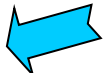


# CSE 5243 INTRO. TO DATA MINING

## Cluster Analysis: Basic Concepts and Methods

Yu Su, CSE@The Ohio State University

# Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: An Introduction 
- Partitioning Methods
- Hierarchical Methods
- Density- and Grid-Based Methods
- Evaluation of Clustering
- Summary

# Introduction

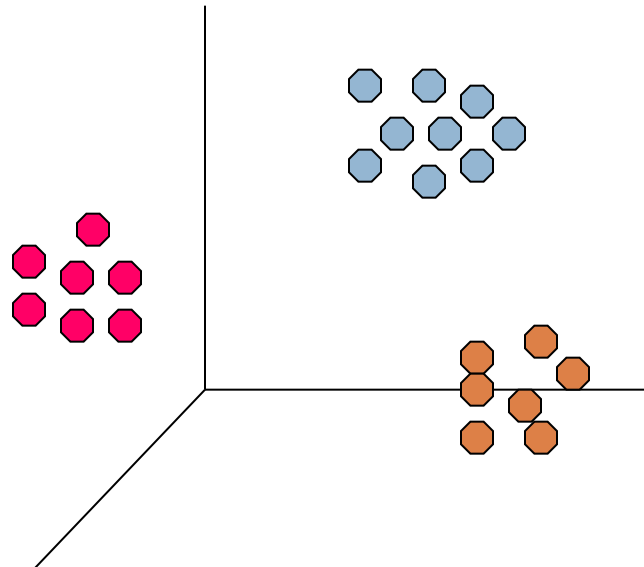
3

- Suppose you are a marketing manager and you have (anonymized) information about users such as demographics and purchase history stored as feature vectors. What to do next towards an effective marketing strategy?

# What is Cluster Analysis?

## □ What is a cluster?

- ▣ A cluster is a collection of data objects which are
  - Similar (or related) to one another within the same group (i.e., cluster)
  - Dissimilar (or unrelated) to the objects in other groups (i.e., clusters)

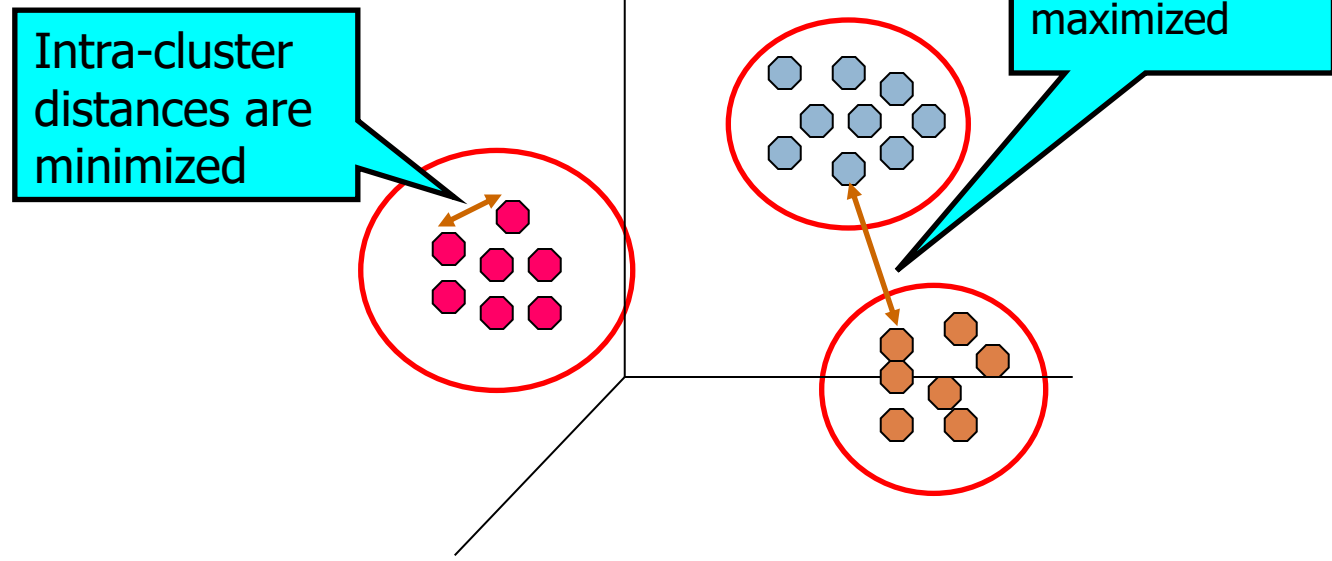


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  - ▣ Given a set of data points, partition them into a set of groups (i.e., clusters), **such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups**

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  - ▣ Given a set of data points, partition them into a set of groups (i.e., clusters), **such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups**
- Cluster analysis is **unsupervised learning** (i.e., no predefined classes)
  - ▣ This contrasts with *classification*, which is supervised learning
- Typical ways to use/apply cluster analysis
  - ▣ As a stand-alone tool to get insight into data distribution, or
  - ▣ As a preprocessing (or intermediate) step for other algorithms

# What is Good Clustering?

- A good clustering method will produce high quality clusters, which should have
  - ▣ **High intra-class similarity:** **Cohesive** within clusters
  - ▣ **Low inter-class similarity:** **Distinctive** between clusters



# What is Good Clustering?

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  - ▣ **High intra-class similarity:** **Cohesive** within clusters
  - ▣ **Low inter-class similarity:** **Distinctive** between clusters
- **Quality function**
  - ▣ There is usually a separate “quality” function that measures the “goodness” of a cluster
  - ▣ It is hard to define “similar enough” or “good enough”
    - The answer is typically highly subjective
- There exist many similarity measures and/or functions for different applications
- **Similarity measure is critical for cluster analysis**

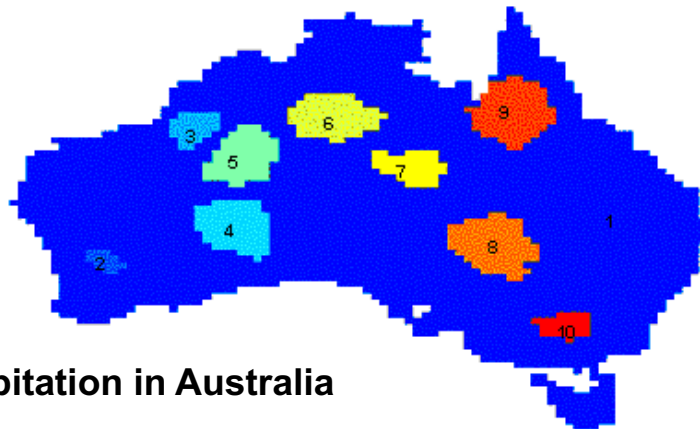
# Cluster Analysis: Applications

## □ Understanding

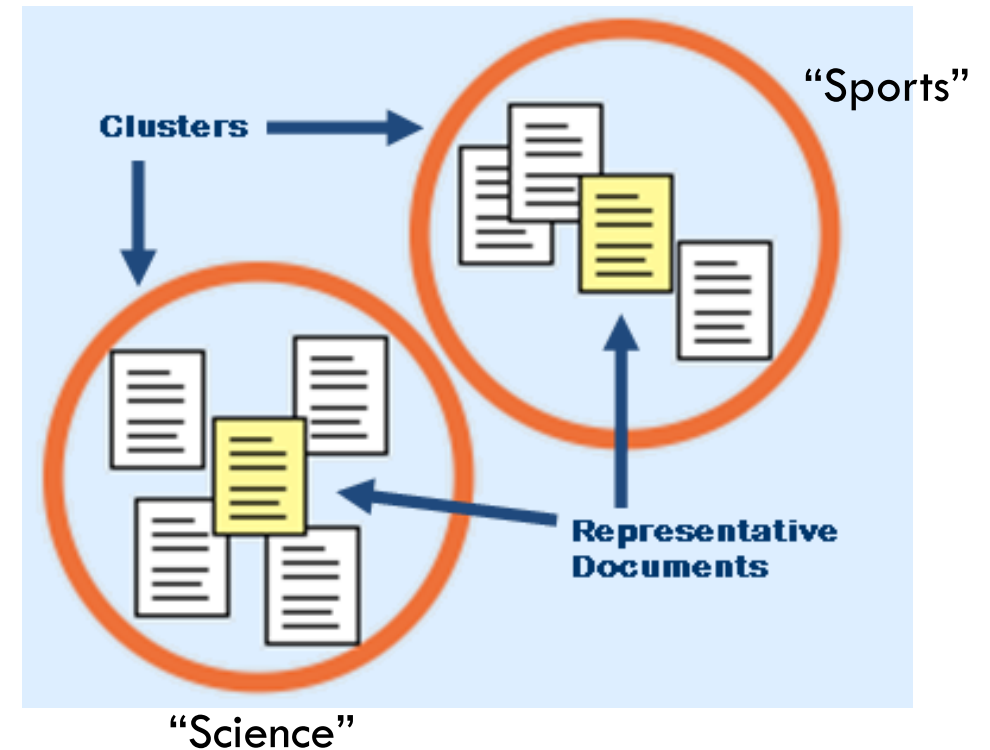
- Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

## □ Summarization

- Reduce the size of large data sets



Clustering precipitation in Australia



# What is not Cluster Analysis?

- Supervised classification
  - ▣ Have class label information
- Simple segmentation
  - ▣ Dividing students into different registration groups alphabetically, by last name
- Results of a query
  - ▣ Groupings are a result of an external specification

# Notion of a Cluster can be Ambiguous

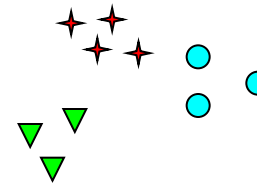


How many clusters?

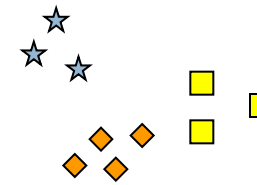
# Notion of a Cluster can be Ambiguous



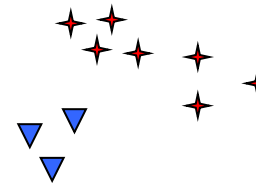
How many clusters?



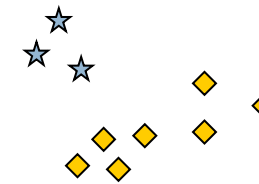
Six Clusters



Two Clusters



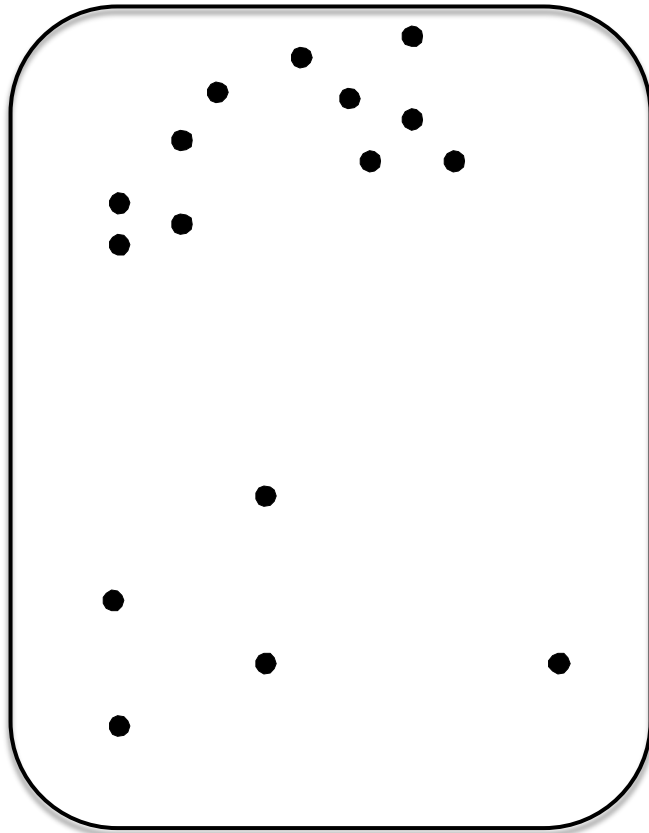
Four Clusters



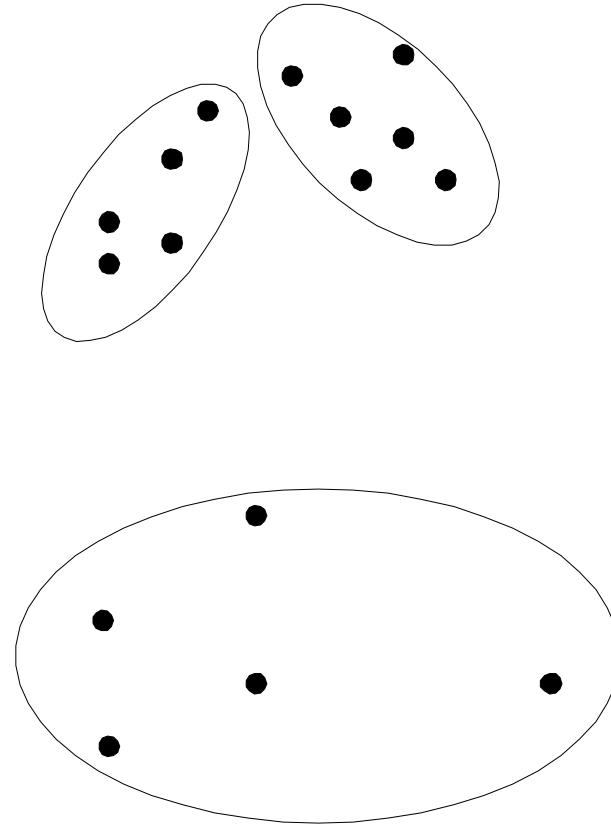
# Types of Clusterings

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

# Partitional Clustering



**Original Points**



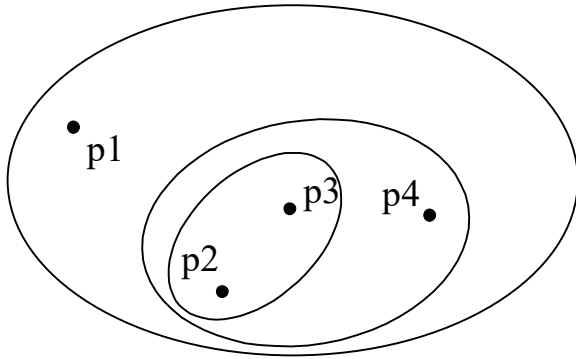
**A Partitional Clustering**

# Types of Clusterings

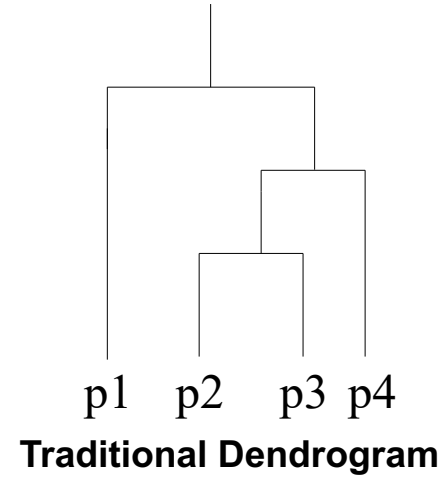
- A **clustering** is a set of clusters
- Important distinction between **hierarchical** and **partitional** sets of clusters
- Partitional Clustering
  - A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  -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



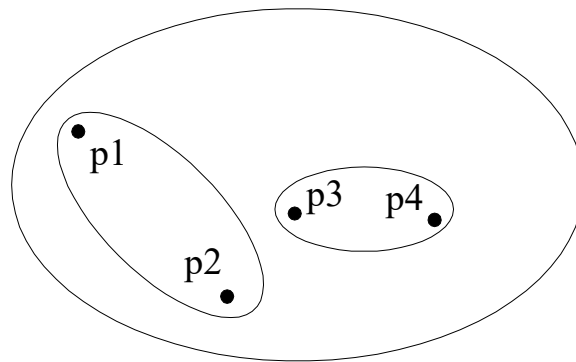
# Hierarchical Clustering



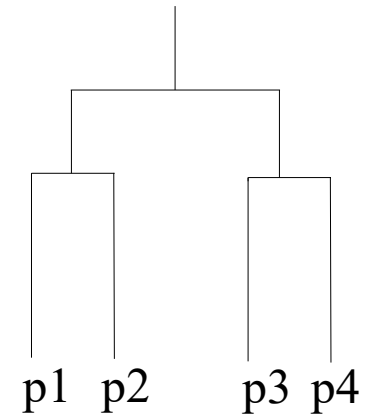
**Traditional Hierarchical Clustering**



**Traditional Dendrogram**



**Non-traditional Hierarchical Clustering**

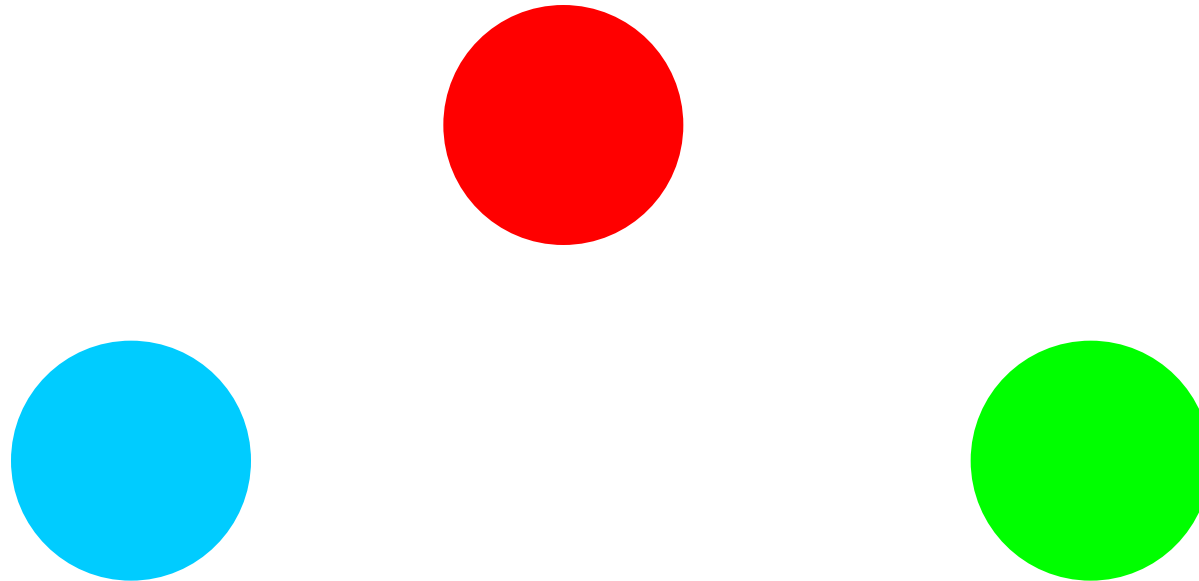


**Non-traditional Dendrogram**

# Types of Clusters: Well-Separated

## □ Well-Separated Clusters:

- A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.

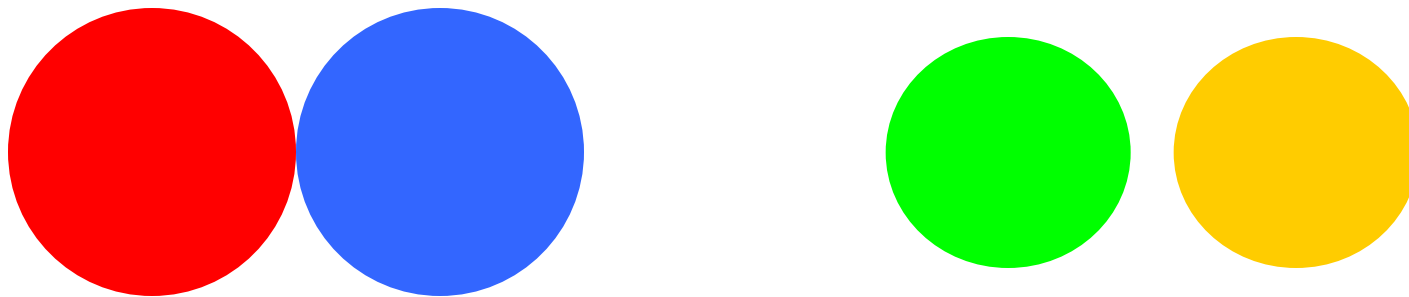


**3 well-separated clusters**

# Types of Clusters: Center-Based

## □ Center-based

- A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
- The center of a cluster is often a **centroid**, the average of all the points in the cluster, or a **medoid**, the most “representative” point of a cluster

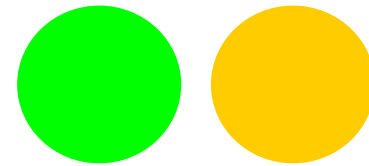
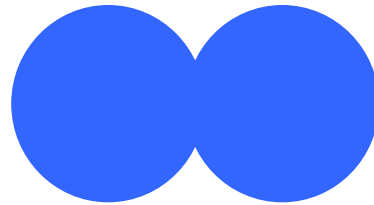
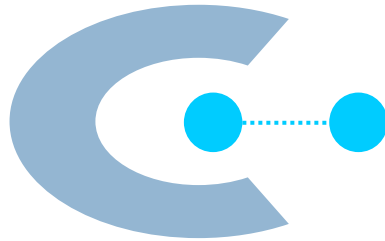
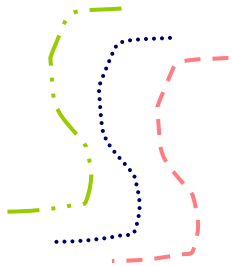


4 center-based clusters

# Types of Clusters: Contiguity-Based

## □ Contiguous Cluster (Nearest neighbor or Transitive)

- A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.

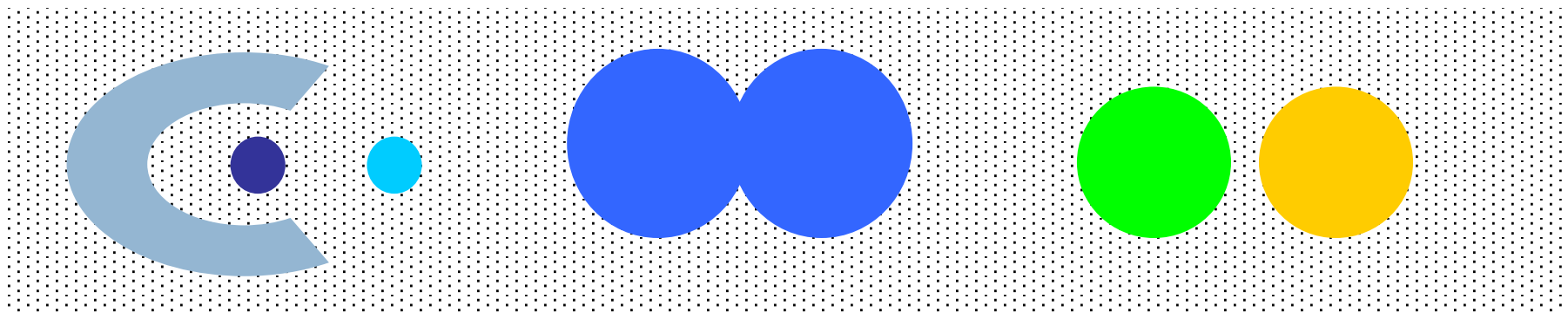


**8 contiguous clusters**

# Types of Clusters: Density-Based

## □ Density-based

- A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
- Used when the clusters are irregular or intertwined, and when noise and outliers are present.



**6 density-based clusters**

# Characteristics of the Input Data Are Important

- Type of proximity or density measure
  - ▣ This is a derived measure, but central to clustering
- Sparseness
  - ▣ Dictates type of similarity
  - ▣ Adds to efficiency
- Attribute type
  - ▣ Dictates type of similarity
- Type of Data
  - ▣ Dictates type of similarity
  - ▣ Other characteristics, e.g., autocorrelation
- Dimensionality
- Noise and Outliers
- Type of Distribution

# Clustering Algorithms

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- K-means and its variants
- Hierarchical clustering
- Density-based clustering

# K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a **centroid** (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters,  $K$ , must be specified
- The basic algorithm is very simple

---

- 1: Select  $K$  points as the initial centroids.
- 2: **repeat**
- 3:   Form  $K$  clusters by assigning all points to the closest centroid.
- 4:   Recompute the centroid of each cluster.
- 5: **until** The centroids don't change

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Often chosen  
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3: Form  $K$  clusters by assigning all points to the closest centroid.

Measured by Euclidean  
distance, cosine similarity,  
etc.

4: Recompute the centroid of each cluster.

5: **until** The centroids don't change

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Typically the mean of  
the points in the cluster

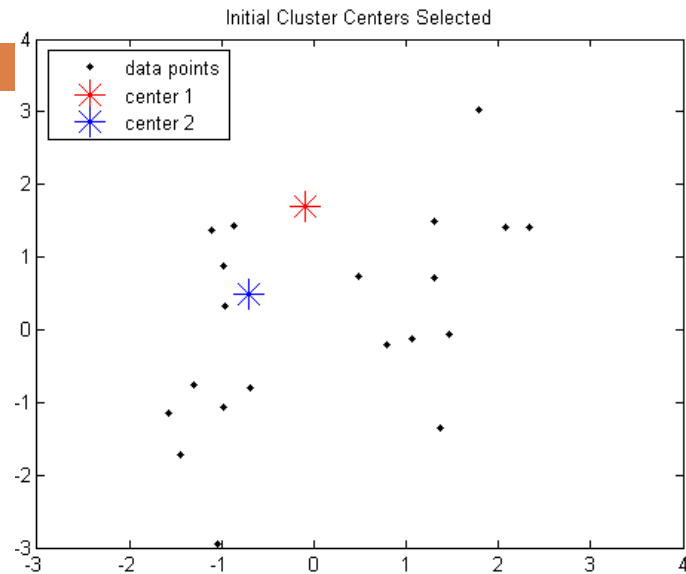
5: **until** The centroids don't change

---

# K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - ▣ Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - ▣ Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is  $O(n * K * I * d)$ 
  - ▣  $n$  = number of points,  $K$  = number of clusters,  
 $I$  = number of iterations,  $d$  = number of attributes

# Example: *K*-Means Clustering



The original data points &  
randomly select  $K = 2$  centroids

## Execution of the *K*-Means Clustering Algorithm

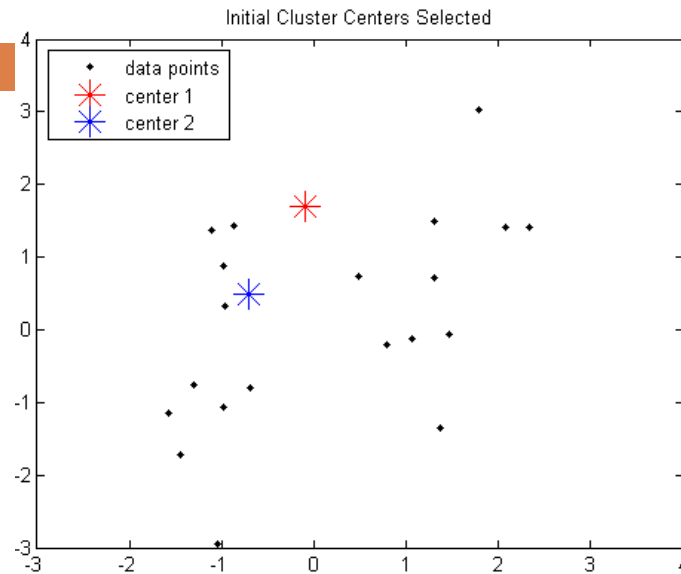
Select  $K$  points as initial centroids

### Repeat

- Form  $K$  clusters by assigning each point to its closest centroid
- Re-compute the centroids (i.e., *mean point*) of each cluster

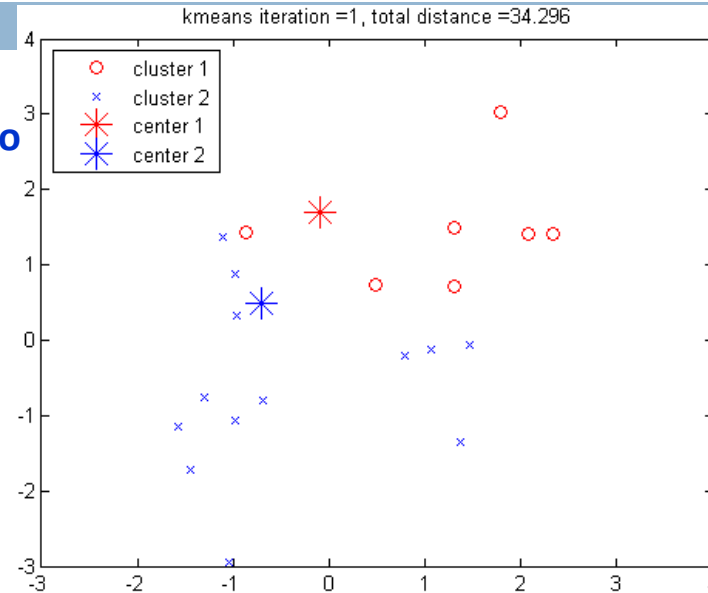
**Until** convergence criterion is satisfied

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The original data points &  
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Assign  
points to  
clusters



## Execution of the *K*-Means Clustering Algorithm

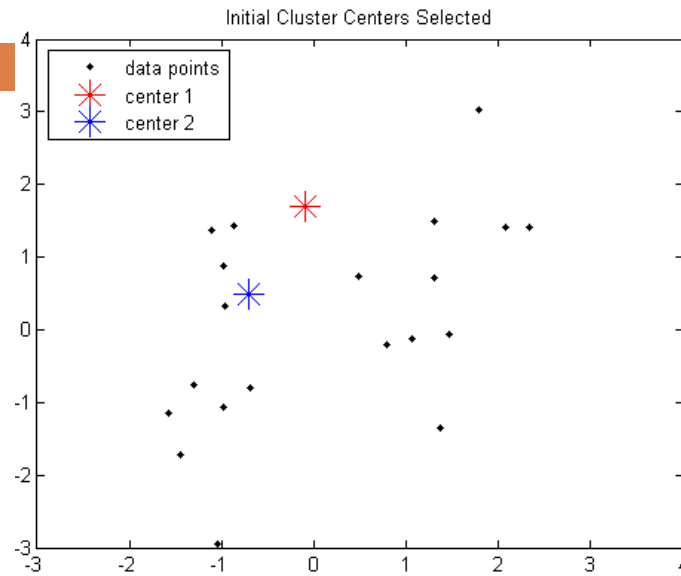
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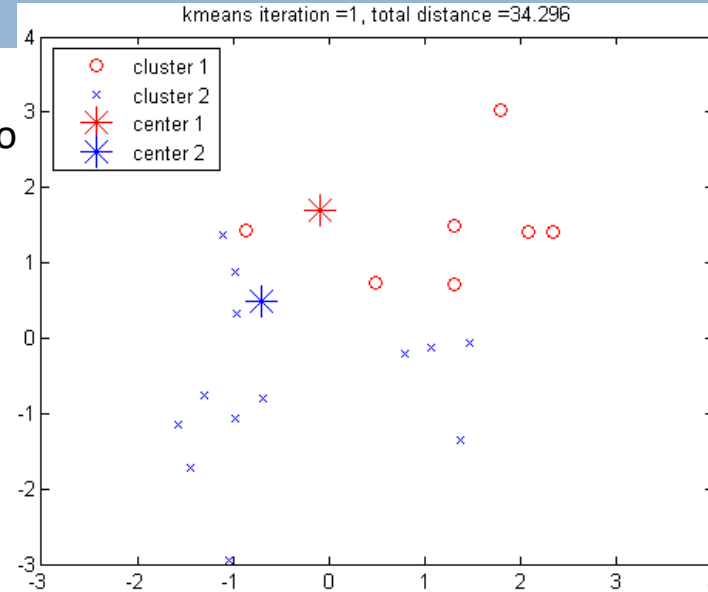
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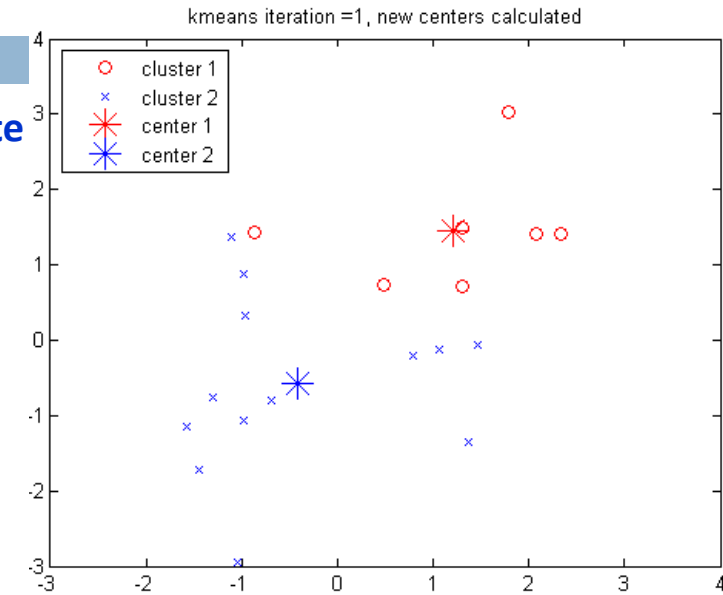


The original data points &  
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Assign  
points to  
clusters



Recompute  
cluster  
centers



## Execution of the *K*-Means Clustering Algorithm

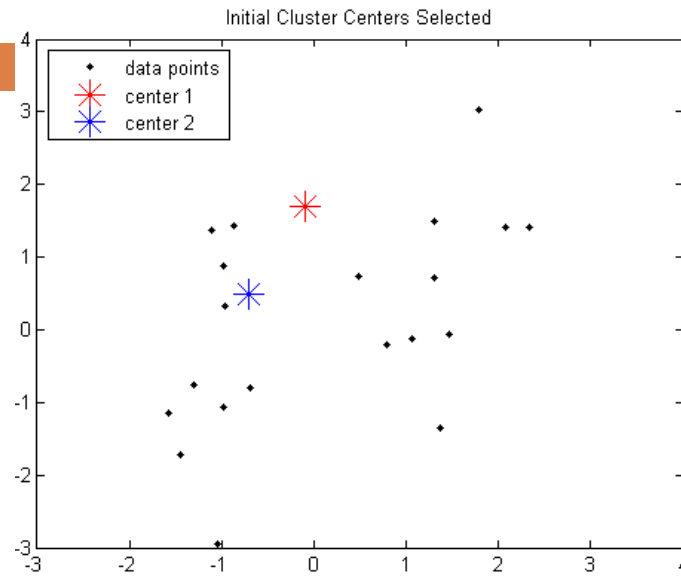
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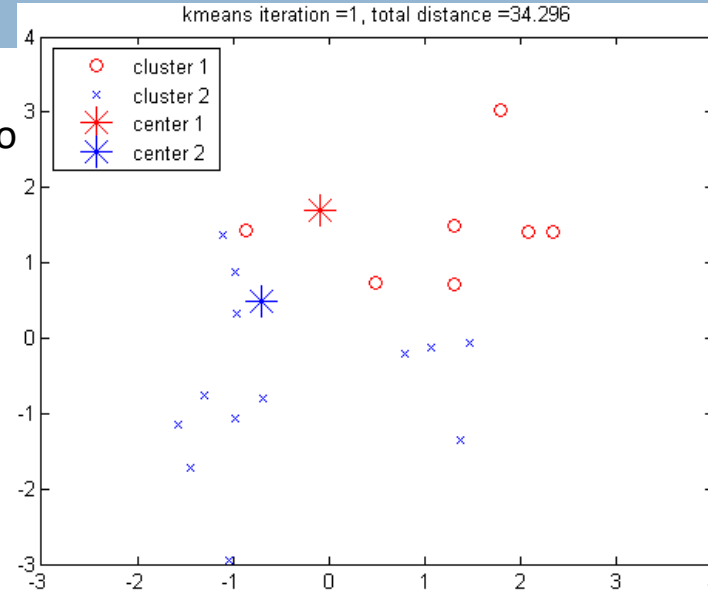
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# Example: *K*-Means Clustering

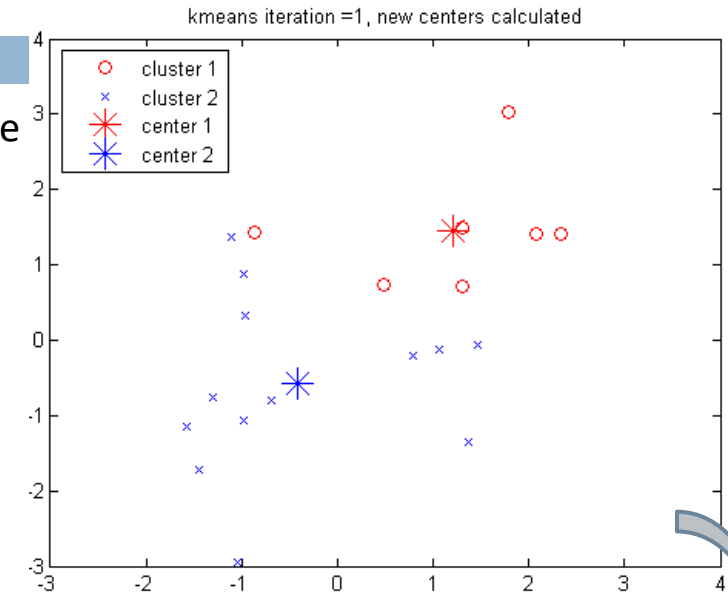


The original data points & randomly select  $K = 2$  centroids

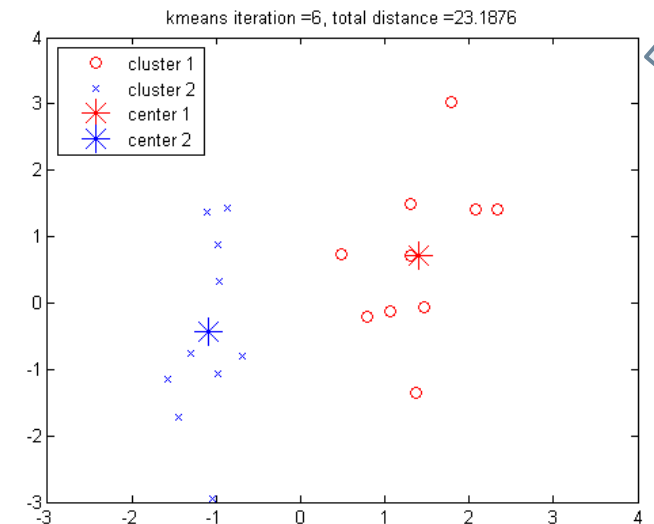
Assign points to clusters



Recompute cluster centers



Redo point assignment



## Execution of the *K*-Means Clustering Algorithm

Select  $K$  points as initial centroids

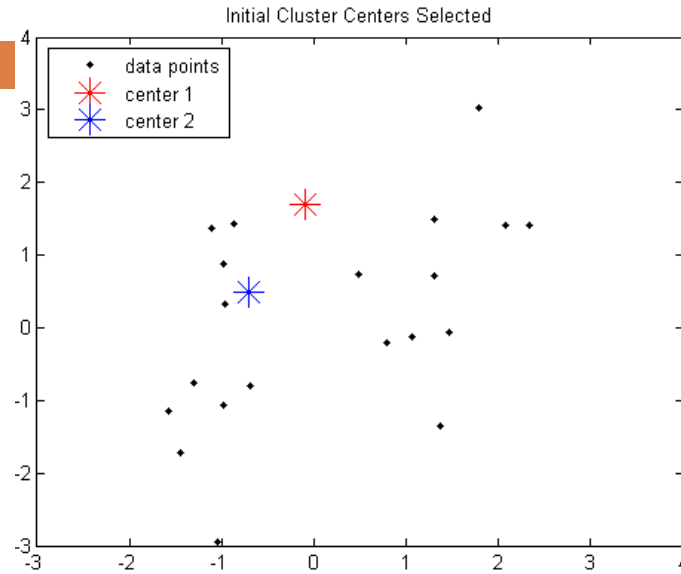
### Repeat

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Until convergence criterion is satisfied

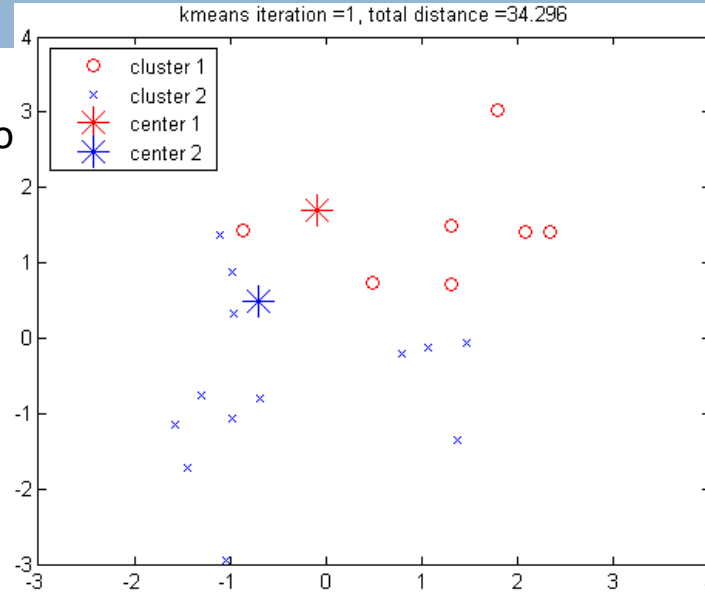


# Example: *K*-Means Clustering



The original data points & randomly select  $K = 2$  centroids

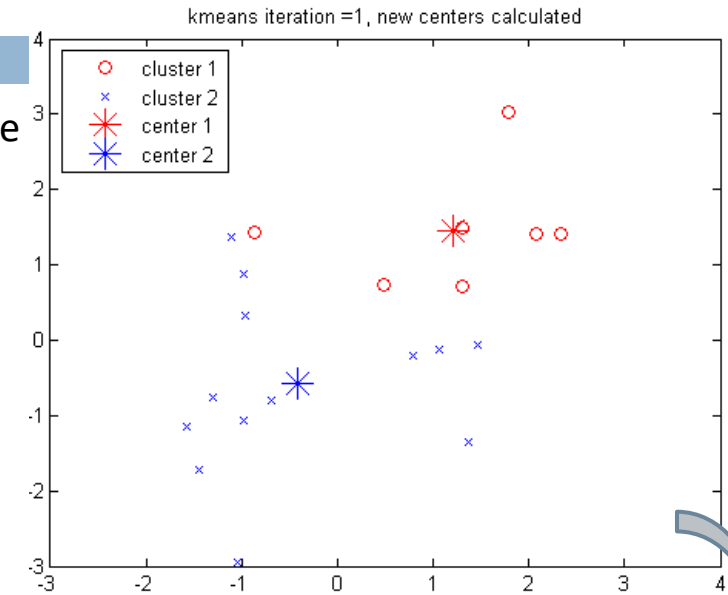
Assign points to clusters



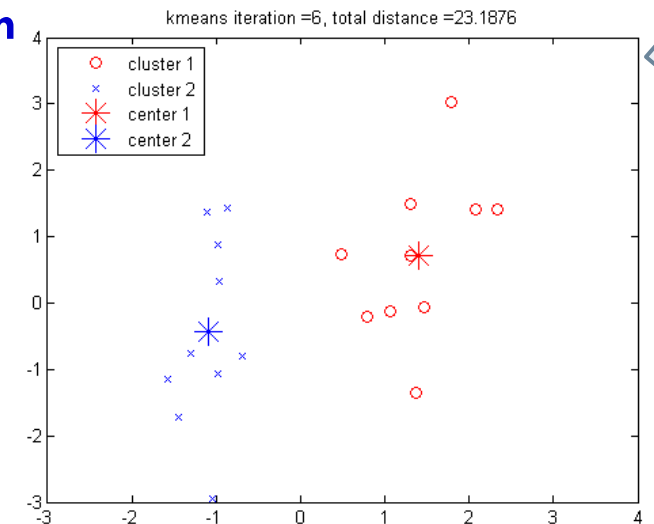
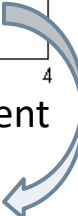
Recompute cluster centers



Next iteration



Redo point assignment



## Execution of the *K*-Means Clustering Algorithm

Select  $K$  points as initial centroids

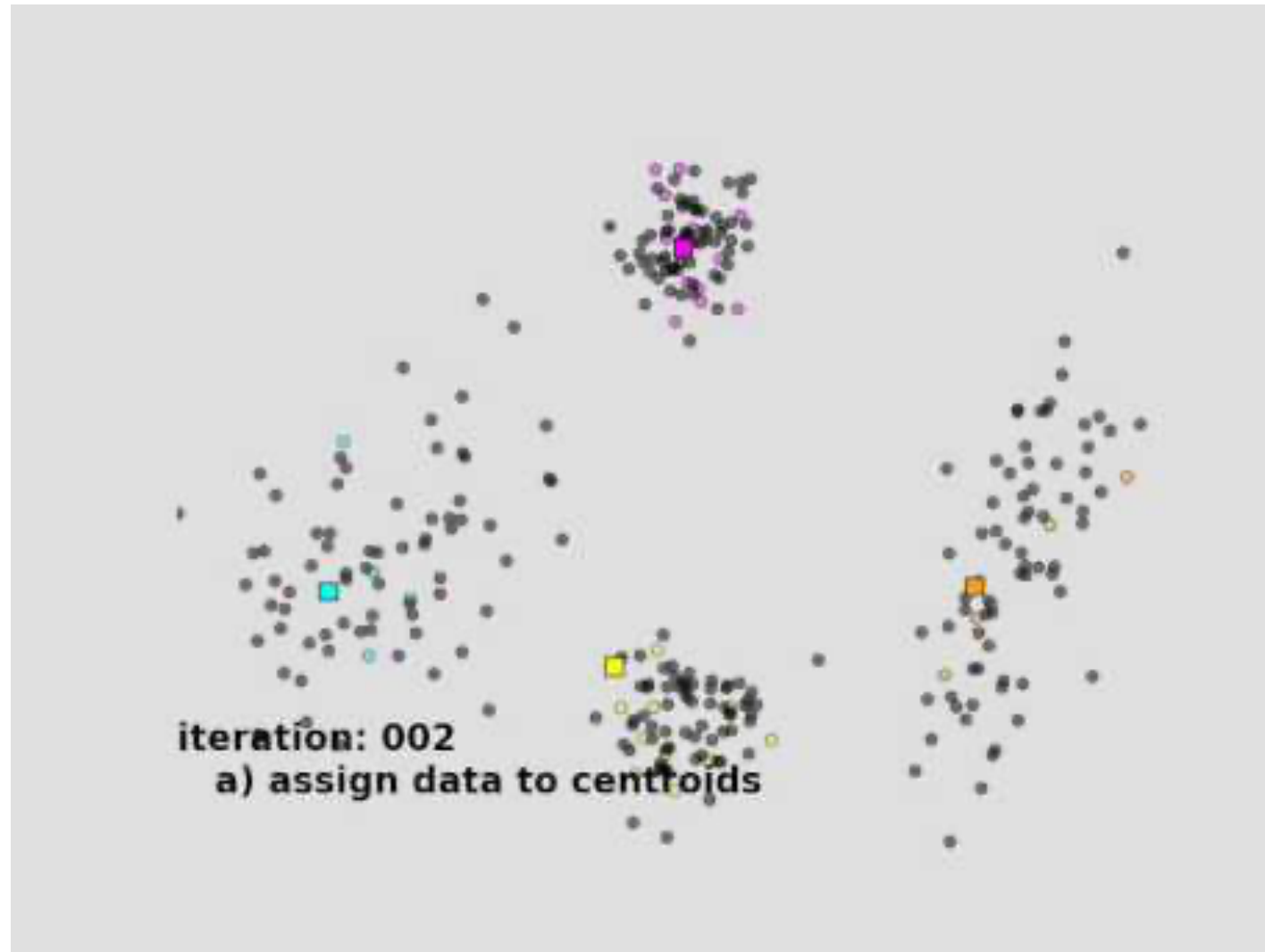
**Repeat**

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- Re-compute the centroids (i.e., *mean point*) of each cluster

**Until** convergence criterion is satisfied

# K-means Example – Animated

34



# Evaluating K-means Clusters

- Why one clustering result is better than the other?

# Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - ▣ For each point, the error is the distance to the nearest cluster
  - ▣ To get SSE, we square these errors and sum them.

$$SSE(C) = \sum_{i=1}^K \sum_{x \in C_i} dist^2(x, c_i)$$

- ▣  $x$  is a data point in cluster  $C_i$  and  $c_i$  is the representative point (e.g., center) of cluster  $C_i$

# Evaluating K-means Clusters

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$$SSE(C) = \sum_{i=1}^K \sum_{x \in C_i} \|x - c_i\|^2$$

Using Euclidean Distance

- ▣  $x$  is a data point in cluster  $C_i$  and  $c_i$  is the representative point (e.g., center) of cluster  $C_i$

# Evaluating K-means Clusters

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- ▣  $x$  is a data point in cluster  $C_i$  and  $c_i$  is the representative point (e.g., center) of cluster  $C_i$
- ▣ Given two clusters, we can choose the one with the smaller error
- ▣ However, one easy way to reduce SSE is to increase  $K$ , the number of clusters
  - A good clustering with smaller  $K$  can have a larger SSE than a poor clustering with larger  $K$
  - Think of the extreme case when  $K = \text{number of data points}$

# Evaluating K-means Clusters

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  - 5: **until** The centroids don't change
- 

=> attempt to minimize SSE

# Derivation of K-means to Minimize SSE

- Example: one-dimensional data

Step 4: how to update centroid

$$\begin{aligned}\frac{\partial}{\partial c_k} \text{SSE} &= \frac{\partial}{\partial c_k} \sum_{i=1}^K \sum_{x \in C_i} (c_i - x)^2 \\ &= \sum_{i=1}^K \sum_{x \in C_i} \frac{\partial}{\partial c_k} (c_i - x)^2 \\ &= \sum_{x \in C_k} 2 \times (c_k - x_k) = 0\end{aligned}$$

$$\sum_{x \in C_k} 2 \times (c_k - x_k) = 0 \Rightarrow m_k c_k = \sum_{x \in C_k} x_k \Rightarrow c_k = \frac{1}{m_k} \sum_{x \in C_k} x_k$$



# Derivation of K-means to Minimize SSE

- Example: What if we choose Manhattan distance?

Step 4: how to update centroid

$$\begin{aligned}\frac{\partial}{\partial c_k} \text{SAE} &= \frac{\partial}{\partial c_k} \sum_{i=1}^K \sum_{x \in C_i} |c_i - x| \\ &= \sum_{i=1}^K \sum_{x \in C_i} \frac{\partial}{\partial c_k} |c_i - x| \\ &= \sum_{x \in C_k} \frac{\partial}{\partial c_k} |c_k - x| = 0\end{aligned}$$

$$\sum_{x \in C_k} \frac{\partial}{\partial c_k} |c_k - x| = 0 \Rightarrow \sum_{x \in C_k} \text{sign}(x - c_k) = 0$$

# Partitioning Algorithms: From Optimization Angle

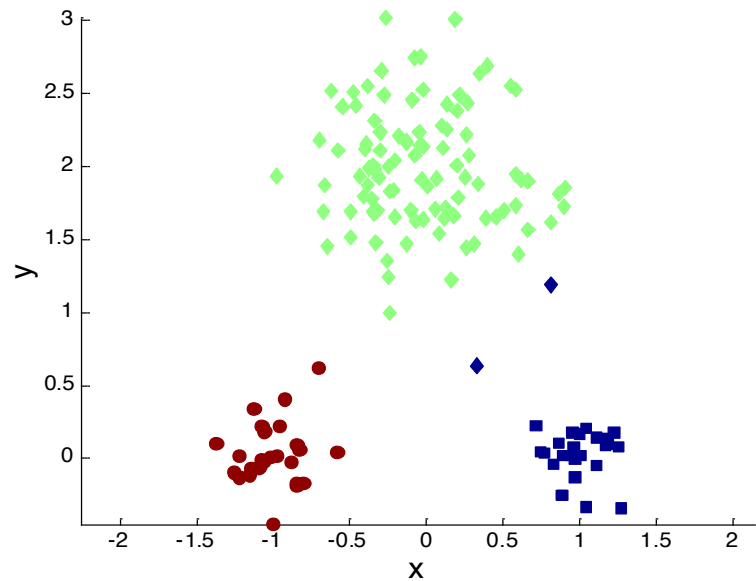
- Partitioning method: Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions
- *K*-partitioning method: Partitioning a dataset ***D*** of ***n*** objects into a set of ***K*** clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where  $c_i$  is the "center" of cluster  $C_i$ )

- A typical objective function: **Sum of Squared Errors (SSE)**

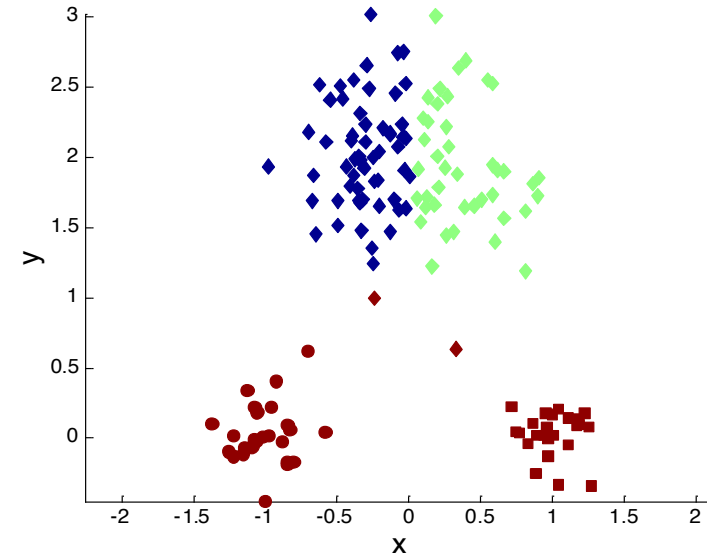
$$SSE(C) = \sum_{i=1}^K \sum_{x \in C_i} \|x - c_i\|^2$$

- Problem definition: **Given *K*, find a partition of *K* clusters that optimizes the chosen partitioning criterion**
  - Global optimum: Needs to exhaustively enumerate all partitions
  - Heuristic methods (i.e., greedy algorithms): *K*-Means, *K*-Medians, *K*-Medoids, etc.

## Two different K-means Clusterings

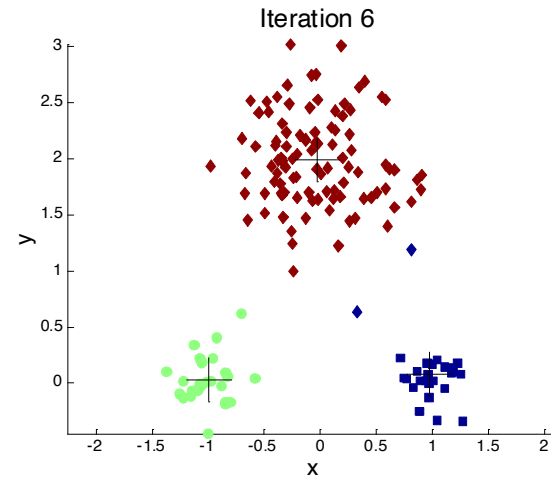
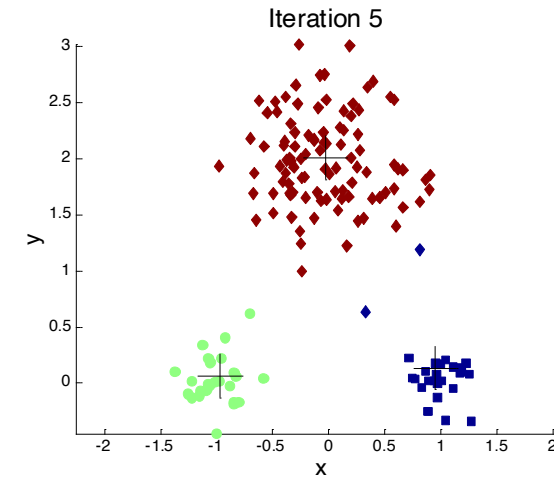
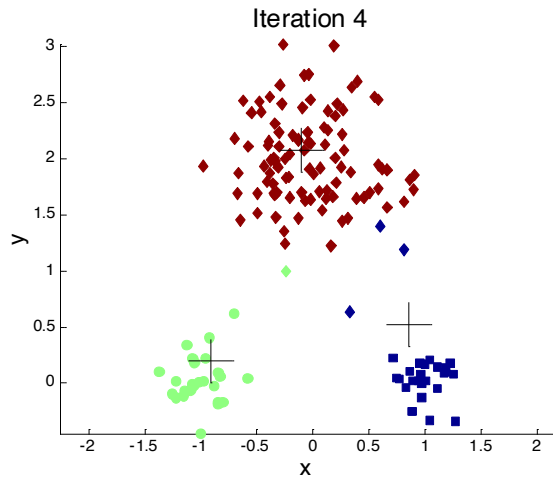
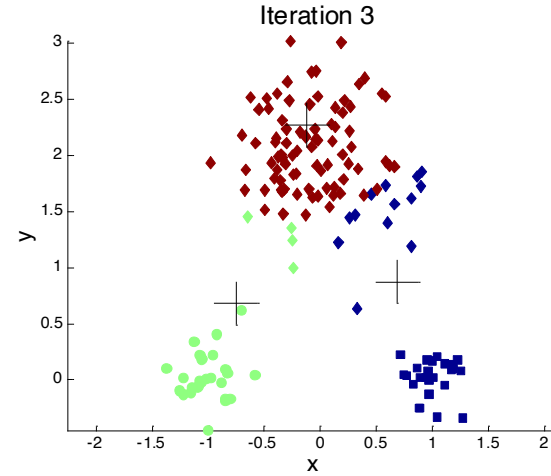
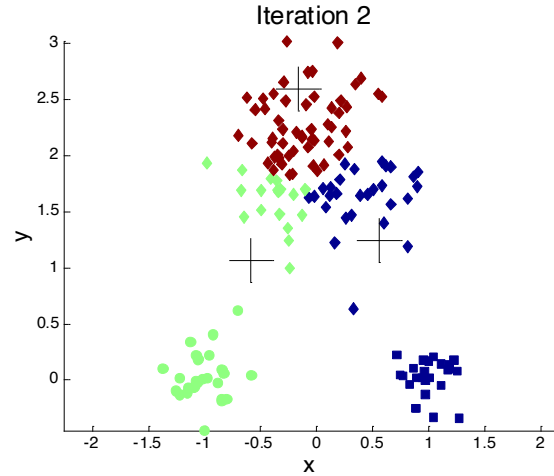
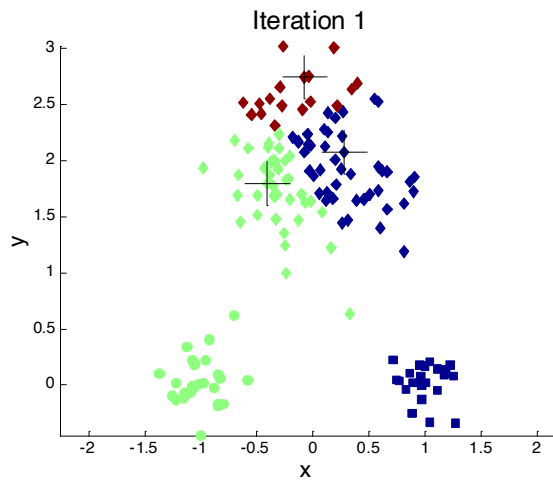


**Optimal Clustering**



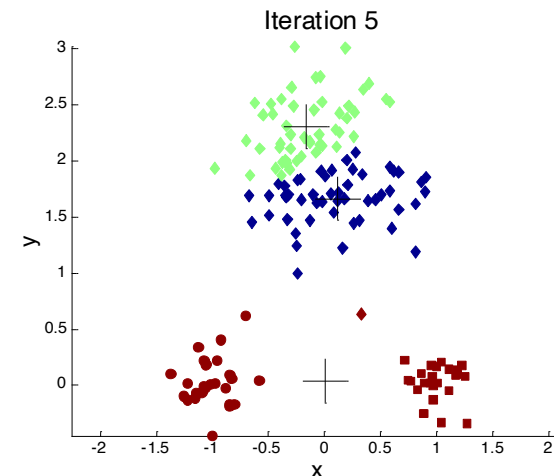
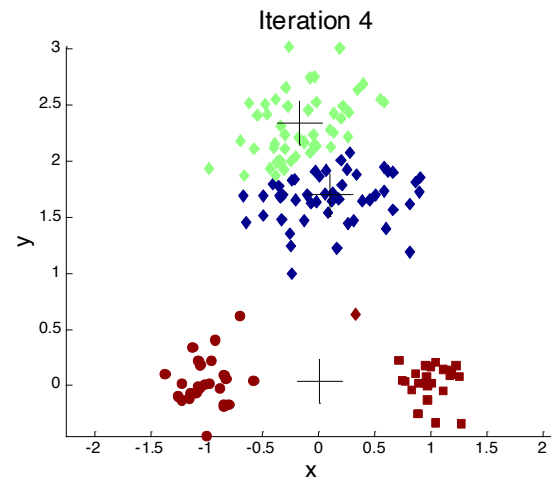
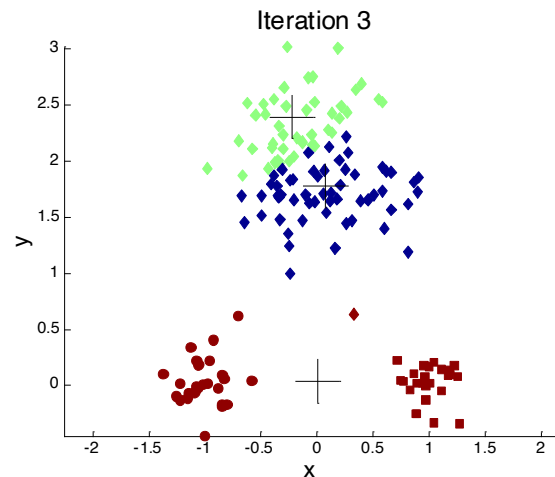
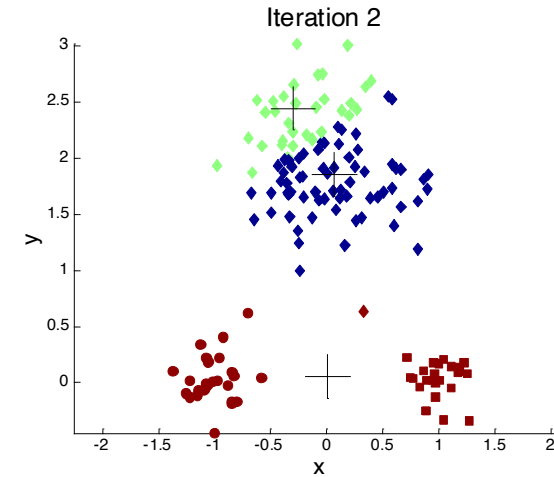
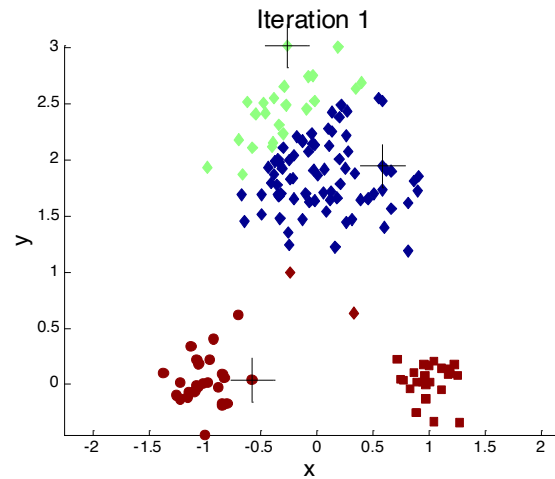
**Sub-optimal Clustering**

# Importance of Choosing Initial Centroids (1)



**Optimal  
Clustering**

## Importance of Choosing Initial Centroids (2)



**Sub-optimal  
Clustering**

# Solutions to Initial Centroids Problem

- **Multiple runs**
  - ▣ Helps, but probability is not on your side
- Select more than  $k$  initial centroids and then select among these initial centroids
  - ▣ Select most widely separated
- General intuition: **spreading out the  $k$  initial centroids is a good thing**

# Pre-processing and Post-processing

- Pre-processing

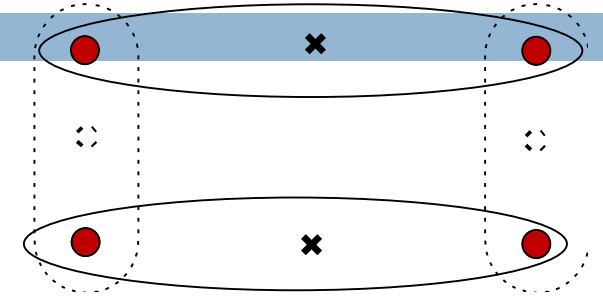
- Normalize the data
- Eliminate outliers

- Post-processing

- Eliminate small clusters that may represent outliers
- Split 'loose' clusters, i.e., clusters with relatively high SSE
- Merge clusters that are 'close' and that have relatively low SSE
- Can use these steps during the clustering process
  - ISODATA

# K-means++

- Original proposal (MacQueen'67): Select  $K$  seeds **randomly**
  - ▣ Need to run the algorithm multiple times using different seeds



- ▣ There are many methods proposed for better initialization of  $k$  seeds
  - ▣ **K-means++** (Arthur & Vassilvitskii'07):
    - ▣ The first centroid is selected at random
    - ▣ **The next centroid selected is the one that is farthest from the currently selected**  
(selection is based on a weighted probability score)
    - ▣ The selection continues until  $K$  centroids are obtained



# K-means++

---

**Algorithm 7.2** K-means++ initialization algorithm.

---

- 1: For the first centroid, pick one of the points at random.
  - 2: **for**  $i = 1$  to *number of trials* **do**
  - 3:   Compute the distance,  $d(x)$ , of each point to its closest centroid.
  - 4:   Assign each point a probability proportional to each point's  $d(x)^2$ .
  - 5:   Pick new centroid from the remaining points using the weighted probabilities.
  - 6: **end for**
-

# K-means vs. K-means++

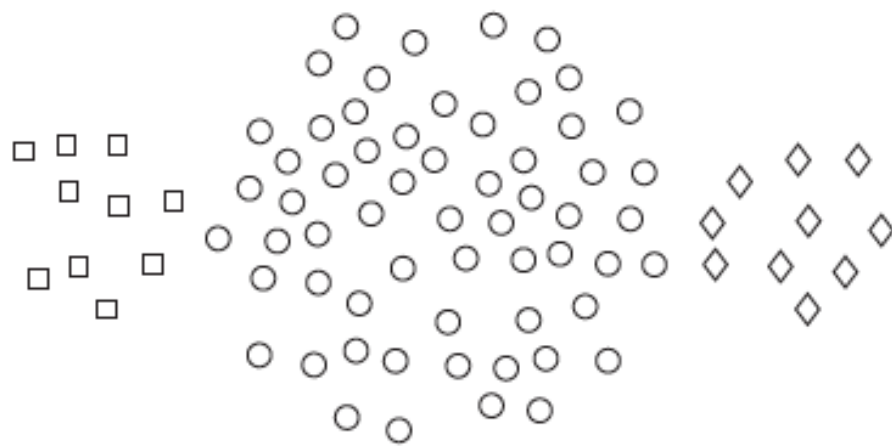
51

- K-means++ is generally preferred over K-means
  - ▣ Even among advanced initialization strategies for K-Means (e.g., Random Partition, Maximin, among others), K-means++ is generally among the best
- K-means++ has better quality guarantee than K-means
  - ▣ For K-means, clusterings can be **arbitrarily worse** than the optimum
  - ▣ K-means++ guarantees an approximation ratio  $O(\log k)$  in expectation
- In practice K-means++ often performs better than K-means in both quality and speed

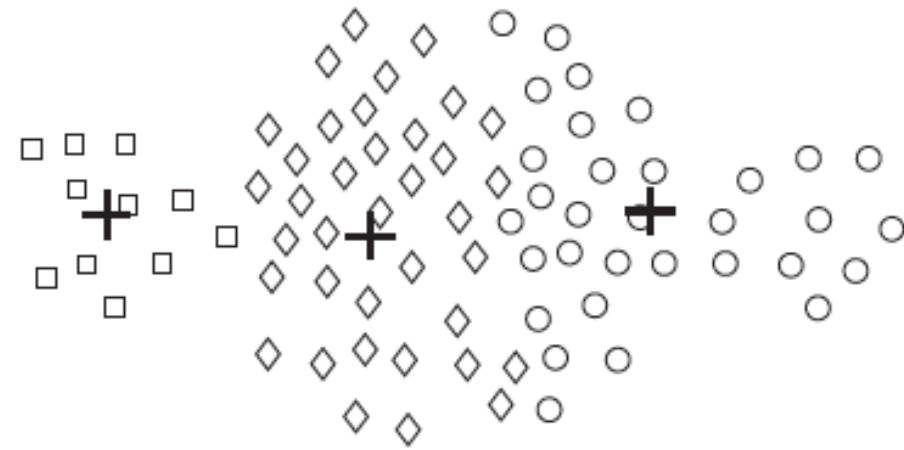
# Limitations of K-means

- K-means has problems when clusters are of differing
  - ▣ Sizes
  - ▣ Densities
  - ▣ Non-globular shapes
- K-means has problems when the data contains outliers.

## Limitations of K-means: Differing Size



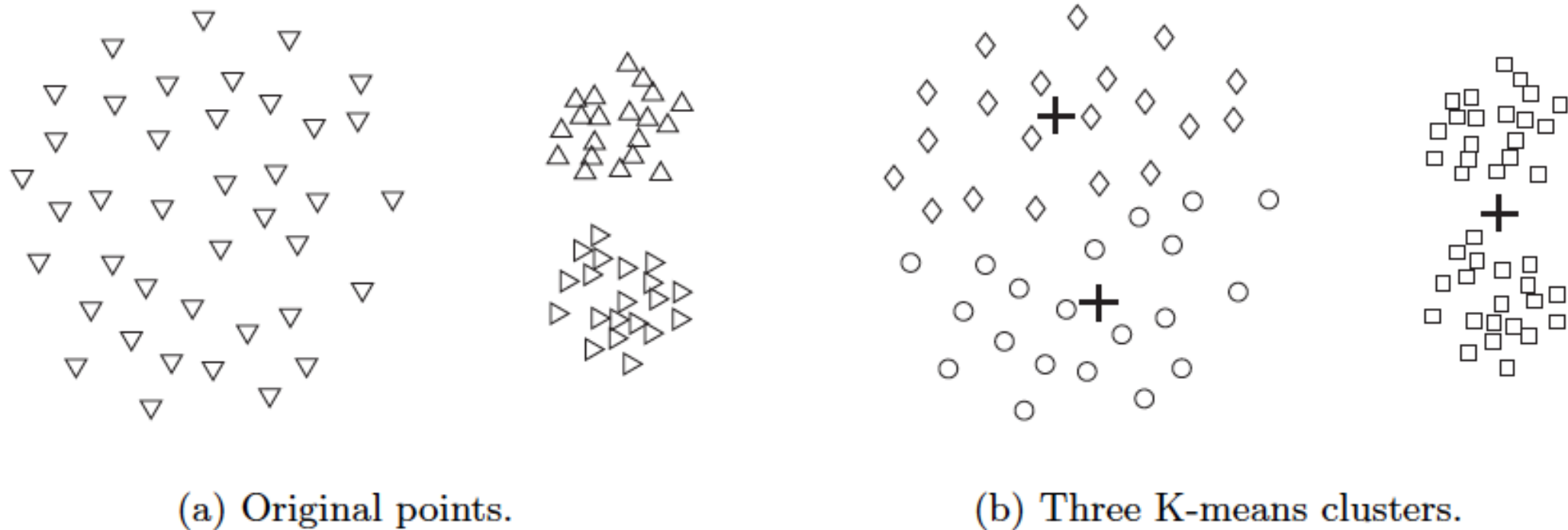
(a) Original points.



(b) Three K-means clusters.

**Figure 7.9.** K-means with clusters of different size.

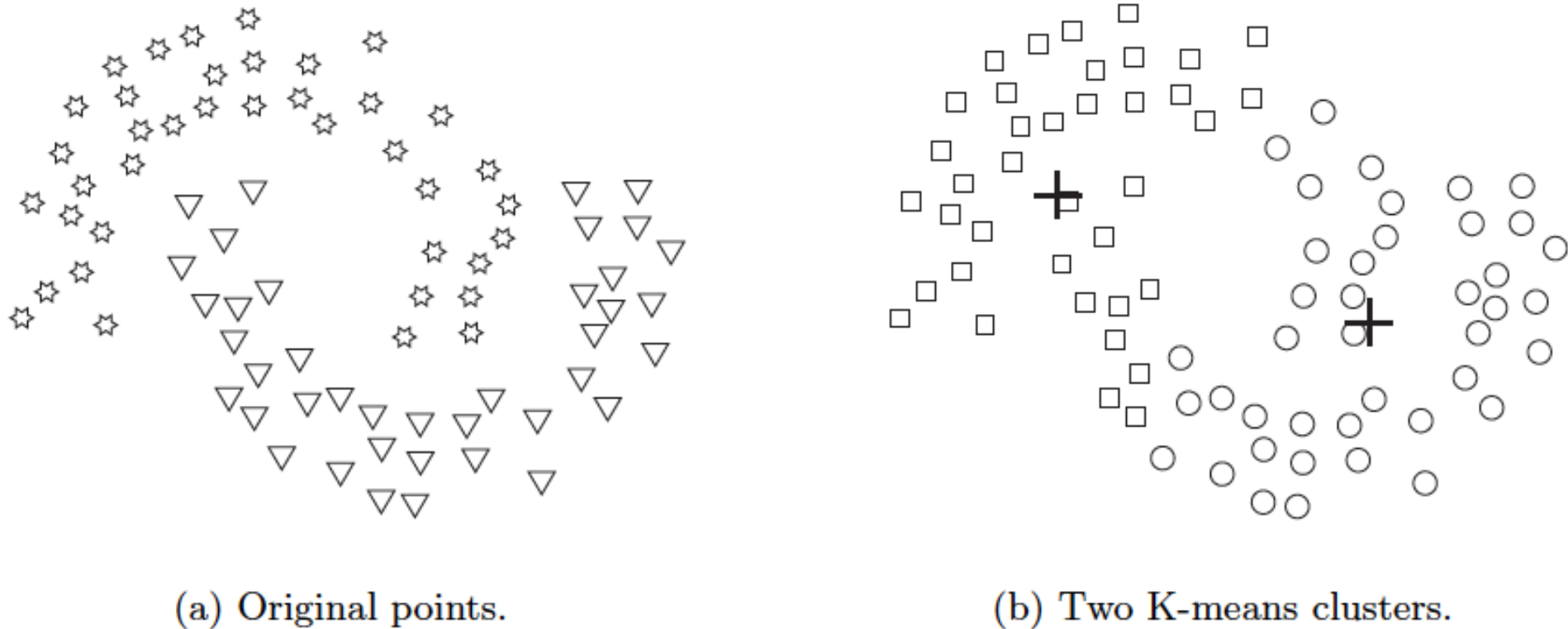
## Limitations of K-means: Differing Density



**Figure 7.10.** K-means with clusters of different density.

[https://www-users.cs.umn.edu/~kumar001/dmbook/ch7\\_clustering.pdf](https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf)

## Limitations of K-means: Non-globular Clusters

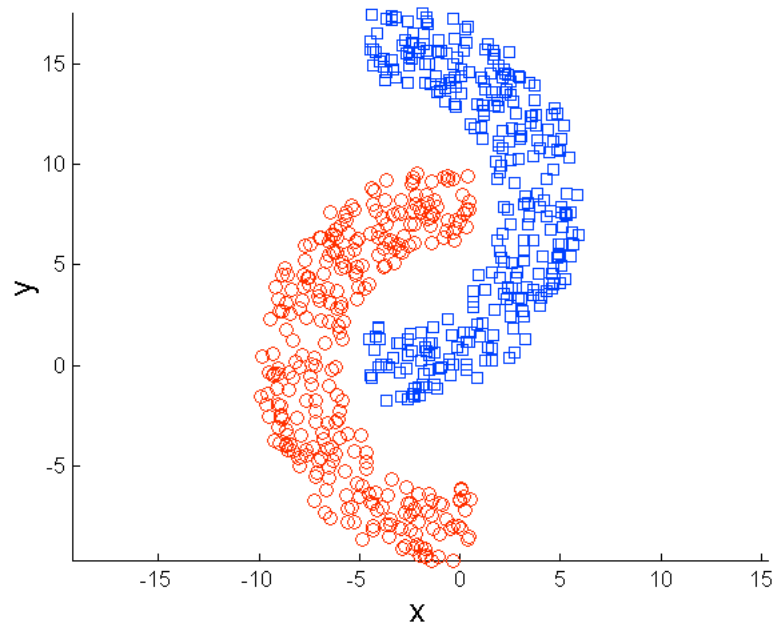


**Figure 7.11.** K-means with non-globular clusters.

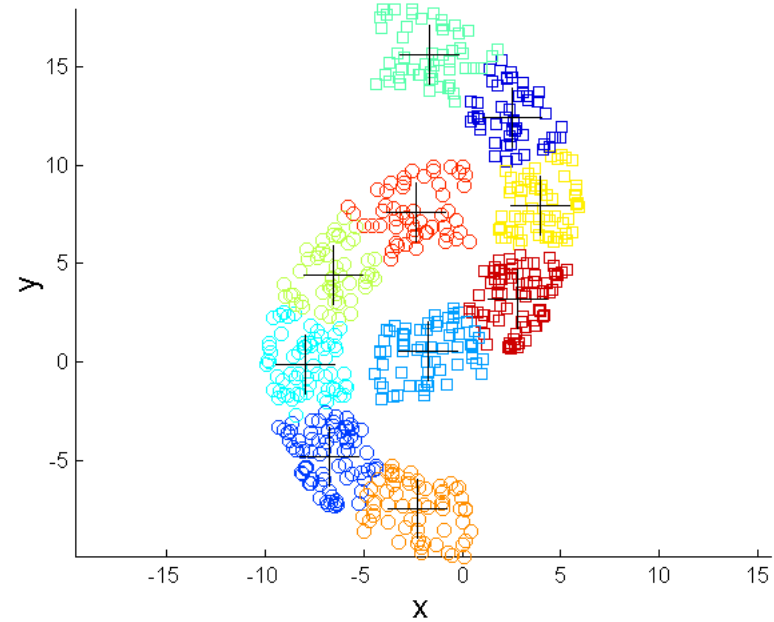
[https://www-users.cs.umn.edu/~kumar001/dmbook/ch7\\_clustering.pdf](https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf)

# Overcoming K-means Limitations:

## Breaking Clusters to Subclusters



**Original Points**



**K-means Clusters**

# *K-Medians: Handling Outliers by Computing Medians*

- Medians are less sensitive to outliers than means
  - ▣ Think of the median salary vs. mean salary of a large firm when adding a few top executives!



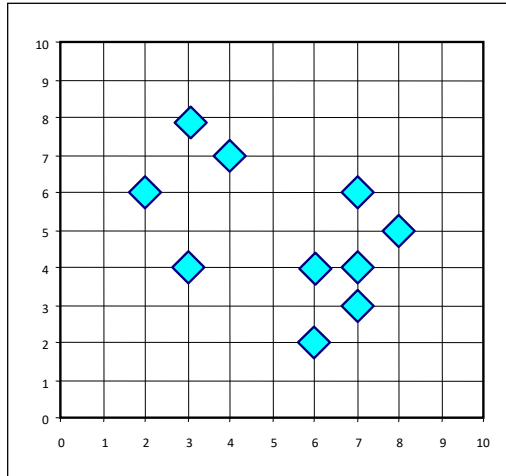
# *K-Medians*: Handling Outliers by Computing Medians

- Medians are less sensitive to outliers than means
  - ▣ Think of the median salary vs. mean salary of a large firm when adding a few top executives!
- ***K-Medians***: Instead of taking the **mean** value of the object in a cluster as a reference point, **medians** are used (corresponding to  $L_1$ -norm as the distance measure)
- The criterion function for the *K-Medians* algorithm:
$$S = \sum_{i=1}^K \sum_{x \in C_i} \sum_{j=1}^D |x_j - med_{ij}|$$
- The *K-Medians* clustering algorithm:
  - Select  $K$  points as the initial representative objects (i.e., as initial  $K$  medians)
  - **Repeat**
    - Assign every point to its nearest median
    - Re-compute the median using the median of each individual feature
  - **Until** convergence criterion is satisfied

# *K-Medoids*: PAM (Partitioning around Medoids)

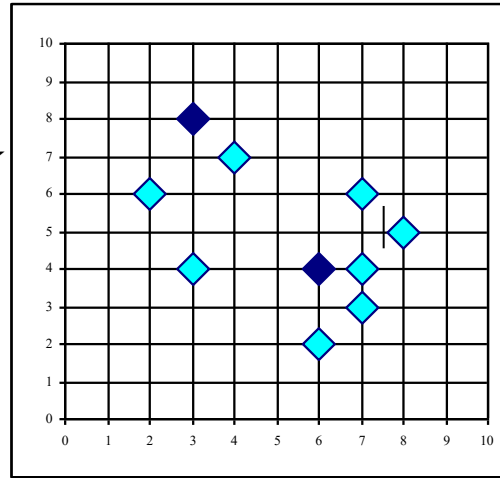
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster
- The *K-Medoids* clustering algorithm: 
$$SSE(C) = \sum_{i=1}^K \sum_{x \in C_i} dist(x, o_i)$$
  - Select  $K$  points as the initial representative objects (i.e., as initial  $K$  medoids)
  - **Repeat**
    - Assigning each point to the cluster with the closest medoid
    - **Randomly select a non-representative object  $o_j$**
    - Compute the total cost  $S$  of swapping the medoid  $m$  with  $o_j$
    - If  $S < 0$ , then swap  $m$  with  $o_j$  to form the new set of medoids
  - **Until** convergence criterion is satisfied

# *K*-Medoids: PAM (Partitioning around Medoids)

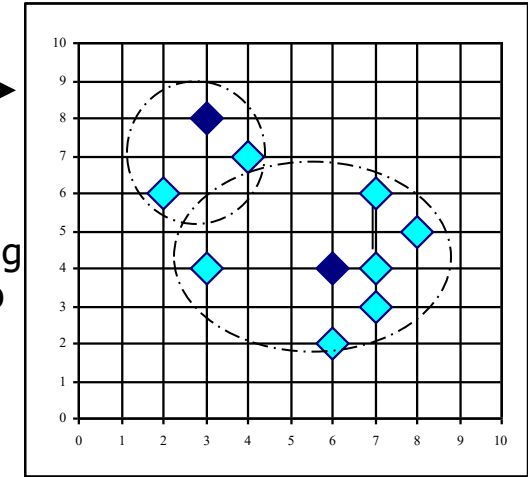


$K = 2$

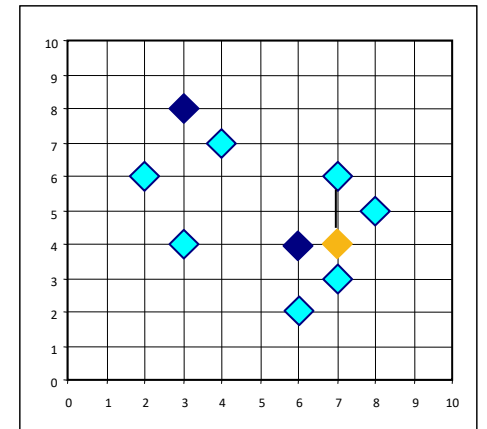
Arbitrary choose  $K$   
object as initial  
medoids



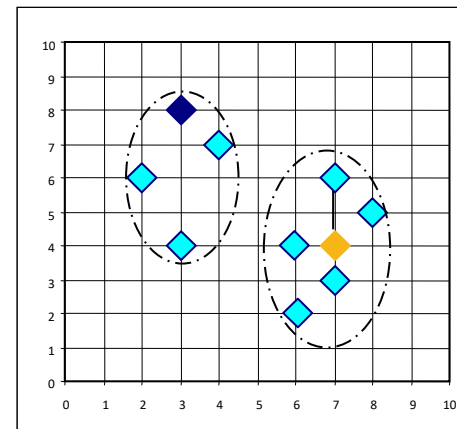
Assign  
each  
remaining  
object to  
nearest  
medoids



Randomly select a non-  
medoid object,  $O_{\text{random}}$



Compute total  
cost of swapping



Swapping  $O$   
and  $O_{\text{random}}$   
If quality is  
improved

Select initial *K*-Medoids randomly

**Repeat**

Object re-assignment

Swap medoid  $m$  with  $o_i$  if it  
improves the clustering quality

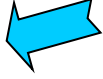
**Until** convergence criterion is satisfied

# Reminder

63

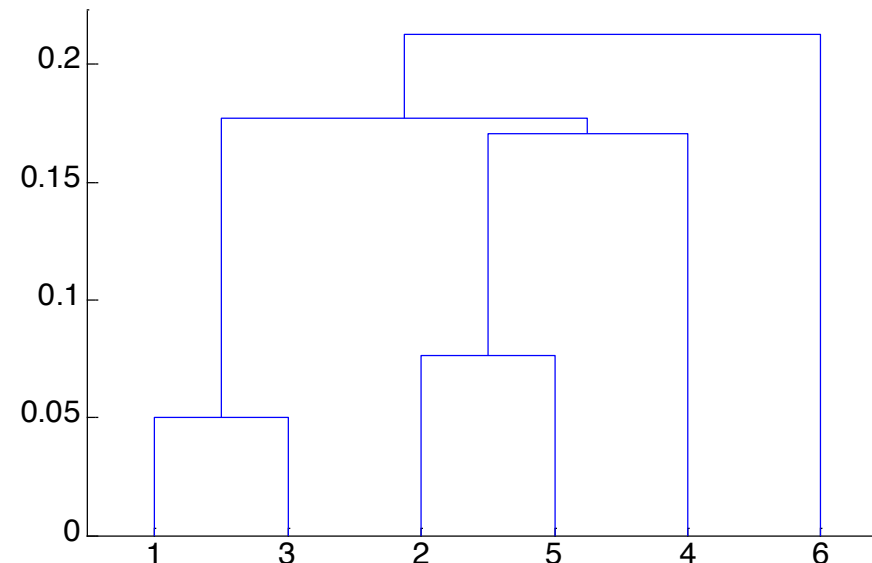
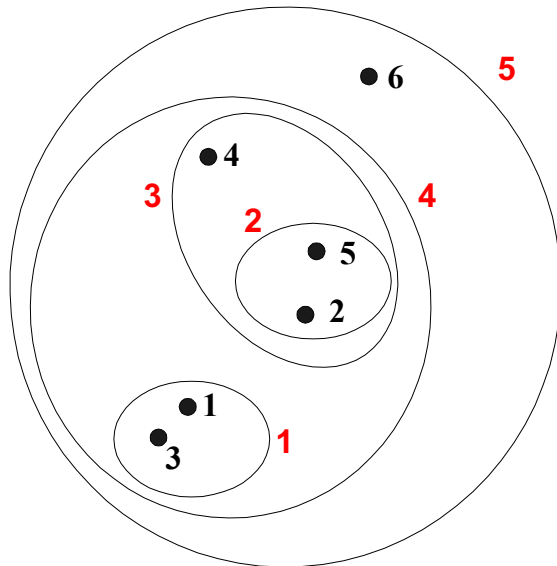
- HW2 due next Wednesday by 11:59PM
  - ▣ Memory issue for the programming task
    - There are **11,314** documents, about **100K** distinct tokens (depending on how you tokenize/lemmatize/etc.), so the feature matrix may have over  $10^9$  entries. An Int could take 4 to 8 bytes, so it could take up to **8GB** memory
    - Solutions
      - Use sparse matrix
      - Truncate the vocabulary by frequency
  - ▣ Make sure your handwriting is readable to TA (if you do not type).

# Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: An Introduction
- Partitioning Methods
- Hierarchical Methods 
- Density- and Grid-Based Methods
- Evaluation of Clustering
- Summary

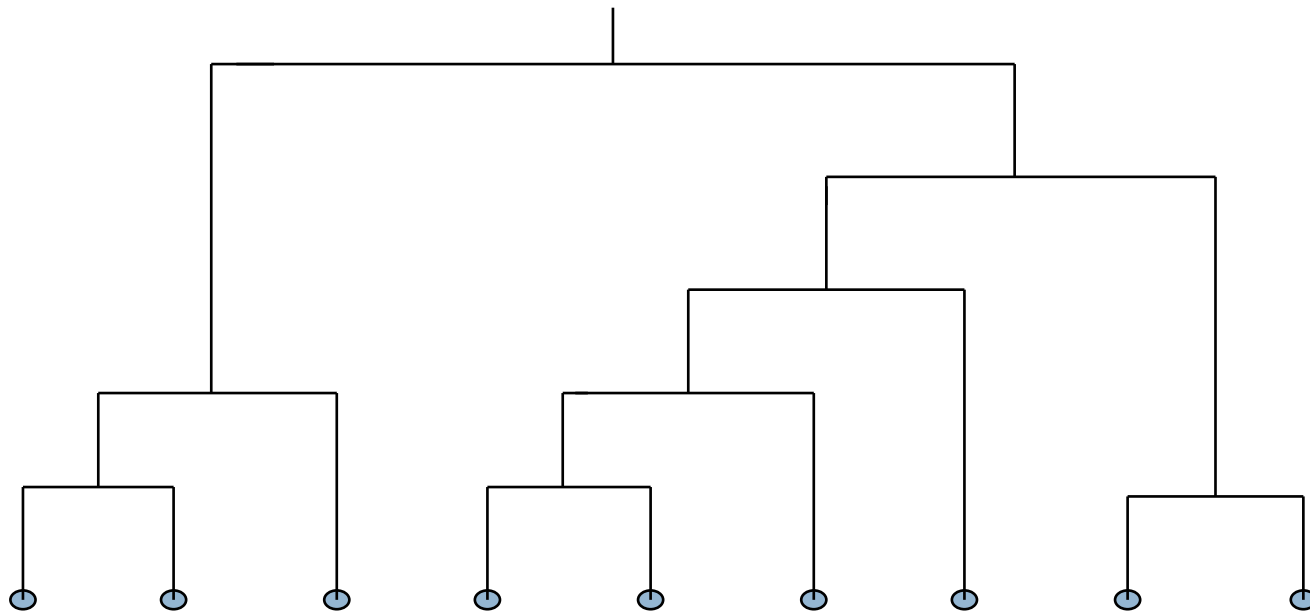
# Hierarchical Clustering

- 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



# Dendrogram: Shows How Clusters are Merged/Splitted

- Dendrogram: Decompose a set of data objects into a tree of clusters by multi-level nested partitioning
- A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster



Hierarchical clustering  
generates a dendrogram  
(a hierarchy of clusters)

# 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 dendrogram at the proper level
- They may correspond to meaningful taxonomies
  - ▣ Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)



# Hierarchical Clustering

- Two main types of hierarchical clustering
  - ▣ Agglomerative:
  - ▣ Divisive:

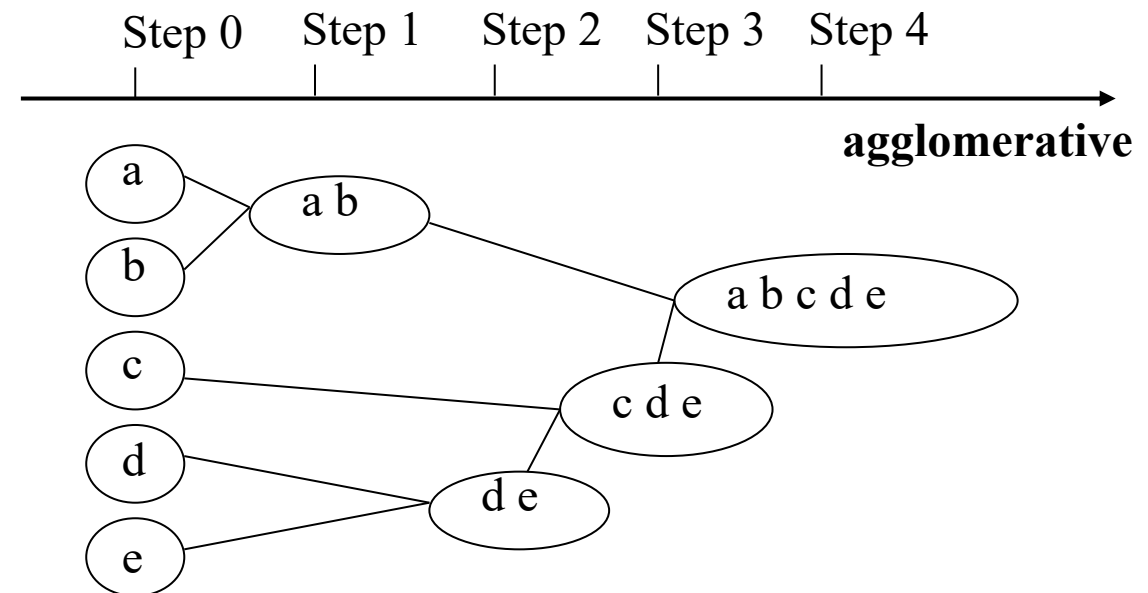
# Hierarchical Clustering

## □ 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
- Build a bottom-up hierarchy of clusters

### ▣ Divisive:



# Hierarchical Clustering

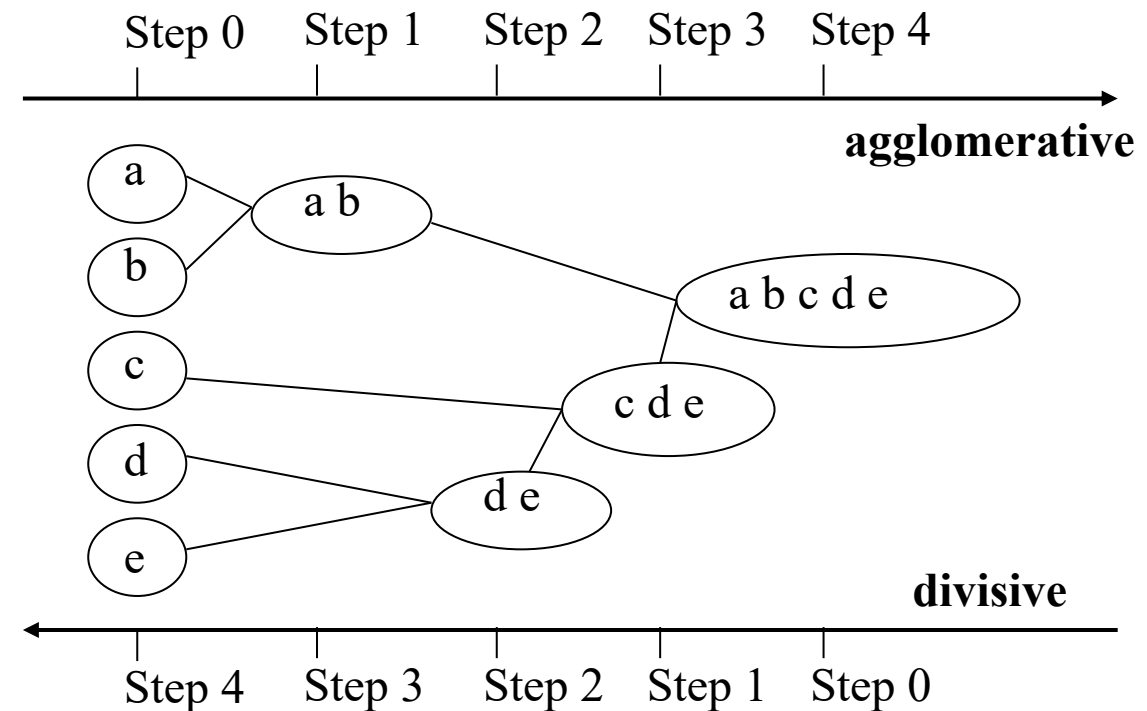
## □ Two main types of hierarchical clustering

### ▣ 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
- Build a bottom-up hierarchy of clusters

### ▣ Divisive:

- Start with one, all-inclusive cluster
- At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Generate a top-down hierarchy of clusters



# Hierarchical Clustering

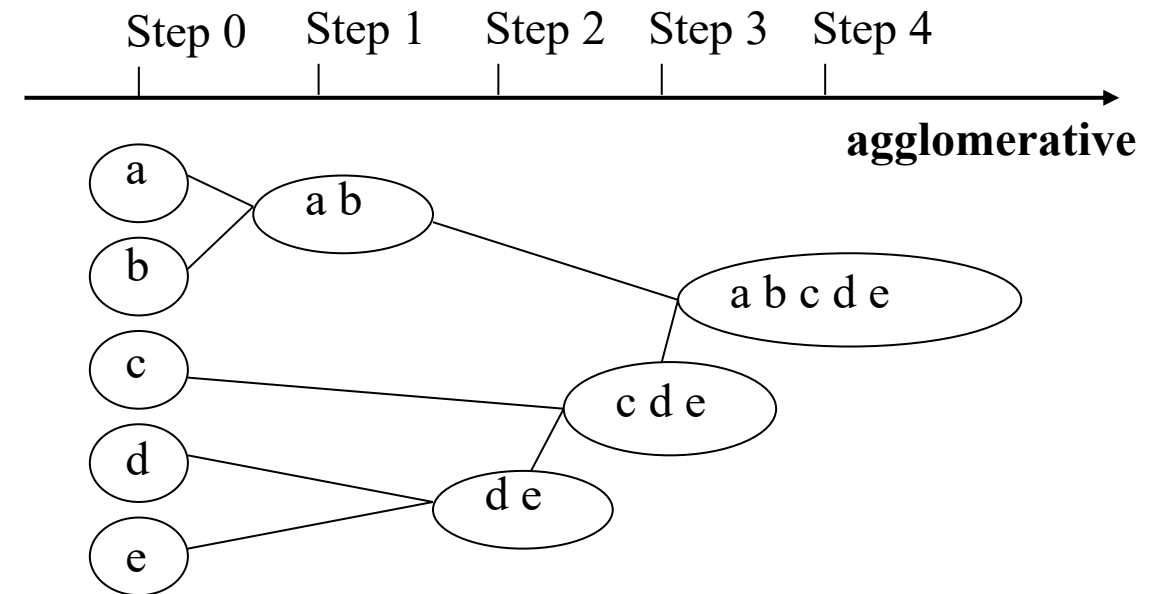
- Two main types of hierarchical clustering
  - ▣ **Agglomerative:**
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or  $k$  clusters) left
  - ▣ **Divisive:**
    - Start with one, all-inclusive cluster
    - At each 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

# 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

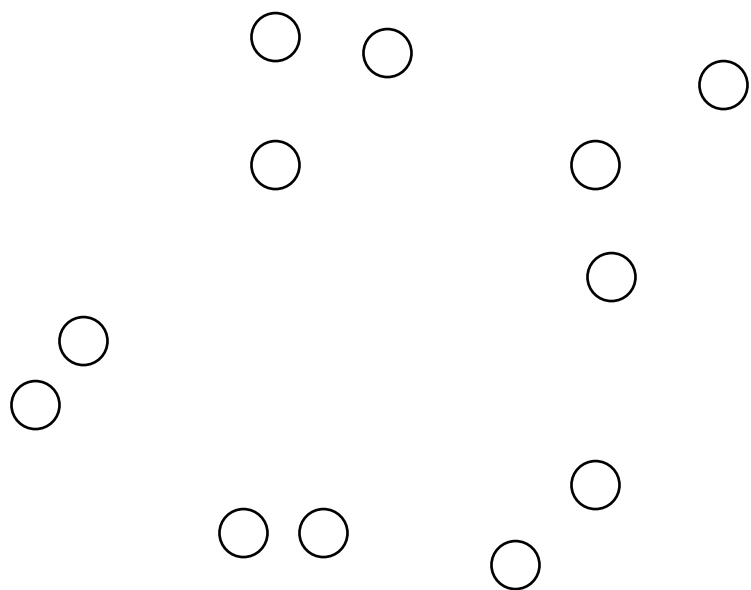


# Agglomerative Clustering Algorithm

- 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/similarity between clusters** distinguish the different algorithms

# Starting Situation

- Start with clusters of individual points and a proximity matrix



12 data points

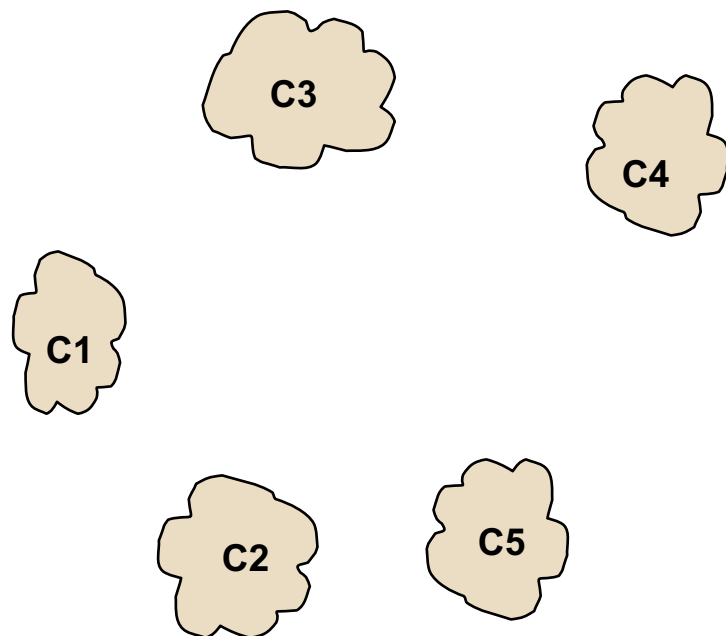
	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



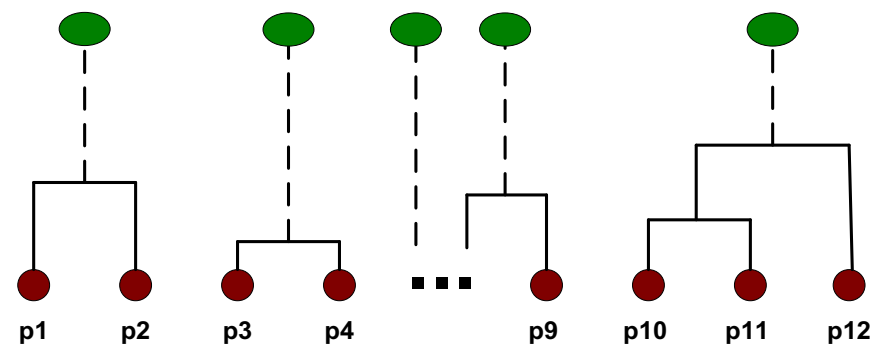
# Intermediate Situation

□ After some merging steps, we have some clusters



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

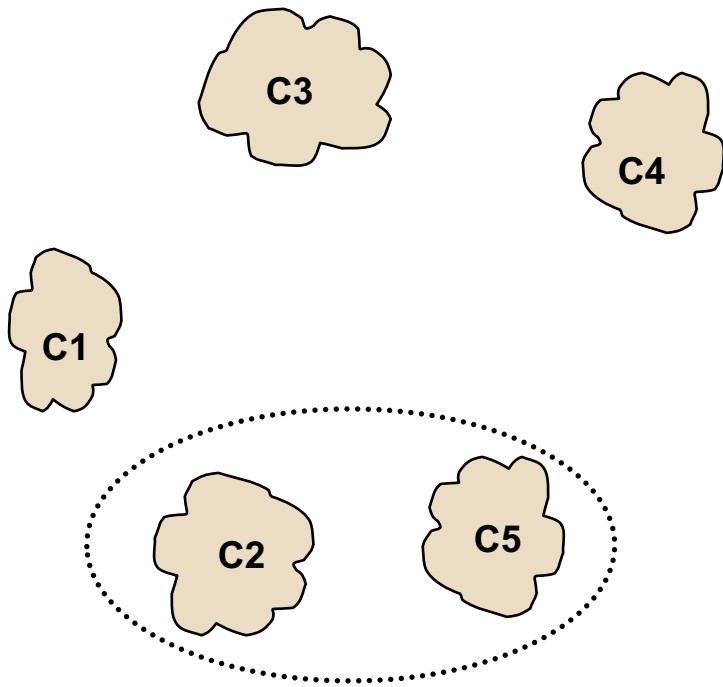
Proximity Matrix





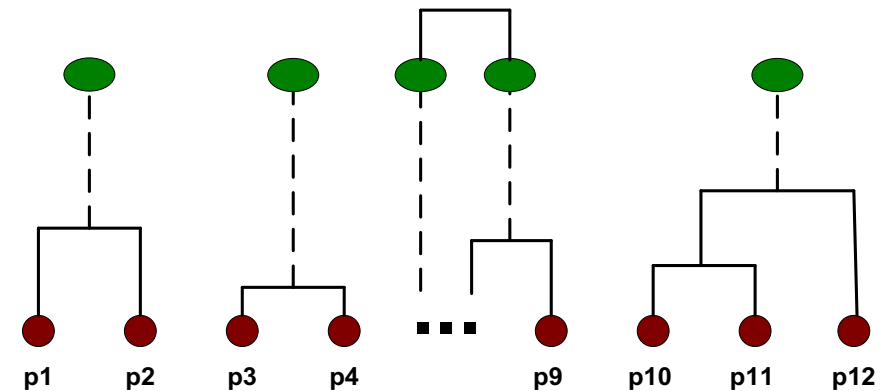
# Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.



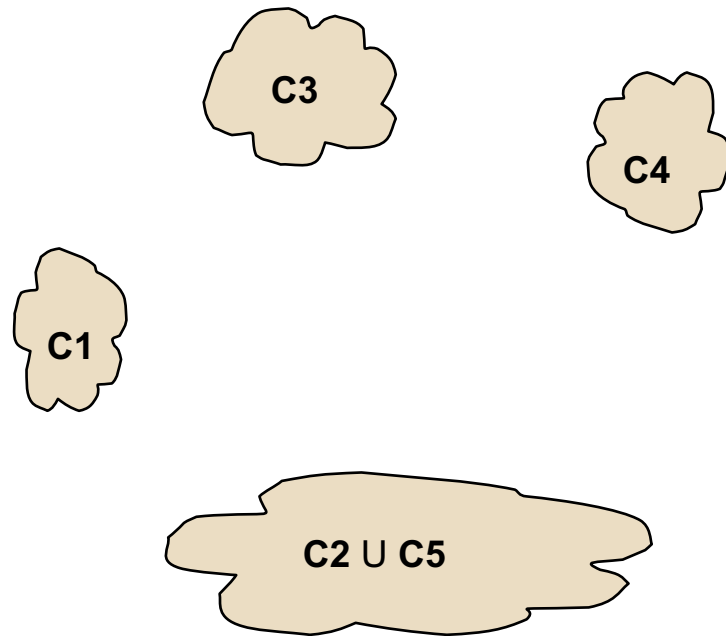
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

**Proximity Matrix**



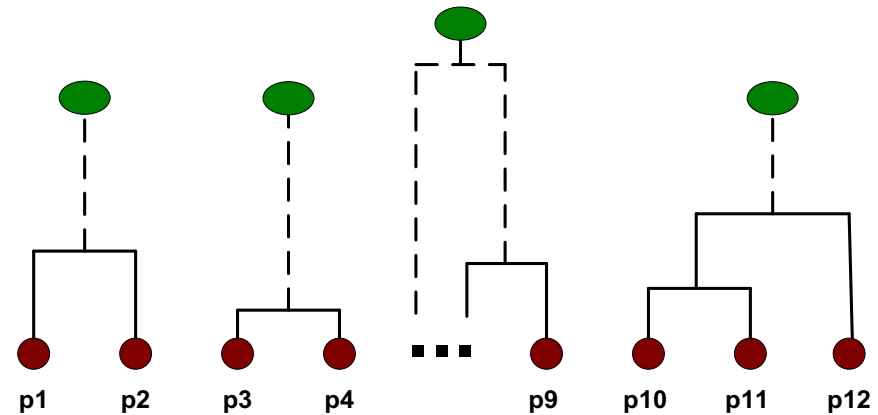
# After Merging

- How do we update the proximity matrix?

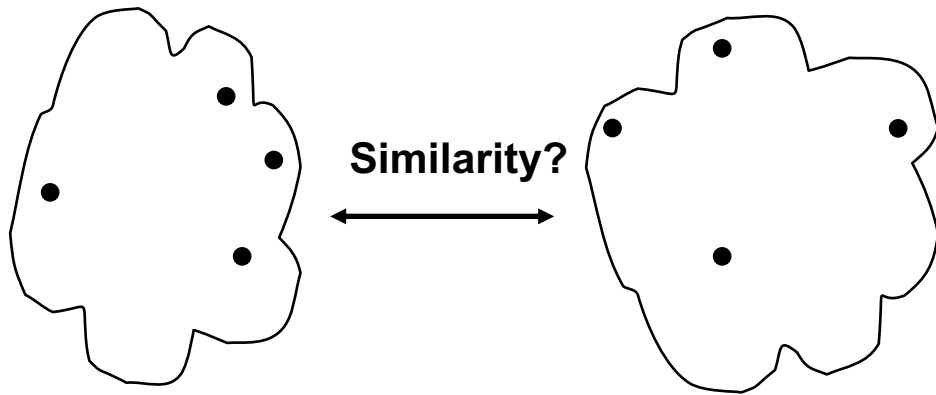


	C1	$C2 \cup C5$	C3	C4
C1		?		
$C2 \cup C5$	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



## How to Define Inter-Cluster Similarity



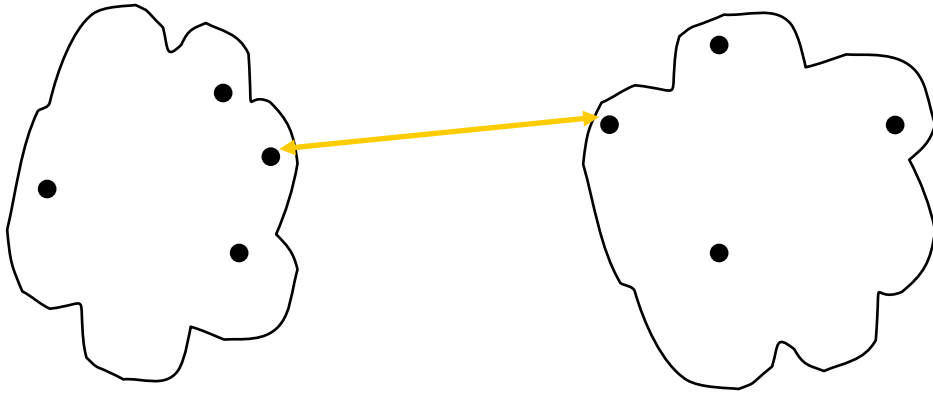
- MIN
- MAX
- Group Average
- Distance Between Centroids

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

**Proximity Matrix**

·  
·

## How to Define Inter-Cluster Similarity



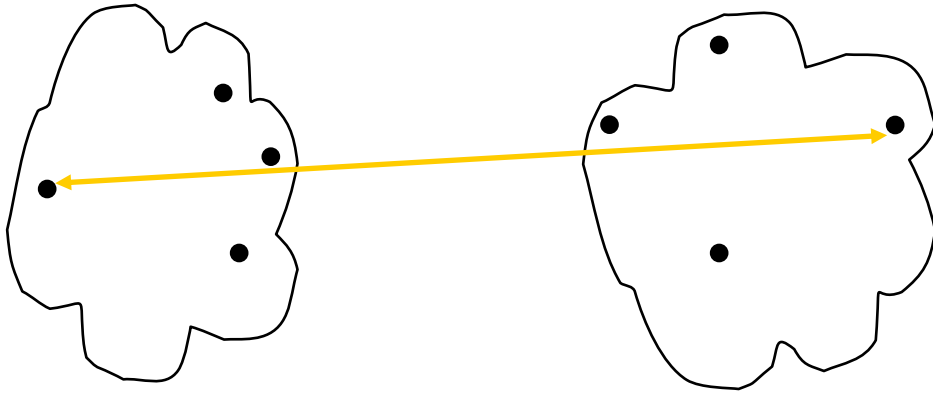
- MIN
- MAX
- Group Average
- Distance Between Centroids

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

**Proximity Matrix**

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## How to Define Inter-Cluster Similarity

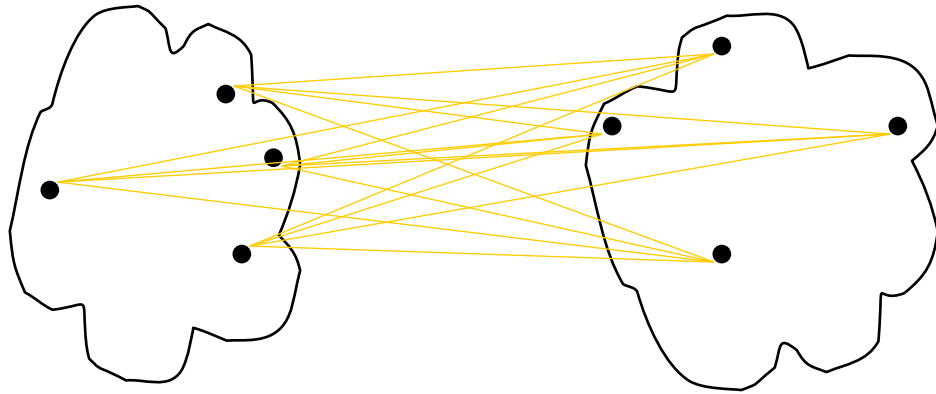


- MIN
- MAX
- Group Average
- Distance Between Centroids

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

**Proximity Matrix**

## How to Define Inter-Cluster Similarity



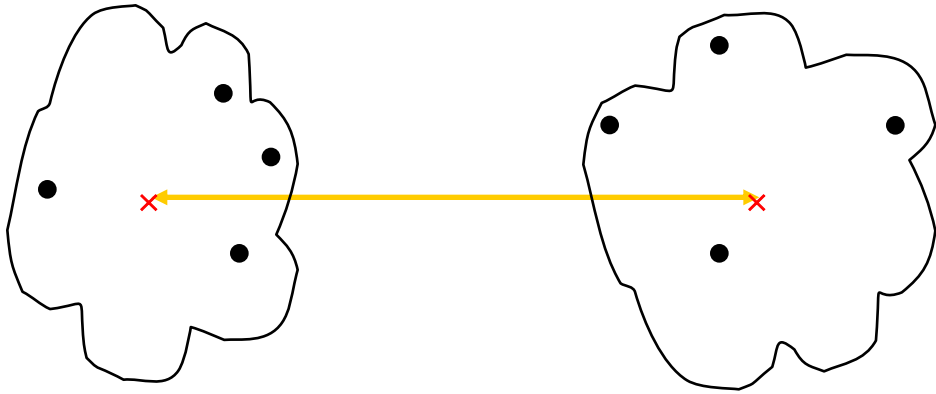
- MIN
- MAX
- **Group Average**
- Distance Between Centroids

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

· **Proximity Matrix**

·

## How to Define Inter-Cluster Similarity



- MIN
- MAX
- Group Average
- Distance Between Centroids

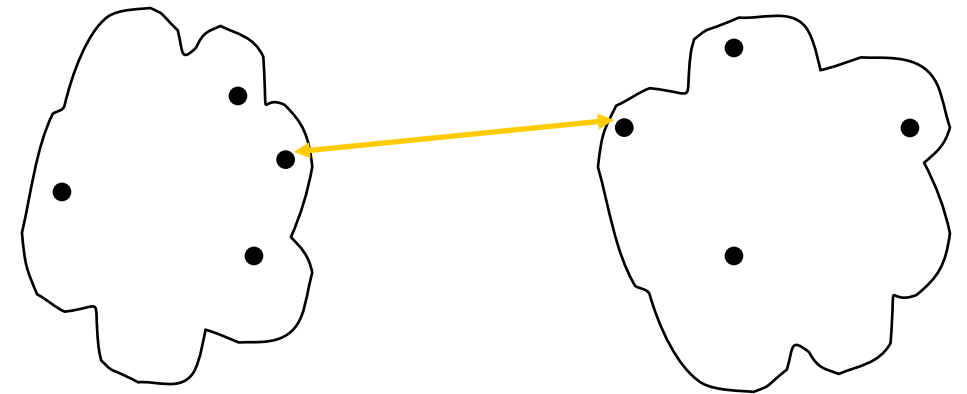
	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						

· **Proximity Matrix**

·

# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters

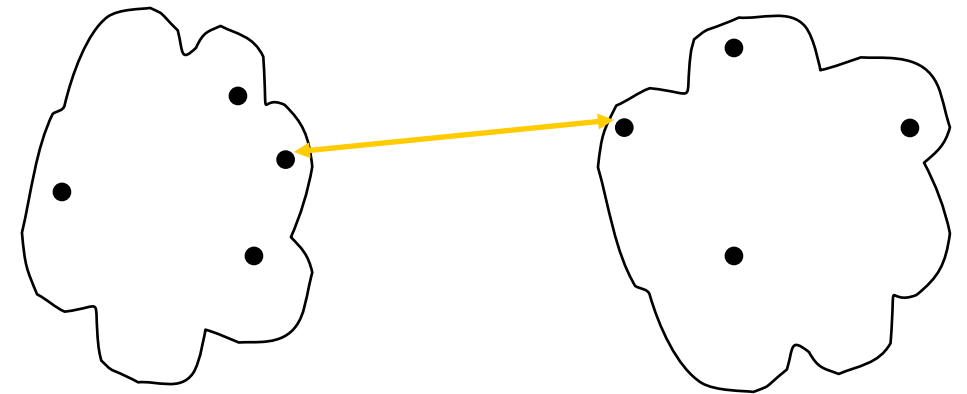


Why single linkage?



# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters



The name comes from the observation that if we connect two points in two clusters within this distance, typically only a single link would exist.

# Cluster Similarity: MIN or Single Linkage

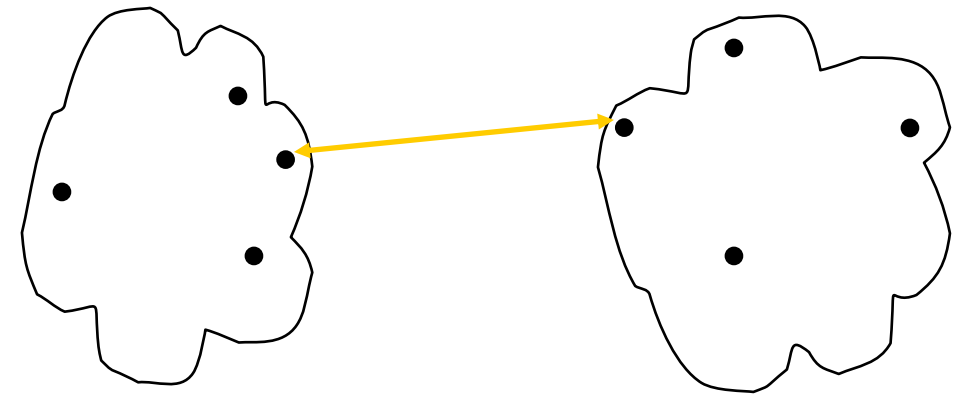
- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters

Let us define the distance between two points using Euclidean distance:

$$\delta(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \left( \sum_{i=1}^d (x_i - y_i)^2 \right)^{1/2}$$

Using single link, the **distance** between two clusters  $C_i$  and  $C_j$  is then:

$$\delta(C_i, C_j) = \underline{\min}\{\delta(\mathbf{x}, \mathbf{y}) \mid \mathbf{x} \in C_i, \mathbf{y} \in C_j\}$$



The name comes from the observation that if we connect two points in two clusters within this distance, typically only a single link would exist.

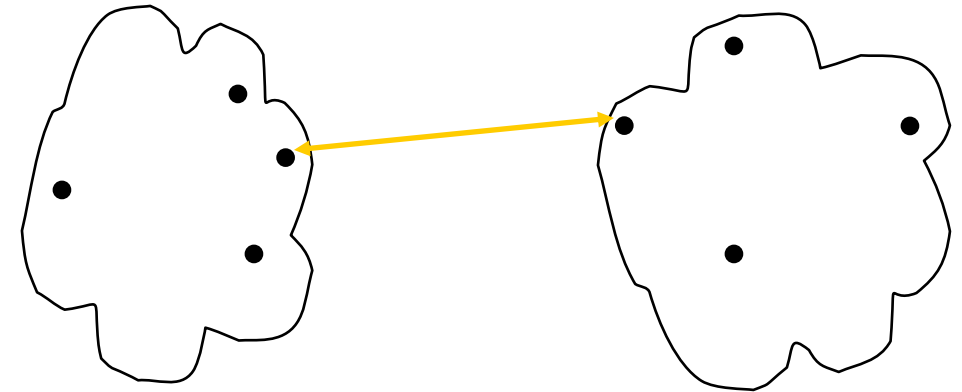
# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters

What if we define the similarity (**not distance**) between two points?

Using single link, the similarity between two clusters  $C_i$  and  $C_j$  is then:

$$\text{Sim}(C_i, C_j) = \underline{\text{max}}\{\text{sim}(x, y) \mid x \text{ in } C_i, y \text{ in } C_j\}$$



The name comes from the observation that if we connect two points in two clusters within this distance, typically only a single link would exist.

# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters

	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 (**Similarity** Matrix)

1	2	3	4	5

# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters

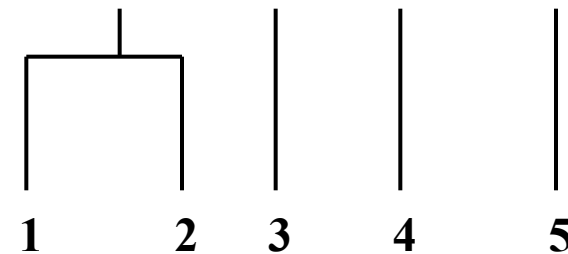
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00

Example (**Similarity** Matrix)

# Cluster Similarity: MIN or Single Linkage

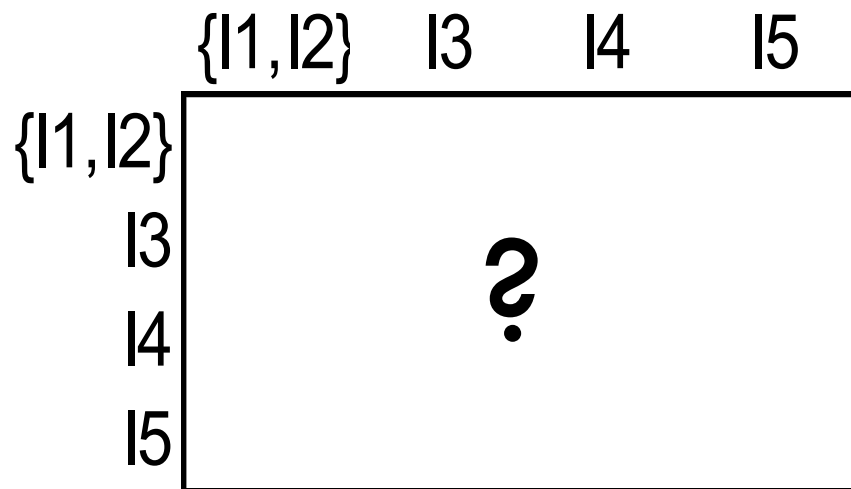
- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters

	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



# Cluster Similarity: MIN or Single Linkage

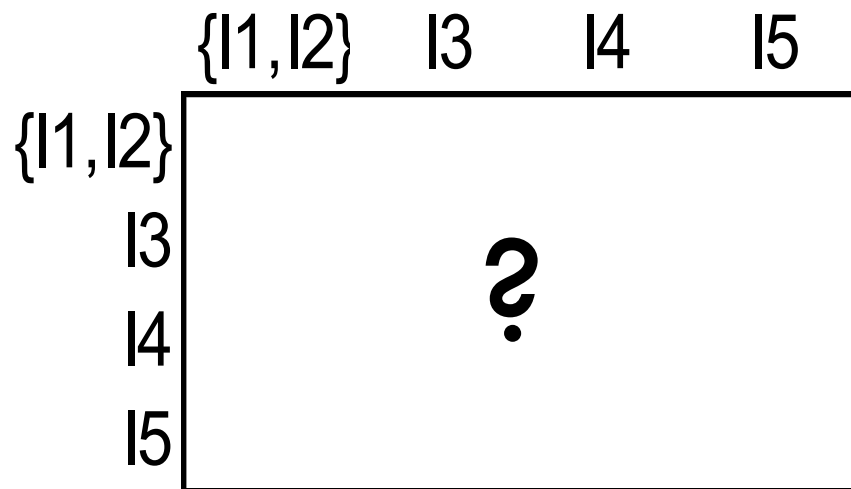
- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters



Update proximity matrix with new cluster  $\{1,1,2\}$

# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters



Update proximity matrix with new cluster  $\{I1, I2\}$

	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

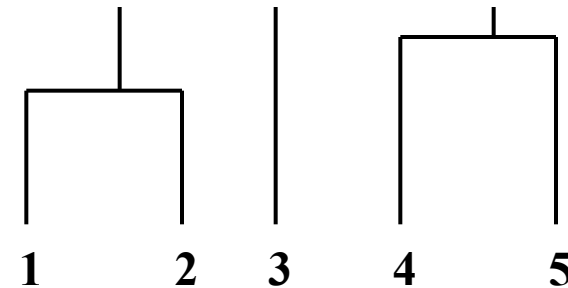


# Cluster Similarity: MIN or Single Linkage

- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters

	{1,2}	3	4	5
{1,2}	1.00	0.70	0.65	0.50
3	0.70	1.00	0.40	0.30
4	0.65	0.40	1.00	0.80
5	0.50	0.30	0.80	1.00

Update proximity matrix with new cluster {1, 2}



# Cluster Similarity: MIN or Single Linkage

- 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**.

	{1,2}	3	{4,5}
{1,2}	1.00	0.70	?
3	0.70	1.00	
{4,5}			

Update proximity matrix with new cluster {1, 2} and {4, 5}

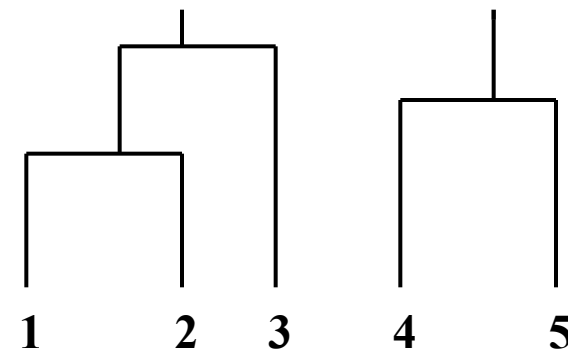
	{1,2}	3	4	5
{1,2}	1.00	0.70	0.65	0.50
3	0.70	1.00	0.40	0.30
4	0.65	0.40	1.00	0.80
5	0.50	0.30	0.80	1.00

# Cluster Similarity: MIN or Single Linkage

- 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**.

	$\{1,2\}$	3	$\{4,5\}$
$\{1,2\}$	1.00	0.70	0.65
3	0.70	1.00	0.40
$\{4,5\}$	0.65	0.40	1.00

Update proximity matrix with new cluster  $\{1, 2\}$  and  $\{4, 5\}$

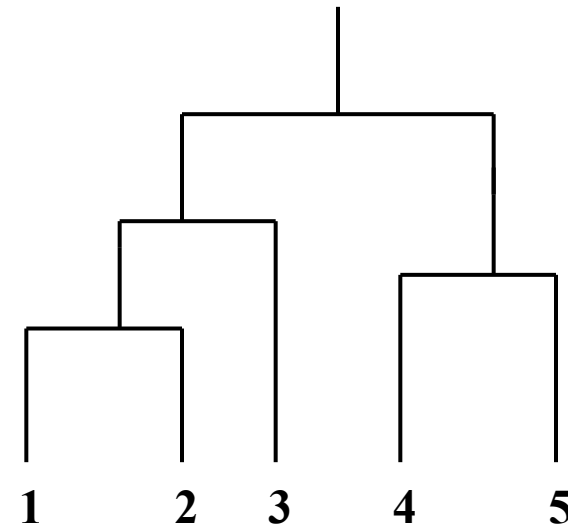


# Cluster Similarity: MIN or Single Linkage

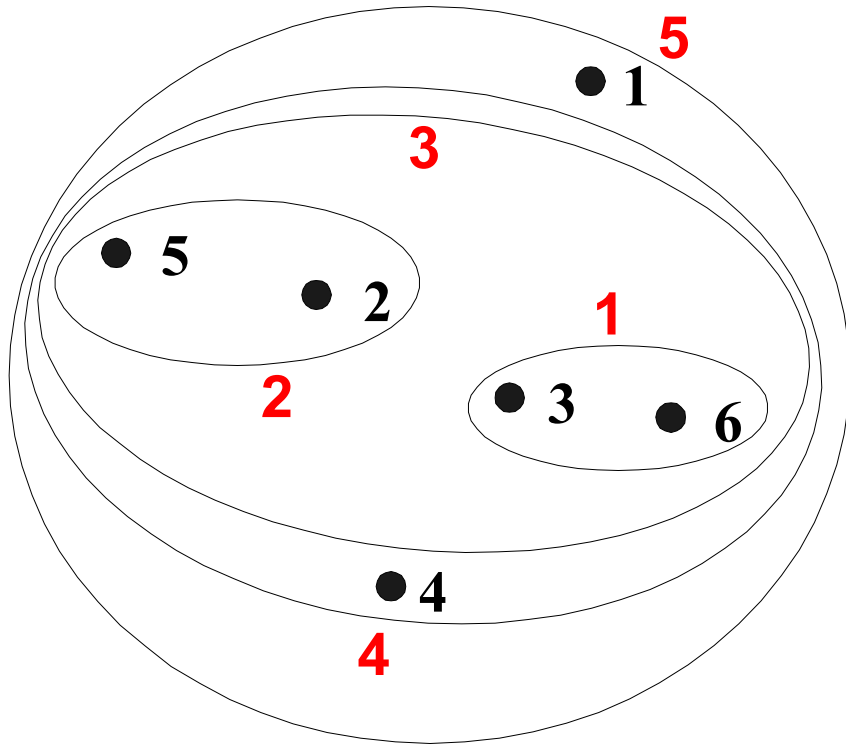
- Similarity of two clusters is based on the **two most similar (closest)** points in the different clusters
  - ▣ Determined by one pair of points, i.e., by **one link in the proximity graph**.

	$\{1, 2, 3\}$	$\{4, 5\}$
$\{1, 2, 3\}$	1.00	0.65
$\{4, 5\}$	0.65	1.00

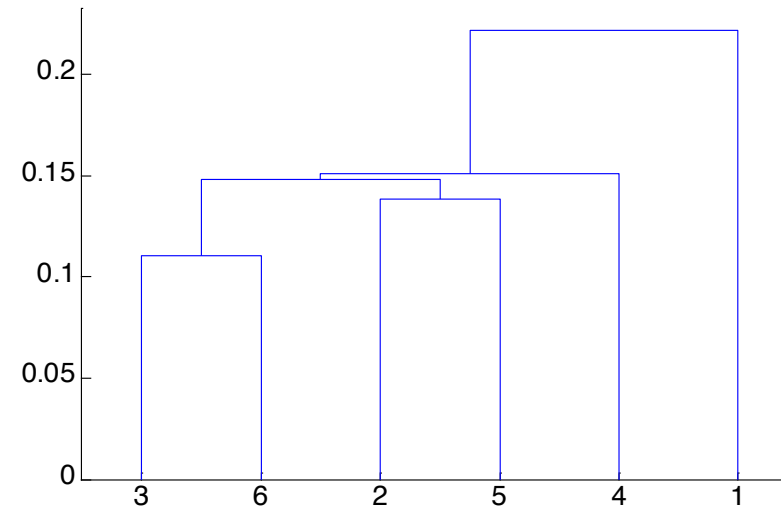
Only two clusters are left.



# Hierarchical Clustering: MIN

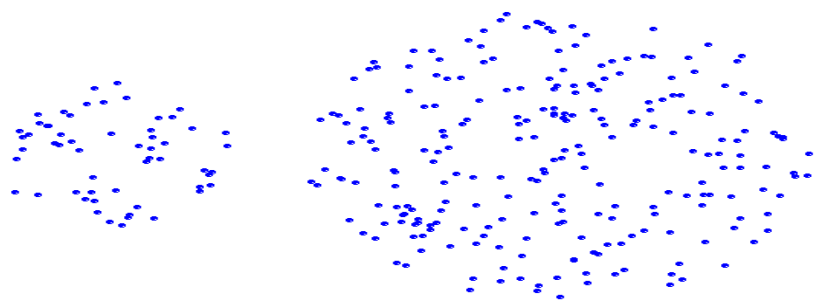


**Nested Clusters**

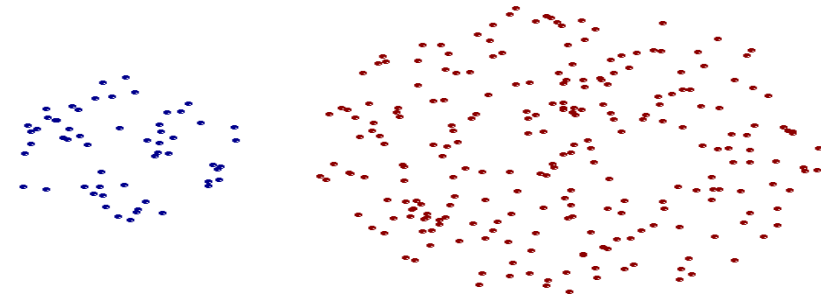


**Dendrogram**

# Strength of MIN



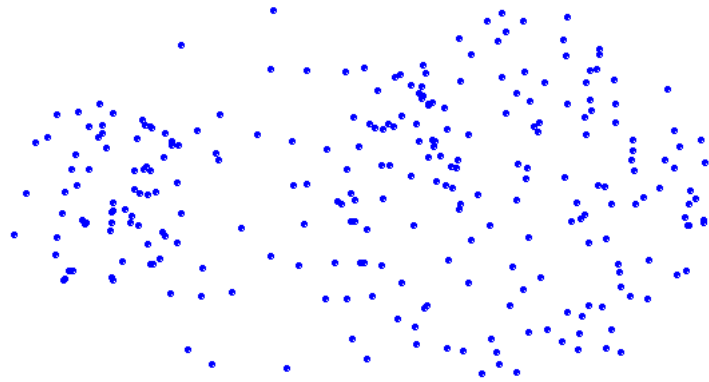
**Original Points**



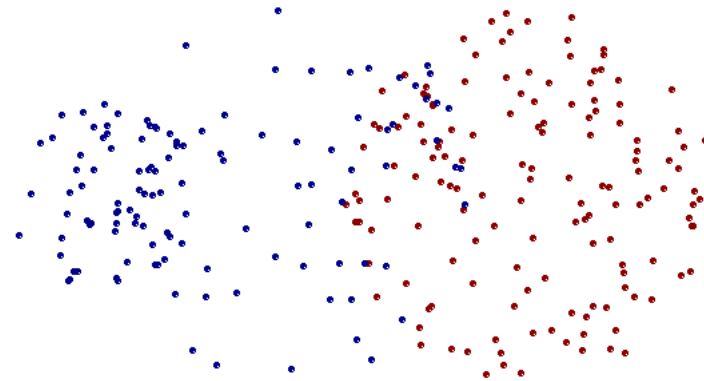
**Two Clusters**

- Can handle non-globular or some irregular shapes

# Limitations of MIN



**Original Points**



**Two Clusters**

- **Sensitive to noise and outliers**

# Cluster Similarity: MAX

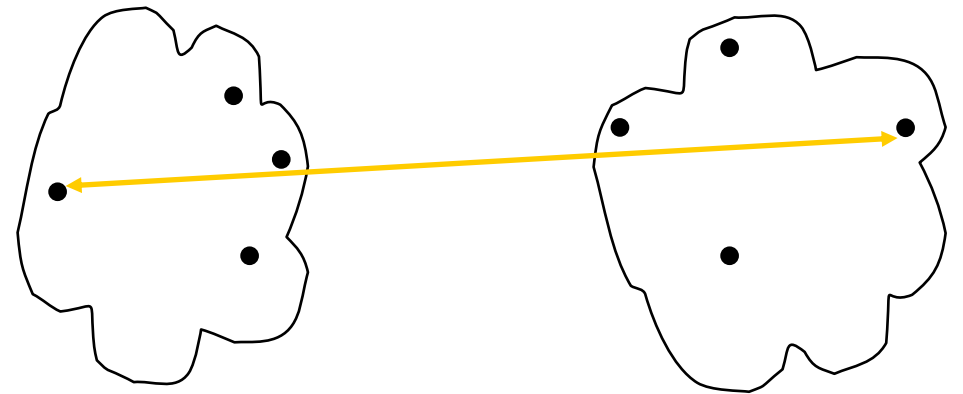
- Similarity of two clusters is based on **the two least similar (most distant)** points in the different clusters
  - ▣ Determined by all pairs of points in the two clusters

Let us define the distance between two points using Euclidean distance:

$$\delta(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \left( \sum_{i=1}^d (x_i - y_i)^2 \right)^{1/2}$$

Using MAX link, the distance between two clusters  $C_i$  and  $C_j$  is then:

$$\delta(C_i, C_j) = \max\{\delta(\mathbf{x}, \mathbf{y}) \mid \mathbf{x} \in C_i, \mathbf{y} \in C_j\}$$





# Cluster Similarity: MAX or Complete Linkage

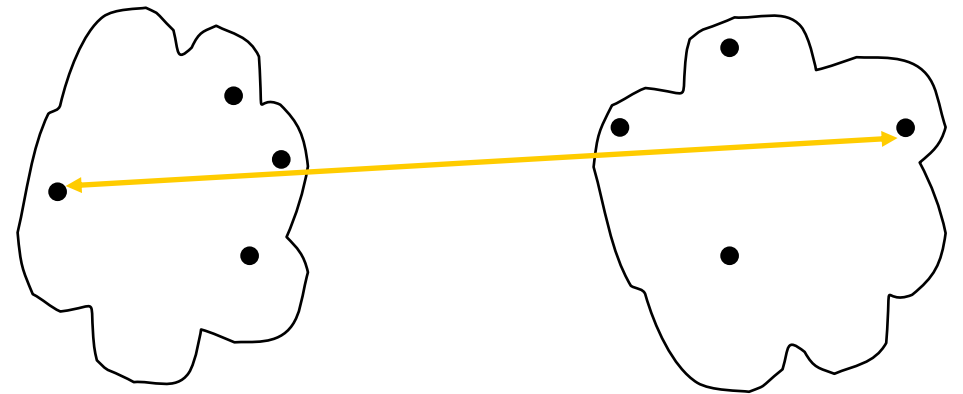
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$$\delta(C_i, C_j) = \max\{\delta(\mathbf{x}, \mathbf{y}) \mid \mathbf{x} \in C_i, \mathbf{y} \in C_j\}$$



Why complete linkage?

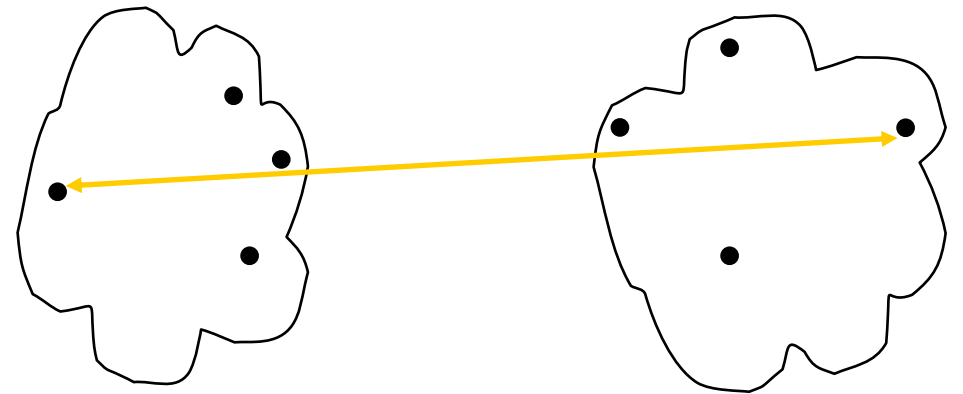
# Cluster Similarity: MAX or Complete Linkage

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  - ▣ Determined by all pairs of points in the two clusters

What if we define the similarity (**not distance**) between two points?

Using MAX link, the similarity between two clusters  $C_i$  and  $C_j$  is then:

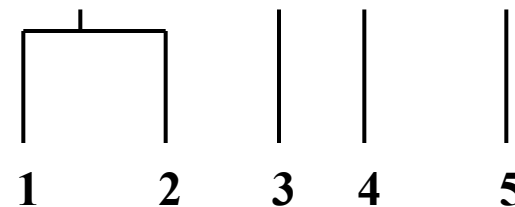
$$\text{Sim}(C_i, C_j) = \min\{\text{sim}(x, y) \mid x \text{ in } C_i, y \text{ in } C_j\}$$



# Cluster Similarity: MAX or Complete Linkage

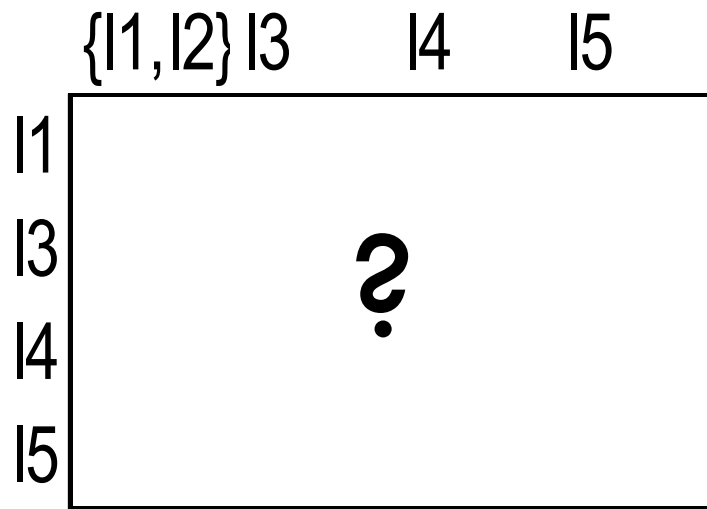
- Similarity of two clusters is based on **the two least similar (most distant)** points in the different clusters
  - ▣ Determined by all pairs of points in the two clusters

	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



# Cluster Similarity: MAX or Complete Linkage

- Similarity of two clusters is based on **the two least similar (most distant)** points in the different clusters
  - ▣ Determined by all pairs of points in the two clusters

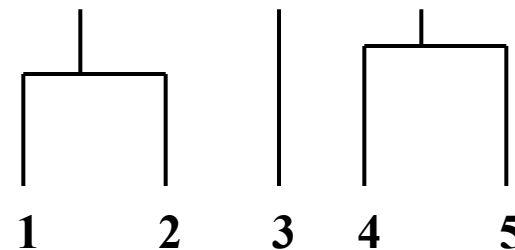


	1	2	3	4	5
1	1.00	0.90	0.10	0.65	0.20
2	0.90	1.00	0.70	0.60	0.50
3	0.10	0.70	1.00	0.40	0.30
4	0.65	0.60	0.40	1.00	0.80
5	0.20	0.50	0.30	0.80	1.00

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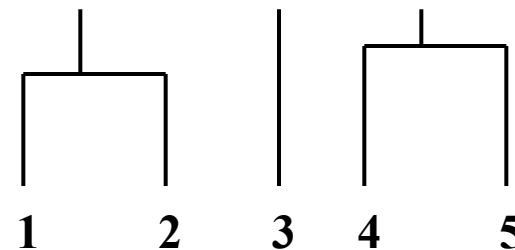
	{1,2}	3	4	5
1	1.00	0.10	0.60	0.20
3	0.10	1.00	0.40	0.30
4	0.60	0.40	1.00	0.80
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## Cluster Similarity: MAX or Complete Linkage

- Similarity of two clusters is based on **the two least similar (most distant)** points in the different clusters
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	{1,2}	3	4	5
1	1.00	0.10	0.60	0.20
3	0.10	1.00	0.40	0.30
4	0.60	0.40	1.00	0.80
5	0.20	0.30	0.80	1.00

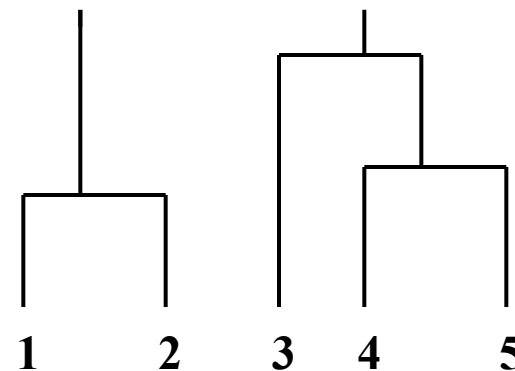


Which two clusters should be merged next?

# Cluster Similarity: MAX or Complete Linkage

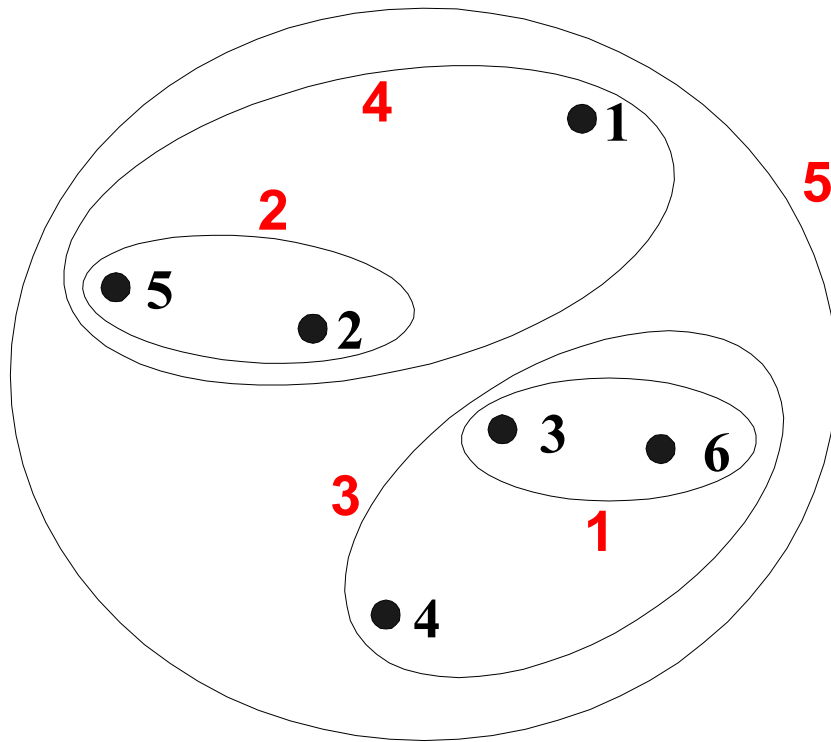
- Similarity of two clusters is based on **the two least similar (most distant)** points in the different clusters
  - ▣ Determined by all pairs of points in the two clusters

	{1,2}	3	4	5
1	1.00	0.10	0.60	0.20
3	0.10	1.00	0.40	0.30
4	0.60	0.40	1.00	0.80
5	0.20	0.30	0.80	1.00

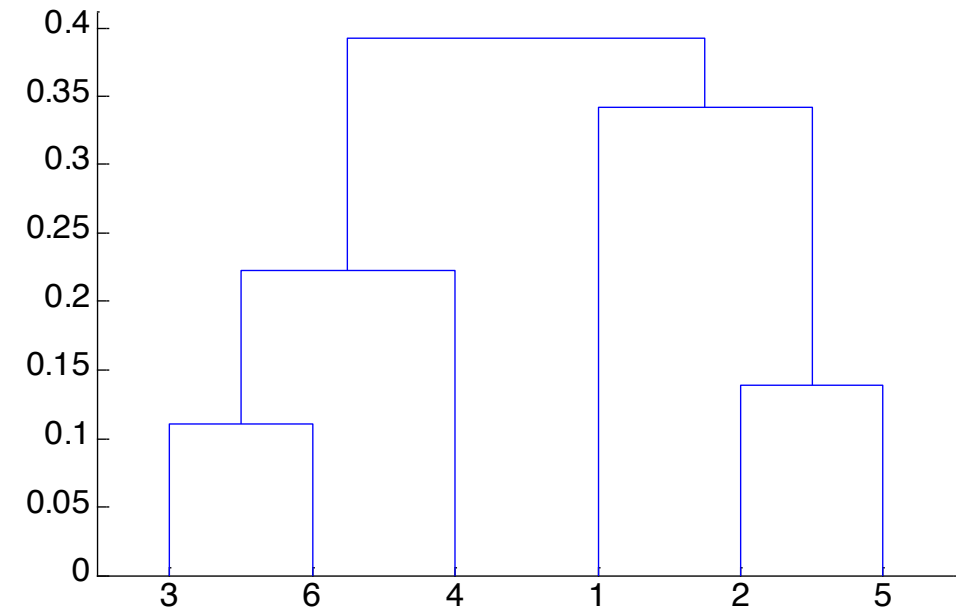


Merge {3} with {4,5}, why?

# Hierarchical Clustering: MAX



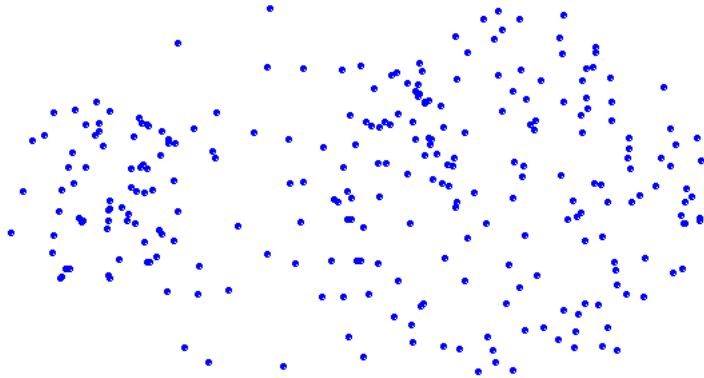
**Nested Clusters**



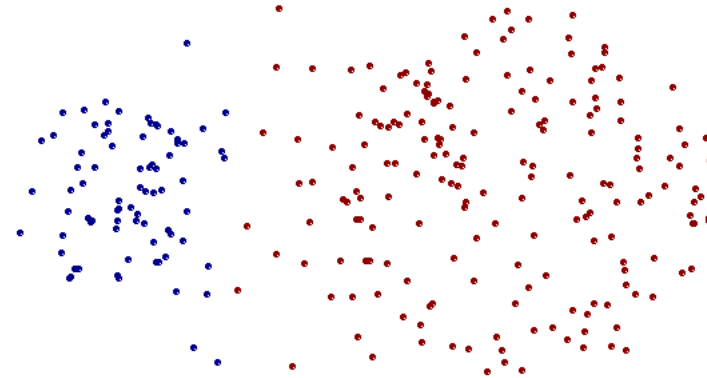
**Dendrogram**



# Strength of MAX



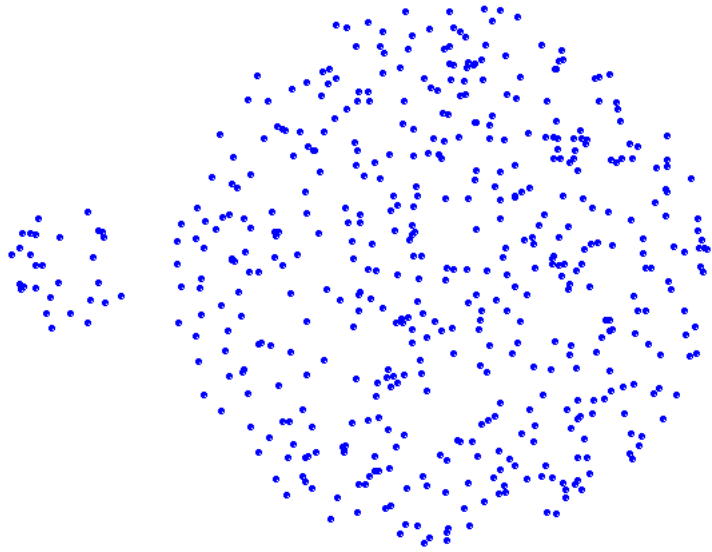
**Original Points**



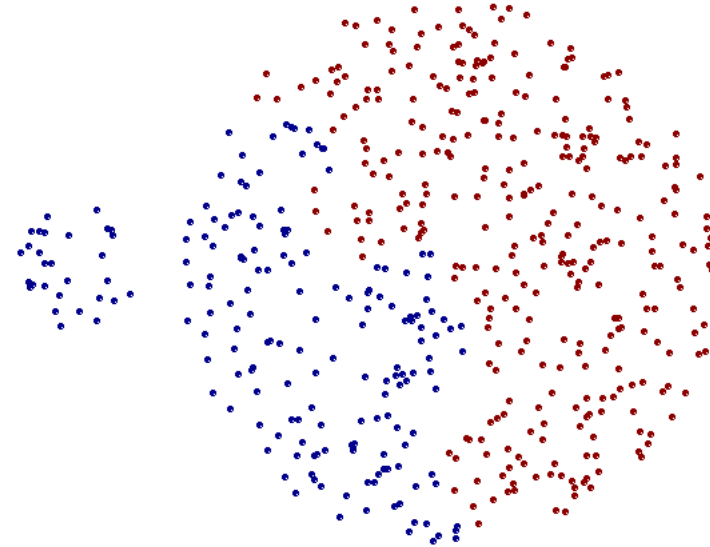
**Two Clusters**

- **Less susceptible to noise and outliers**

# Limitations of MAX



**Original Points**



**Two Clusters**

- Tends to break large clusters
- Biased towards globular clusters

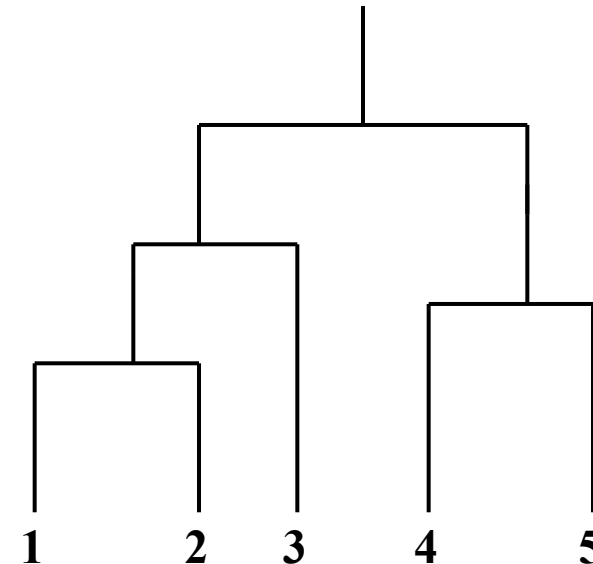
# Cluster Similarity: Group Average

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

$$\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| * |\text{Cluster}_j|}$$

- Need to use average connectivity for scalability since total proximity favors large clusters

	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



# Hierarchical Clustering: Problems and Limitations

- Once a decision is made to combine two clusters, it cannot be undone
- No objective function is directly minimized
- Different schemes have problems with one or more of the following:
  - ▣ Sensitivity to noise and outliers
  - ▣ Difficulty handling different sized clusters and convex shapes
  - ▣ Breaking large clusters

# Hierarchical Clustering: Time and Space requirements

□ Space complexity?

A.  $O(N^2)$

B.  $O(N)$

C.  $O(N \cdot \log(N))$

# Hierarchical Clustering: Time and Space requirements

- Space complexity?

- A.  $O(N^2)$

- B.  $O(N)$

- C.  $O(N \log(N))$

- Time complexity?

- ▣ N: the number of data points.  $O(N^3)$  time in many cases, as there are N steps and at each step the proximity matrix (of size  $N^2$ ) must be updated and searched

- ▣ Complexity can be reduced to  $O(N^2 \log(N))$  time for some approaches

# Clustering Algorithms

---

- K-means and its variants
- Hierarchical clustering
- Density-based clustering

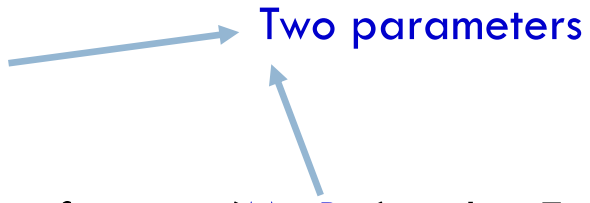
# Density-Based Clustering Methods

- Clustering based on density (a local cluster criterion), such as density-connected points
- Major features:
  - ▣ Discover clusters of arbitrary shape
  - ▣ Handle noise
  - ▣ One scan (only examine the local region to justify density)
  - ▣ Need density parameters as termination condition
- Several interesting studies:
  - ▣ DBSCAN: Ester, et al. (KDD'96)
  - ▣ OPTICS: Ankerst, et al (SIGMOD'99)
  - ▣ DENCLUE: Hinneburg & D. Keim (KDD'98)
  - ▣ CLIQUE: Agrawal, et al. (SIGMOD'98) (also, grid-based)



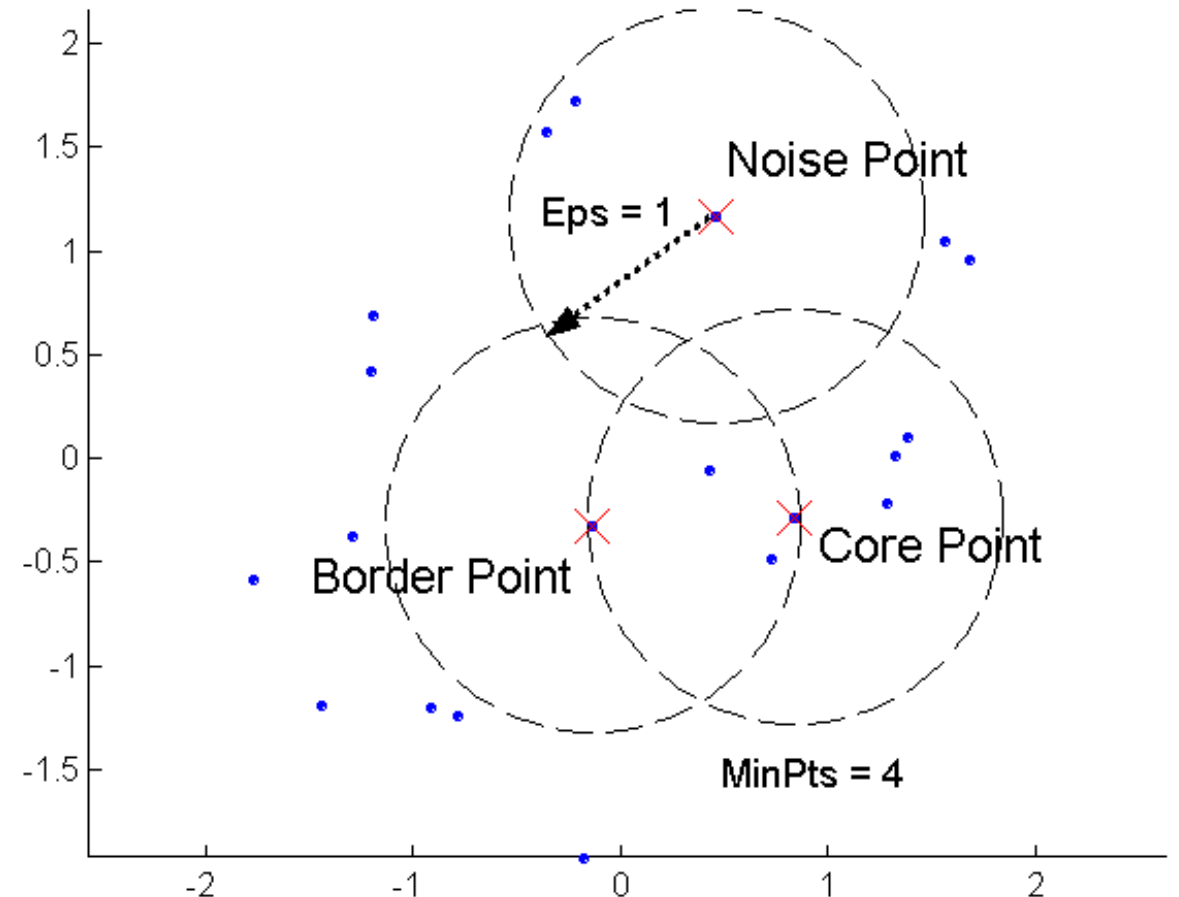


# DBSCAN

- DBSCAN (M. Ester, H.-P. Kriegel, J. Sander, and X. Xu, KDD'96)
  - ▣ Discovers clusters of arbitrary shape: Density-Based Spatial Clustering of Applications with Noise
  
- DBSCAN is a density-based algorithm.
  - ▣ Density = number of points within a specified radius (Eps) 
  - ▣ A point is a **core point** if it has at least a specified number of points (MinPts) within Eps
    - These are points that are at the interior of a cluster
  - ▣ A **border point** has fewer than MinPts within Eps, but is in the neighborhood of a core point
  - ▣ A **noise point** is any point that is not a core point or a border point.

## DBSCAN: Core, Border, and Noise Points

1. A point is a **core point** if it has at least a specified number of points (MinPts) within Eps
2. A **border point** has fewer than MinPts within Eps, but is in the neighborhood of a core point
3. A **noise point** is any point that is not a core point or a border point.



# DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points

$current\_cluster\_label \leftarrow 1$

**for** all core points **do**

**if** the core point has no cluster label **then**

$current\_cluster\_label \leftarrow current\_cluster\_label + 1$

        Label the current core point with cluster label  $current\_cluster\_label$

**end if**

**for** all points in the Eps-neighborhood, except  $i^{th}$  the point itself **do**

**if** the point does not have a cluster label **then**

            Label the point with cluster label  $current\_cluster\_label$

**end if**

**end for**

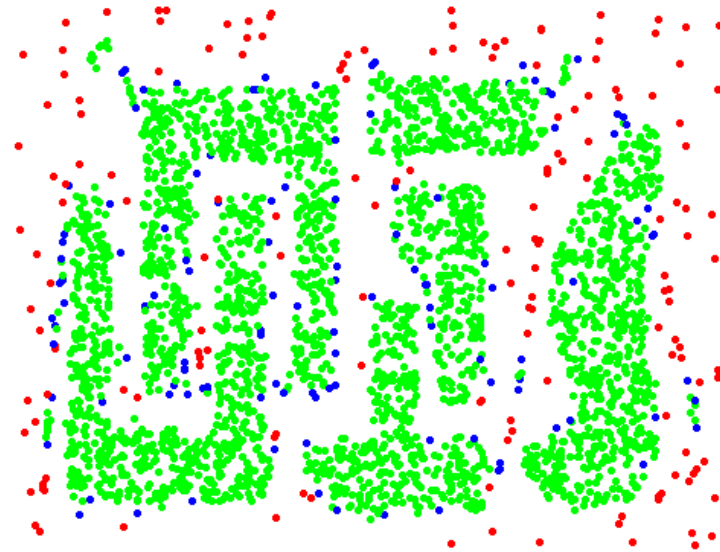
**end for**

**The Eps-neighborhood of a point  $q$ :**  
 $N_{Eps}(q): \{p \text{ belongs to } D \mid \text{dist}(p, q) \leq Eps\}$

## DBSCAN: Core, Border and Noise Points



Original Points



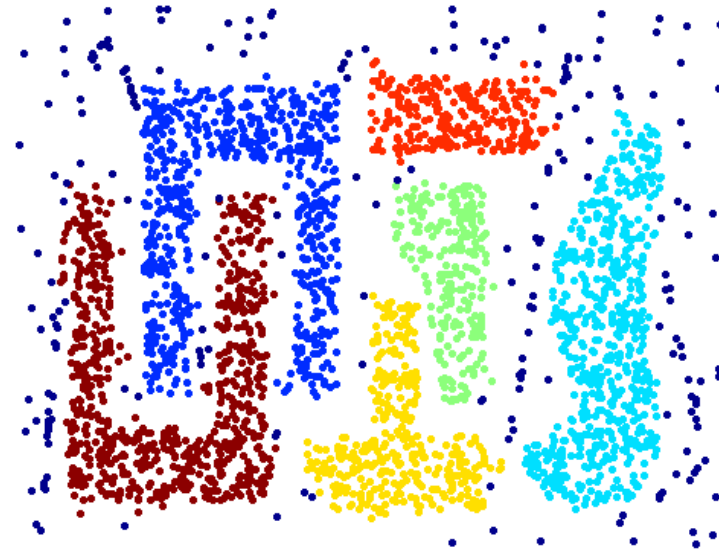
Point types: **core**, **border** and **noise**

Eps = 10, MinPts = 4

## When DBSCAN Works Well



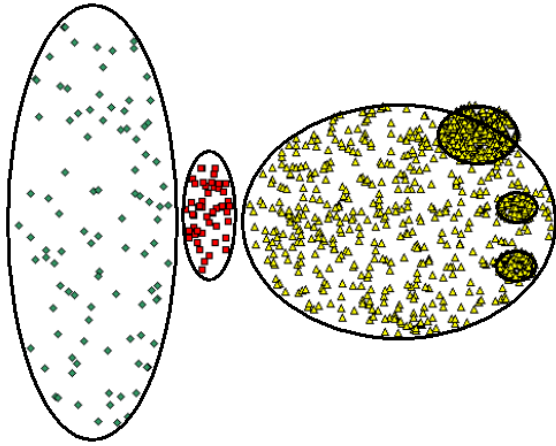
Original Points



Clusters

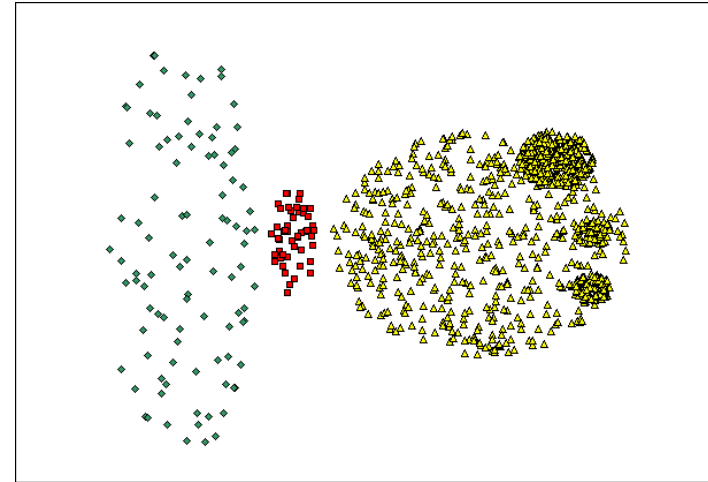
- Resistant to Noise
- Can handle clusters of different shapes and sizes

# When DBSCAN Does NOT Work Well

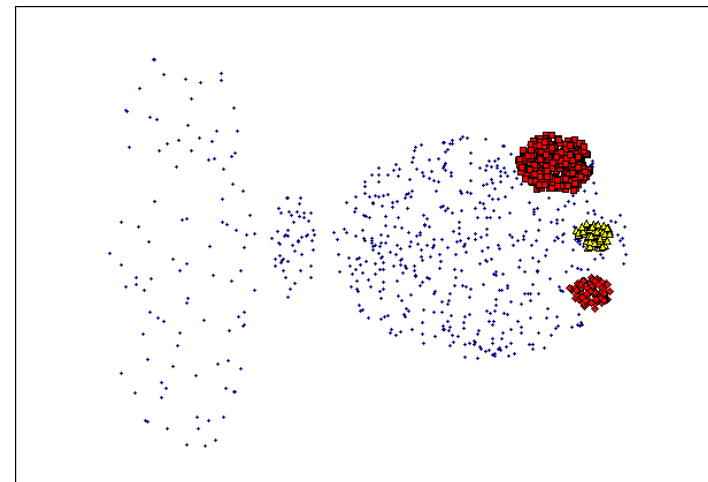


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)



Sensitive to  
parameters!

# 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?**
  - **One measure mentioned before...**

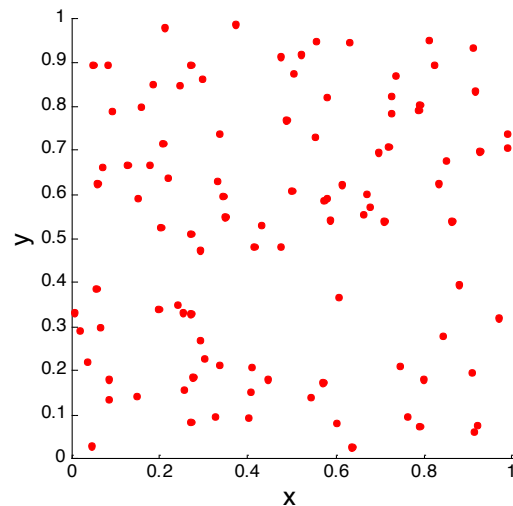
# Cluster Validity

- 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?
- But “clusters are in the eye of the beholder”!
- 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



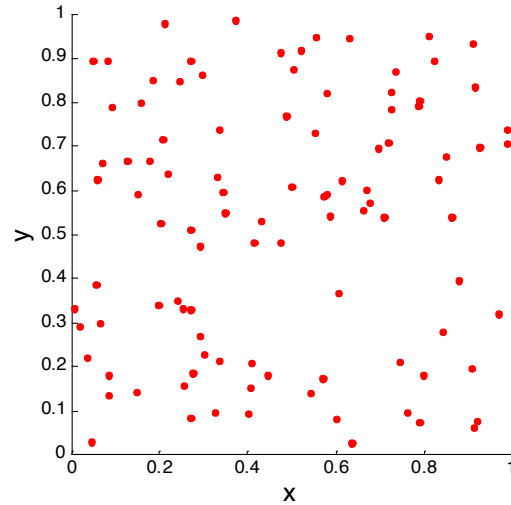
# Clusters found in Random Data

Random  
Points

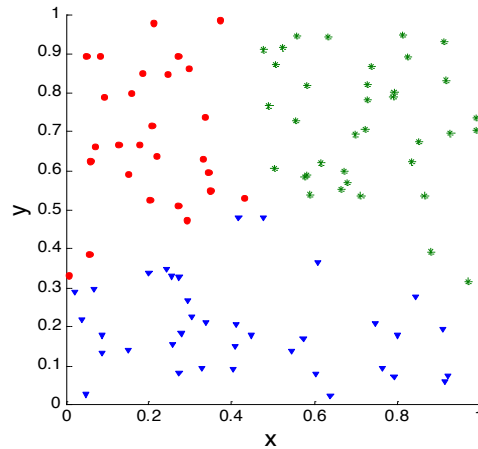


# Clusters found in Random Data

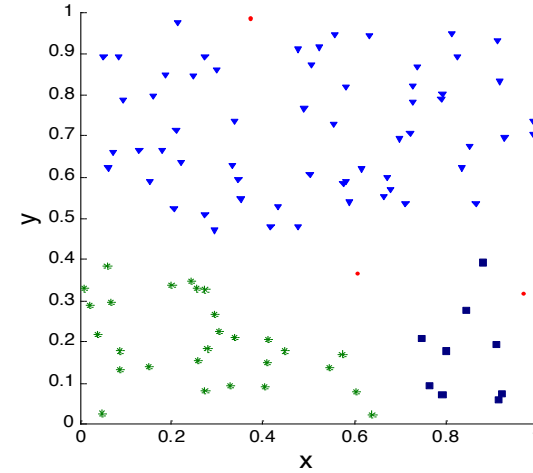
**Random Points**



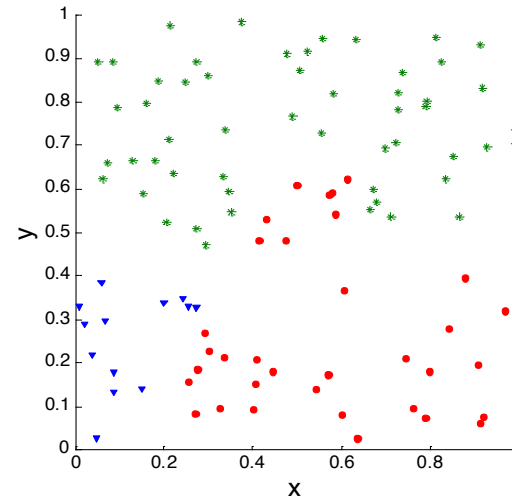
**K-means**



**DBSCAN**

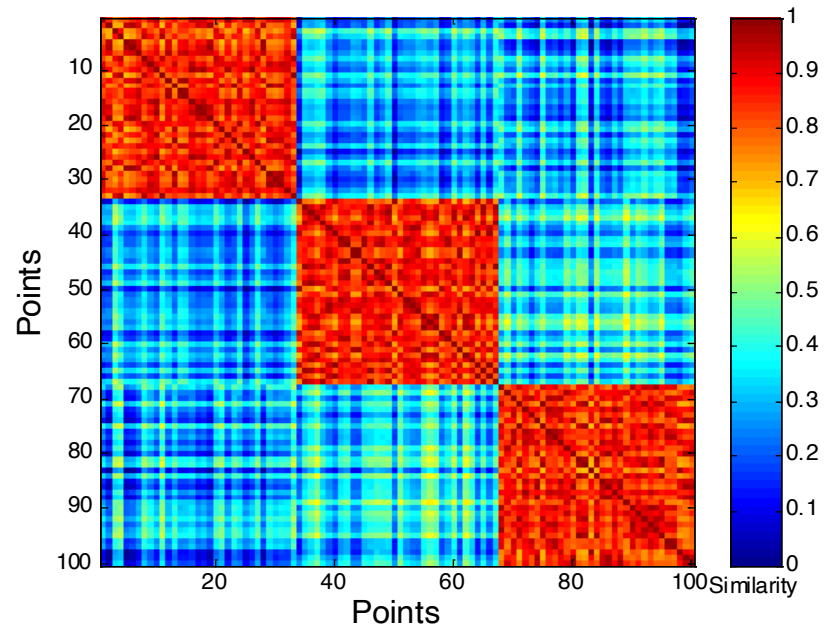
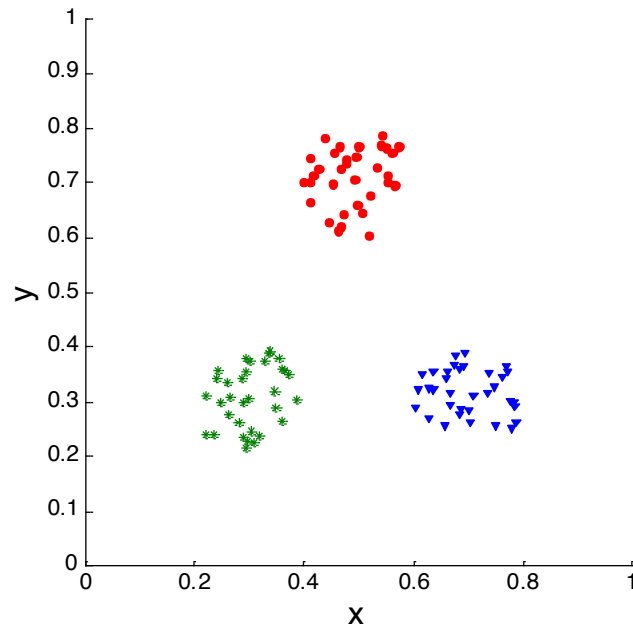


**Complete Link**



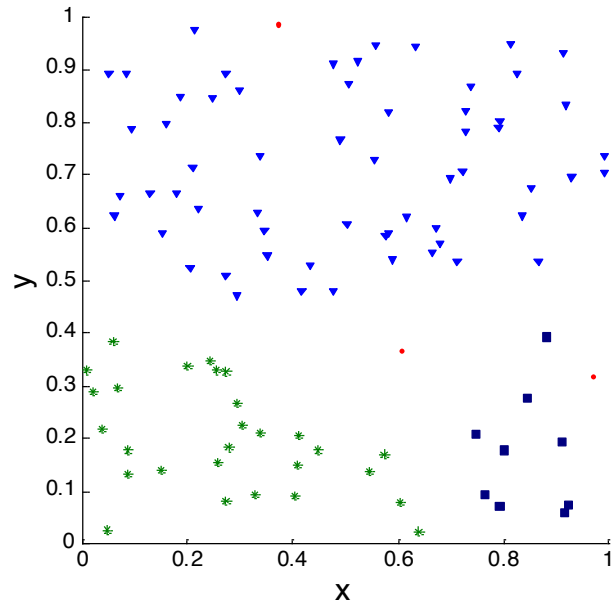
## Using Similarity Matrix for Cluster Validation

- Order the similarity matrix with respect to cluster labels and inspect visually.



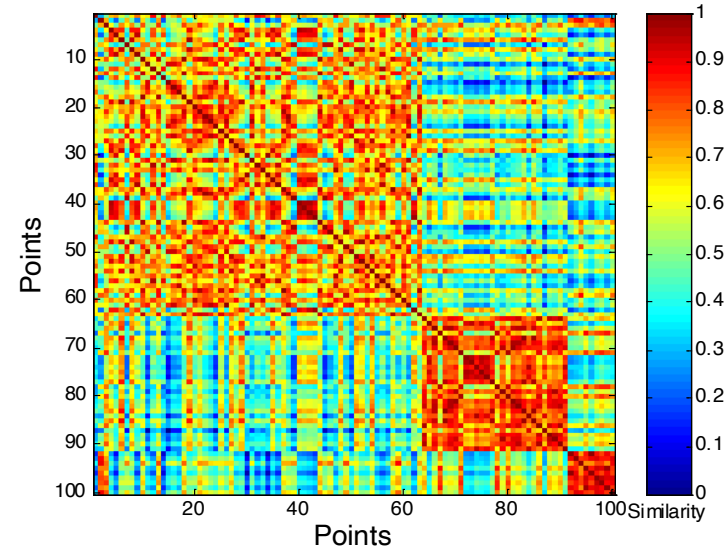
# Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

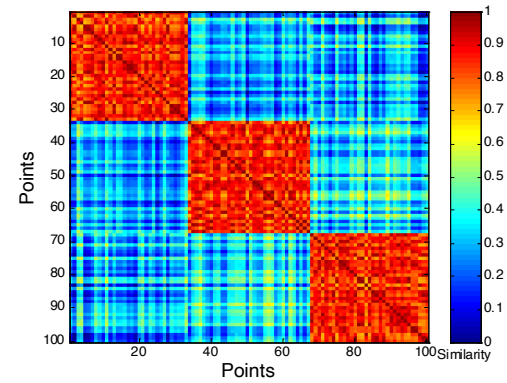


**DBSCAN**

Visualization



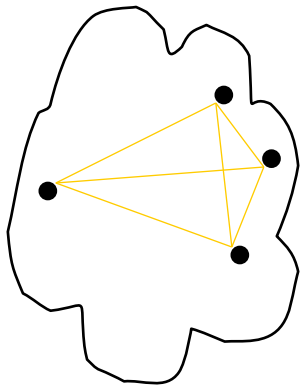
Visualization of Similarity Matrix



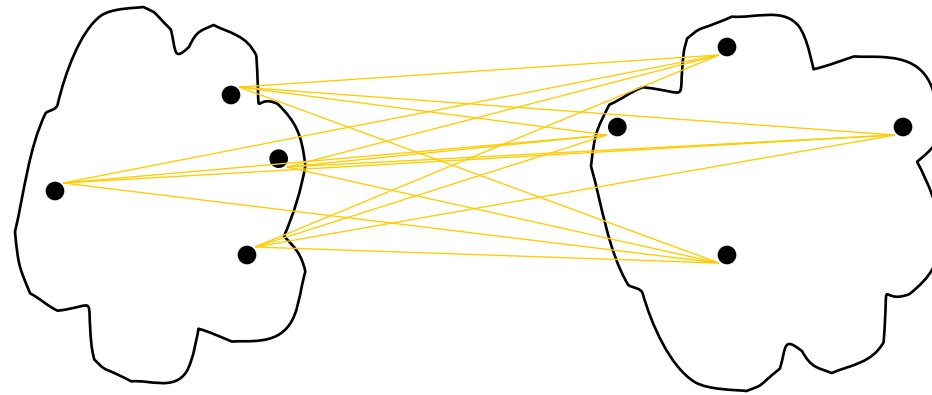
What good clustering results look like...

# Cohesion and Separation

- A proximity graph based approach can also be used for cohesion and separation.
  - ▣ Cluster cohesion is the sum of the weight of all links within a cluster.
  - ▣ Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion



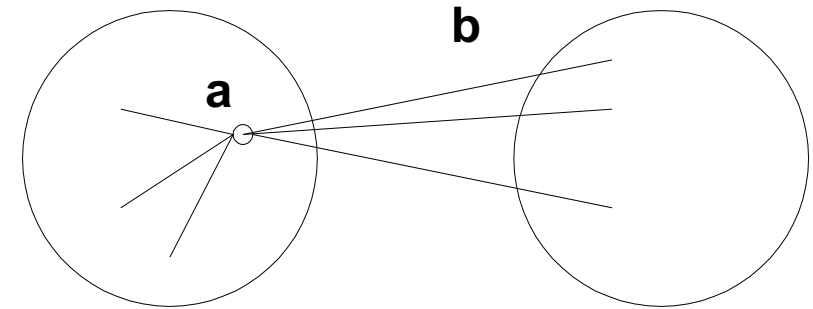
separation

# Silhouette Coefficient

- Silhouette Coefficient **combine ideas of both cohesion and separation**, but for individual points, as well as clusters and clusterings
- For an individual point,  $i$ 
  - ▣ Calculate  $a$  = average distance of  $i$  to the points in its cluster
  - ▣ Calculate  $b$  = min (average distance of  $i$  to points in another cluster)
  - ▣ The silhouette coefficient for a point is then given by

$$s = 1 - a/b \quad \text{if } a < b, \quad (\text{or } s = b/a - 1 \quad \text{if } a > b, \text{ not the usual case})$$

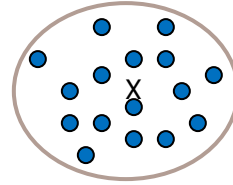
- ▣ **Typically between 0 and 1.**
- ▣ The closer to 1 the better.



- Can calculate the Average Silhouette width for a cluster or a clustering

# Measures of Cluster: Centroid, Radius and Diameter

- Centroid:  $\vec{x}_0$ 
  - the “middle” of a cluster
  - $n$ : number of points in a cluster
  - $\vec{x}_i$  is the  $i$ -th point in the cluster



$$\vec{x}_0 = \frac{\sum_i^n \vec{x}_i}{n}$$

- Radius:  $R$ 
  - Average distance from member objects to the centroid
  - The square root of average distance from any point of the cluster to its centroid

$$R = \sqrt{\frac{\sum_i^n (\vec{x}_i - \vec{x}_0)^2}{n}}$$

- Diameter:  $D$ 
  - Average pairwise distance within a cluster
  - The square root of average mean squared distance between all pairs of points in the cluster

$$D = \sqrt{\frac{\sum_i^n \sum_j^n (\vec{x}_i - \vec{x}_j)^2}{n(n-1)}}$$

## Other Measures of Cluster Validity

### □ Entropy/Gini (Please review how to calculate it)

- If **there is a class label** – you can use the entropy/gini of the class label – similar to what we did for classification (Check problem III in sample midterm)
- If **there is no class label** – one can compute the entropy w.r.t each attribute (dimension) and sum up or weighted average to compute the disorder within a cluster

### □ Classification Error

- If there is a class label one can compute this in a similar manner