

# Web Mining (網路探勘)

## Unsupervised Learning (非監督式學習)

1011WM04

TLMXM1A

Wed 8,9 (15:10-17:00) U705

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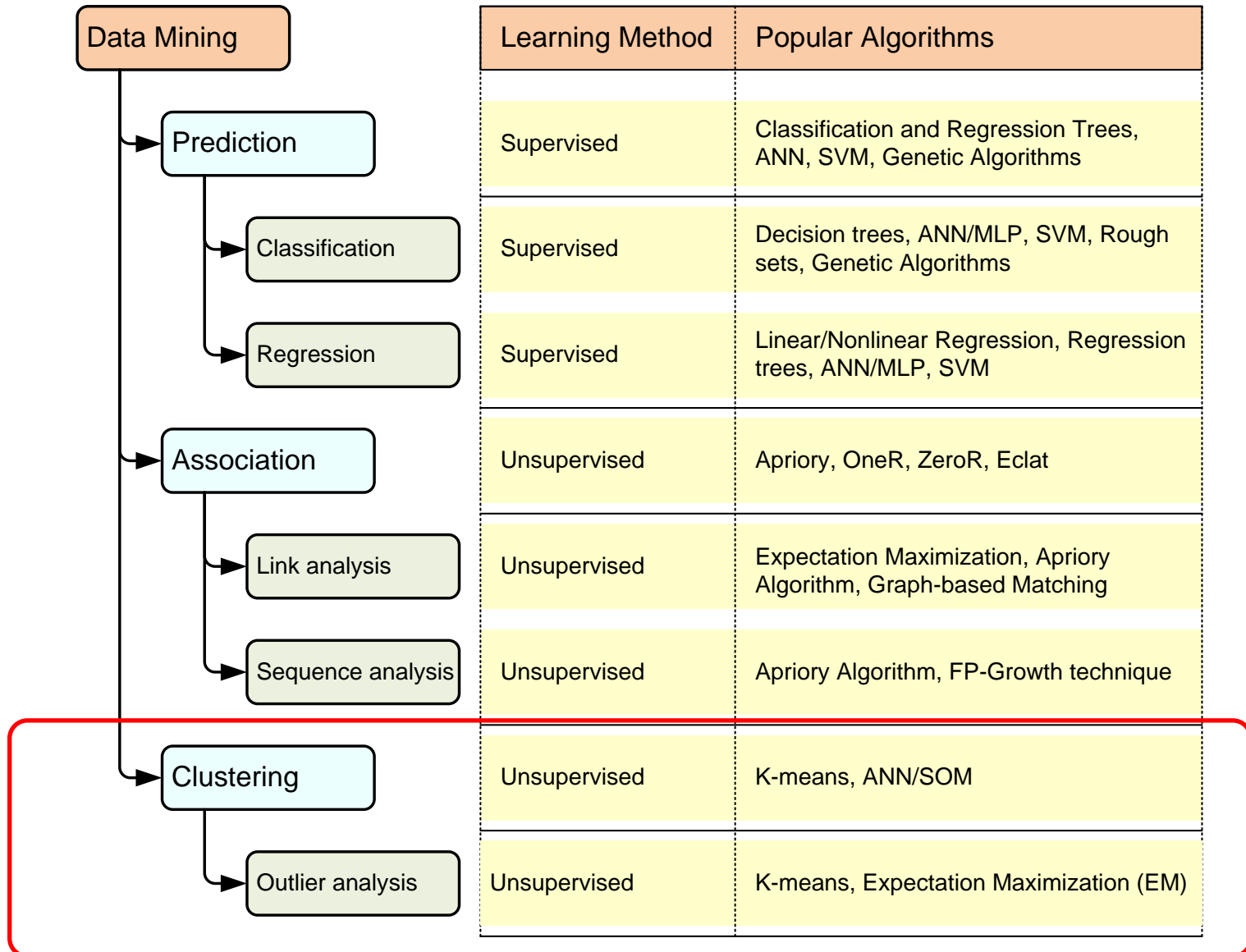
# 課程大綱 (Syllabus)

週次	日期	內容 (Subject/Topics)
1	101/09/12	Introduction to Web Mining (網路探勘導論)
2	101/09/19	Association Rules and Sequential Patterns (關聯規則和序列模式)
3	101/09/26	Supervised Learning (監督式學習)
4	101/10/03	Unsupervised Learning (非監督式學習)
5	101/10/10	國慶紀念日(放假一天)
6	101/10/17	Paper Reading and Discussion (論文研讀與討論)
7	101/10/24	Partially Supervised Learning (部分監督式學習)
8	101/10/31	Information Retrieval and Web Search (資訊檢索與網路搜尋)
9	101/11/07	Social Network Analysis (社會網路分析)

# 課程大綱 (Syllabus)

週次	日期	內容 (Subject/Topics)
10	101/11/14	Midterm Presentation (期中報告)
11	101/11/21	Web Crawling (網路爬行)
12	101/11/28	Structured Data Extraction (結構化資料擷取)
13	101/12/05	Information Integration (資訊整合)
14	101/12/12	Opinion Mining and Sentiment Analysis (意見探勘與情感分析)
15	101/12/19	Paper Reading and Discussion (論文研讀與討論)
16	101/12/26	Web Usage Mining (網路使用挖掘)
17	102/01/02	Project Presentation 1 (期末報告1)
18	102/01/09	Project Presentation 2 (期末報告2)

# A Taxonomy for Data Mining Tasks



# Outline

- Unsupervised Learning
  - Clustering
- Cluster Analysis
- k-Means Clustering Algorithm
- Similarity and Distance Functions
- Cluster Evaluation

# Supervised learning vs. unsupervised learning

- **Supervised learning:**  
discover patterns in the data that relate data attributes with a target (class) attribute.
  - These patterns are then utilized to predict the values of the target attribute in future data instances.
- **Unsupervised learning:**  
The data have no target attribute.
  - We want to explore the data to find some intrinsic structures in them.

# Clustering

- Clustering is a technique for finding **similarity groups** in data, called **clusters**. I.e.,
  - it groups data instances that are similar to (near) each other in one cluster and data instances that are very different (far away) from each other into different clusters.
- Clustering is often called an **unsupervised learning** task as no class values denoting an *a priori* grouping of the data instances are given, which is the case in supervised learning.
- Due to historical reasons, clustering is often considered synonymous with unsupervised learning.
  - In fact, association rule mining is also unsupervised

# Outline

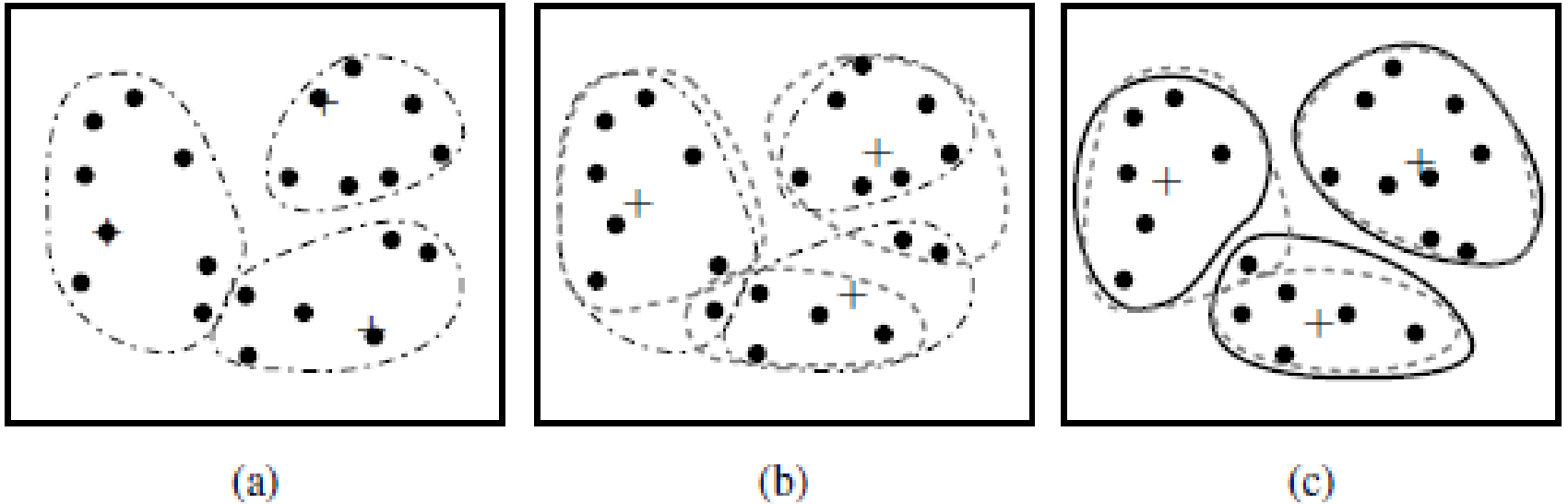
- Unsupervised Learning
  - Clustering
- Cluster Analysis
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- Similarity and Distance Functions
- Cluster Evaluation



# Cluster Analysis

- Used for automatic identification of natural groupings of things
- Part of the machine-learning family
- Employ unsupervised learning
- Learns the clusters of things from past data, then assigns new instances
- There is not an output variable
- Also known as segmentation

# Cluster Analysis

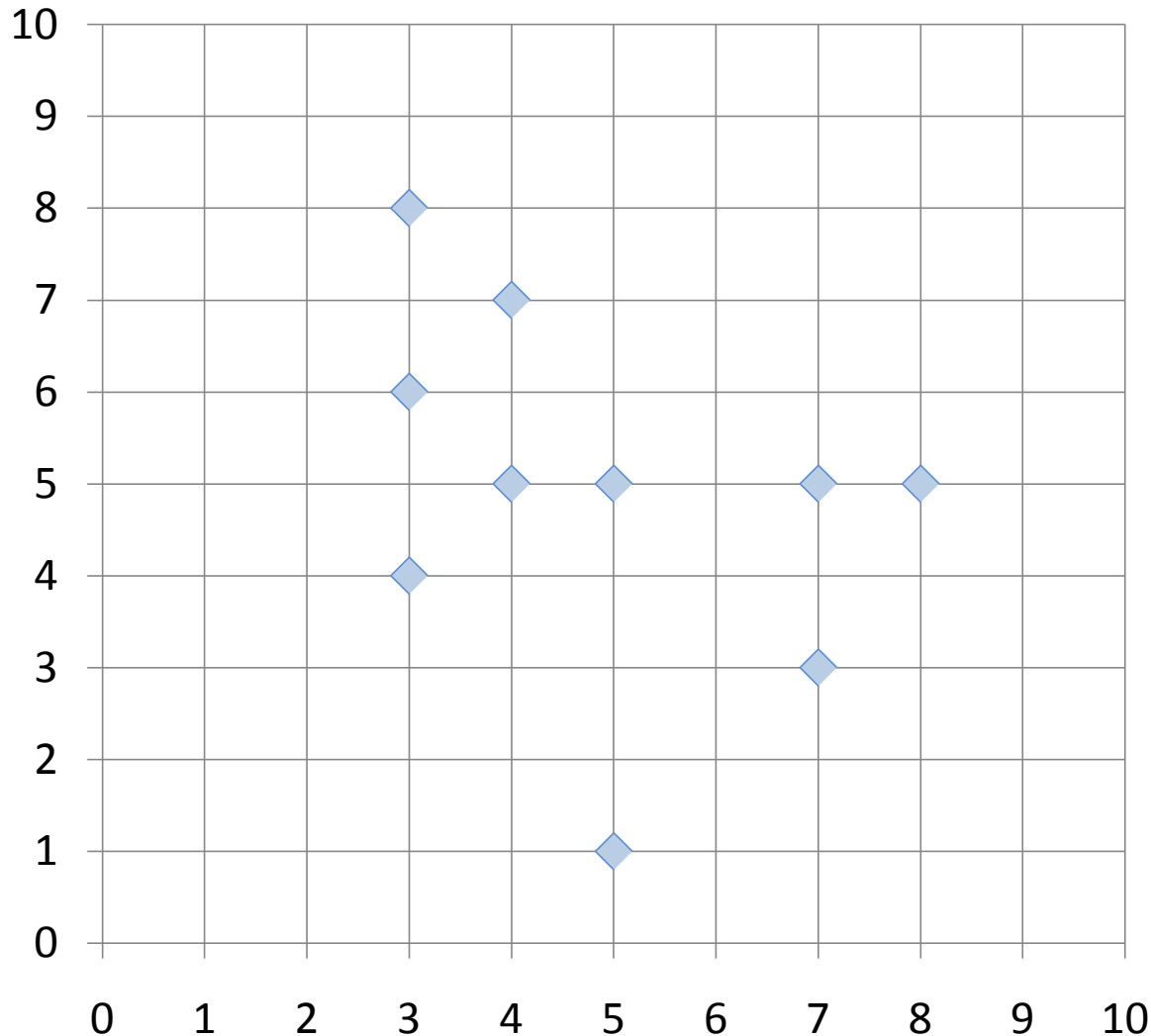


Clustering of a set of objects based on the *k-means method*.  
(The mean of each cluster is marked by a “+”.)

# Cluster Analysis

- Clustering results may be used to
  - Identify natural groupings of customers
  - Identify rules for assigning new cases to classes for targeting/diagnostic purposes
  - Provide characterization, definition, labeling of populations
  - Decrease the size and complexity of problems for other data mining methods
  - Identify outliers in a specific domain (e.g., rare-event detection)

# Example of Cluster Analysis



Point	P	P(x,y)
p01	a	(3, 4)
p02	b	(3, 6)
p03	c	(3, 8)
p04	d	(4, 5)
p05	e	(4, 7)
p06	f	(5, 1)
p07	g	(5, 5)
p08	h	(7, 3)
p09	i	(7, 5)
p10	j	(8, 5)

# Cluster Analysis for Data Mining

- Analysis methods
  - Statistical methods  
(including both hierarchical and nonhierarchical),  
such as *k*-means, *k*-modes, and so on
  - Neural networks  
(adaptive resonance theory [ART],  
self-organizing map [SOM])
  - Fuzzy logic (e.g., fuzzy c-means algorithm)
  - Genetic algorithms
- Divisive versus Agglomerative methods

# Cluster Analysis for Data Mining

- **How many clusters?**
  - There is not a “truly optimal” way to calculate it
  - Heuristics are often used
    1. Look at the sparseness of clusters
    2. **Number of clusters =  $(n/2)^{1/2}$**  (n: no of data points)
    3. Use Akaike information criterion (AIC)
    4. Use Bayesian information criterion (BIC)
- Most cluster analysis methods involve the use of a **distance measure** to calculate the closeness between pairs of items
  - **Euclidian** versus **Manhattan** (rectilinear) **distance**

# Outline

- Unsupervised Learning
  - Clustering
- Cluster Analysis
- **k-Means Clustering Algorithm**
- Similarity and Distance Functions
- Cluster Evaluation

# ***k*-Means Clustering Algorithm**

- $k$  : pre-determined number of clusters
- Algorithm (**Step 0**: determine value of  $k$ )

**Step 1**: Randomly generate  $k$  random points as initial cluster centers

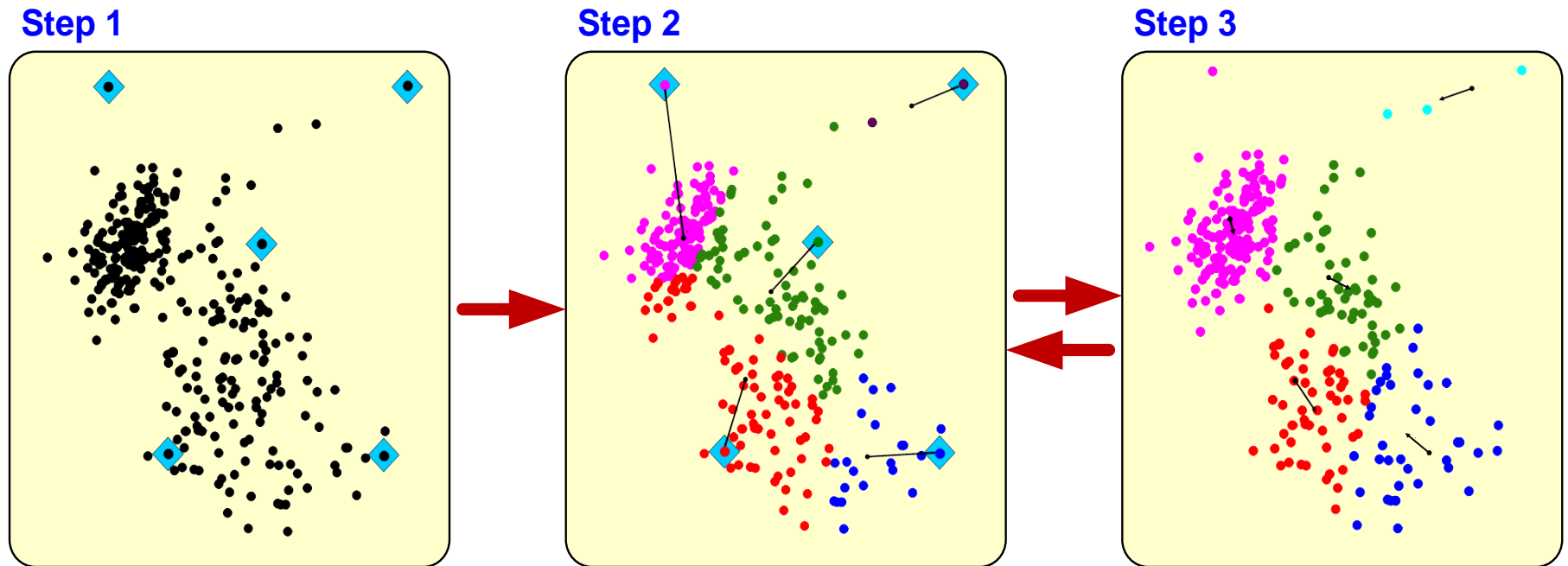
**Step 2**: Assign each point to the nearest cluster center

**Step 3**: Re-compute the new cluster centers

**Repetition step**: Repeat steps 2 and 3 until some convergence criterion is met (usually that the assignment of points to clusters becomes stable)



# Cluster Analysis for Data Mining - *k*-Means Clustering Algorithm



# Similarity and Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
- Some popular ones include: *Minkowski distance*:

$$d(i, j) = \sqrt[q]{(|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \dots + |x_{ip} - x_{jp}|^q)}$$

where  $i = (x_{i1}, x_{i2}, \dots, x_{ip})$  and  $j = (x_{j1}, x_{j2}, \dots, x_{jp})$  are two  $p$ -dimensional data objects, and  $q$  is a positive integer

- If  $q = 1$ ,  $d$  is **Manhattan distance**

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

# Similarity and Dissimilarity Between Objects (Cont.)

- If  $q = 2$ ,  $d$  is **Euclidean distance**:

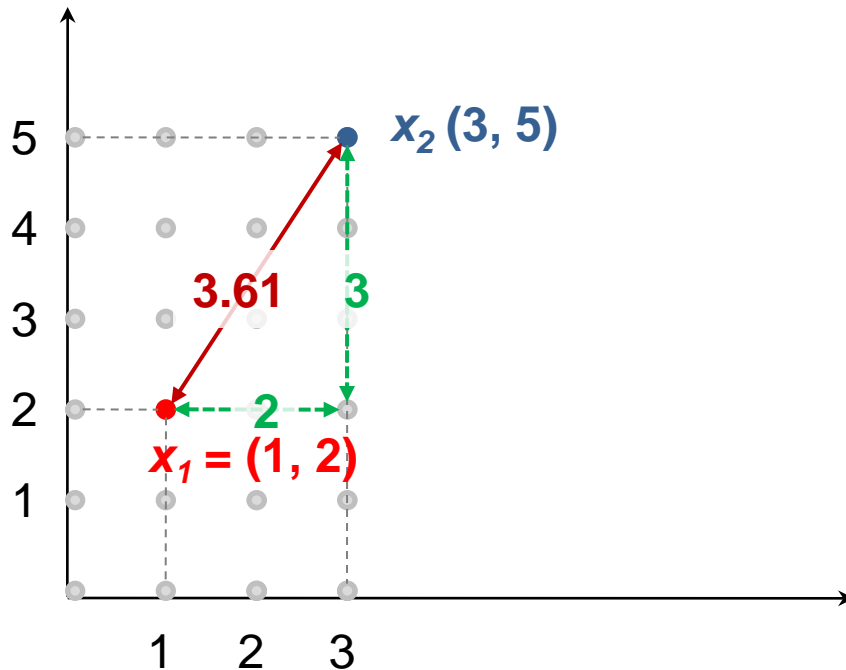
$$d(i, j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + \dots + |x_{i_p} - x_{j_p}|^2)}$$

– Properties

- $d(i, j) \geq 0$
  - $d(i, i) = 0$
  - $d(i, j) = d(j, i)$
  - $d(i, j) \leq d(i, k) + d(k, j)$
- Also, one can use weighted distance, parametric Pearson product moment correlation, or other dissimilarity measures

# Euclidean distance vs Manhattan distance

- Distance of two point  $x_1 = (1, 2)$  and  $x_2 (3, 5)$



Euclidean distance:

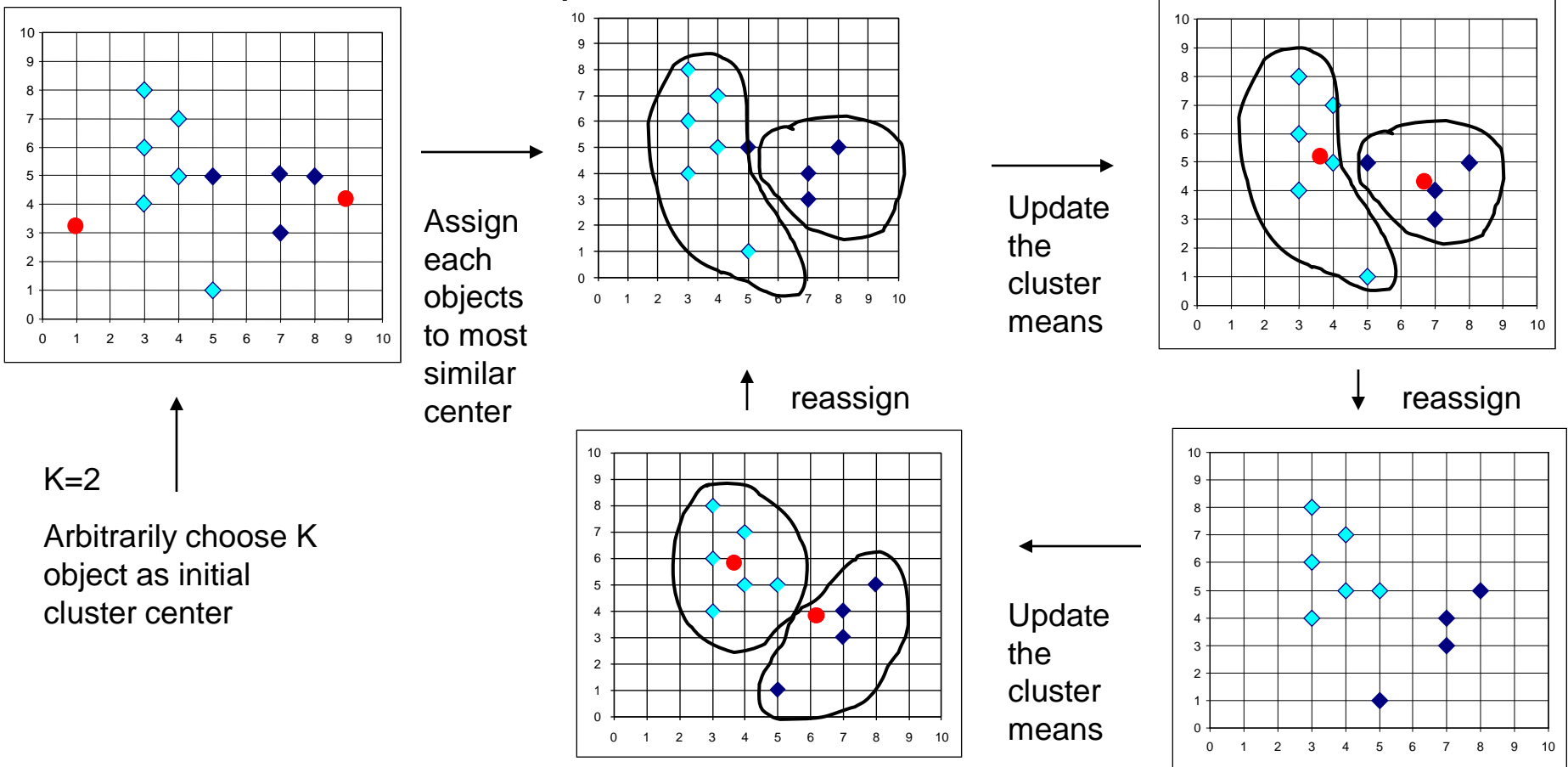
$$\begin{aligned} &= ((3-1)^2 + (5-2)^2)^{1/2} \\ &= (2^2 + 3^2)^{1/2} \\ &= (4 + 9)^{1/2} \\ &= (13)^{1/2} \\ &= 3.61 \end{aligned}$$

Manhattan distance:

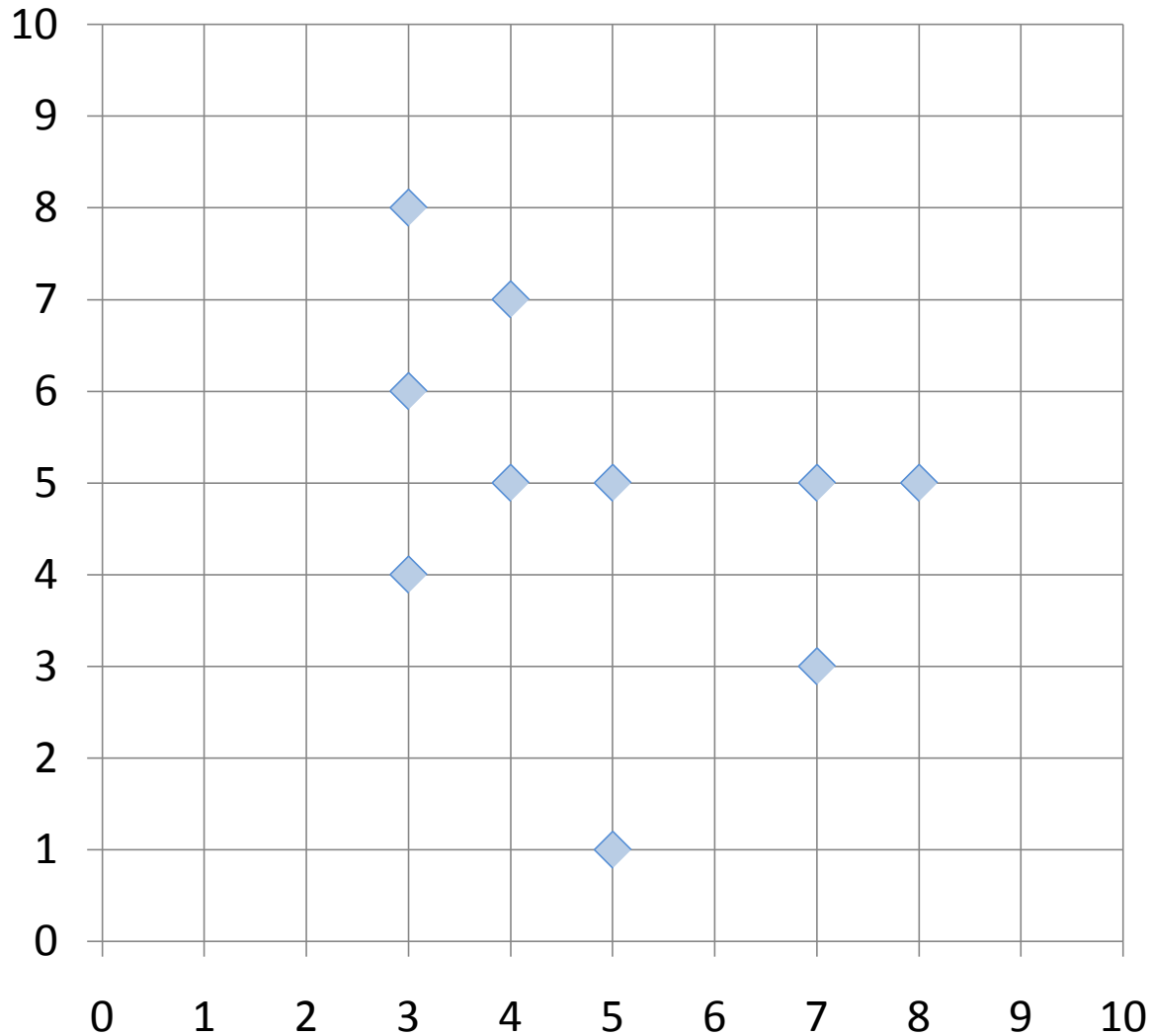
$$\begin{aligned} &= (3-1) + (5-2) \\ &= 2 + 3 \\ &= 5 \end{aligned}$$

# The *K-Means* Clustering Method

- Example



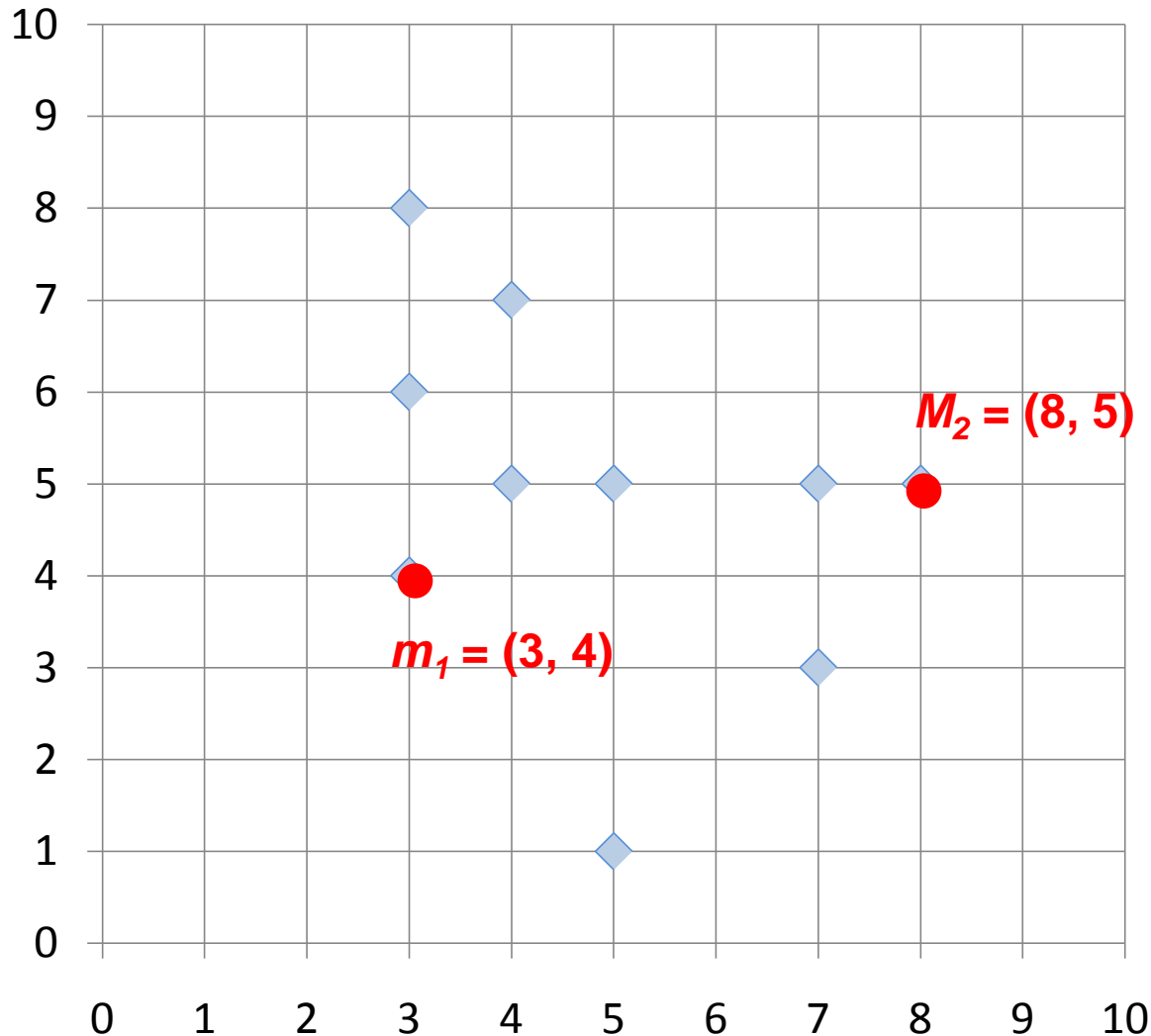
# *K-Means* Clustering Step by Step



Point	P	P(x,y)
p01	a	(3, 4)
p02	b	(3, 6)
p03	c	(3, 8)
p04	d	(4, 5)
p05	e	(4, 7)
p06	f	(5, 1)
p07	g	(5, 5)
p08	h	(7, 3)
p09	i	(7, 5)
p10	j	(8, 5)

# K-Means Clustering

Step 1: K=2, Arbitrarily choose K object as initial cluster center

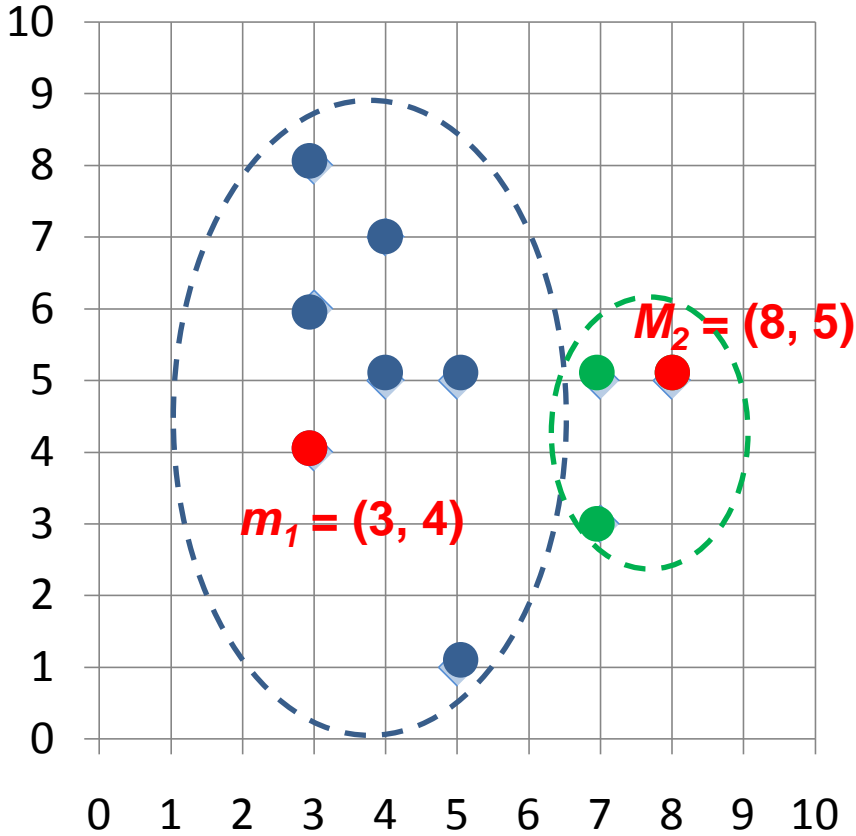


Point	P	P(x,y)
p01	a	(3, 4)
p02	b	(3, 6)
p03	c	(3, 8)
p04	d	(4, 5)
p05	e	(4, 7)
p06	f	(5, 1)
p07	g	(5, 5)
p08	h	(7, 3)
p09	i	(7, 5)
p10	j	(8, 5)

Initial  $m_1$  (3, 4)  
Initial  $m_2$  (8, 5)

**Step 2: Compute seed points as the centroids of the clusters of the current partition**

**Step 3: Assign each objects to most similar center**



Point	P	P(x,y)	m1 distance	m2 distance	Cluster
p01	a	(3, 4)	0.00	5.10	Cluster1
p02	b	(3, 6)	2.00	5.10	Cluster1
p03	c	(3, 8)	4.00	5.83	Cluster1
p04	d	(4, 5)	1.41	4.00	Cluster1
p05	e	(4, 7)	3.16	4.47	Cluster1
p06	f	(5, 1)	3.61	5.00	Cluster1
p07	g	(5, 5)	2.24	3.00	Cluster1
p08	h	(7, 3)	4.12	2.24	Cluster2
p09	i	(7, 5)	4.12	1.00	Cluster2
p10	j	(8, 5)	5.10	0.00	Cluster2

# K-Means Clustering

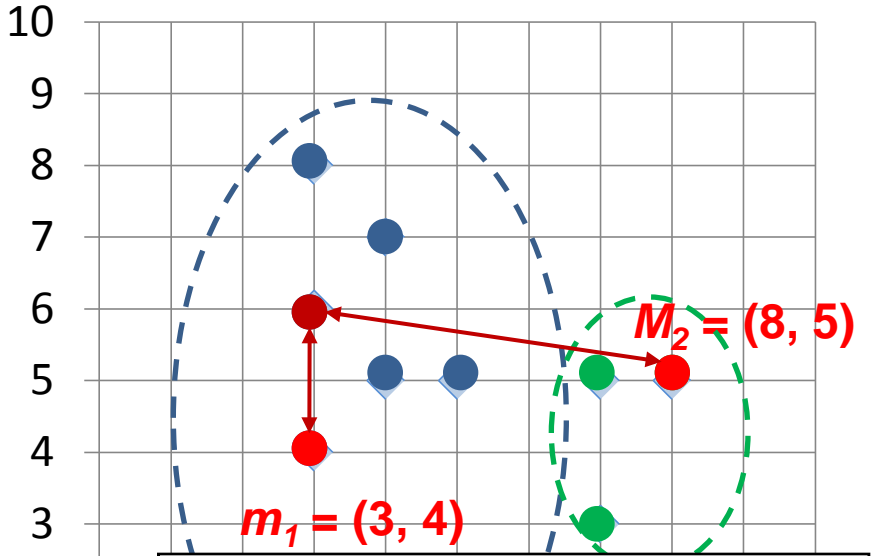
Initial m1 (3, 4)

Initial m2 (8, 5)



**Step 2: Compute seed points as the centroids of the clusters of the current partition**

**Step 3: Assign each objects to most similar center**



Point	P	P(x,y)	m1 distance	m2 distance	Cluster
p01	a	(3, 4)	0.00	5.10	Cluster1
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p03	c	(3, 8)	4.00	5.83	Cluster1
p04	d	(4, 5)	1.41	4.00	Cluster1

**K-1**

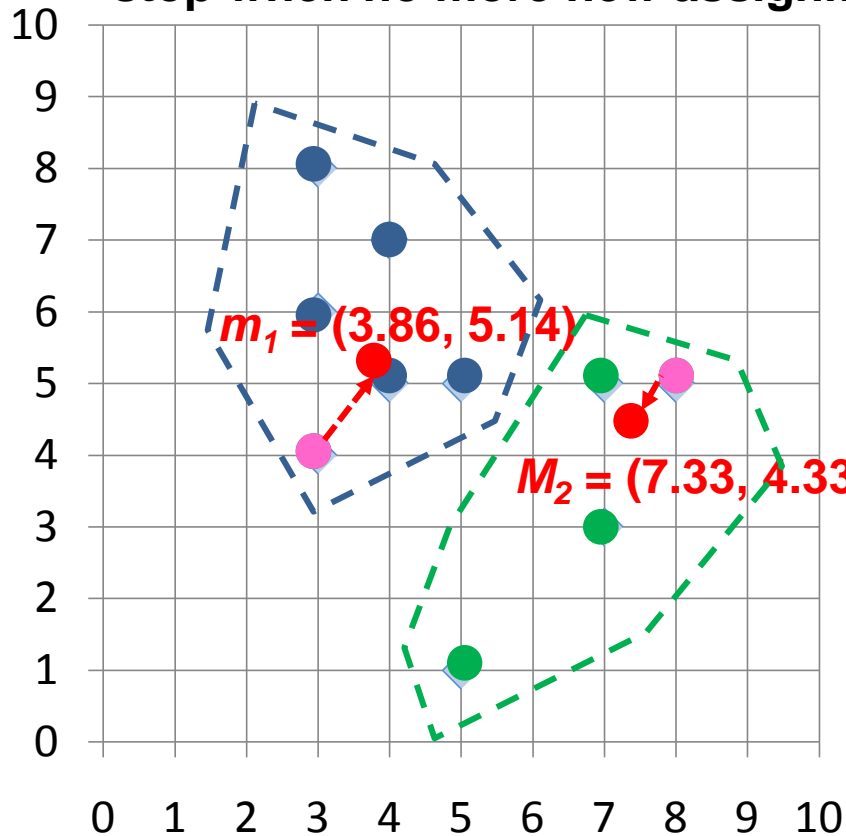
Euclidean distance  
 $b(3,6) \leftrightarrow m1(3,4)$   
 $= ((3-3)^2 + (4-6)^2)^{1/2}$   
 $= (0^2 + (-2)^2)^{1/2}$   
 $= (0 + 4)^{1/2}$   
 $= (4)^{1/2}$   
 $= 2.00$

Euclidean distance  
 $b(3,6) \leftrightarrow m2(8,5)$   
 $= ((8-3)^2 + (5-6)^2)^{1/2}$   
 $= (5^2 + (-1)^2)^{1/2}$   
 $= (25 + 1)^{1/2}$   
 $= (26)^{1/2}$   
 $= 5.10$

Initial m1 (3, 4)

Initial m2 (8, 5)

**Step 4: Update the cluster means,  
Repeat Step 2, 3,  
stop when no more new assignment**



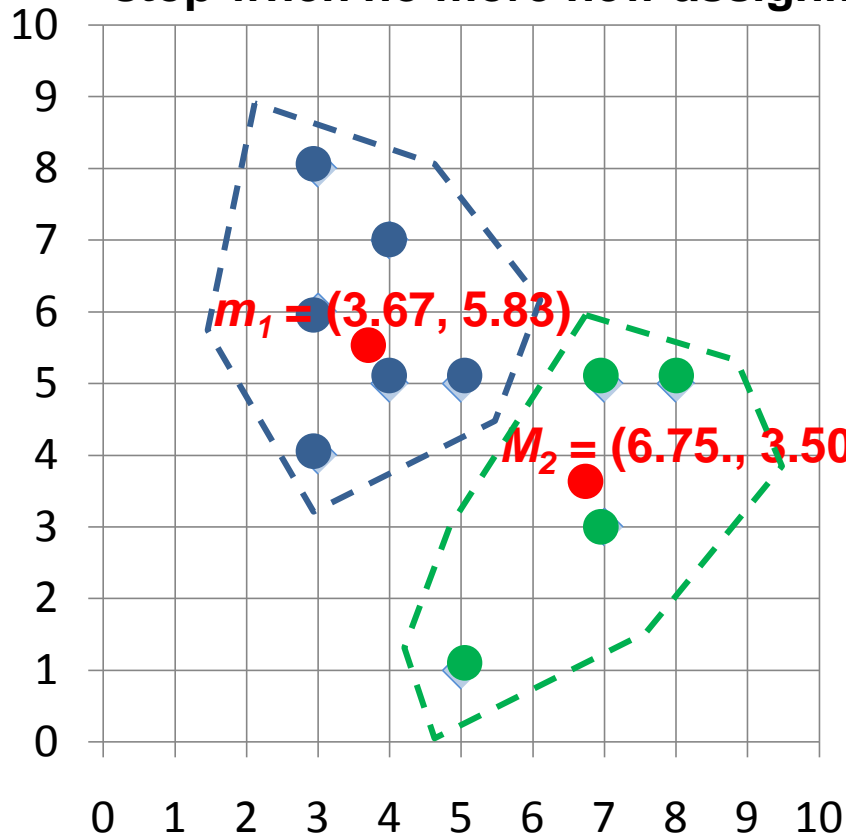
Point	P	P(x,y)	m1 distance	m2 distance	Cluster
p01	a	(3, 4)	1.43	4.34	Cluster1
p02	b	(3, 6)	1.22	4.64	Cluster1
p03	c	(3, 8)	2.99	5.68	Cluster1
p04	d	(4, 5)	0.20	3.40	Cluster1
p05	e	(4, 7)	1.87	4.27	Cluster1
p06	f	(5, 1)	4.29	4.06	Cluster2
p07	g	(5, 5)	1.15	2.42	Cluster1
p08	h	(7, 3)	3.80	1.37	Cluster2
p09	i	(7, 5)	3.14	0.75	Cluster2
p10	j	(8, 5)	4.14	0.95	Cluster2

m1 (3.86, 5.14)

m2 (7.33, 4.33)

## ***K-Means* Clustering**

**Step 4: Update the cluster means,  
Repeat Step 2, 3,  
stop when no more new assignment**



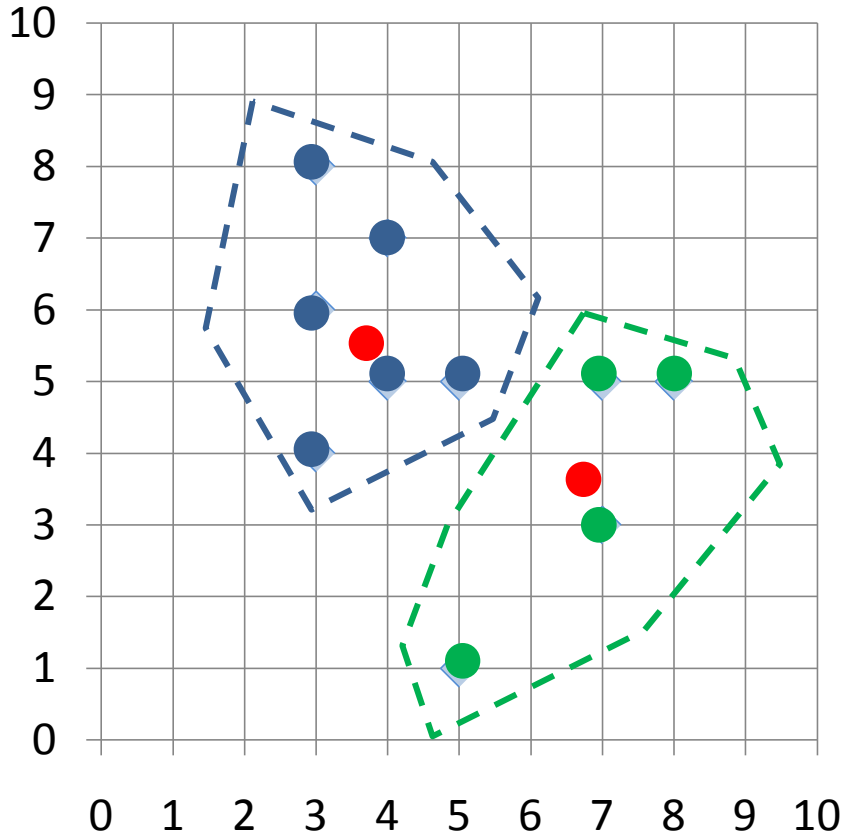
Point	P	P(x,y)	m1 distance	m2 distance	Cluster
p01	a	(3, 4)	1.95	3.78	Cluster1
p02	b	(3, 6)	0.69	4.51	Cluster1
p03	c	(3, 8)	2.27	5.86	Cluster1
p04	d	(4, 5)	0.89	3.13	Cluster1
p05	e	(4, 7)	1.22	4.45	Cluster1
p06	f	(5, 1)	5.01	3.05	Cluster2
p07	g	(5, 5)	1.57	2.30	Cluster1
p08	h	(7, 3)	4.37	0.56	Cluster2
p09	i	(7, 5)	3.43	1.52	Cluster2
p10	j	(8, 5)	4.41	1.95	Cluster2

$m_1$  (3.67, 5.83)

$m_2$  (6.75, 3.50)

## ***K-Means* Clustering**

**stop when no more new assignment**



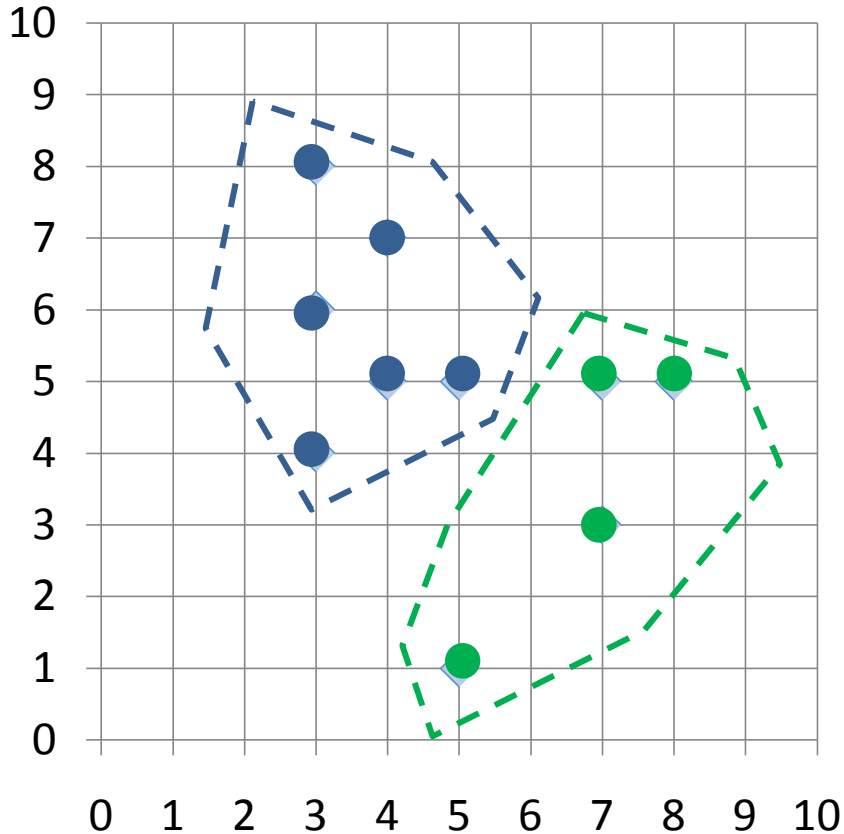
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p09	i	(7, 5)	3.43	1.52	Cluster2
p10	j	(8, 5)	4.41	1.95	Cluster2

m1 (3.67, 5.83)

m2 (6.75, 3.50)

# K-Means Clustering

**stop when no more new assignment**



Point	P	P(x,y)	m1 distance	m2 distance	Cluster
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p08	h	(7, 3)	4.37	0.56	Cluster2
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p10	j	(8, 5)	4.41	1.95	Cluster2

m1 (3.67, 5.83)

m2 (6.75, 3.50)

# K-Means Clustering

# Outline

- Unsupervised Learning
  - Clustering
- Cluster Analysis
- k-Means Clustering Algorithm
- Similarity and Distance Functions
- Cluster Evaluation

# Distance functions

- Key to clustering. “similarity” and “dissimilarity” can also commonly used terms.
- There are numerous distance functions for
  - Different types of data
    - Numeric data
    - Nominal data
  - Different specific applications

# Distance functions for numeric attributes

- Most commonly used functions are
  - Euclidean distance and
  - Manhattan (city block) distance
- We denote distance with:  $dist(\mathbf{x}_i, \mathbf{x}_j)$ , where  $\mathbf{x}_i$  and  $\mathbf{x}_j$  are data points (vectors)
- They are special cases of **Minkowski distance**.  
h is positive integer.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \left( (x_{i1} - x_{j1})^h + (x_{i2} - x_{j2})^h + \dots + (x_{ir} - x_{jr})^h \right)^{\frac{1}{h}}$$



# Euclidean distance and Manhattan distance

- If  $h = 2$ , it is the **Euclidean distance**

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ir} - x_{jr})^2}$$

- If  $h = 1$ , it is the **Manhattan distance**

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ir} - x_{jr}|$$

- **Weighted Euclidean distance**

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{w_1(x_{i1} - x_{j1})^2 + w_2(x_{i2} - x_{j2})^2 + \dots + w_r(x_{ir} - x_{jr})^2}$$

# Squared distance and Chebychev distance

- **Squared Euclidean distance**: to place progressively greater weight on data points that are further apart.

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ir} - x_{jr})^2$$

- **Chebychev distance**: one wants to define two data points as "different" if they are different on any one of the attributes.

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = \max(|x_{i1} - x_{j1}|, |x_{i2} - x_{j2}|, \dots, |x_{ir} - x_{jr}|)$$

# Distance functions for binary and nominal attributes

- **Binary attribute**: has two values or states but no ordering relationships, e.g.,
  - Gender: male and female.
- We use a confusion matrix to introduce the distance functions/measures.
- Let the  $i$ th and  $j$ th data points be  $\mathbf{x}_i$  and  $\mathbf{x}_j$  (vectors)

# Confusion matrix

		Data point $j$		
		1	0	
Data point $i$	1	$a$	$b$	$a+b$
	0	$c$	$d$	$c+d$
		$a+c$	$b+d$	$a+b+c+d$

(10)

- $a$ : the number of attributes with the value of 1 for both data points.
- $b$ : the number of attributes for which  $x_{if} = 1$  and  $x_{jf} = 0$ , where  $x_{if}$  ( $x_{jf}$ ) is the value of the  $f$ th attribute of the data point  $\mathbf{x}_i$  ( $\mathbf{x}_j$ ).
- $c$ : the number of attributes for which  $x_{if} = 0$  and  $x_{jf} = 1$ .
- $d$ : the number of attributes with the value of 0 for both data points.

# Symmetric binary attributes

- A binary attribute is **symmetric** if both of its states (0 and 1) have equal importance, and carry the same weights, e.g., male and female of the attribute Gender
- Distance function: **Simple Matching Coefficient**, proportion of mismatches of their values

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = \frac{b + c}{a + b + c + d}$$

# Symmetric binary attributes: example

$\mathbf{x}_1$	1	1	1	0	1	0	0
$\mathbf{x}_2$	0	1	1	0	0	1	0

$$\text{dist}(\mathbf{x}_1, \mathbf{x}_2) = \frac{2+1}{2+2+1+2} = \frac{3}{7} = 0.429$$

# Asymmetric binary attributes

- **Asymmetric**: if one of the states is more important or more valuable than the other.
  - By convention, state 1 represents the more important state, which is typically the rare or infrequent state.

- **Jaccard coefficient** is a popular measure

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{b + c}{a + b + c}$$

- We can have some variations, adding weights

# Nominal attributes

- **Nominal attributes**: with more than two states or values.
  - the commonly used distance measure is also based on the **simple matching method**.
  - Given two data points  $\mathbf{x}_i$  and  $\mathbf{x}_j$ , let the number of attributes be  $r$ , and the number of values that match in  $\mathbf{x}_i$  and  $\mathbf{x}_j$  be  $q$ .

$$\text{dist}(\mathbf{x}_i, \mathbf{x}_j) = \frac{r - q}{r}$$



# Distance function for text documents

- A text document consists of a sequence of sentences and each sentence consists of a sequence of words.
- To simplify: a document is usually considered a “bag” of words in document clustering.
  - Sequence and position of words are ignored.
- A document is represented with a vector just like a normal data point.
- It is common to use similarity to compare two documents rather than distance.
  - The most commonly used similarity function is the **cosine similarity**.

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# Cluster Evaluation: hard problem

- The quality of a clustering is very hard to evaluate because
  - We do not know the correct clusters
- Some methods are used:
  - User inspection
    - Study centroids, and spreads
    - Rules from a decision tree.
    - For text documents, one can read some documents in clusters.

# Cluster evaluation: ground truth

- We use some labeled data (for classification)
- **Assumption**: Each class is a cluster.
- After clustering, a confusion matrix is constructed. From the matrix, we compute various measurements, entropy, purity, precision, recall and F-score.
  - Let the classes in the data  $D$  be  $C = (c_1, c_2, \dots, c_k)$ . The clustering method produces  $k$  clusters, which divides  $D$  into  $k$  disjoint subsets,  $D_1, D_2, \dots, D_k$ .

# Evaluation measures: Entropy

**Entropy:** For each cluster, we can measure its entropy as follows:

$$\text{entropy}(D_i) = -\sum_{j=1}^k \text{Pr}_i(c_j) \log_2 \text{Pr}_i(c_j), \quad (29)$$

where  $\text{Pr}_i(c_j)$  is the proportion of class  $c_j$  data points in cluster  $i$  or  $D_i$ . The total entropy of the whole clustering (which considers all clusters) is

$$\text{entropy}_{total}(D) = \sum_{i=1}^k \frac{|D_i|}{|D|} \times \text{entropy}(D_i) \quad (30)$$

# Evaluation measures: purity

**Purity:** This again measures the extent that a cluster contains only one class of data. The purity of each cluster is computed with

$$purity(D_i) = \max_j (\Pr_i(c_j)) \quad (31)$$

The total purity of the whole clustering (considering all clusters) is

$$purity_{total}(D) = \sum_{i=1}^k \frac{|D_i|}{|D|} \times purity(D_i) \quad (32)$$

# An example

**Example 14:** Assume we have a text collection  $D$  of 900 documents from three topics (or three classes), Science, Sports, and Politics. Each class has 300 documents. Each document in  $D$  is labeled with one of the topics (classes). We use this collection to perform clustering to find three clusters. Note that class/topic labels are not used in clustering. After clustering, we want to measure the effectiveness of the clustering algorithm.

Cluster	Science	Sports	Politics		Entropy	Purity
1	250	20	10		0.589	0.893
2	20	180	80		1.198	0.643
3	30	100	210		1.257	0.617
Total	300	300	300		1.031	0.711

# A remark about ground truth evaluation

- Commonly used to compare different clustering algorithms.
- A real-life data set for clustering has no class labels.
  - Thus although an algorithm may perform very well on some labeled data sets, no guarantee that it will perform well on the actual application data at hand.
- The fact that it performs well on some label data sets does give us some confidence of the quality of the algorithm.
- This evaluation method is said to be based on **external data** or information.



# Evaluation based on internal information

- **Intra-cluster cohesion (compactness):**
  - Cohesion measures how near the data points in a cluster are to the cluster centroid.
  - Sum of squared error (SSE) is a commonly used measure.
- **Inter-cluster separation (isolation):**
  - Separation means that different cluster centroids should be far away from one another.
- In most applications, expert judgments are still the key.

# Indirect evaluation

- In some applications, clustering is **not the primary task**, but used to help perform another task.
- We can use the performance on the primary task to compare clustering methods.
- For instance, in an application, the primary task is to provide recommendations on book purchasing to online shoppers.
  - If we can cluster books according to their features, we might be able to provide better recommendations.
  - We can evaluate different clustering algorithms based on how well they help with the recommendation task.
  - Here, we assume that the recommendation can be reliably evaluated.

# Summary

- Unsupervised Learning
  - Clustering
- Cluster Analysis
- k-Means Clustering Algorithm
- Similarity and Distance Functions
- Cluster Evaluation

# References

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