CSE 5243 INTRO. TO DATA MINING

Cluster Analysis: Basic Concepts and Methods

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Slides adapted from UIUC CS412 by Prof. Jiawei Han and OSU CSE5243 by Prof. Huan Sun

Chapter 10. Cluster Analysis: Basic Concepts and Methods

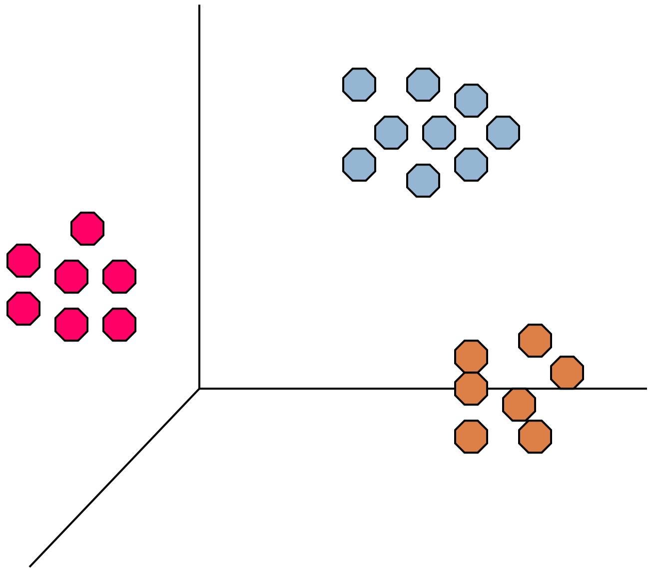
- Cluster Analysis: An Introduction
- Partitioning Methods
- Hierarchical Methods
- Density- and Grid-Based Methods
- Evaluation of Clustering
- Summary

Introduction

- 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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- **Cluster analysis** (or ***clustering***, ***data segmentation***, …)
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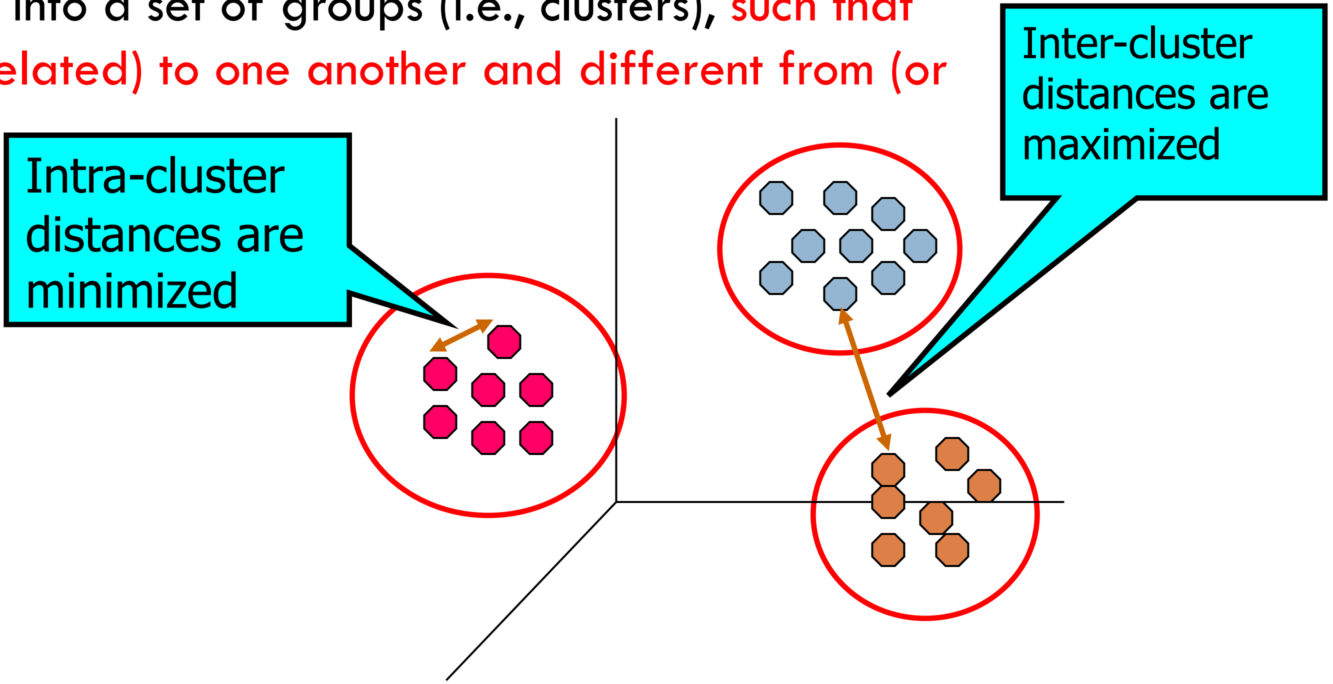

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- Cluster analysis is **unsupervised learning** (i.e., no predefined classes)
  - This contrasts with *classification, which is supervised learning*
- Typical ways to use/apply cluster analysis
  - As a stand-alone tool to get insight into data distribution, 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

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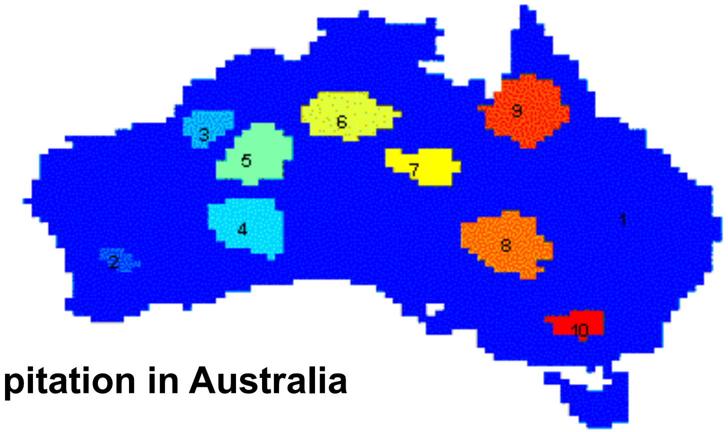
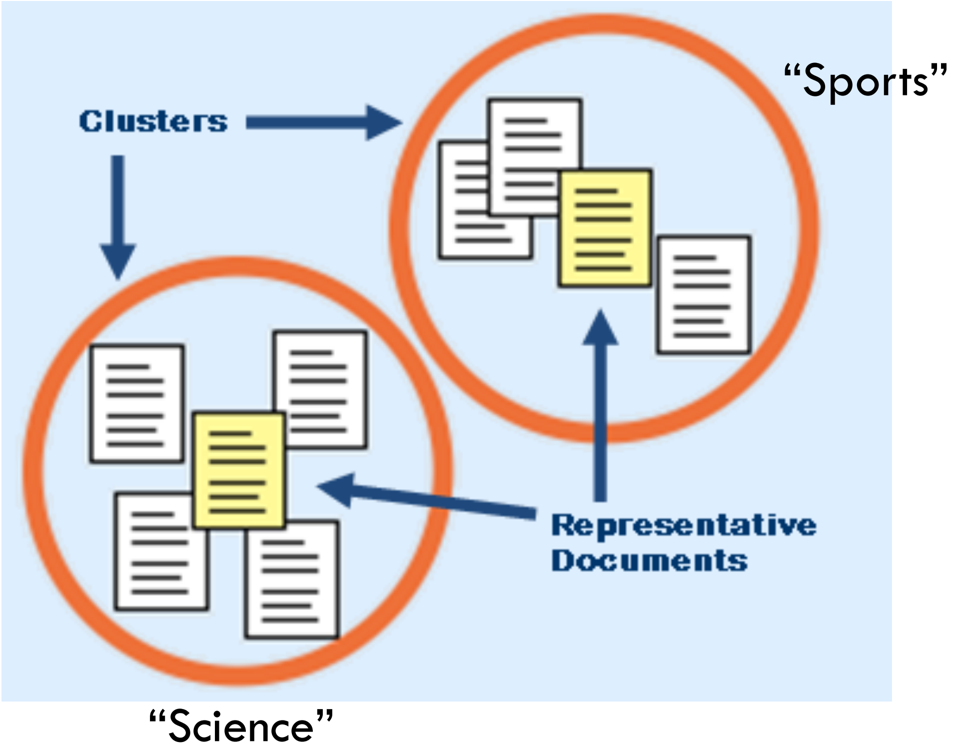
- **Quality function**
  - There is usually a separate "quality" function that measures the "goodness" of a cluster
  - It is hard to define "similar enough" or "good enough"
    - The answer is typically highly subjective
- There exist many similarity measures and/or functions for different applications
- 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

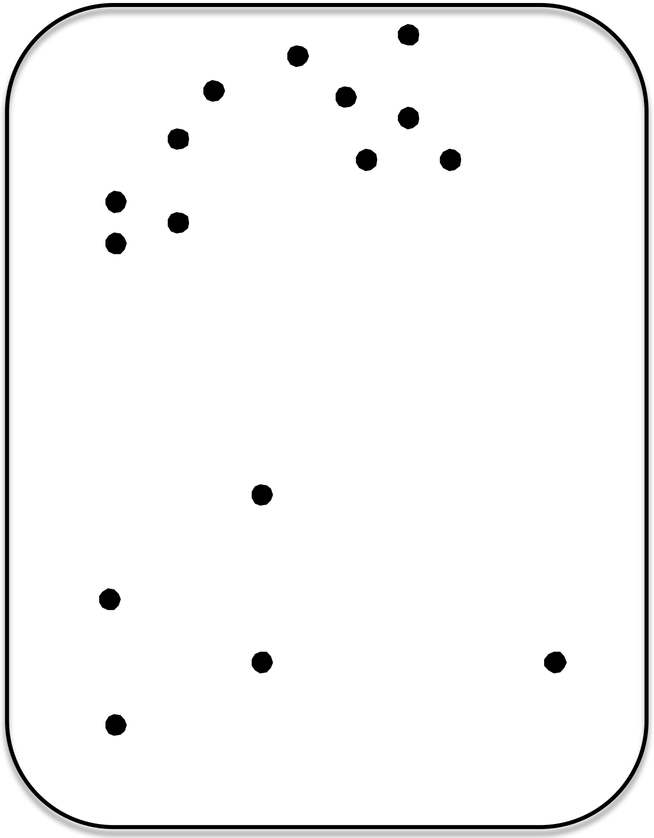
Two Clusters

Four Clusters

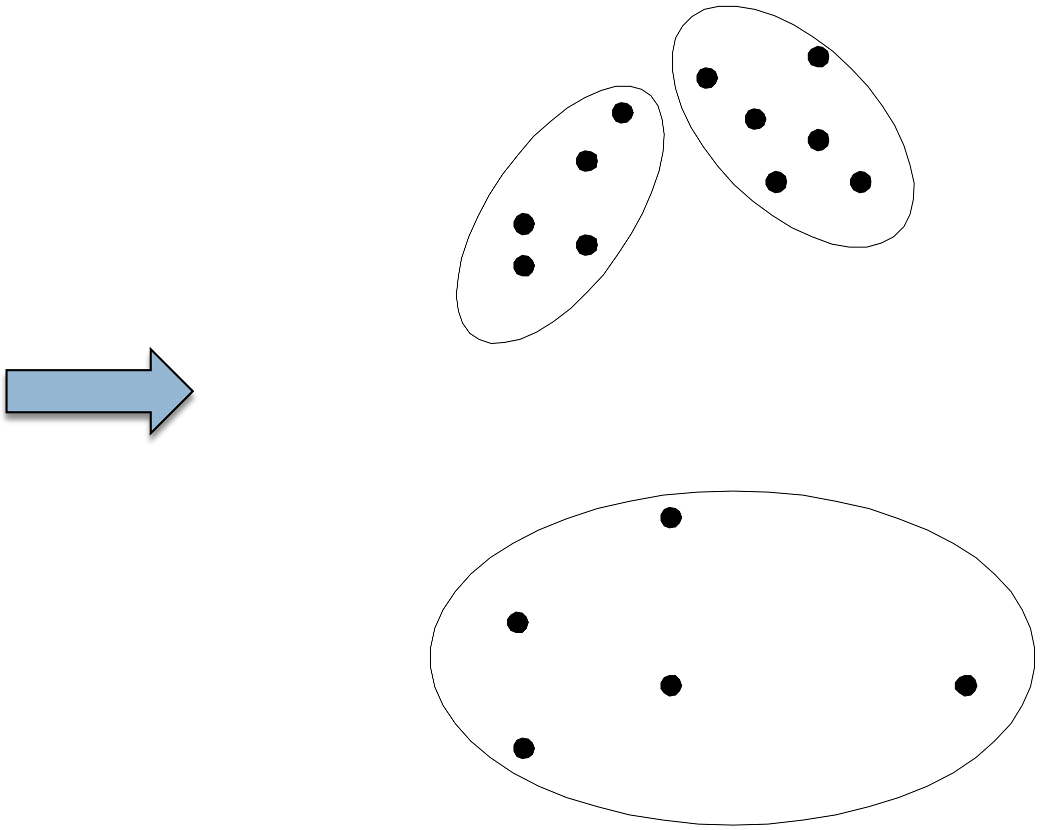
Types of Clusterings

- 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 <u>each data object is in exactly one subset</u>

Partitional Clustering



Original Points

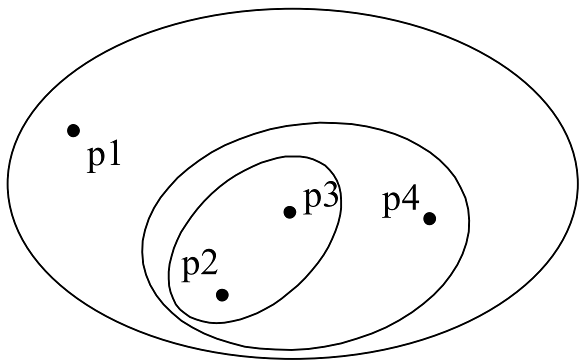


A Partitional Clustering

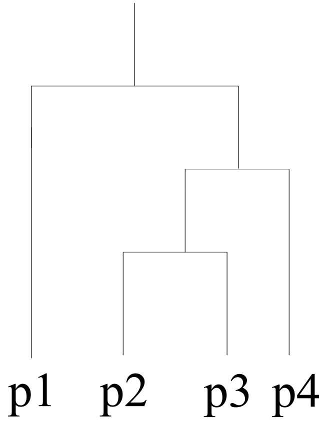
Types of Clusterings

- 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

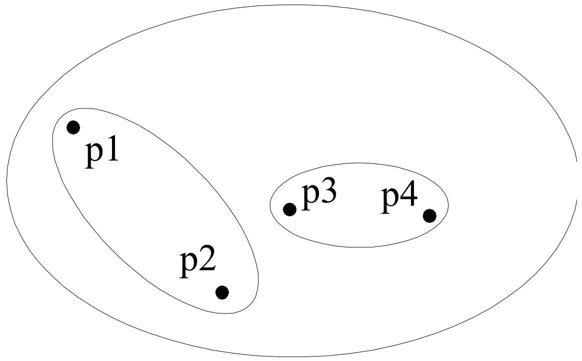
Hierarchical Clustering



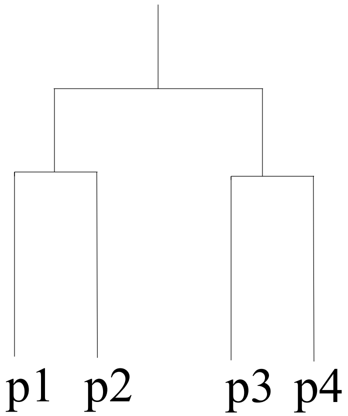
Traditional Hierarchical Clustering



Traditional Dendrogram



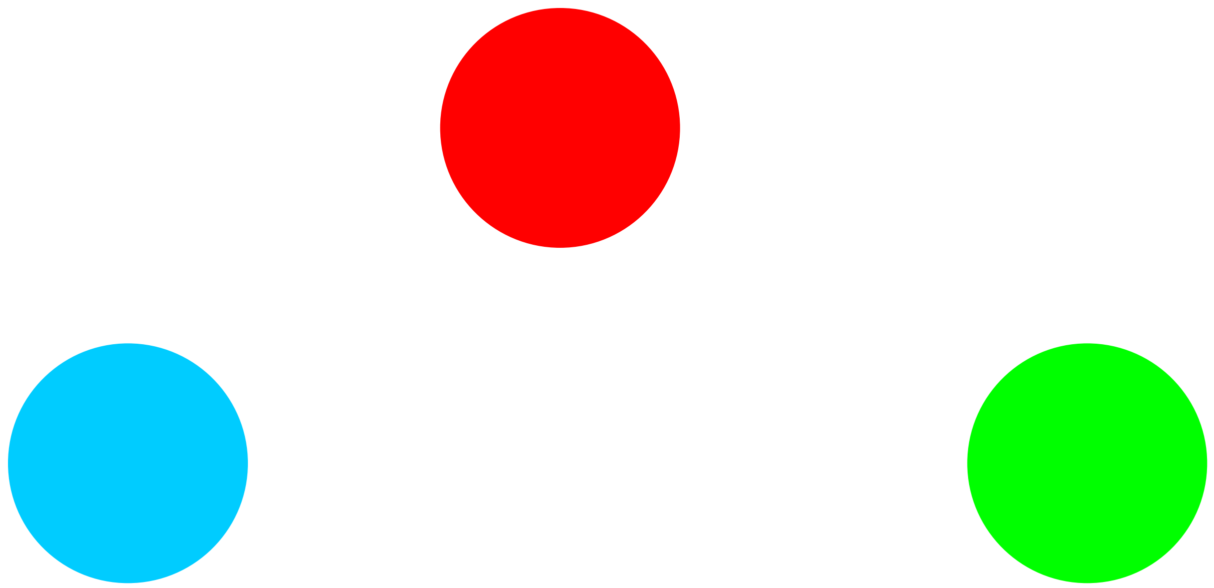
Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Types of Clusters: Well-Separated

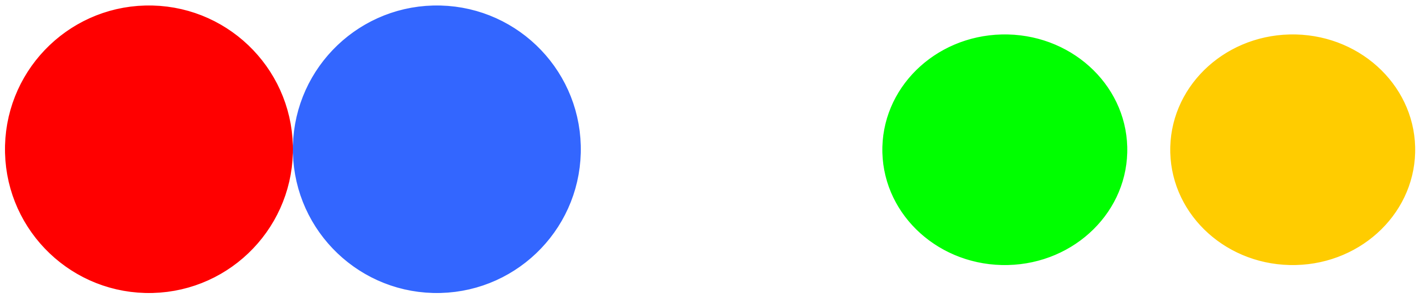
- Well-Separated Clusters:
  - A cluster is a set of points such that <u>any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster</u>.



3 well-separated clusters

Types of Clusters: Center-Based

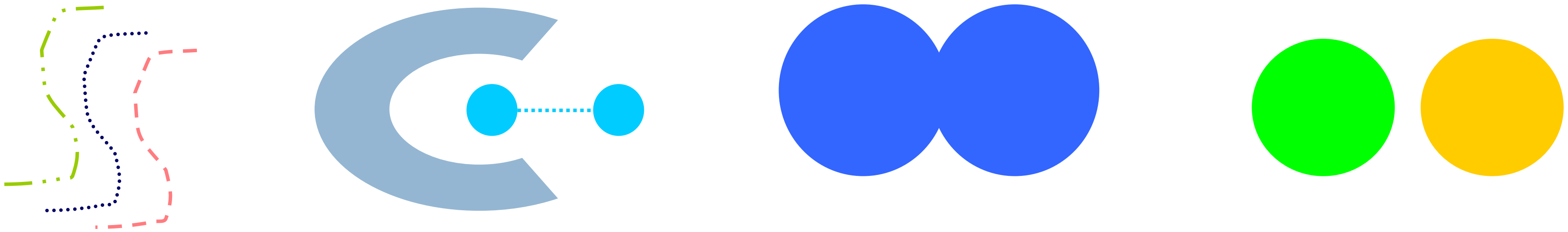
- Center-based
  - A cluster is a set of objects such that <u>an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster</u>
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative" point of a cluster



4 center-based clusters

Types of Clusters: Contiguity-Based

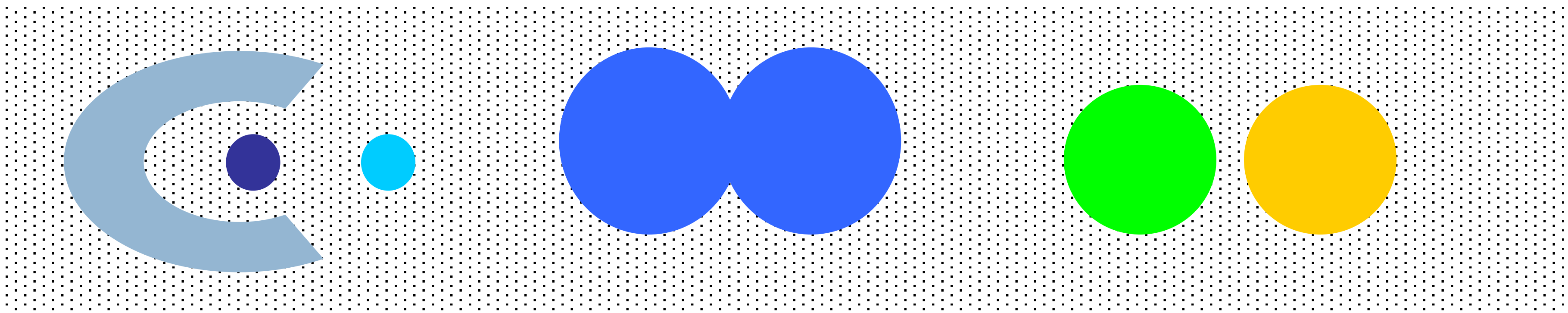
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



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

- 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

```
Select K points as the initial centroids.
repeat
    Form K clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
until The centroids don't change
```

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Often chosen randomly

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Measured by Euclidean distance, cosine similarity, etc.

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Typically the mean of the points in the cluster

K-means Clustering – Details

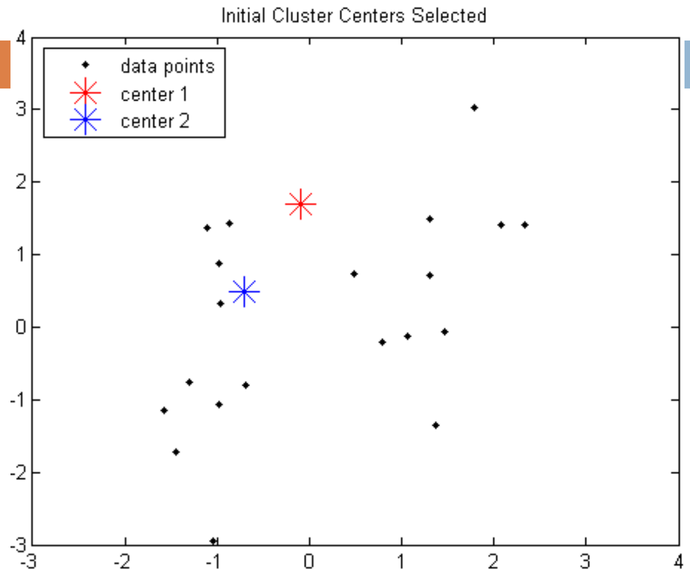
- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.

- 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**

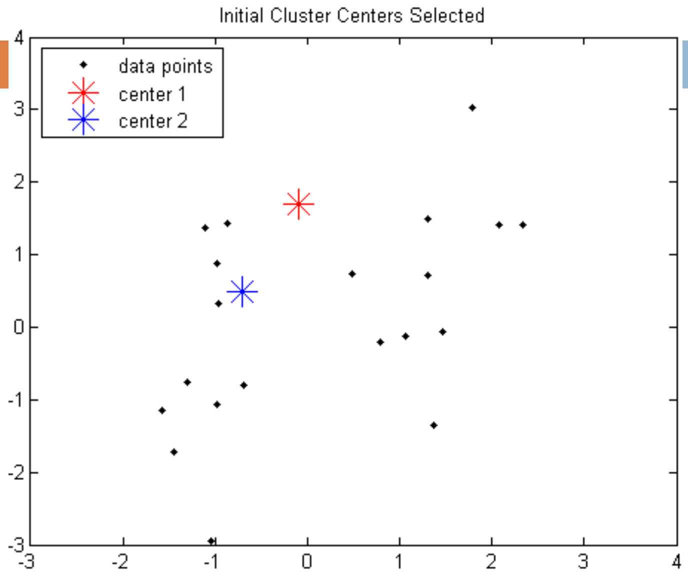
Select *K* points as initial centroids

Repeat

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

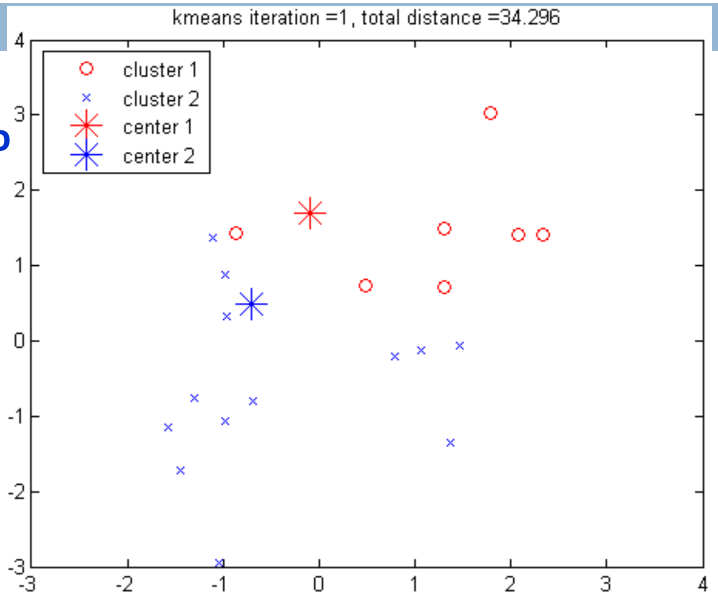
Until convergence criterion is satisfied

Example: *K-Means* Clustering



The original data points & randomly select K = 2 centroids

Assign points to clusters



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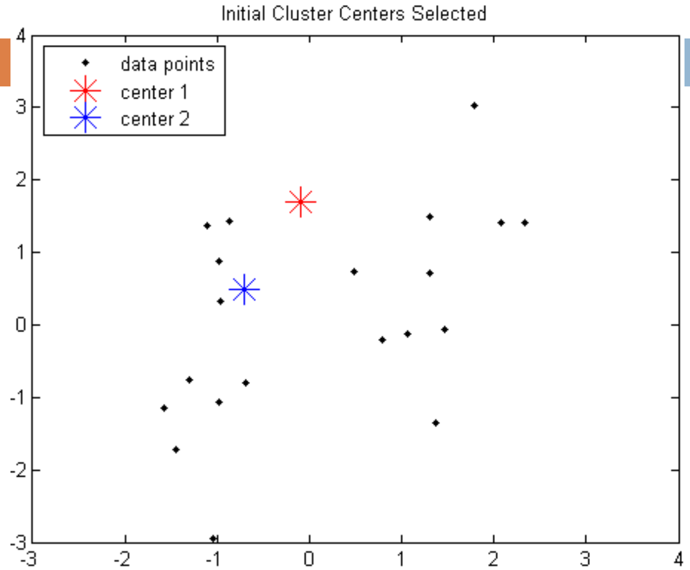

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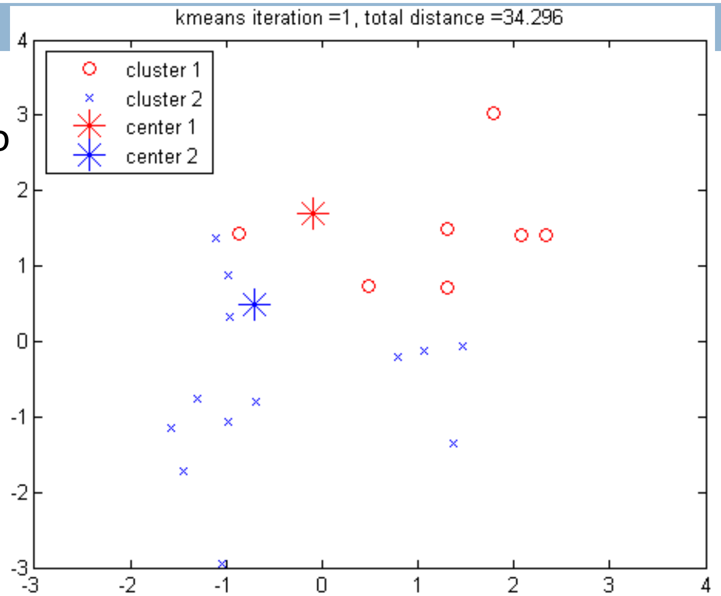
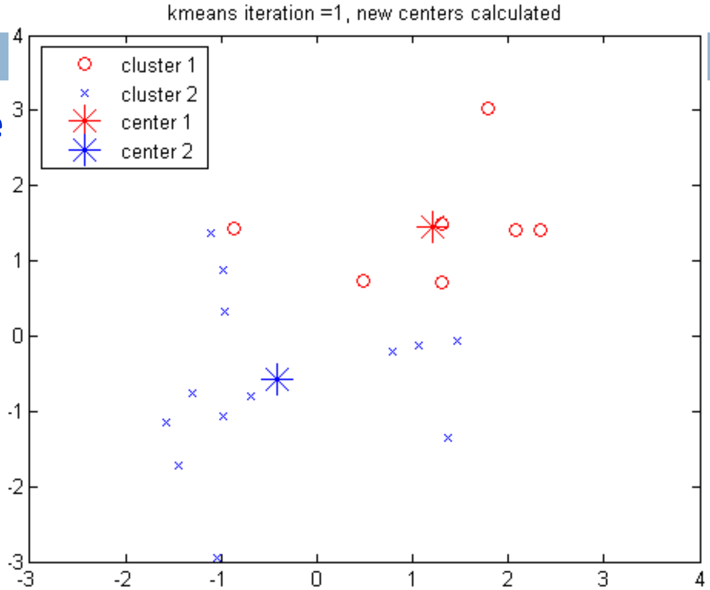


Recompute cluster centers



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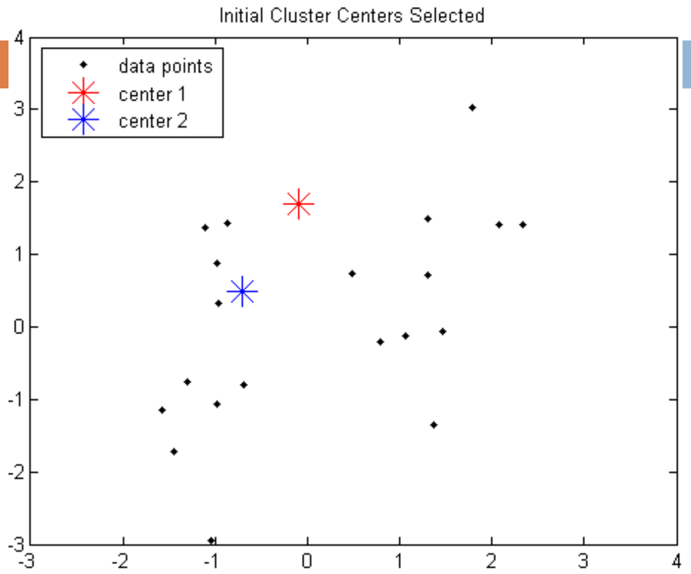
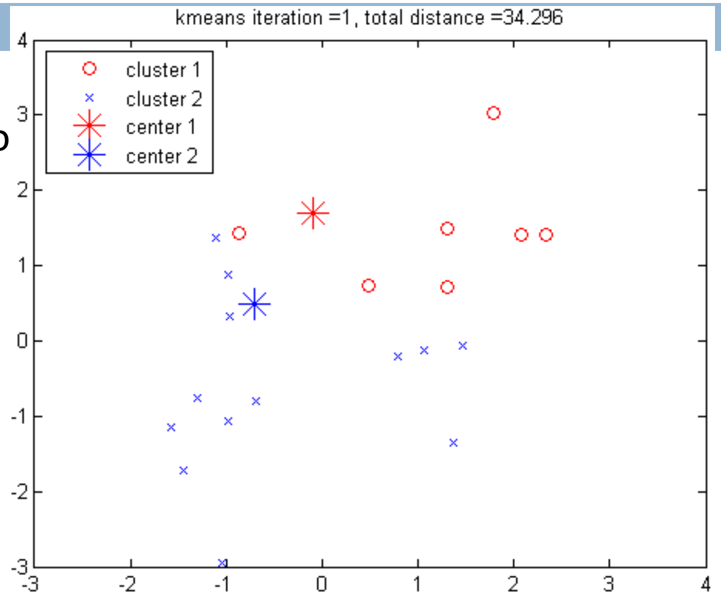


The original data points & randomly select K = 2 centroids

Assign points to clusters



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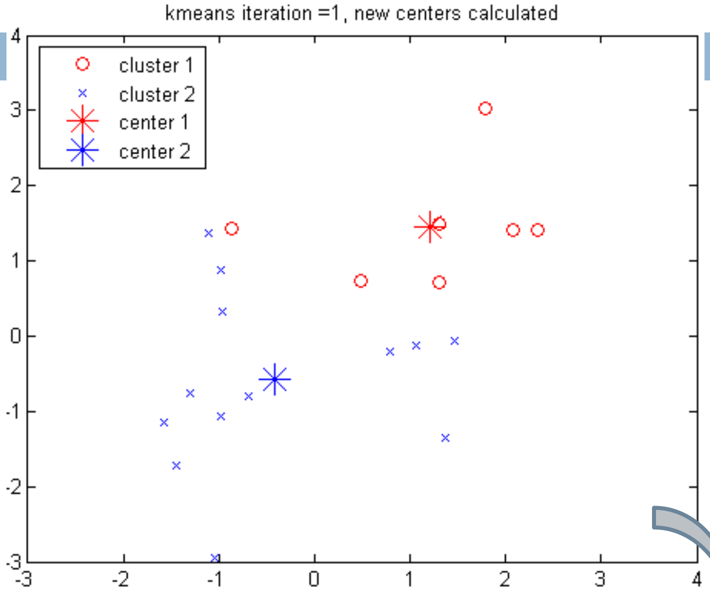
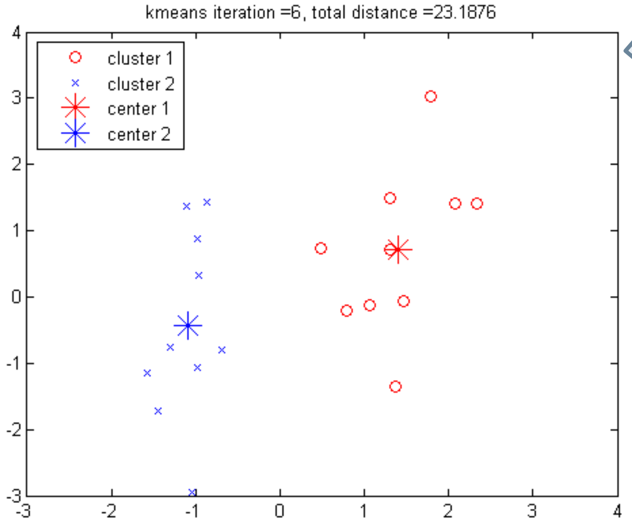


Redo point assignment



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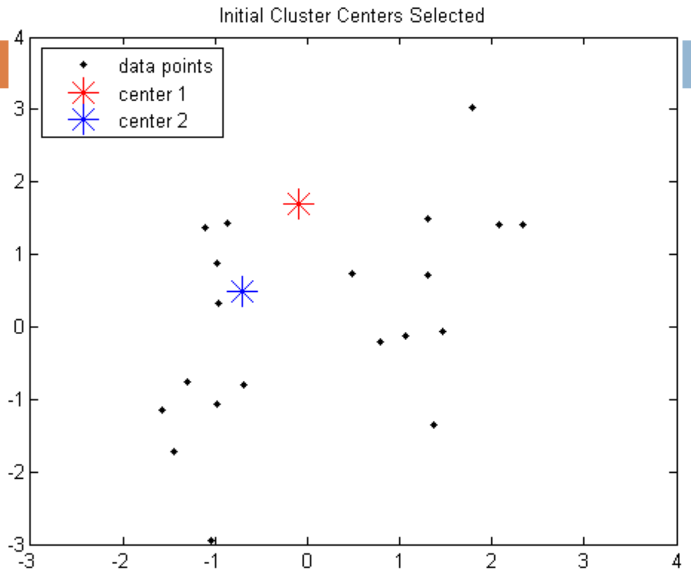

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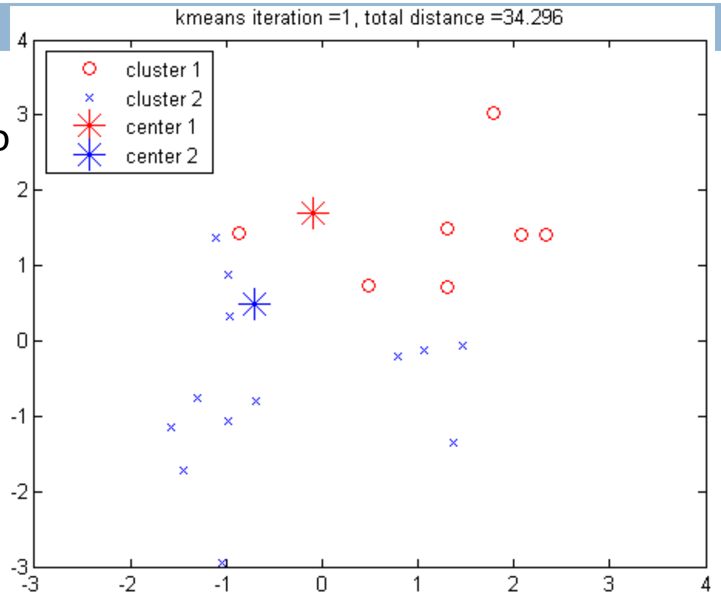
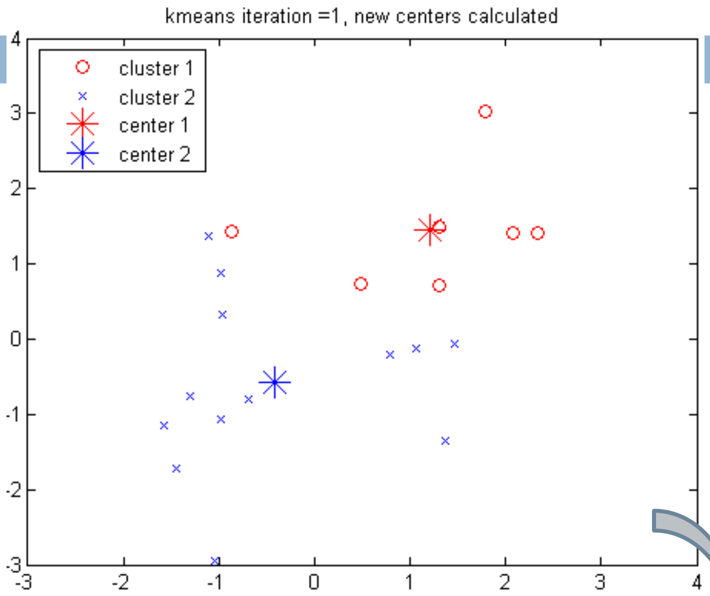
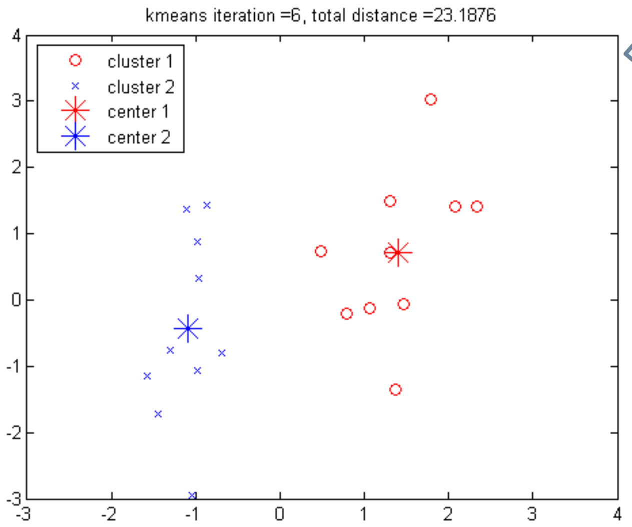


Recompute cluster centers



Redo point assignment

Next iteration



Execution of the K-Means Clustering Algorithm

Select K points as initial centroids

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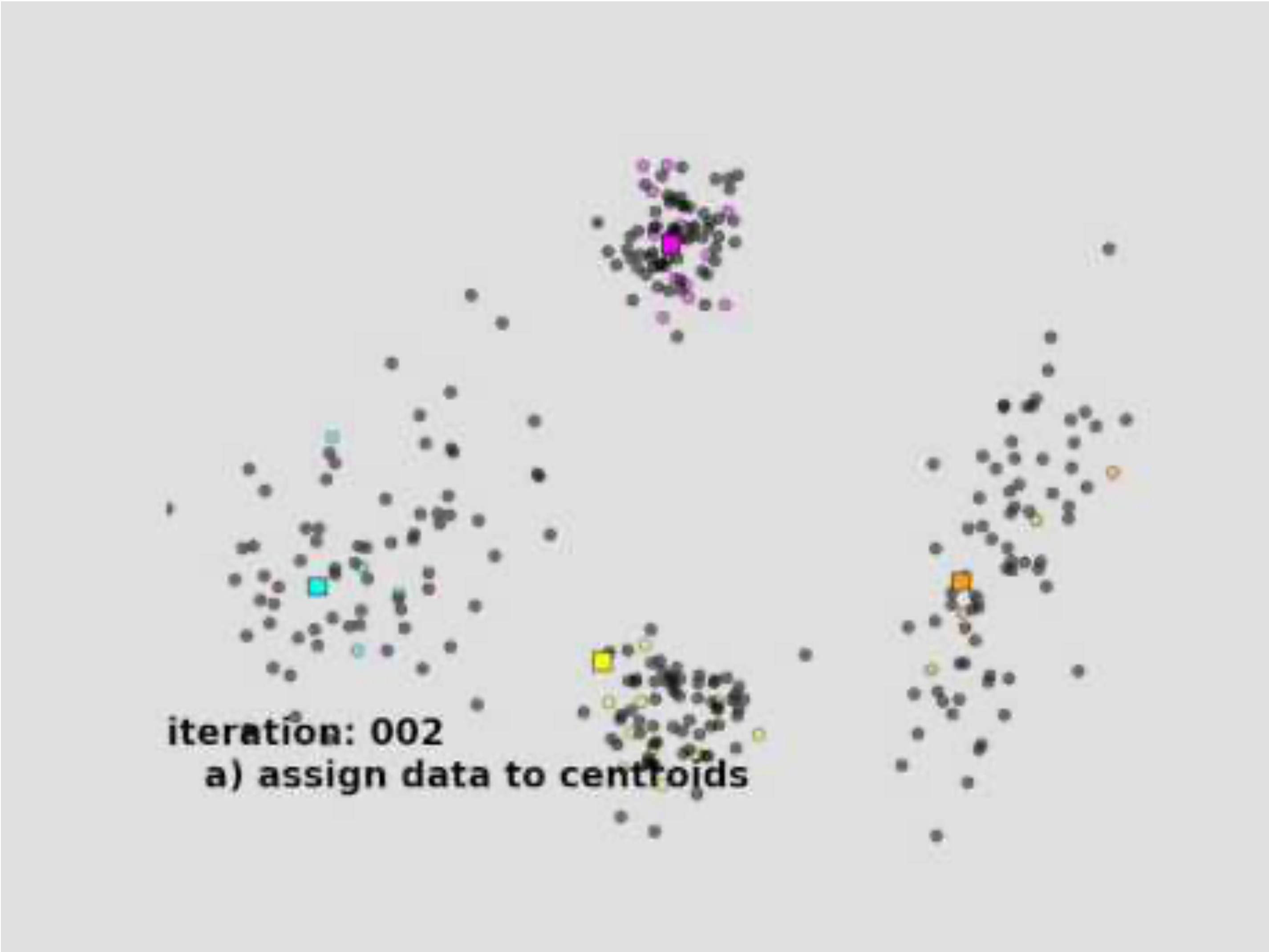
Until convergence criterion is satisfied

K-means Example – Animated



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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  - 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 = number of data points

Evaluating K-means Clusters

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4:     Recompute the centroid of each cluster.
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

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

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

Derivation of K-means to Minimize SSE

- Example: What if we choose Manhattan distance?

Step 4: how to update centroid

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

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

Partitioning Algorithms: From Optimization Angle

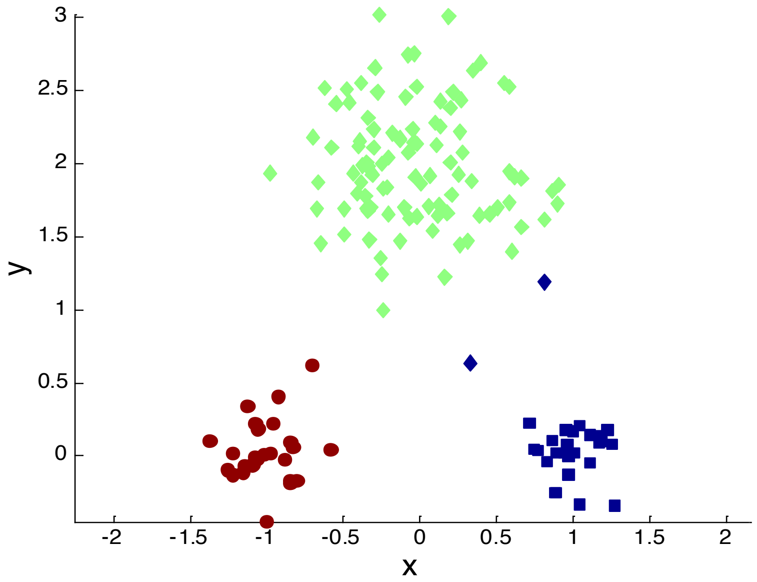
- Partitioning method: Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions

- *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**)

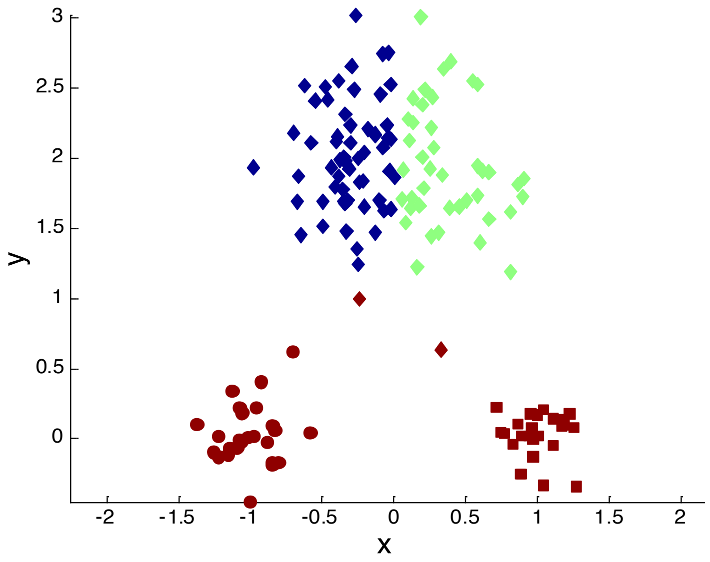
$$SSE(C) = \sum_{i=1}^{K} \sum_{x \in C_i} \|x - c_i\|^2$$

- 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

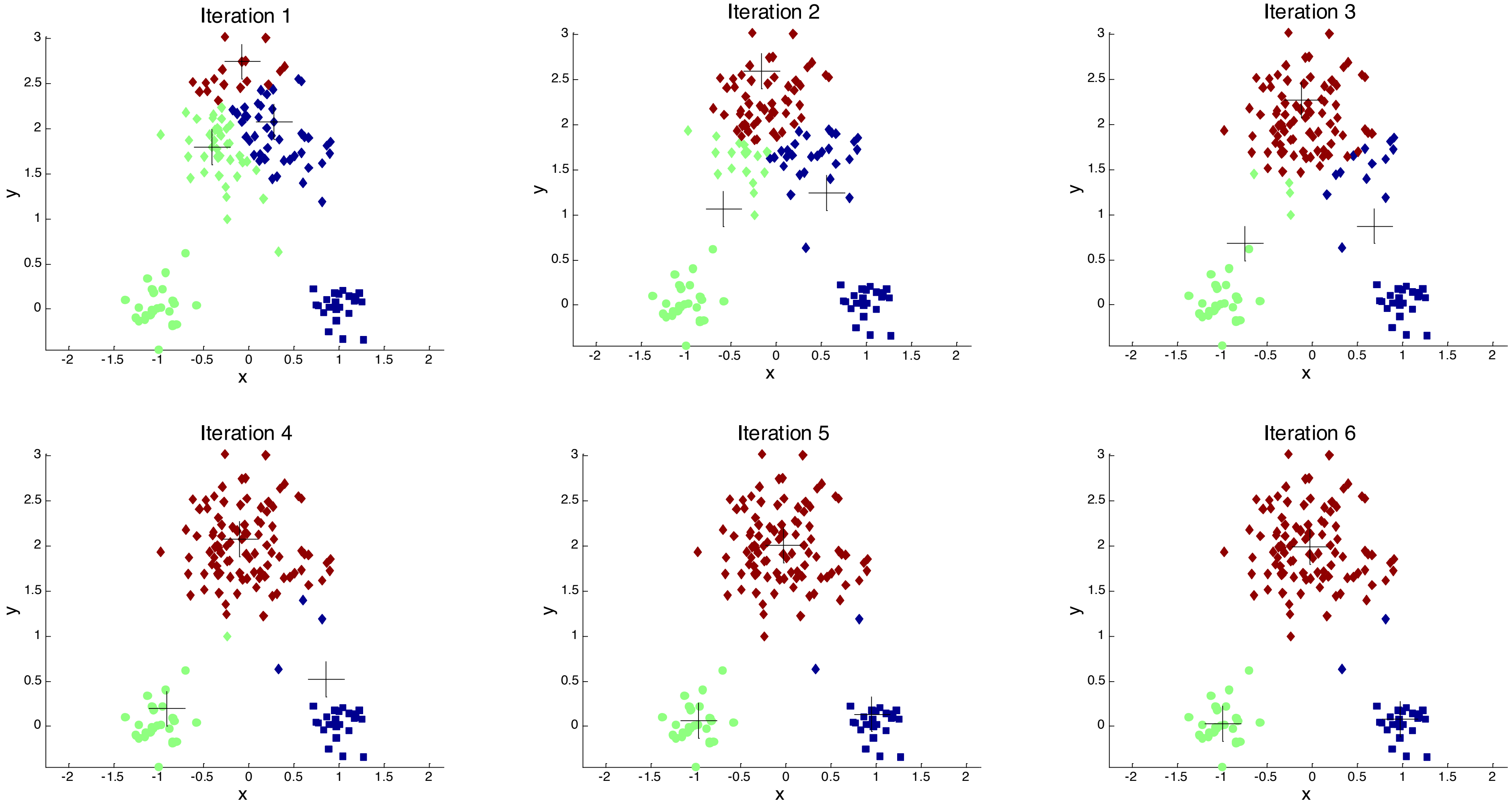


Optimal Clustering



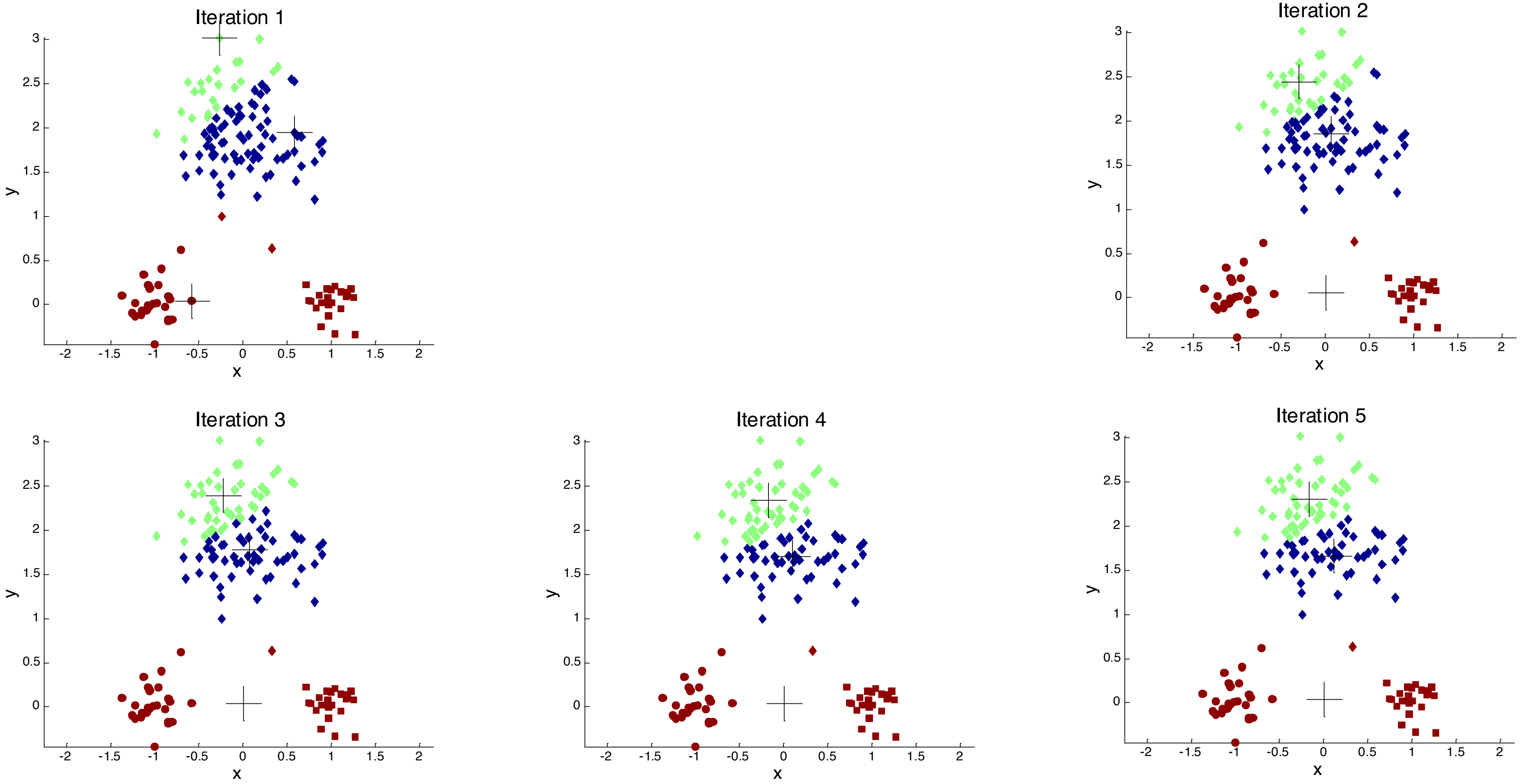
Sub-optimal Clustering

Importance of Choosing Initial Centroids (1)



Optimal Clustering

Importance of Choosing Initial Centroids (2)



Sub-optimal Clustering

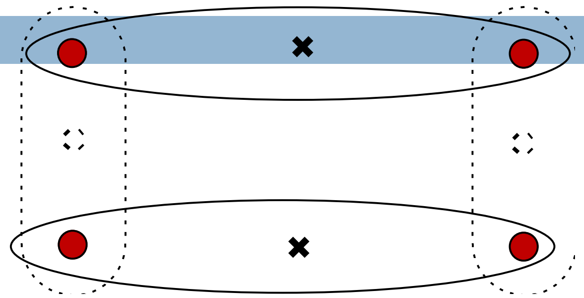
Solutions to Initial Centroids Problem

- 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++

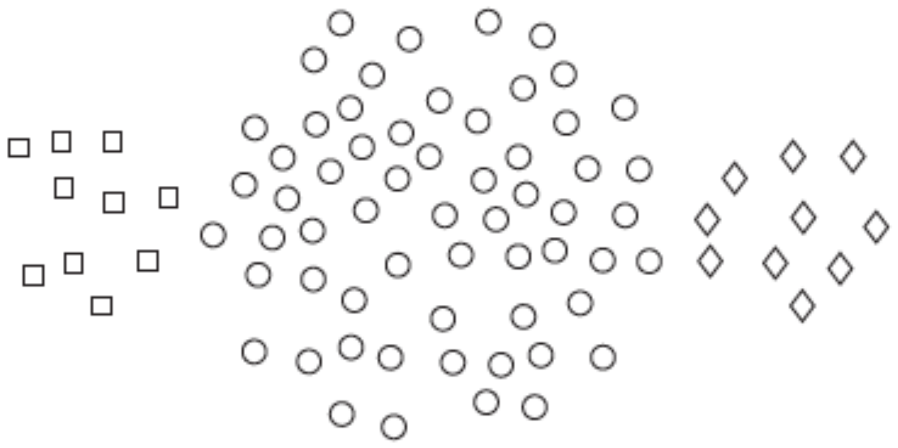
- K-means++ is generally preferred over K-means
  - Even among advanced initialization strategies for K-Means (e.g., Random Partition, Maximin, among others), K-means++ is generally among the best
- K-means++ has better quality guarantee than K-means
  - For K-means, clusterings can be **arbitrarily 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

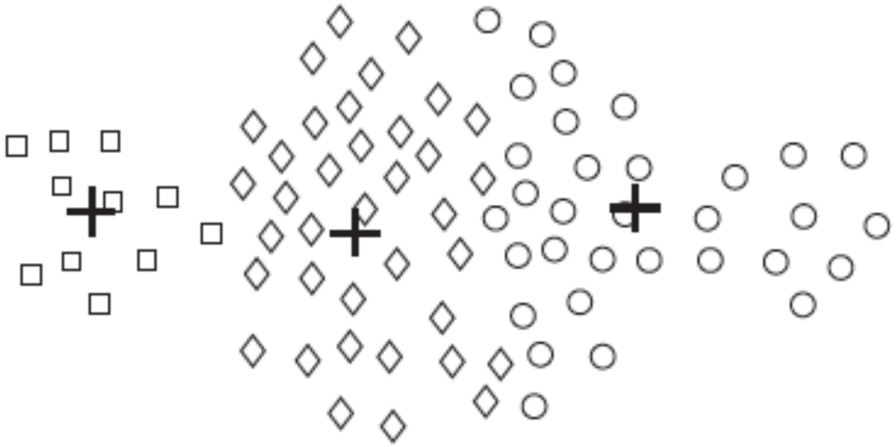
- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes

- K-means has problems when the data contains outliers.

Limitations of K-means: Differing Size



(a) Original points.

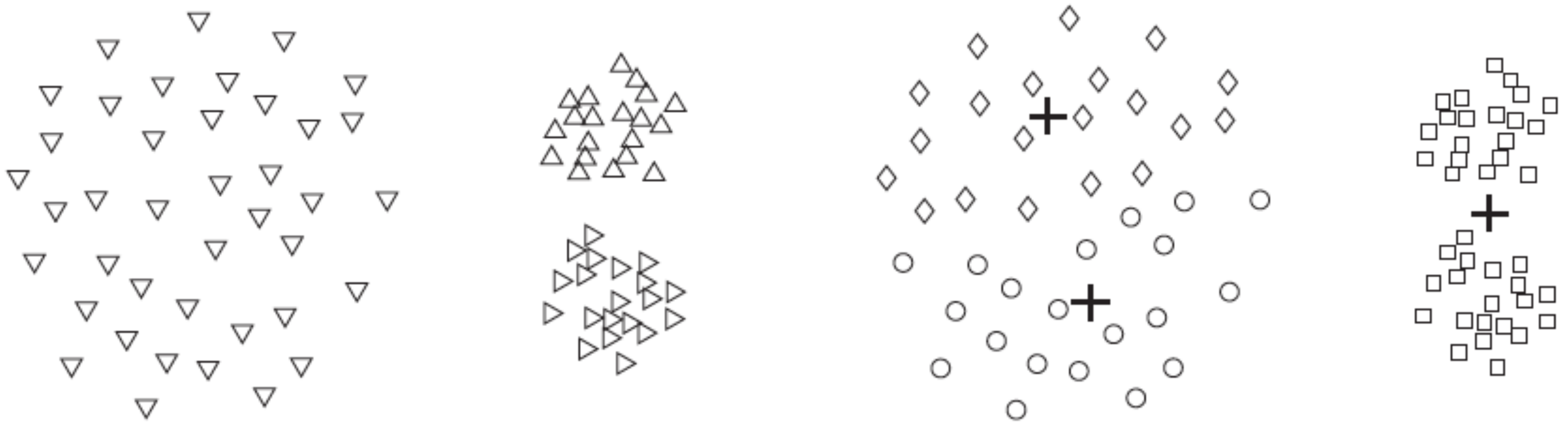


(b) Three K-means clusters.

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

https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf

Limitations of K-means: Differing Density

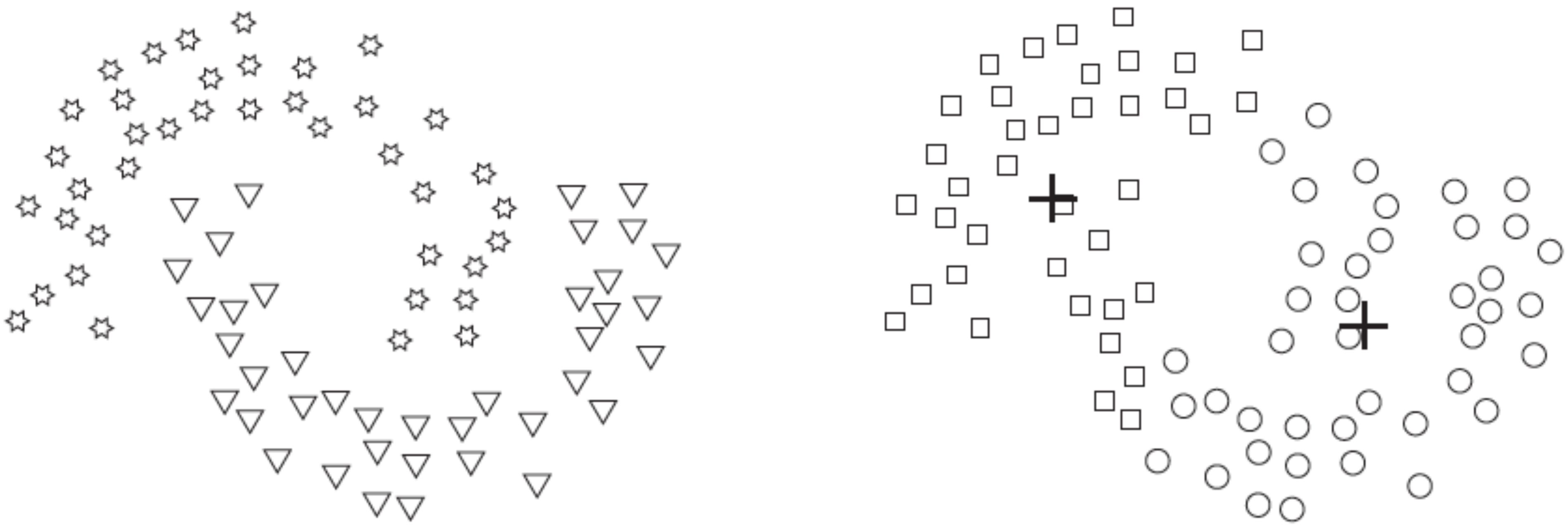


(a) Original points. (b) Three K-means clusters.

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

https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf

Limitations of K-means: Non-globular Clusters



(a) Original points.

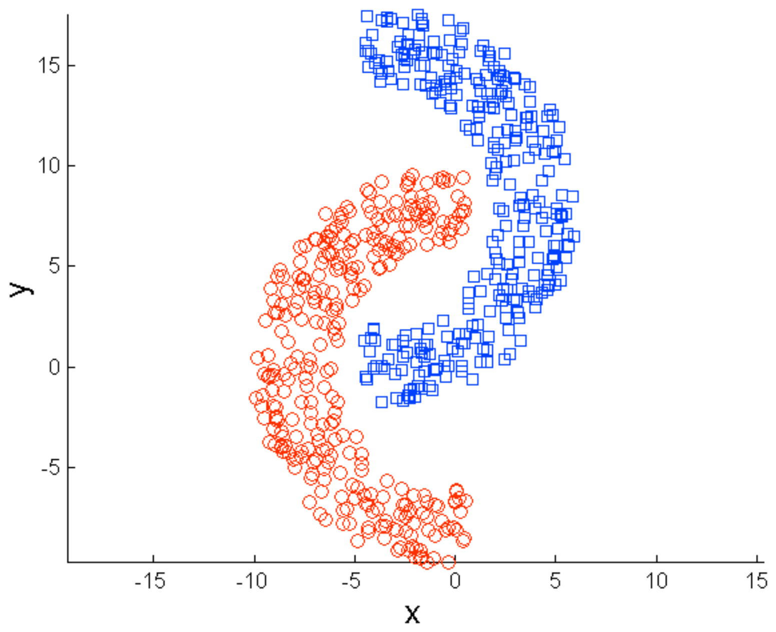
(b) Two K-means clusters.

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

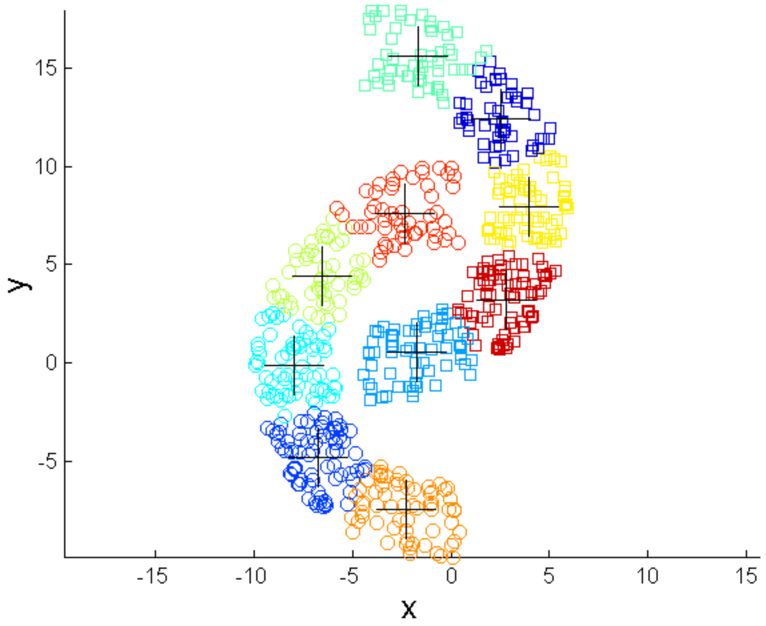
https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf

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:

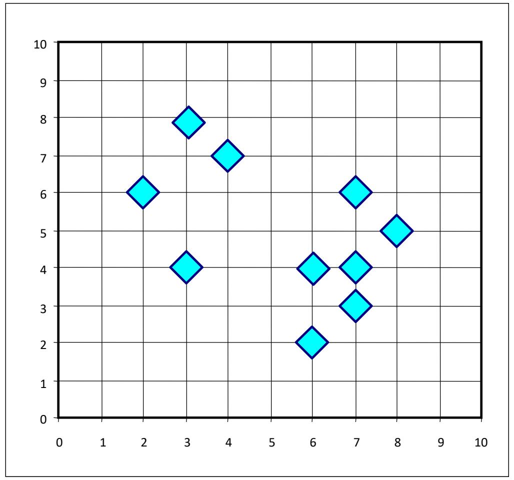
$$S = \sum_{i=1}^{K} \sum_{x \in C_i} \sum_{j=1}^{D} \left| x_j - med_{ij} \right|$$

- 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)

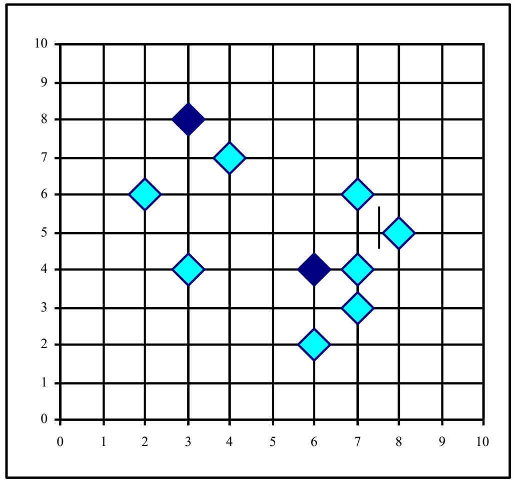
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster
- The *K-Medoids* clustering algorithm: $SSE(C) = \sum_{i=1}^{K} \sum_{x \in C_i} dist(x, o_i)$
  - Select *K* points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

K-Medoids: PAM (Partitioning around Medoids)

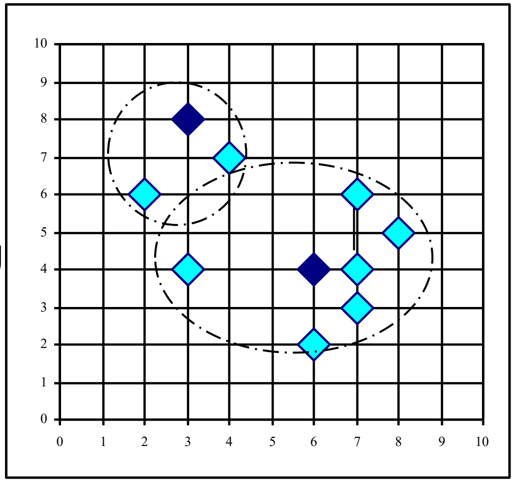


$K = 2$

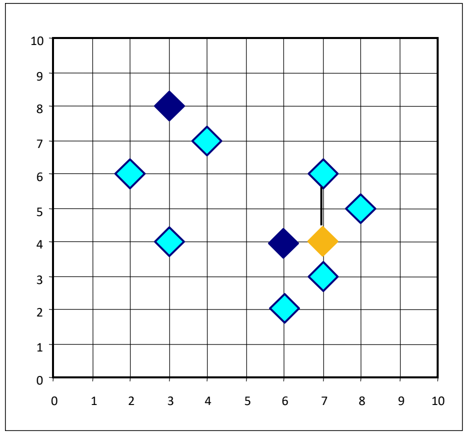
Arbitrary choose K object as initial medoids



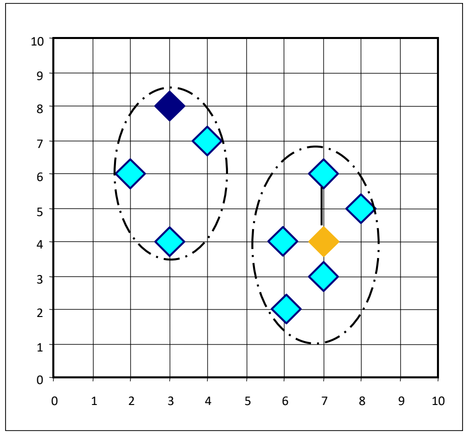
Assign each remaining object to nearest medoids



Randomly select a non-medoid object, O_{ramdom}



Compute total cost of swapping



Swapping O and O_{ramdom}

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

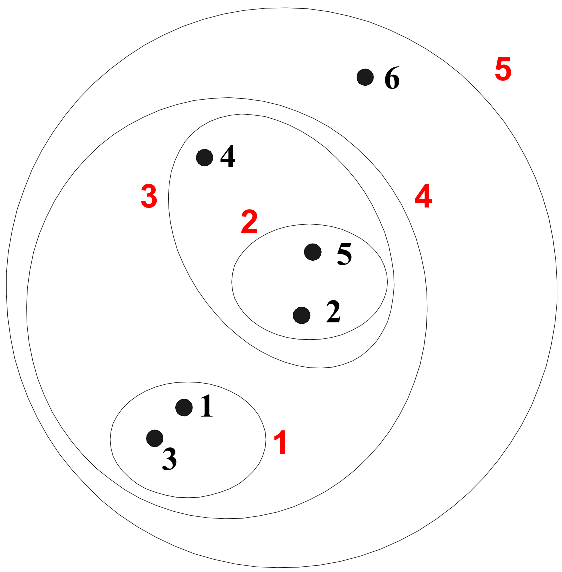
Until convergence criterion is satisfied

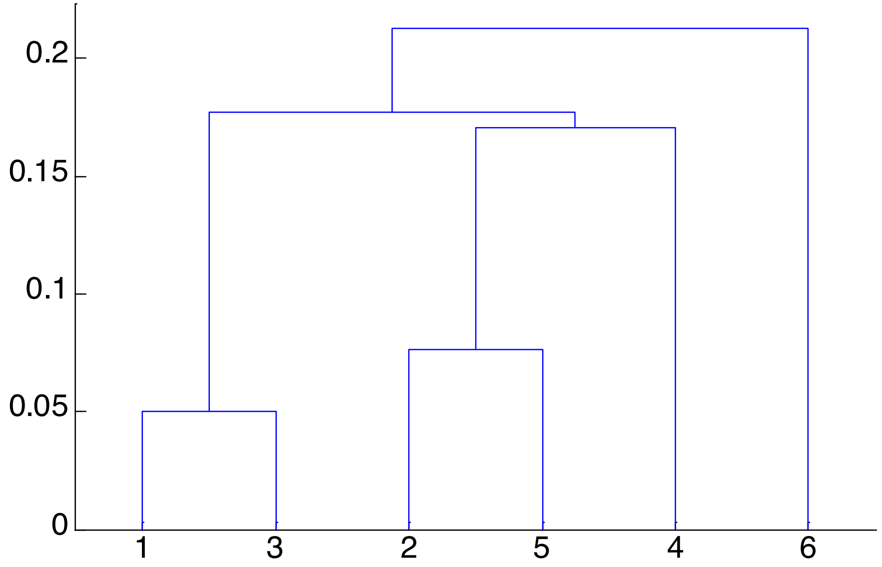
Chapter 10. Cluster Analysis: Basic Concepts and Methods

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

Hierarchical Clustering

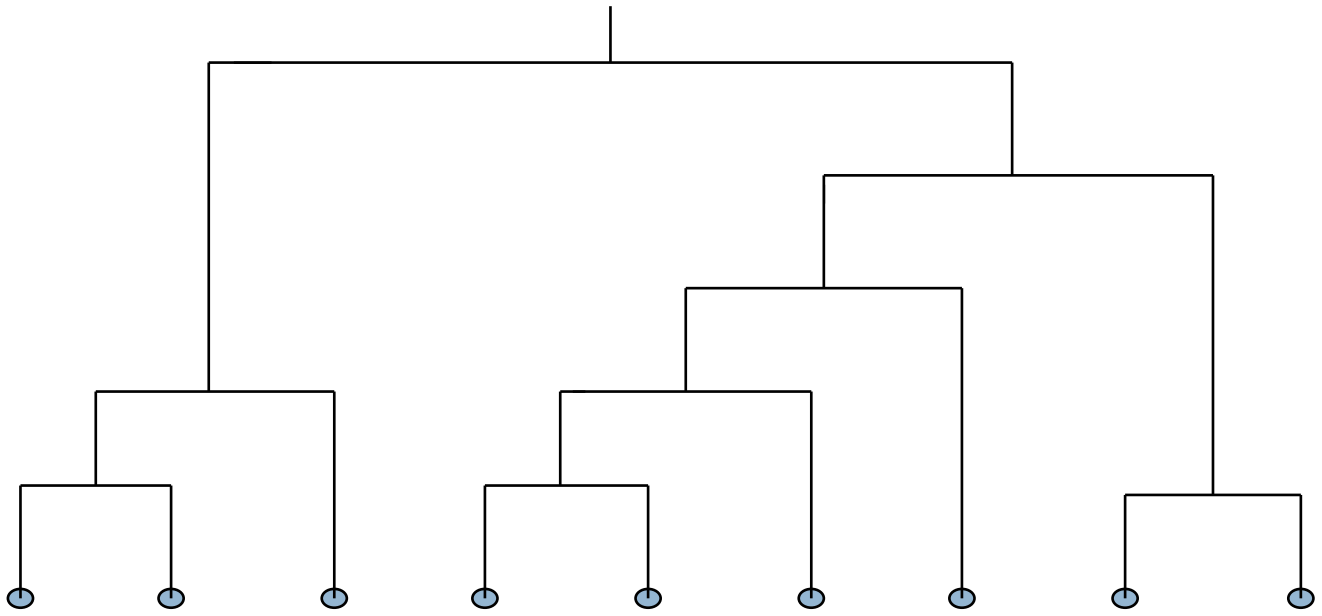
- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - A tree-like diagram that records the sequences of merges or splits





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

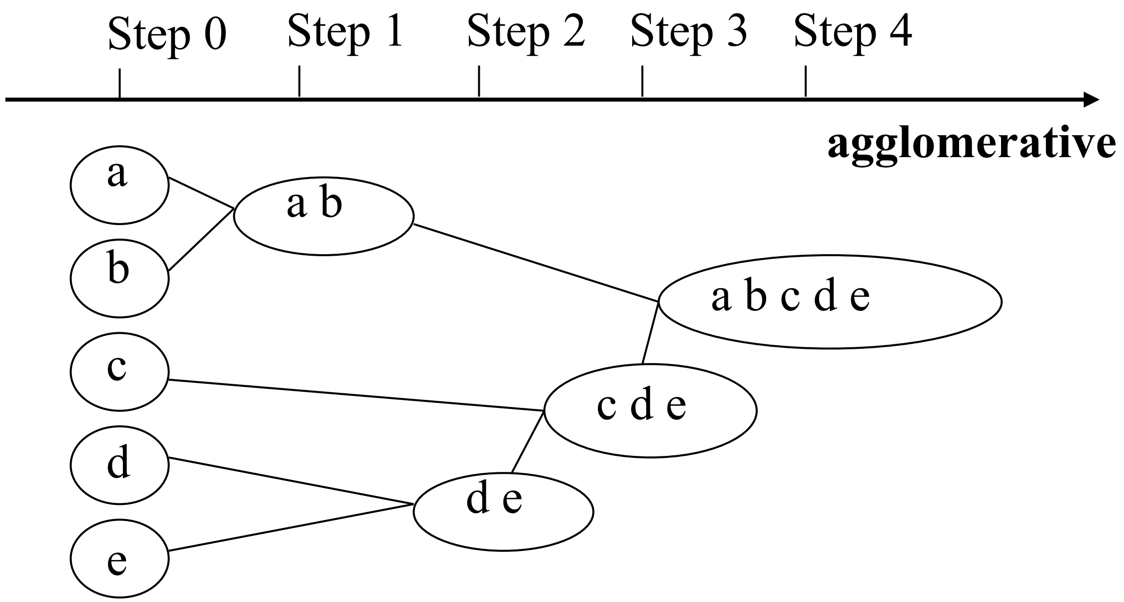
- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by ‘cutting’ the dendogram at the proper level
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Hierarchical Clustering

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

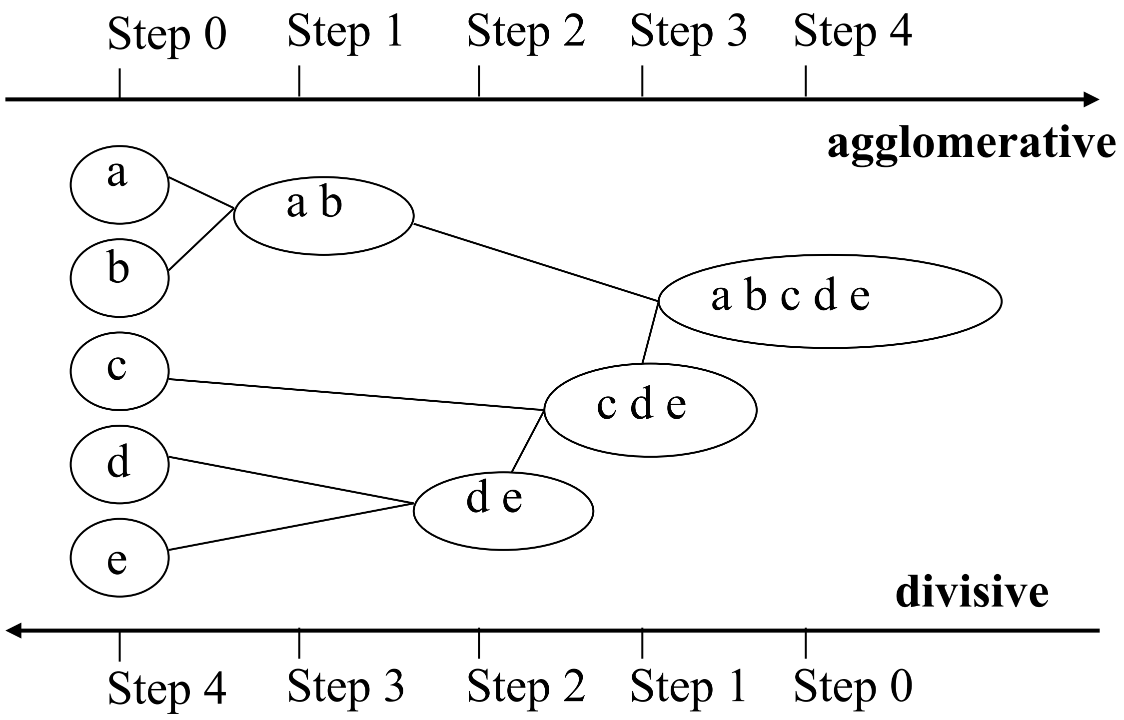
Hierarchical Clustering

- 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

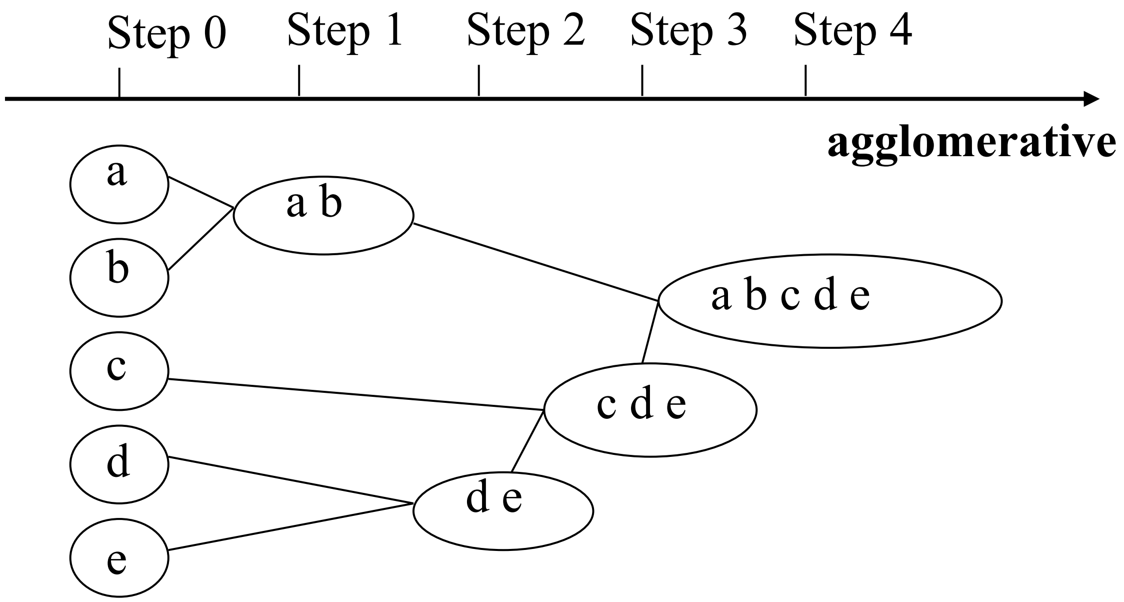


Hierarchical Clustering

- 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

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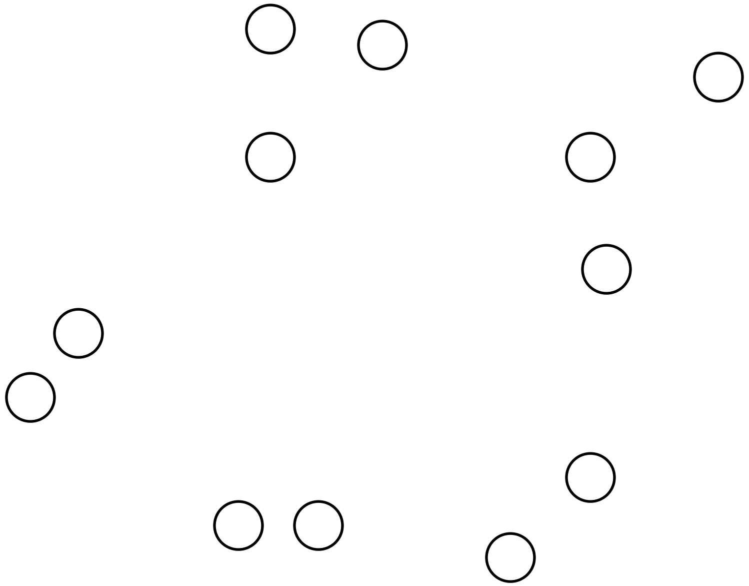
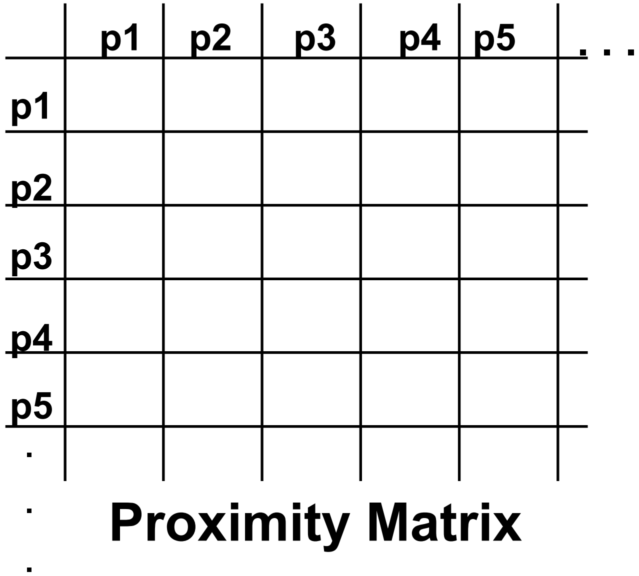
- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. **Repeat**
  4. Merge the two closest clusters
  5. Update the proximity matrix
  6. **Until** only a single cluster remains
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance/similarity between clusters distinguish the different algorithms

Starting Situation

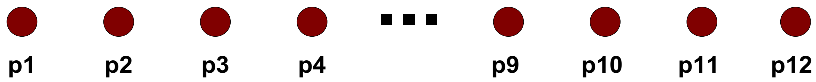
- Start with clusters of individual points and a proximity matrix



12 data points

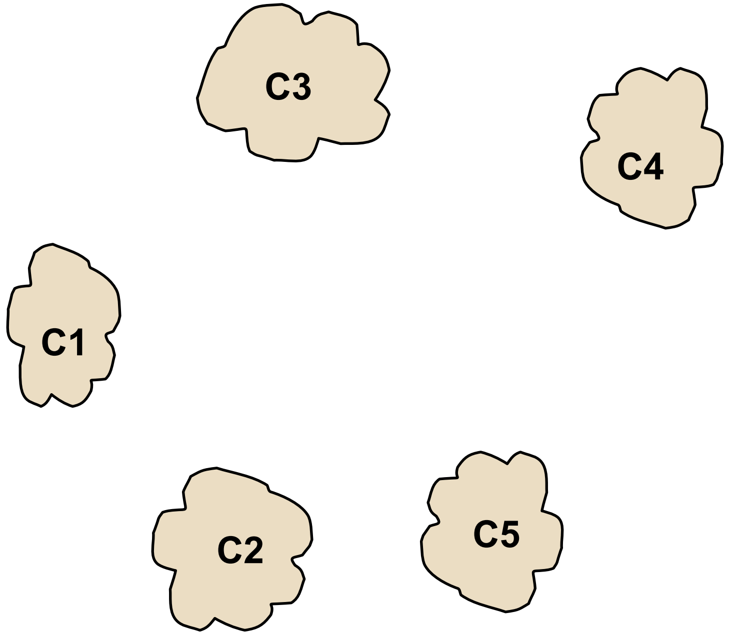


Proximity Matrix



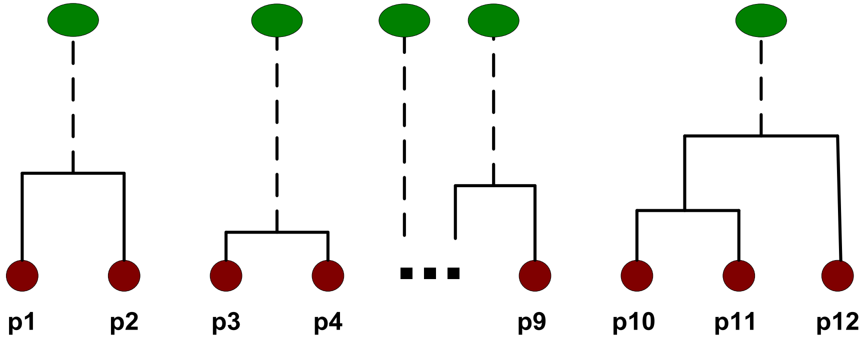
Intermediate Situation

- After some merging steps, we have some clusters



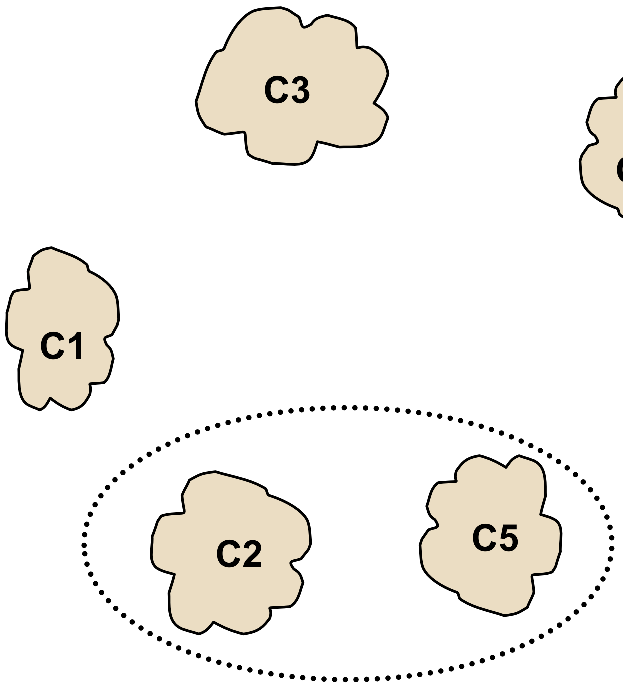
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

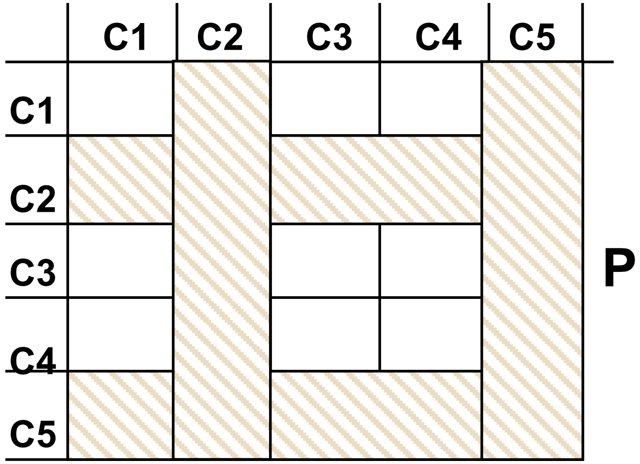
Proximity Matrix



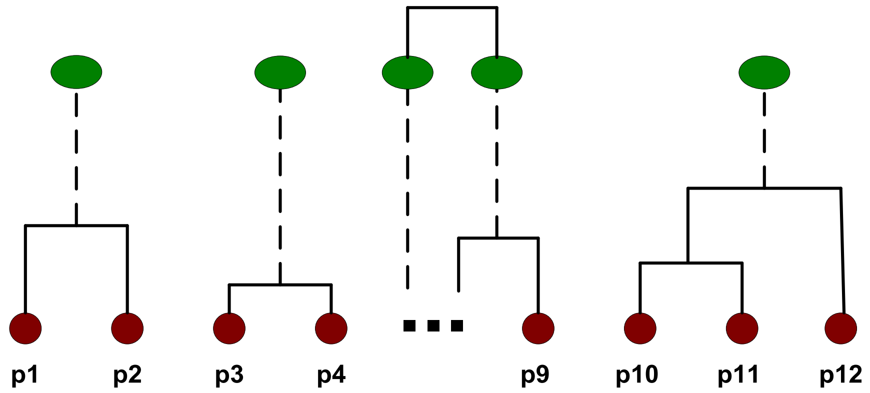
Intermediate Situation

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



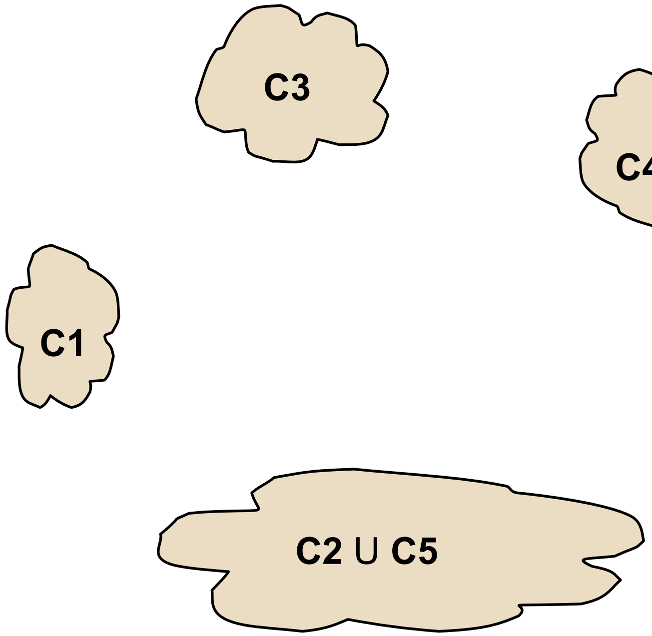


Proximity Matrix



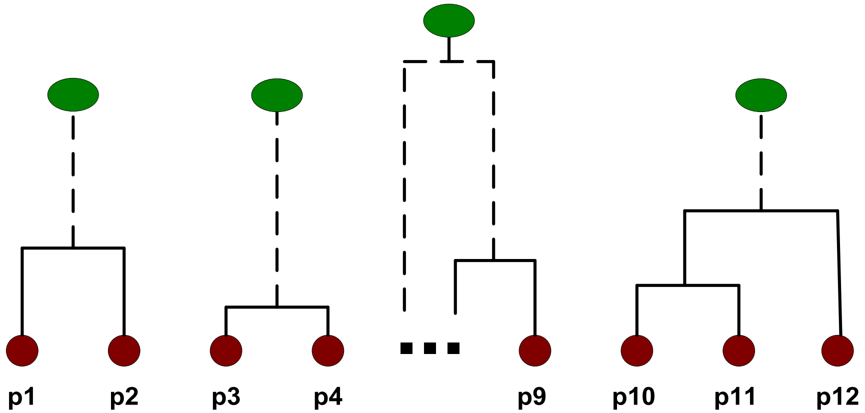
After Merging

- How do we update the proximity matrix?

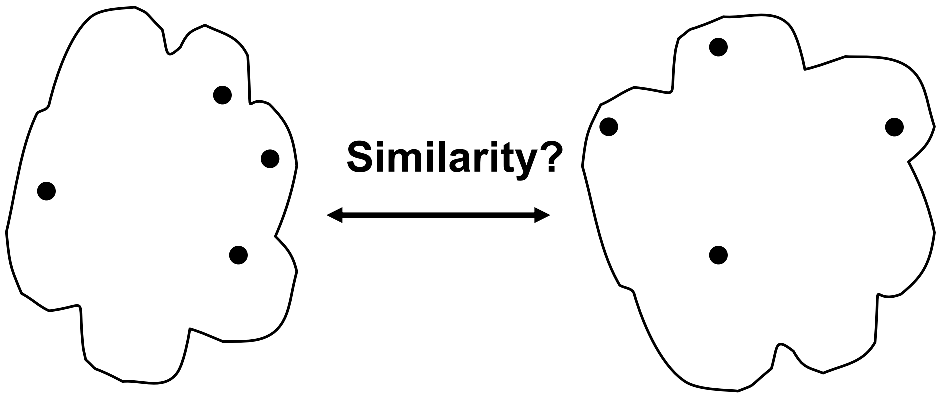


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Similarity

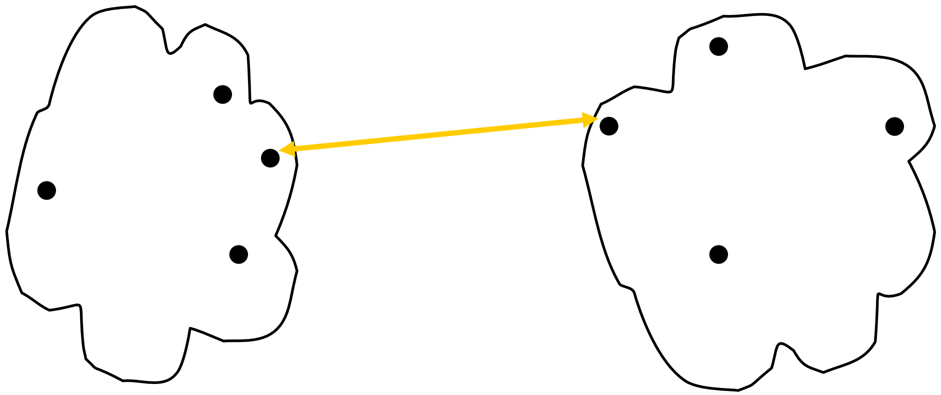


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

How to Define Inter-Cluster Similarity

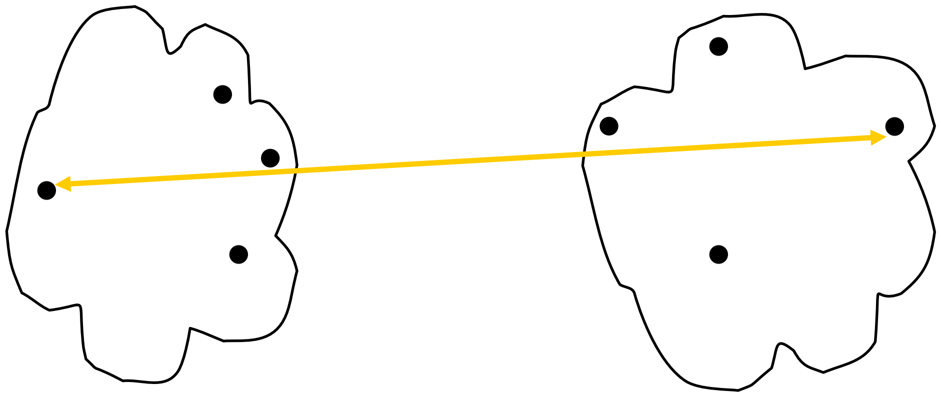


- MIN
- MAX
- Group Average
- Distance Between Centroids

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

Proximity Matrix

How to Define Inter-Cluster Similarity

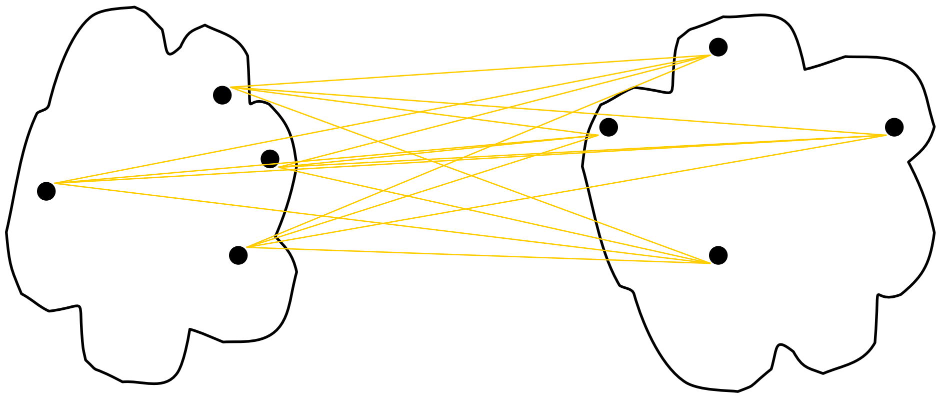


- MIN
- MAX
- Group Average
- Distance Between Centroids

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

Proximity Matrix

How to Define Inter-Cluster Similarity



- MIN
- MAX
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- Distance Between Centroids

	p1	p2	p3	p4	p5	. . .
p1						
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.						
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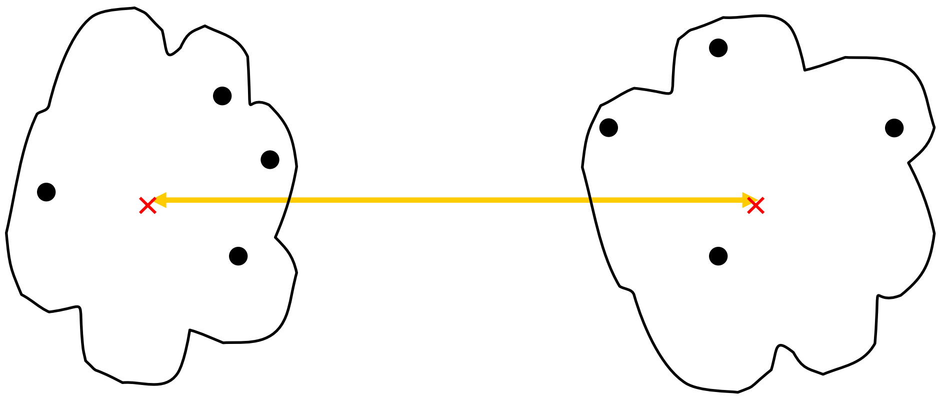
Proximity Matrix

How to Define Inter-Cluster Similarity



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

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

Cluster Similarity: MIN or Single Link

- 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.

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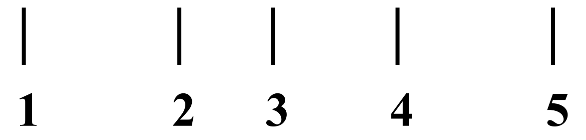
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



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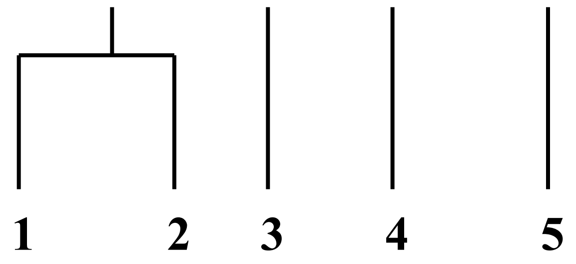
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1.00	$\boxed{0.90}$	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 Link

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

	I1	I2	I3	I4	I5
I1	1.00	$\boxed{0.90}$	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



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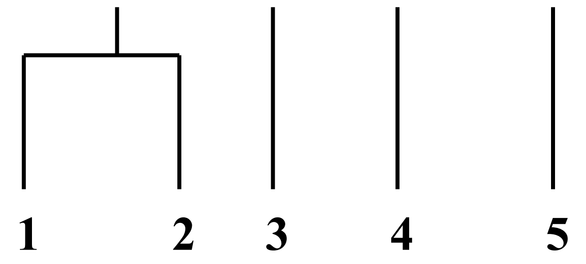
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1.00	$\boxed{0.90}$	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 Link

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

	{I1,I2}	I3	I4	I5
{I1,I2}	1.00	0.70	0.65	0.50
I3	0.70	1.00	0.40	0.30
I4	0.65	0.40	1.00	0.80
I5	0.50	0.30	0.80	1.00

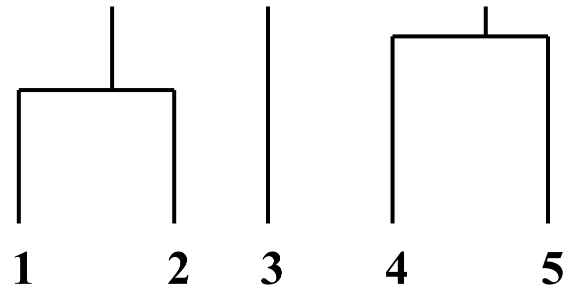
Update proximity matrix with new cluster {I1, I2}

Cluster Similarity: MIN or Single Link

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

	{I1,I2}	I3	I4	I5
{I1,I2}	1.00	0.70	0.65	0.50
I3	0.70	1.00	0.40	0.30
I4	0.65	0.40	1.00	0.80
I5	0.50	0.30	$\boxed{0.80}$	1.00

Update proximity matrix with new cluster {I1, I2}

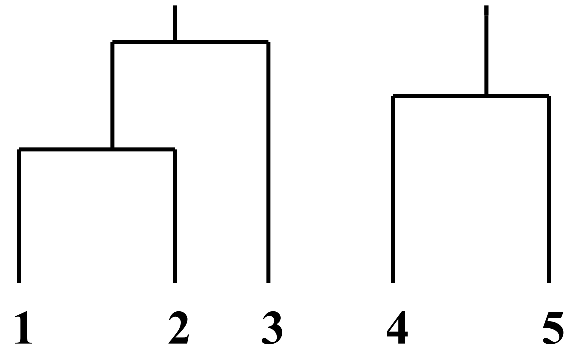


Cluster Similarity: MIN or Single Link

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

	{I1,I2}	I3	{I4,I5}
{I1,I2}	1.00	$\boxed{0.70}$	0.65
I3	0.70	1.00	0.40
{I4,I5}	0.65	0.40	1.00

Update proximity matrix with new cluster {I1, I2} and {I4, I5}

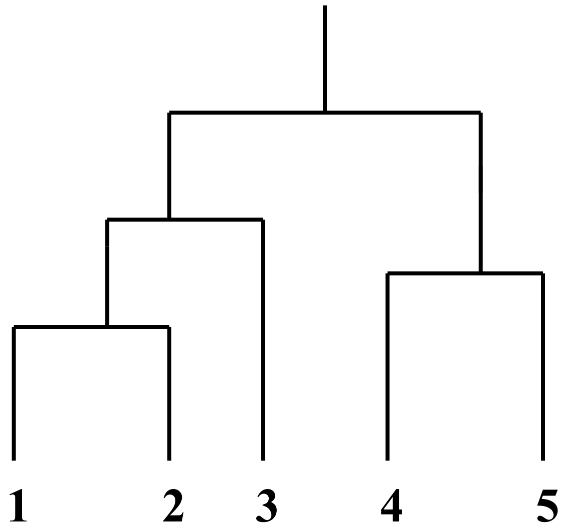


Cluster Similarity: MIN or Single Link

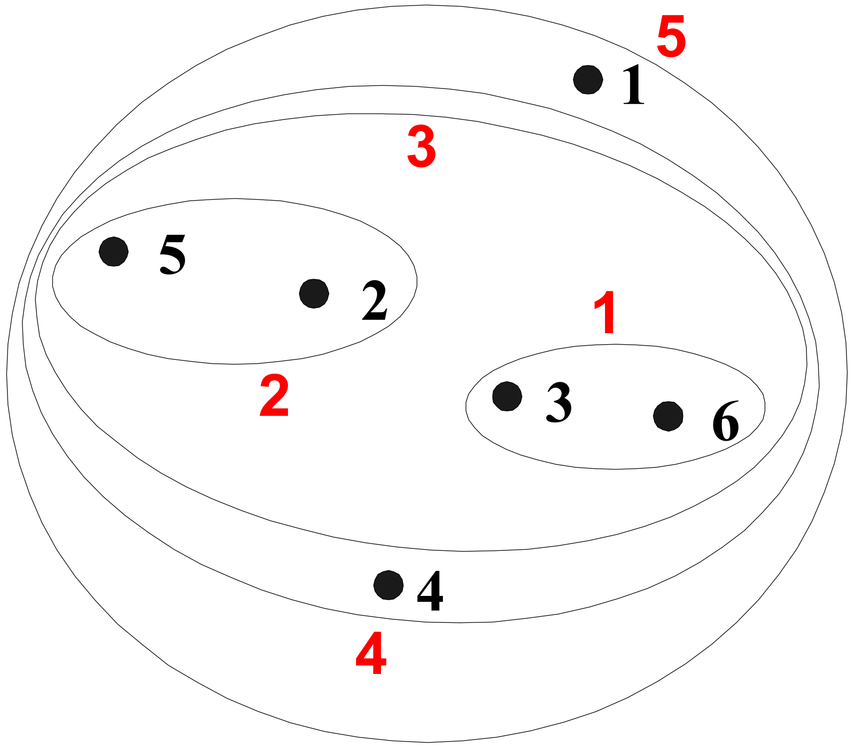
- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	{I1,I2, I3}	{I4,I5}
{I1,I2, I3}	1.00	0.65
{I4,I5}	0.65	1.00

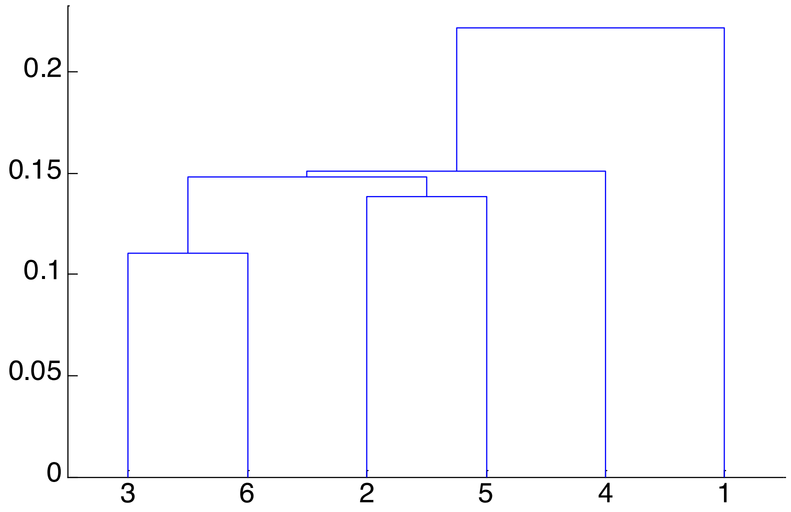
Only two clusters are left.



Hierarchical Clustering: MIN

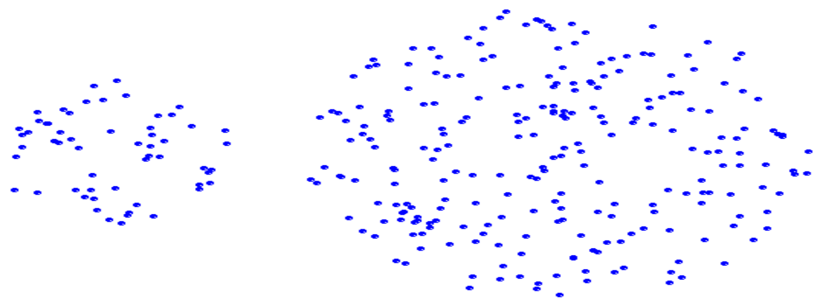


Nested Clusters

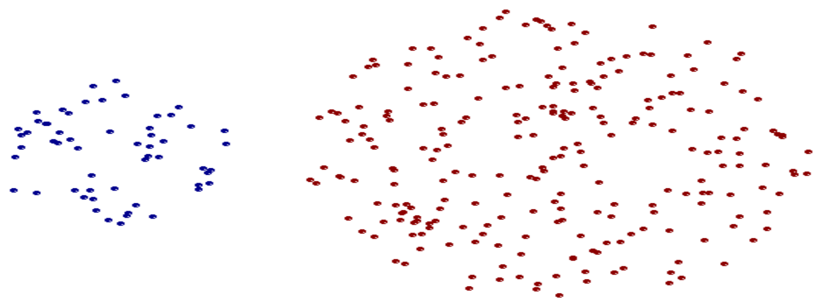


Dendrogram

Strength of MIN



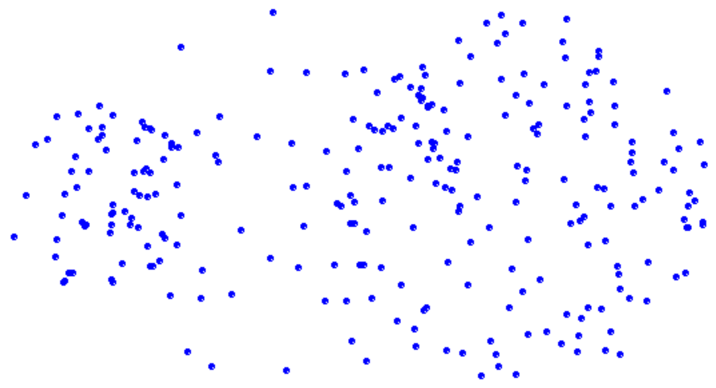
Original Points



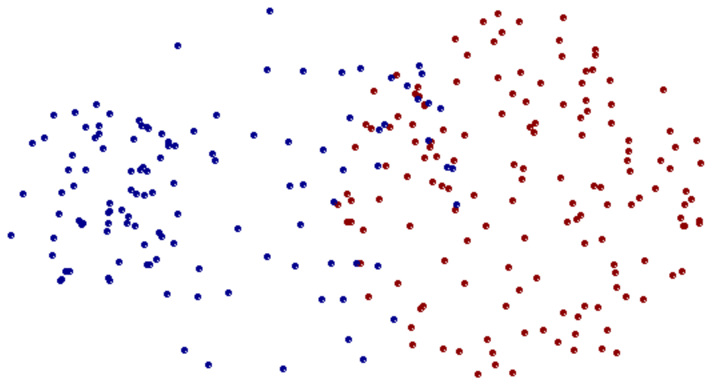
Two Clusters

- **Can handle non-elliptical shapes**

Limitations of MIN



Original Points



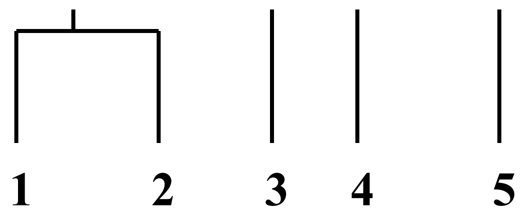
Two Clusters

- **Sensitive to noise and outliers**

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

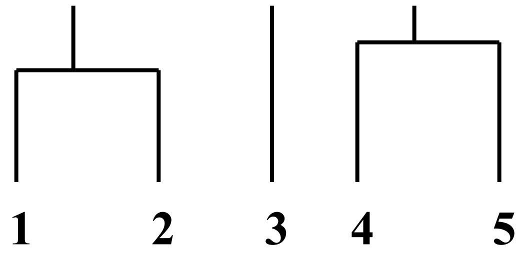
	I1	I2	I3	I4	I5
I1	1.00	$\boxed{0.90}$	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



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

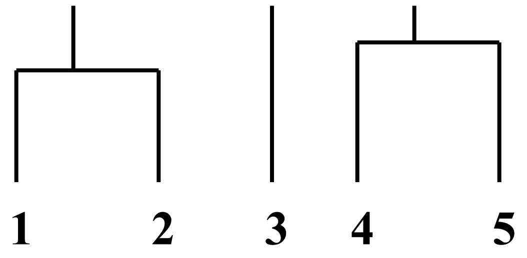
	{I1,I2}	I3	I4	I5
I1	1.00	0.10	0.60	0.20
I3	0.10	1.00	0.40	0.30
I4	0.60	0.40	1.00	0.80
I5	0.20	0.30	$\boxed{0.80}$	1.00



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

	{I1,I2}	I3	I4	I5
I1	1.00	0.10	0.60	0.20
I3	0.10	1.00	0.40	0.30
I4	0.60	0.40	1.00	0.80
I5	0.20	0.30	0.80	1.00

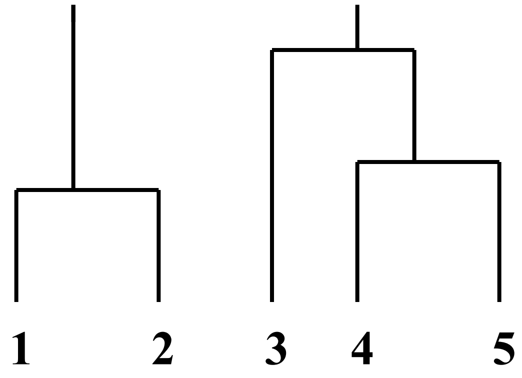


Which two clusters should be merged next?

Cluster Similarity: MAX or Complete Linkage

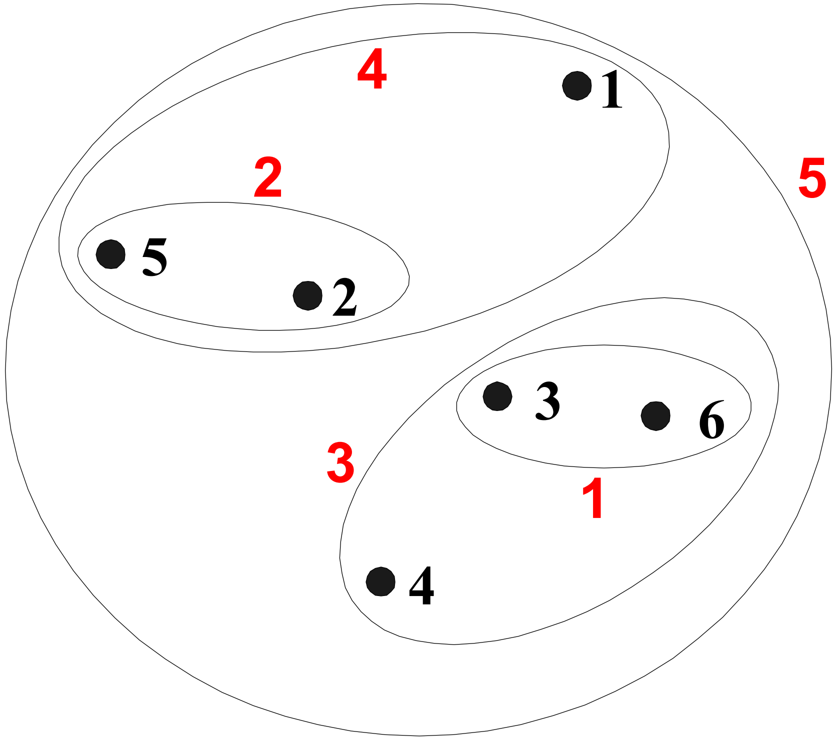
- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

	{I1,I2}	I3	I4	I5
I1	1.00	0.10	0.60	0.20
I3	0.10	1.00	0.40	0.30
I4	0.60	0.40	1.00	0.80
I5	0.20	0.30	0.80	1.00

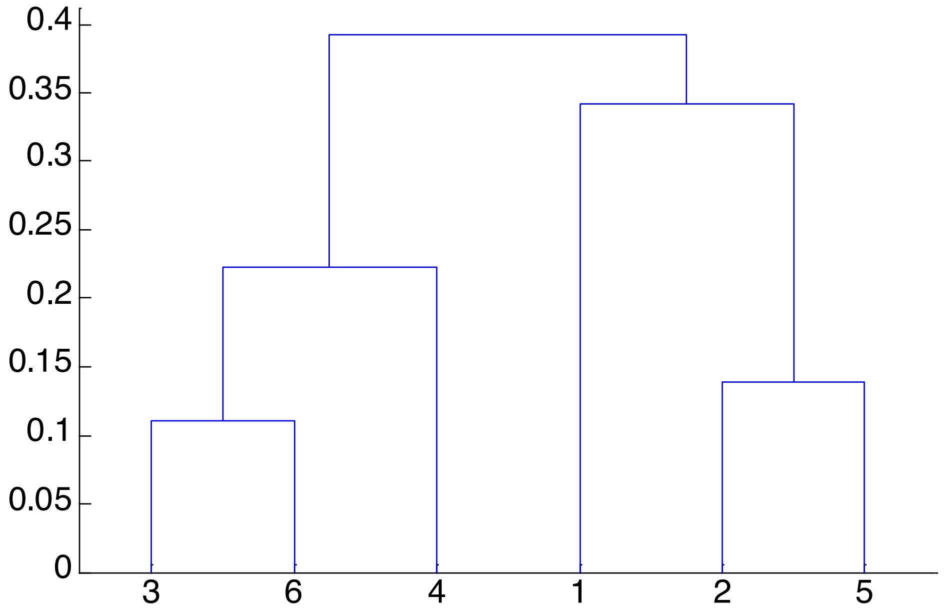


Merge {3} with {4,5}, why?

Hierarchical Clustering: MAX

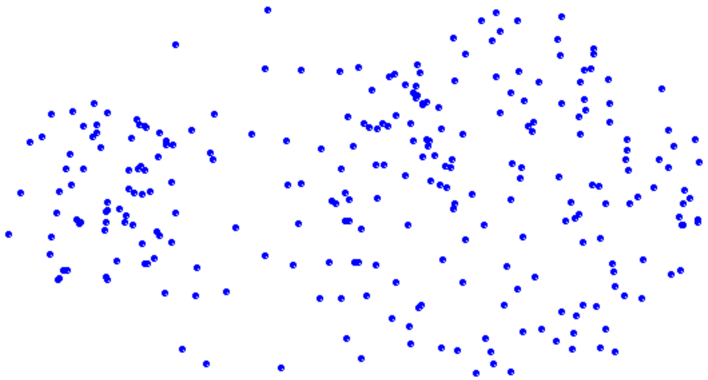


Nested Clusters

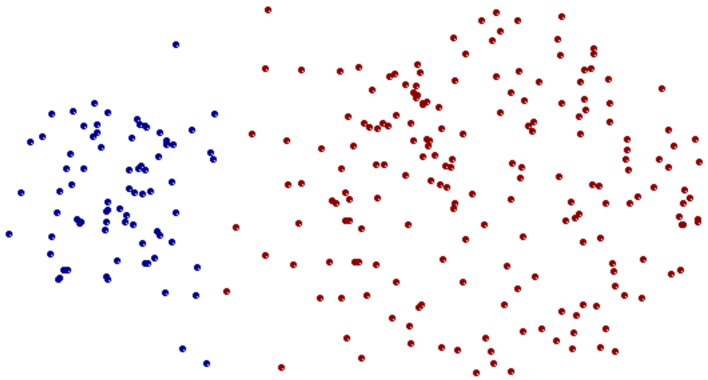


Dendrogram

Strength of MAX



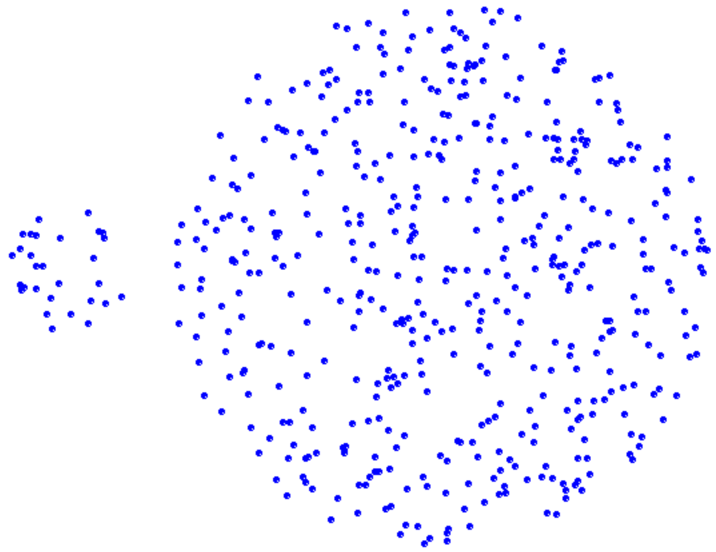
Original Points



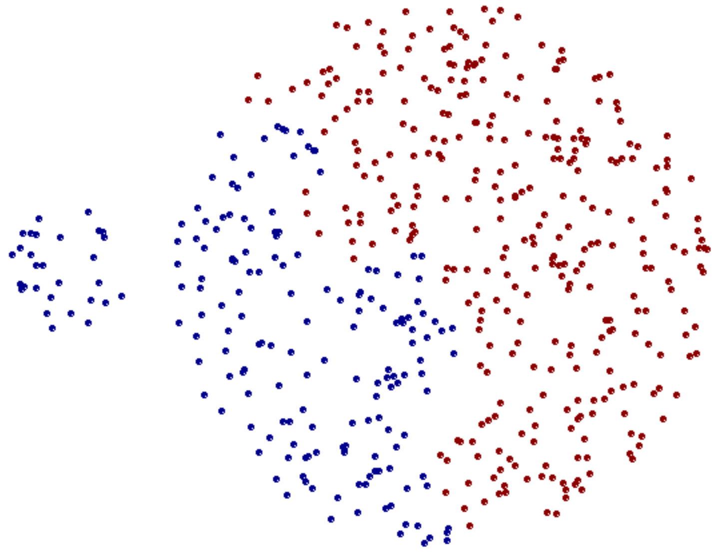
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

- **Tends to break large clusters**
- **Biased towards globular clusters**

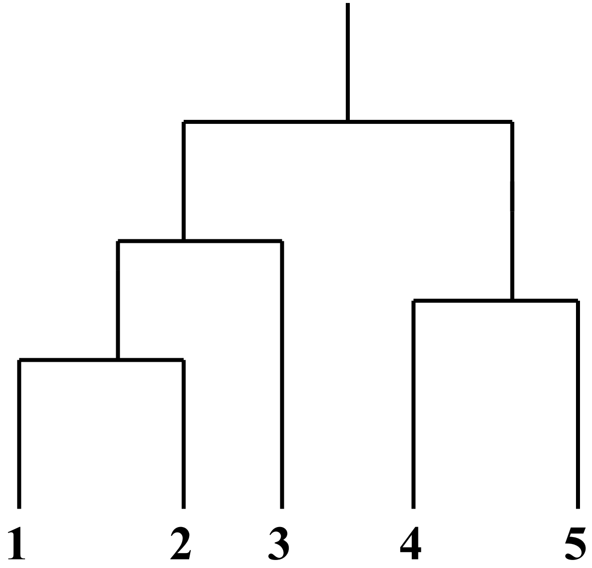
Cluster Similarity: Group Average

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

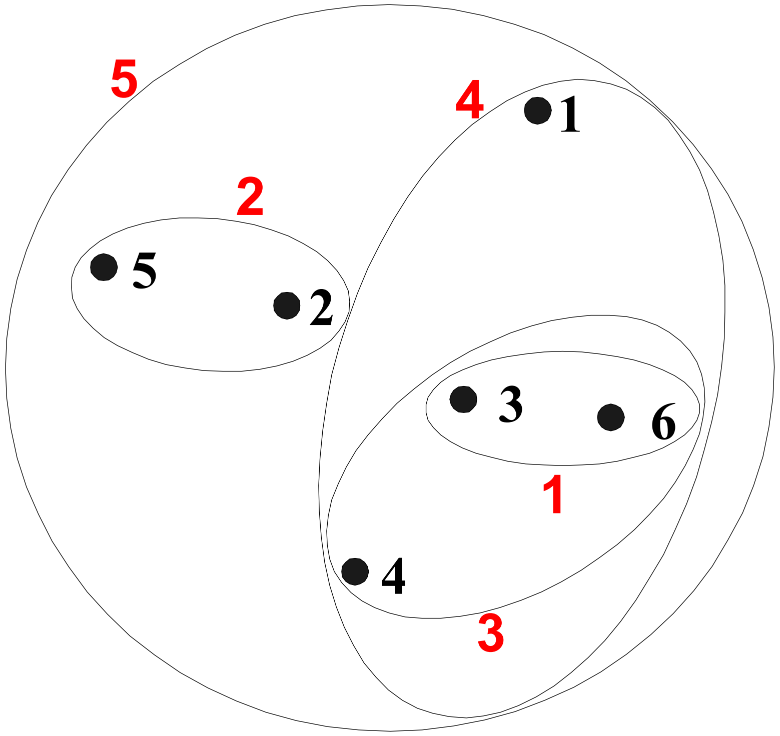
$$\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum\limits_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| * |\text{Cluster}_j|}$$

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

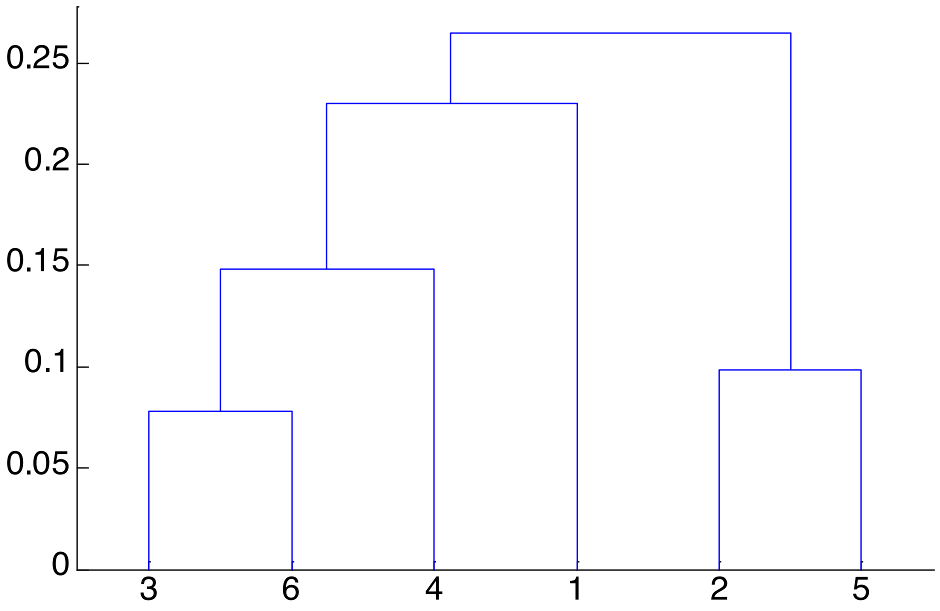
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link

- Strengths
  - Less susceptible to noise and outliers

- Limitations
  - Biased towards globular clusters

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 for some approaches

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