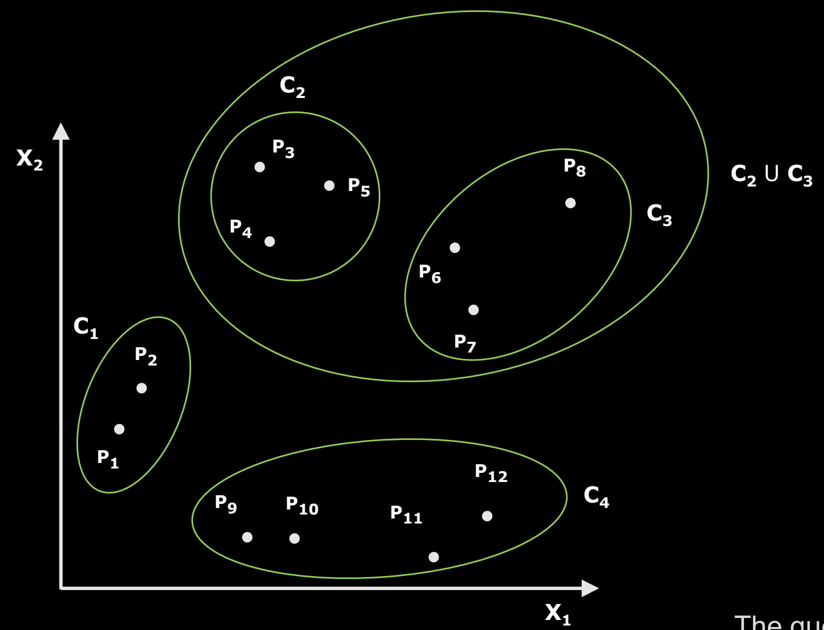


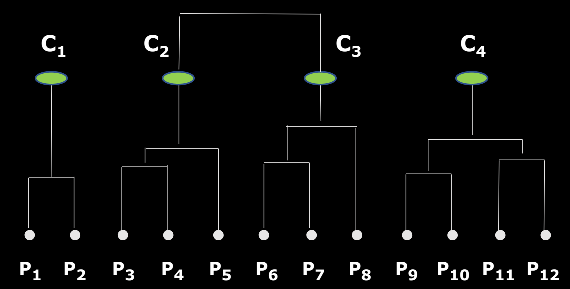

We want to merge the two closest clusters ($C_2$ and $C_3$) and update the proximity matrix.

## AGGLOMERATIVE CLUSTERING



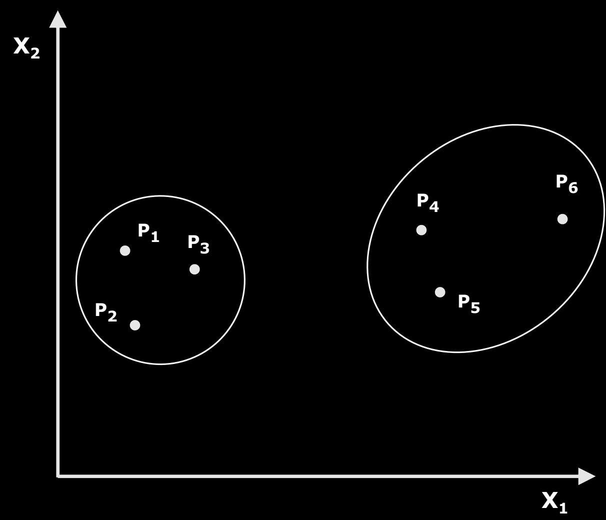

| | C1 | C2 C3 | C4 |
|---|---|---|---|
| C1 | | ? | |
| C2 C3 | ? | ? | ? |
| C4 | | ? | |

**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

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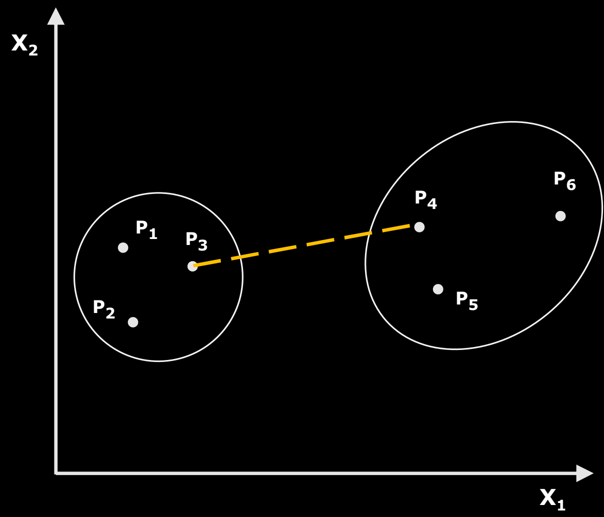


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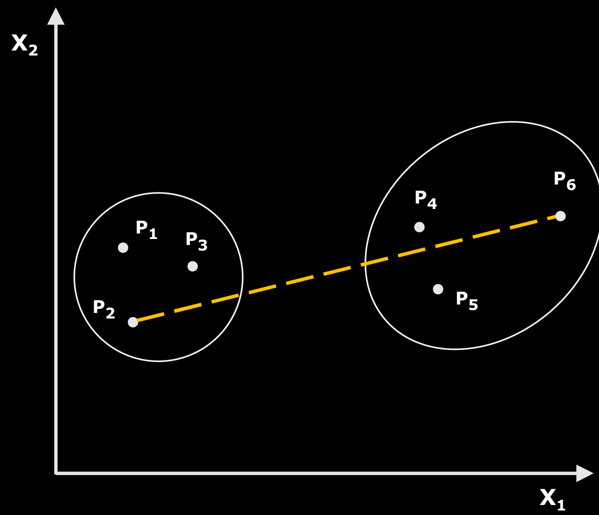


| | C1 | C2 | C3 | C4 |
|---|---|---|---|---|
| C1 | | | | |
| C2 | | | | |
| C3 | | | | |
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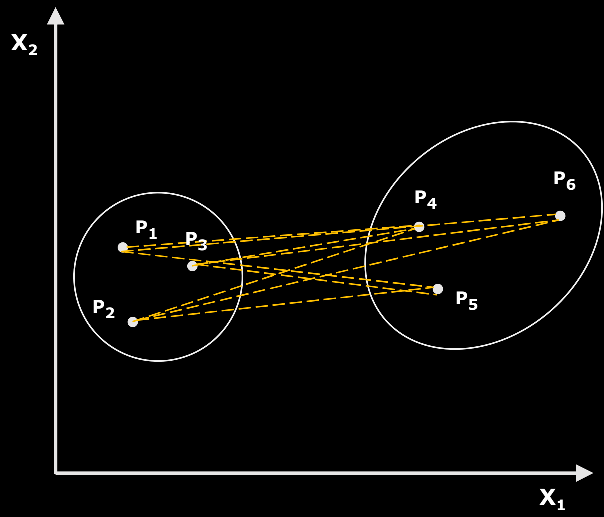


| | C1 | C2 | C3 | C4 |
|---|---|---|---|---|
| C1 | | | | |
| C2 | | | | |
| C3 | | | | |
| C4 | | | | |

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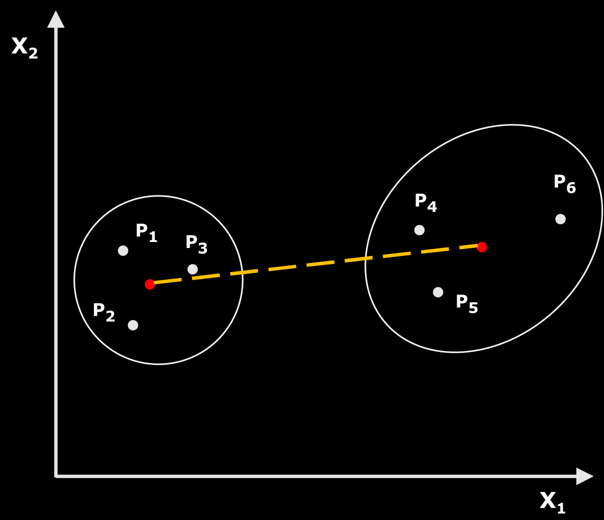
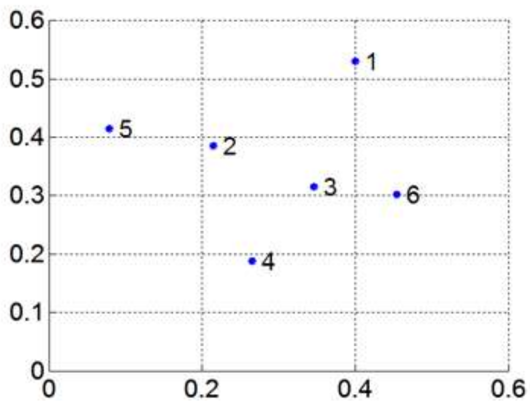



- MIN
- MAX
- Group Average
- **Distance Between Centroids**
- Other methods driven by an objective function
  - Ward's method uses squared error

## 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 |

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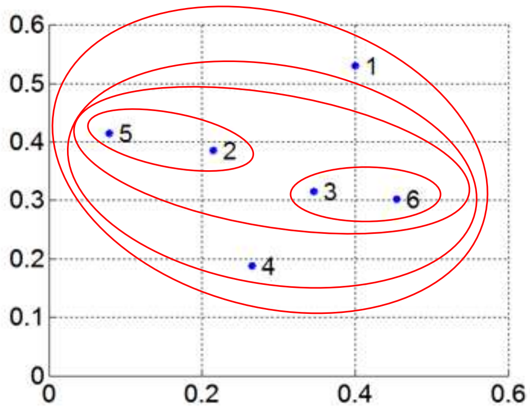
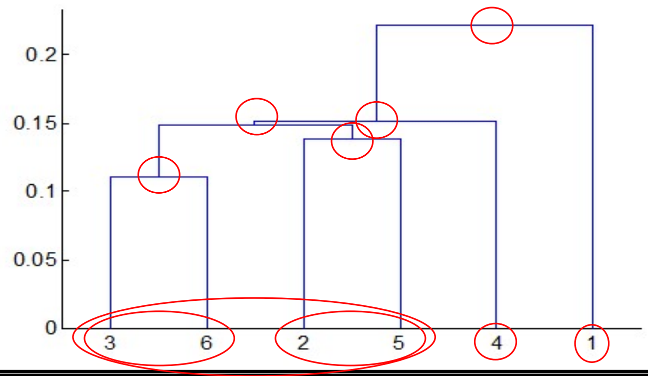
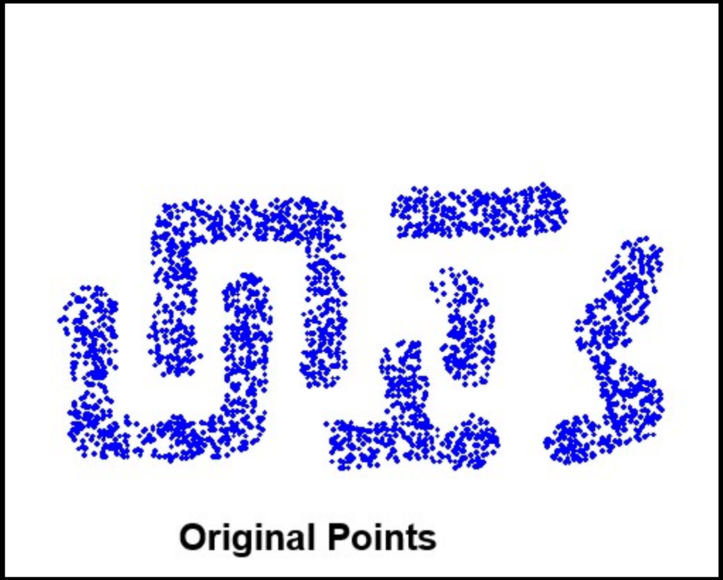


## MIN OR SINGLE LINKAGE (STRENGTHS)



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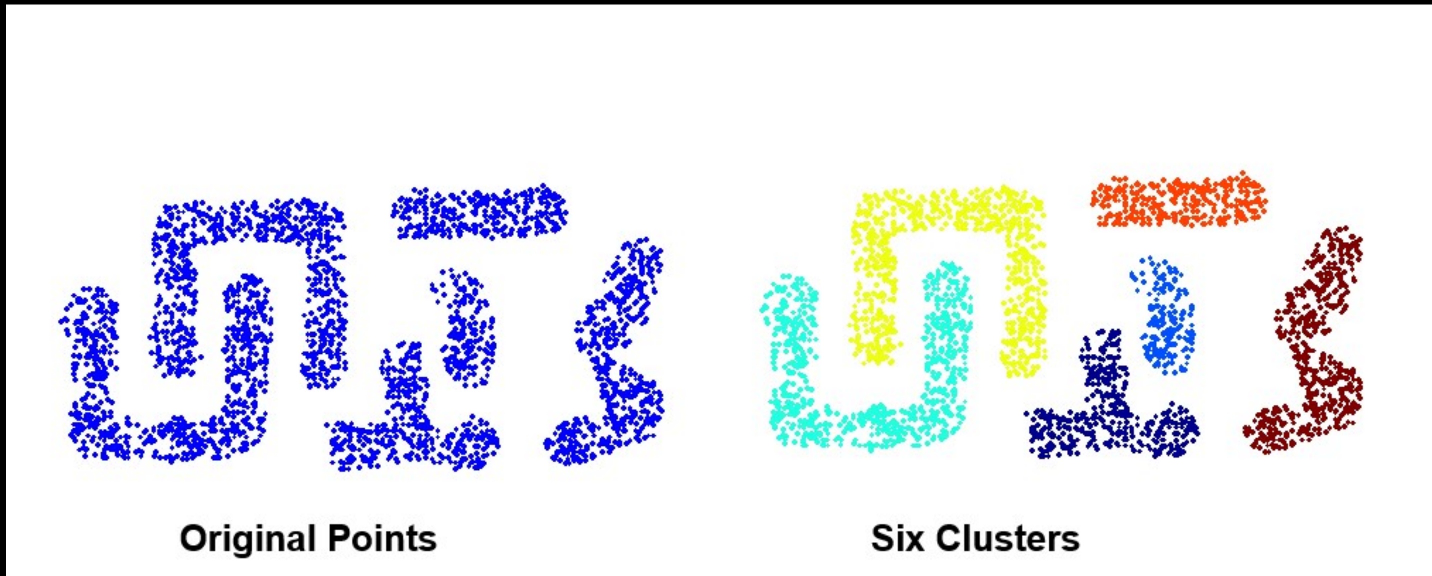
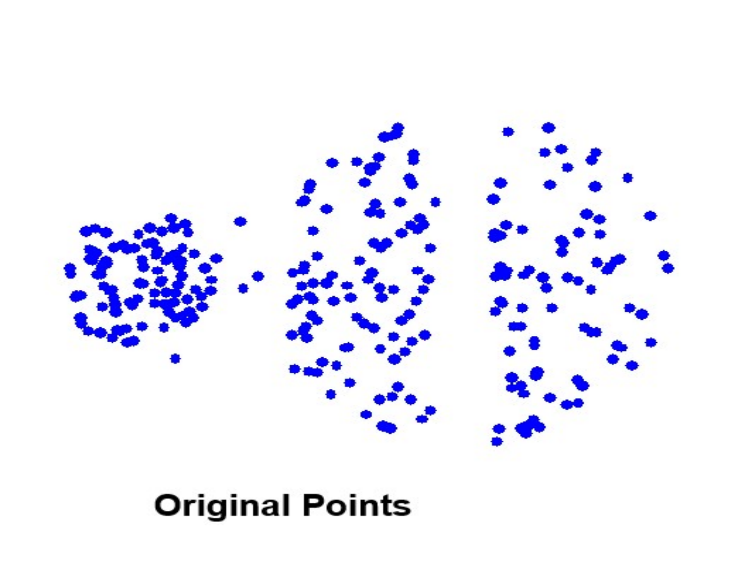



Can handle non-elliptical shapes

## MIN OR SINGLE LINKAGE (LIMITATIONS)



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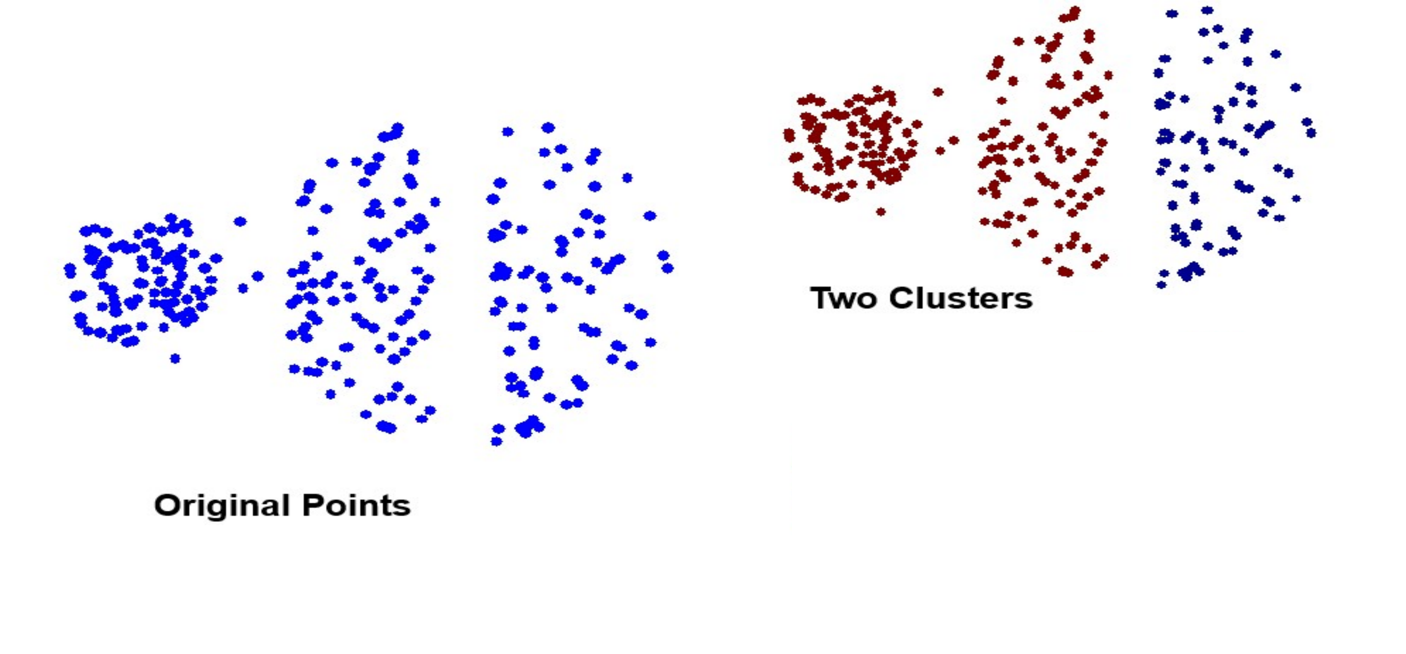

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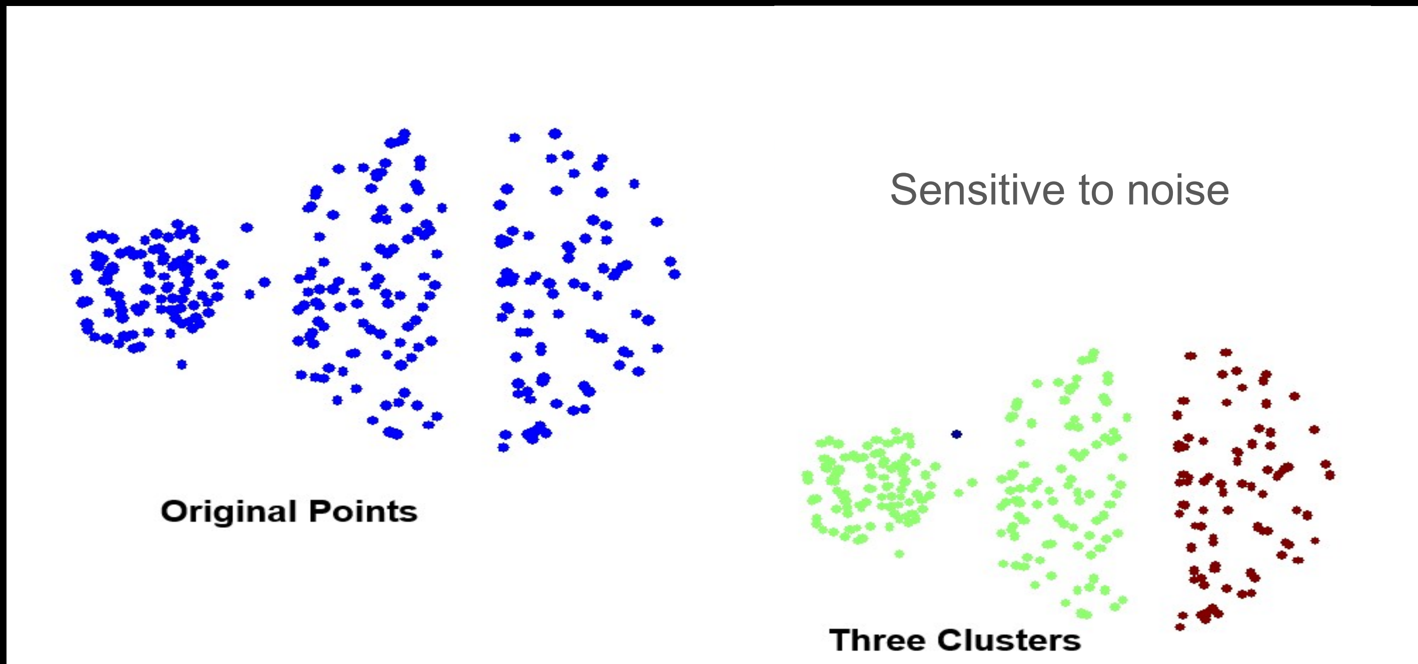
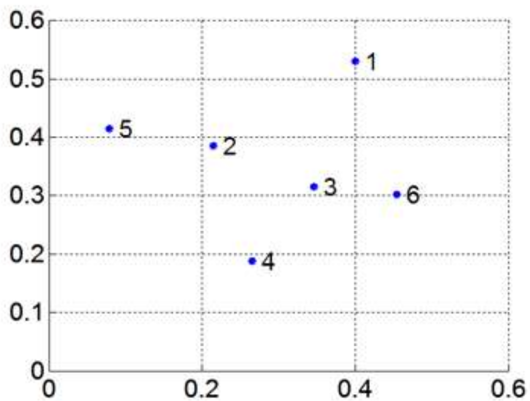


## MAX OR COMPLETE LINKAGE

- 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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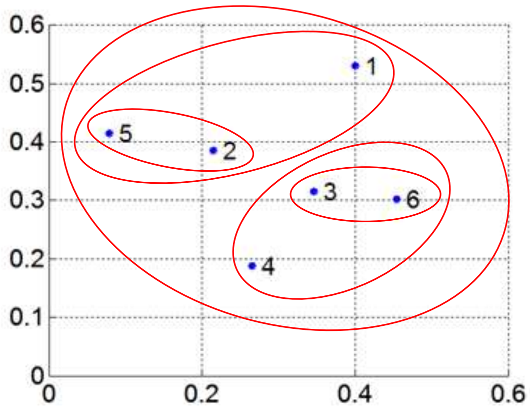
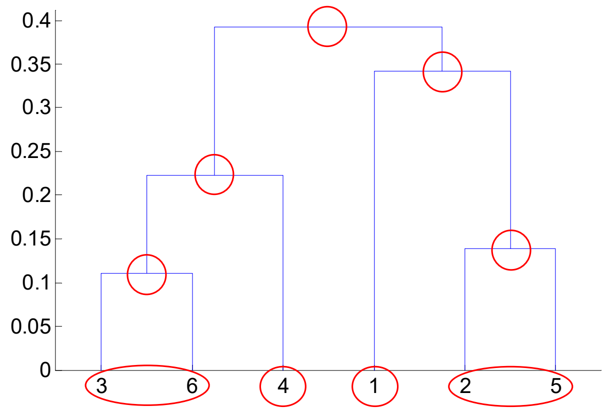
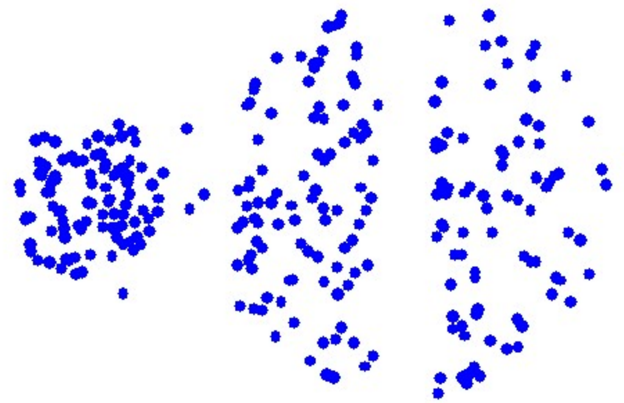
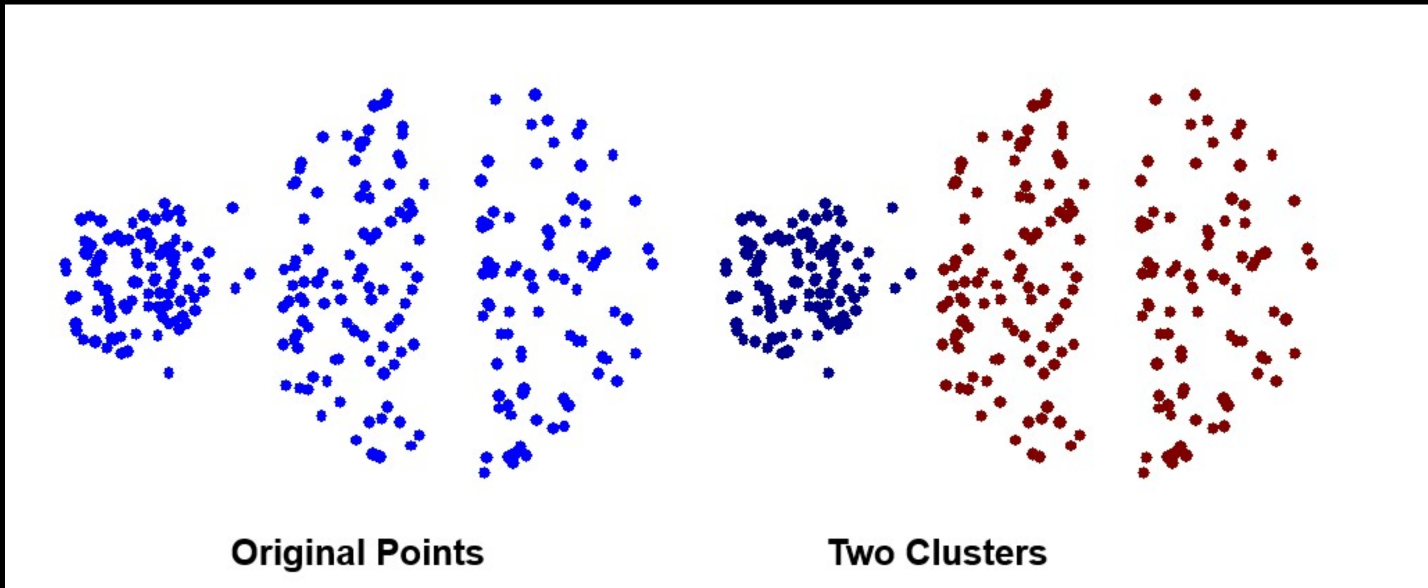


## MAX OR COMPLETE LINKAGE (STRENGHTS)

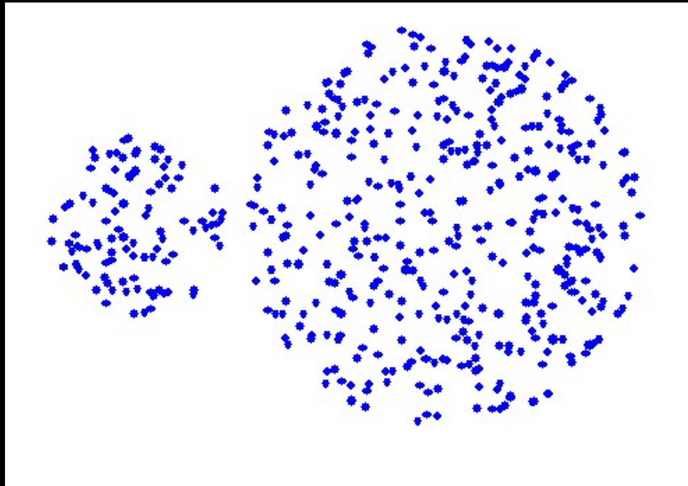

Original Points

## MAX OR COMPLETE LINKAGE (STRENGHTS)




Less susceptible to noise

## MAX OR COMPLETE LINKAGE (LIMITATIONS)



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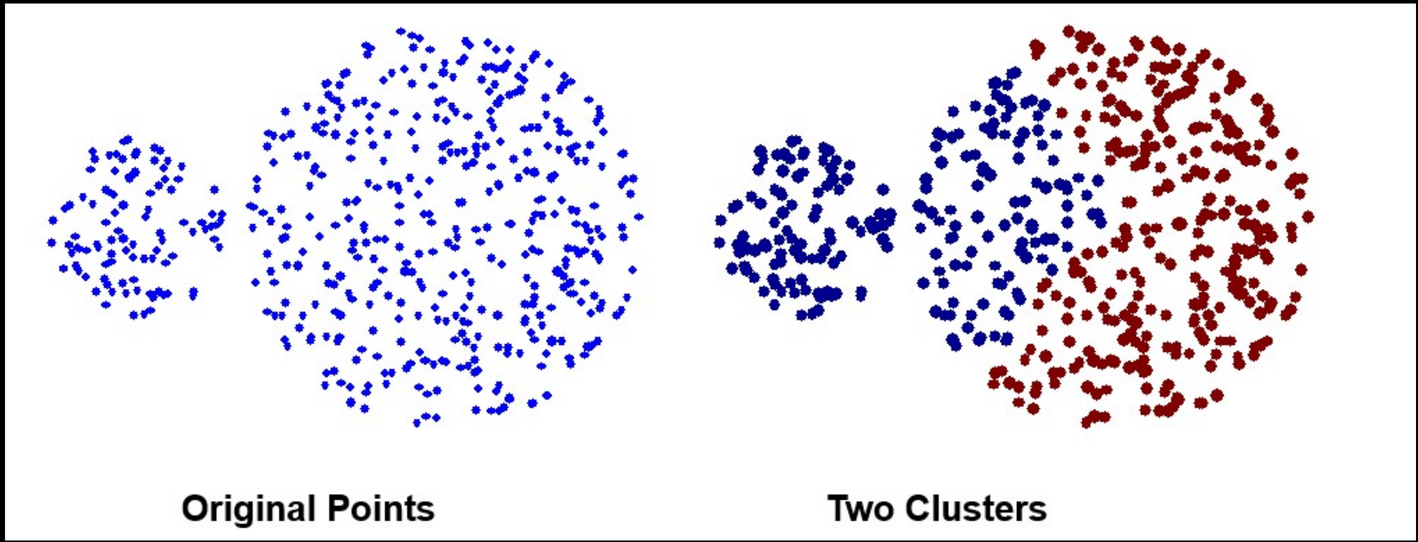
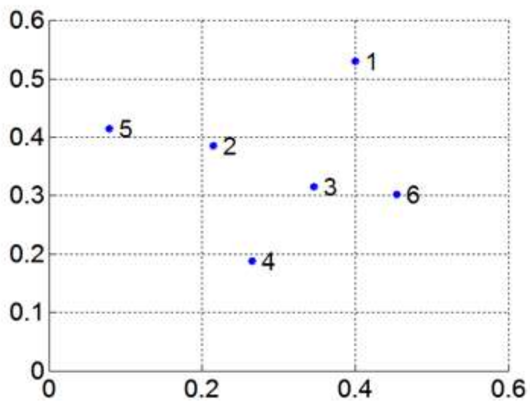



- Tends to break large clusters
- Biased towards globular clusters

## 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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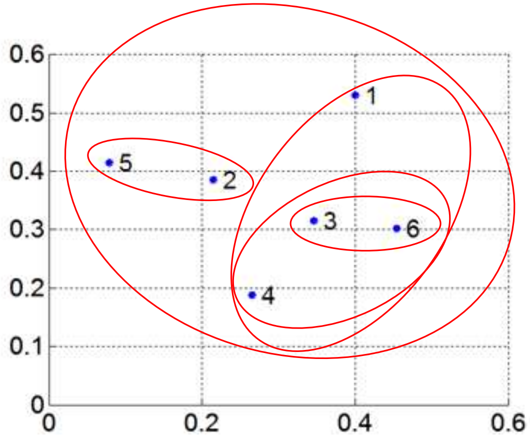
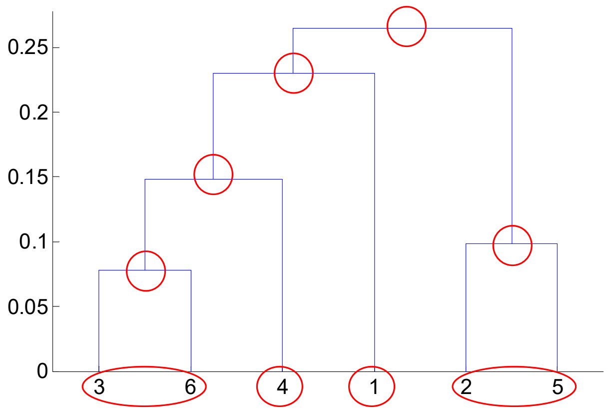
## GROUP AVERAGE



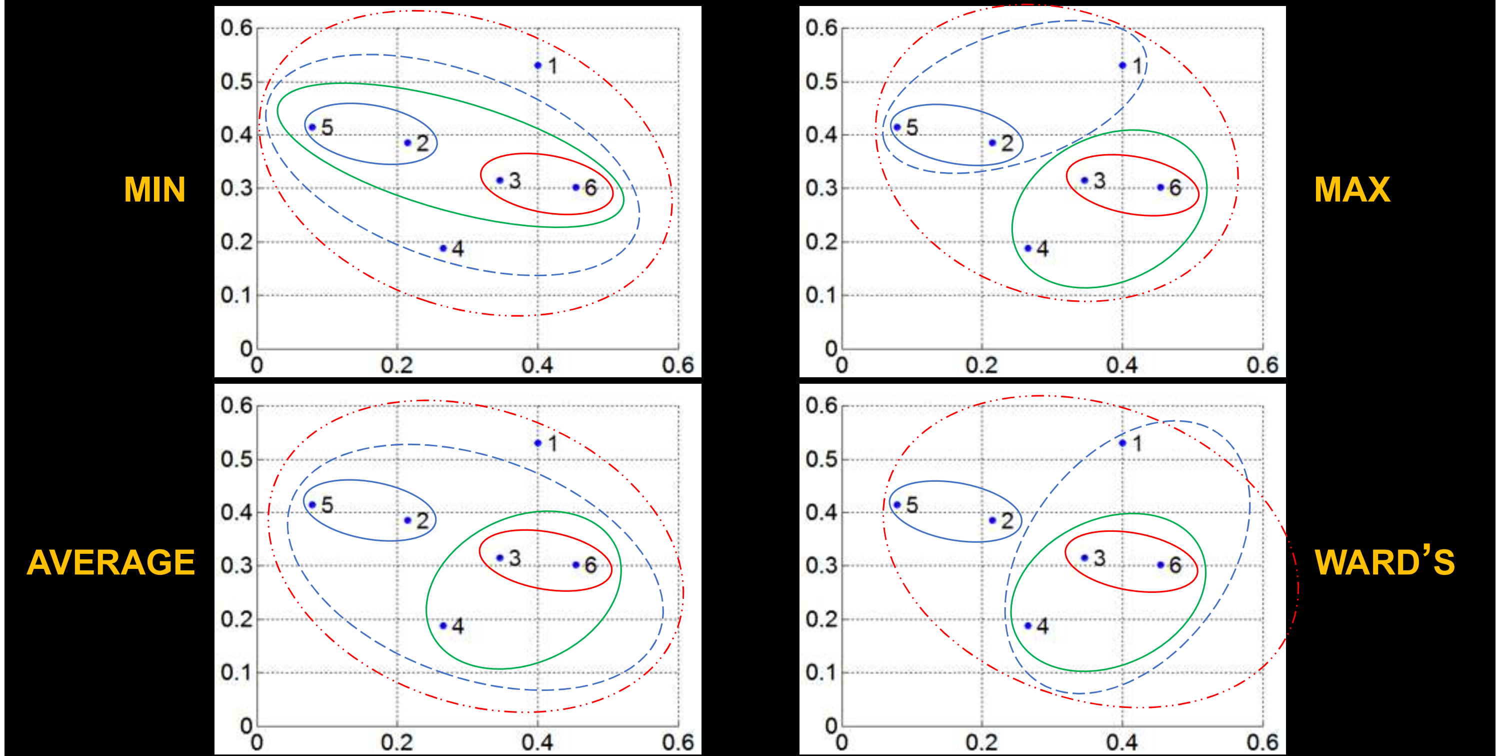



## GROUP AVERAGE

- 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
1
2
3
4
5
6
0.6
0.5
0.4
0.3
0.2
0.1
0
0.2
0.4
0.6

## 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

- Concept
- Strengths
- Types
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    - single linkage
    - complete linkage
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    - Ward's method
  - Divisive
- Complexity
- Limitations