Tamkang University

Data Mining
資料探勘

分群分析
(Cluster Analysis)

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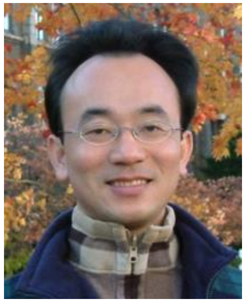
Wed, 7,8 (14:10-16:00) (B130)



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2015-03-18

課程大綱 (Syllabus)

週次 (Week)	日期 (Date)	內容 (Subject/Topics)
1	2015/02/25	資料探勘導論 (Introduction to Data Mining)
2	2015/03/04	關連分析 (Association Analysis)
3	2015/03/11	分類與預測 (Classification and Prediction)
4	2015/03/18	分群分析 (Cluster Analysis)
5	2015/03/25	個案分析與實作一 (SAS EM 分群分析)： Case Study 1 (Cluster Analysis – K-Means using SAS EM)
6	2015/04/01	教學行政觀摩日 (Off-campus study)
7	2015/04/08	個案分析與實作二 (SAS EM 關連分析)： Case Study 2 (Association Analysis using SAS EM)
8	2015/04/15	個案分析與實作三 (SAS EM 決策樹、模型評估)： Case Study 3 (Decision Tree, Model Evaluation using SAS EM)

課程大綱 (Syllabus)

週次 (Week)	日期 (Date)	內容 (Subject/Topics)
9	2015/04/22	期中報告 (Midterm Project Presentation)
10	2015/04/29	期中考試週 (Midterm Exam)
11	2015/05/06	個案分析與實作四 (SAS EM 迴歸分析、類神經網路)：Case Study 4 (Regression Analysis, Artificial Neural Network using SAS EM)
12	2015/05/13	海量資料分析 (Big Data Analytics)
13	2015/05/20	文字探勘與網頁探勘 (Text and Web Mining)
14	2015/05/27	期末報告 (Final Project Presentation)
15	2015/06/03	畢業考試週 (Final Exam)

A Taxonomy for Data Mining Tasks

Data Mining	Learning Method	Popular Algorithms
Prediction	Supervised	Classification and Regression Trees, ANN, SVM, Genetic Algorithms
Classification	Supervised	Decision trees, ANN/MLP, SVM, Rough sets, Genetic Algorithms
Regression	Supervised	Linear/Nonlinear Regression, Regression trees, ANN/MLP, SVM
Association	Unsupervised	Apriory, OneR, ZeroR, Eclat
Link analysis	Unsupervised	Expectation Maximization, Apriory Algorithm, Graph-based Matching
Sequence analysis	Unsupervised	Apriory Algorithm, FP-Growth technique
Clustering	Unsupervised	K-means, ANN/SOM
Outlier analysis	Unsupervised	K-means, Expectation Maximization (EM)

Source: Turban et al. (2011), Decision Support and Business Intelligence Systems

Outline

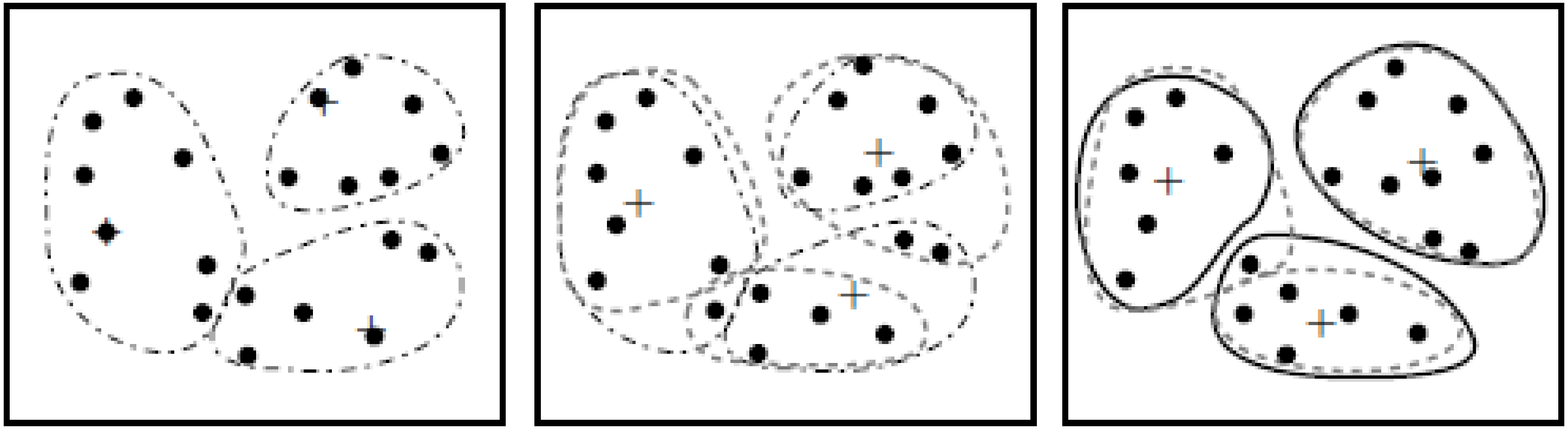
- Cluster Analysis
- *K-Means* Clustering

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

Source: Turban et al. (2011), Decision Support and Business Intelligence Systems

Cluster Analysis



(a) (b) (c)

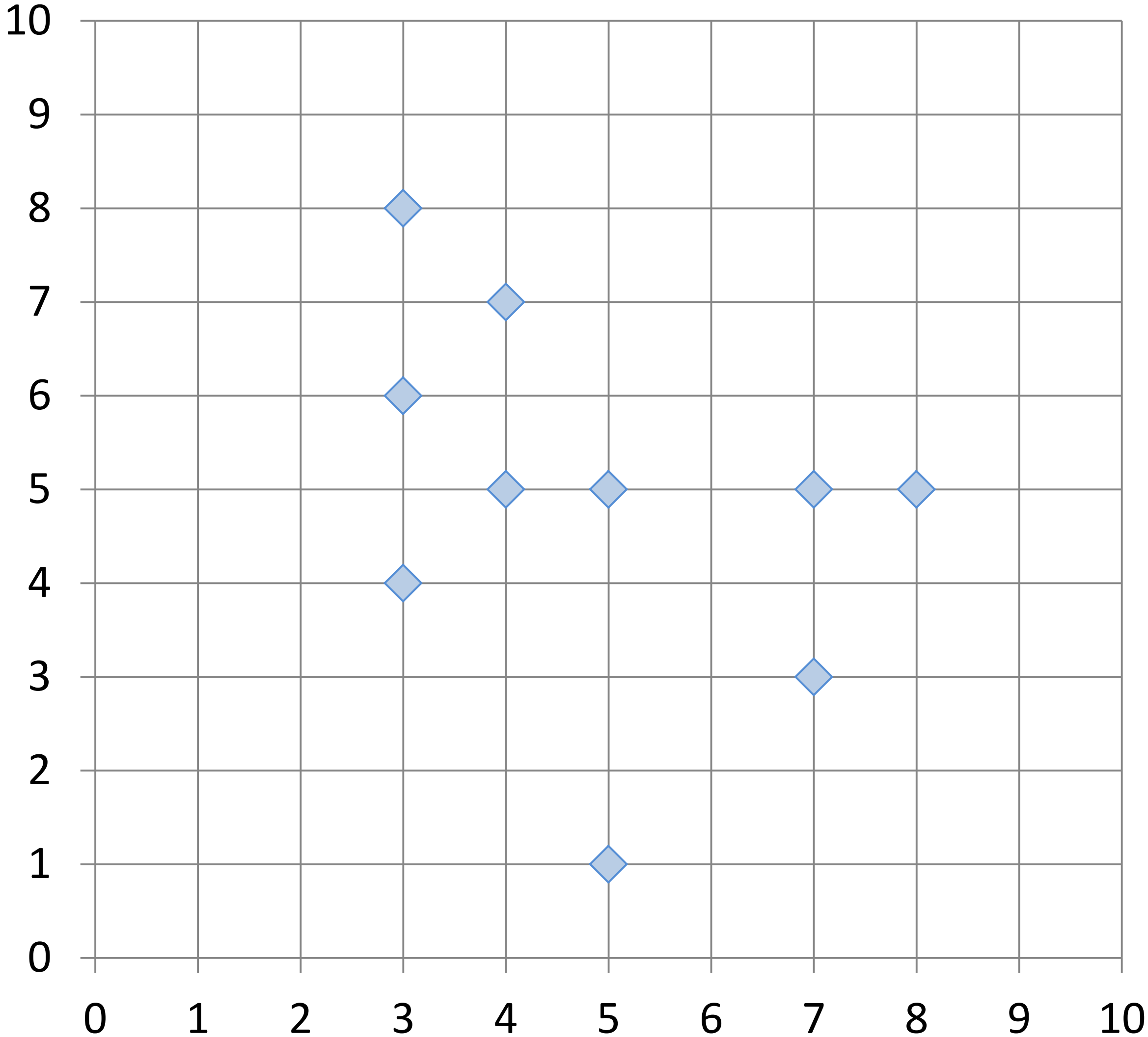
Clustering of a set of objects based on the *k-means method.*
(The mean of each cluster is marked by a "+".)

Source: Han & Kamber (2006)

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



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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

Source: Turban et al. (2011), Decision Support and Business Intelligence Systems

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

Source: Turban et al. (2011), Decision Support and Business Intelligence Systems

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

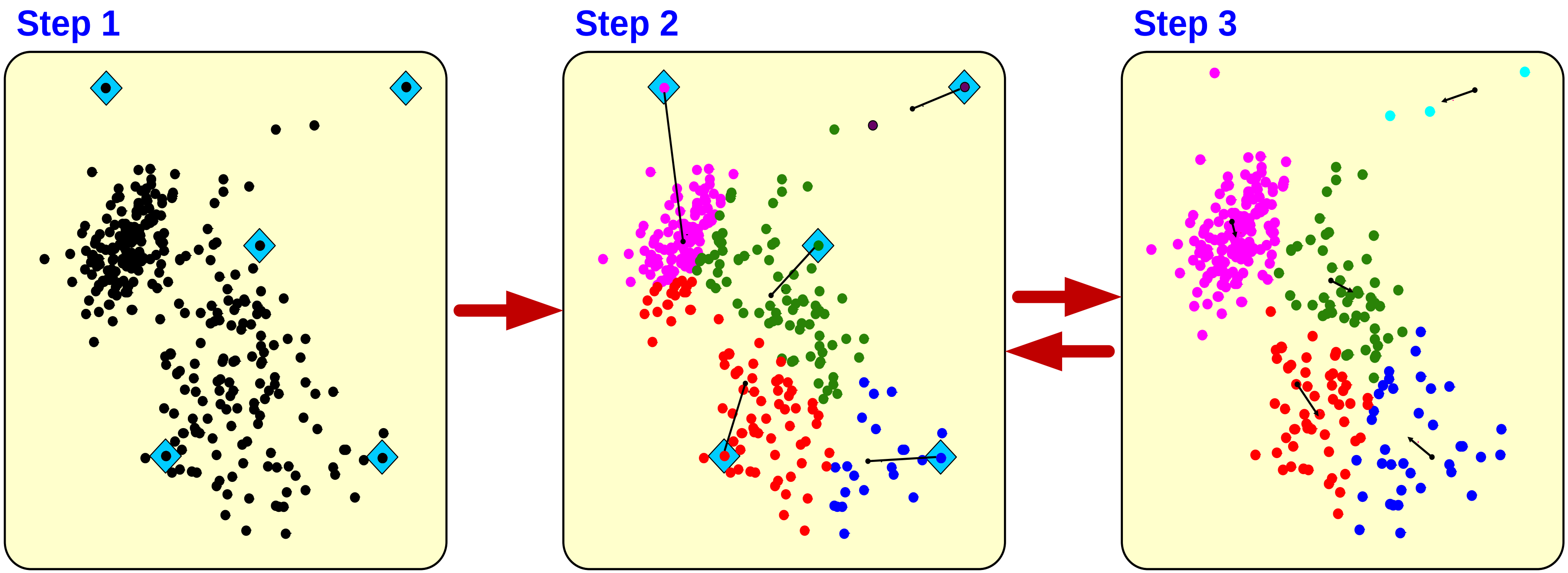
Step 2: Assign each point to the nearest cluster center

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)

Source: Turban et al. (2011), Decision Support and Business Intelligence Systems

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*:

$$d(i,j) = \sqrt[q]{(|x_{i_1} - x_{j_1}|^q + |x_{i_2} - x_{j_2}|^q + \ldots + |x_{i_p} - x_{j_p}|^q)}$$

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

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

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

Source: Han & Kamber (2006)

Similarity and Dissimilarity Between Objects (Cont.)

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

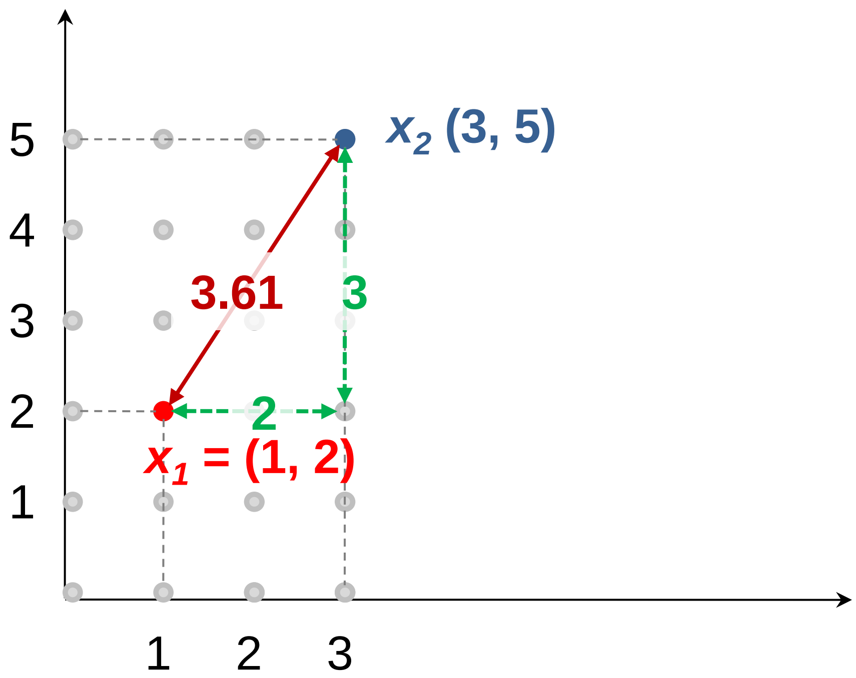
$$d(i,j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + \ldots + |x_{i_p} - x_{j_p}|^2)}$$

  - 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 disimilarity measures

Source: Han & Kamber (2006)

Euclidean distance vs Manhattan distance

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

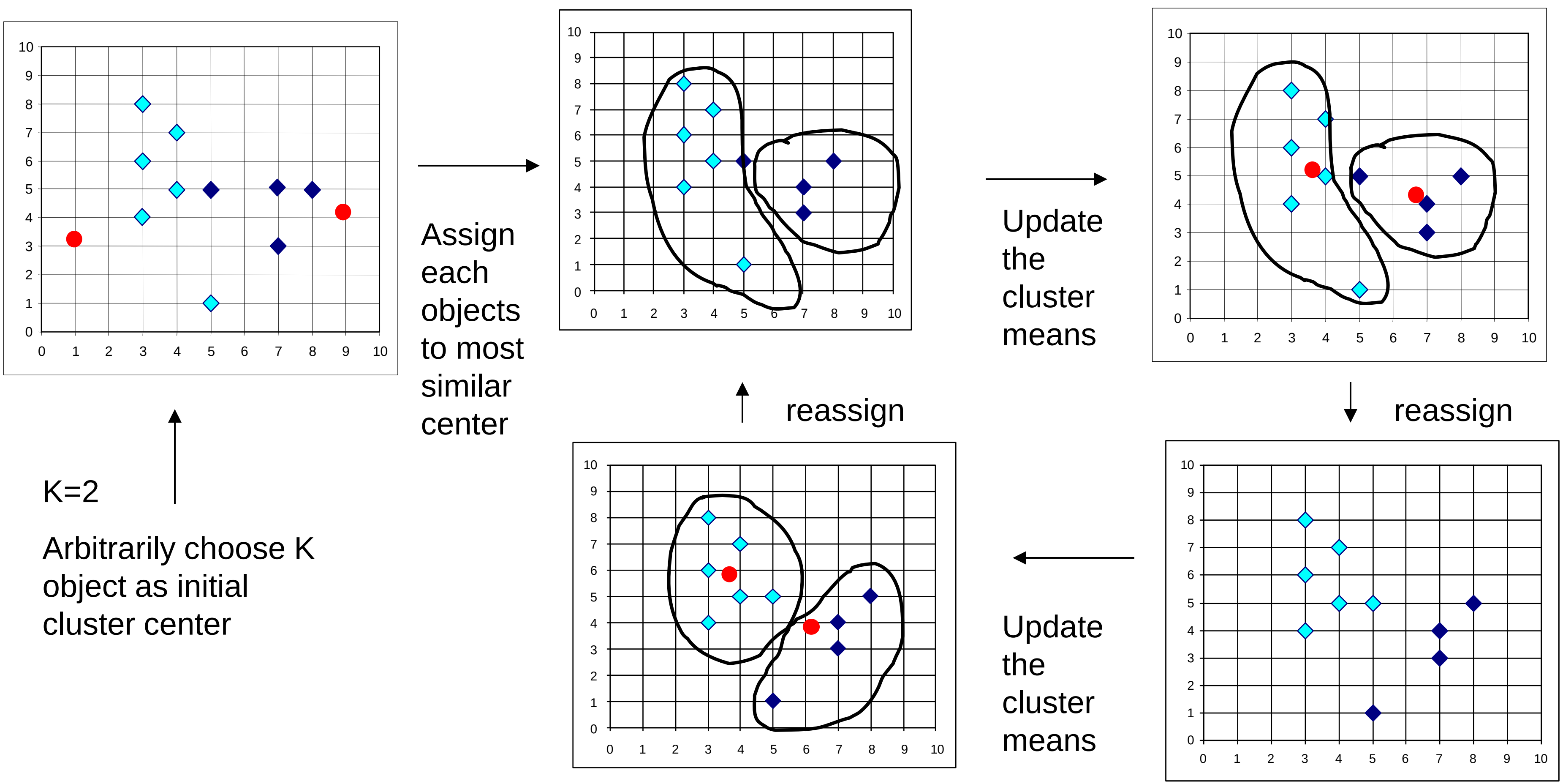


Euclidean distance:
$= ((3-1)^2 + (5-2)^2)^{1/2}$
$= (2^2 + 3^2)^{1/2}$
$= (4 + 9)^{1/2}$
$= (13)^{1/2}$
$= 3.61$

Manhattan distance:
$= (3-1) + (5-2)$
$= 2 + 3$
$= 5$

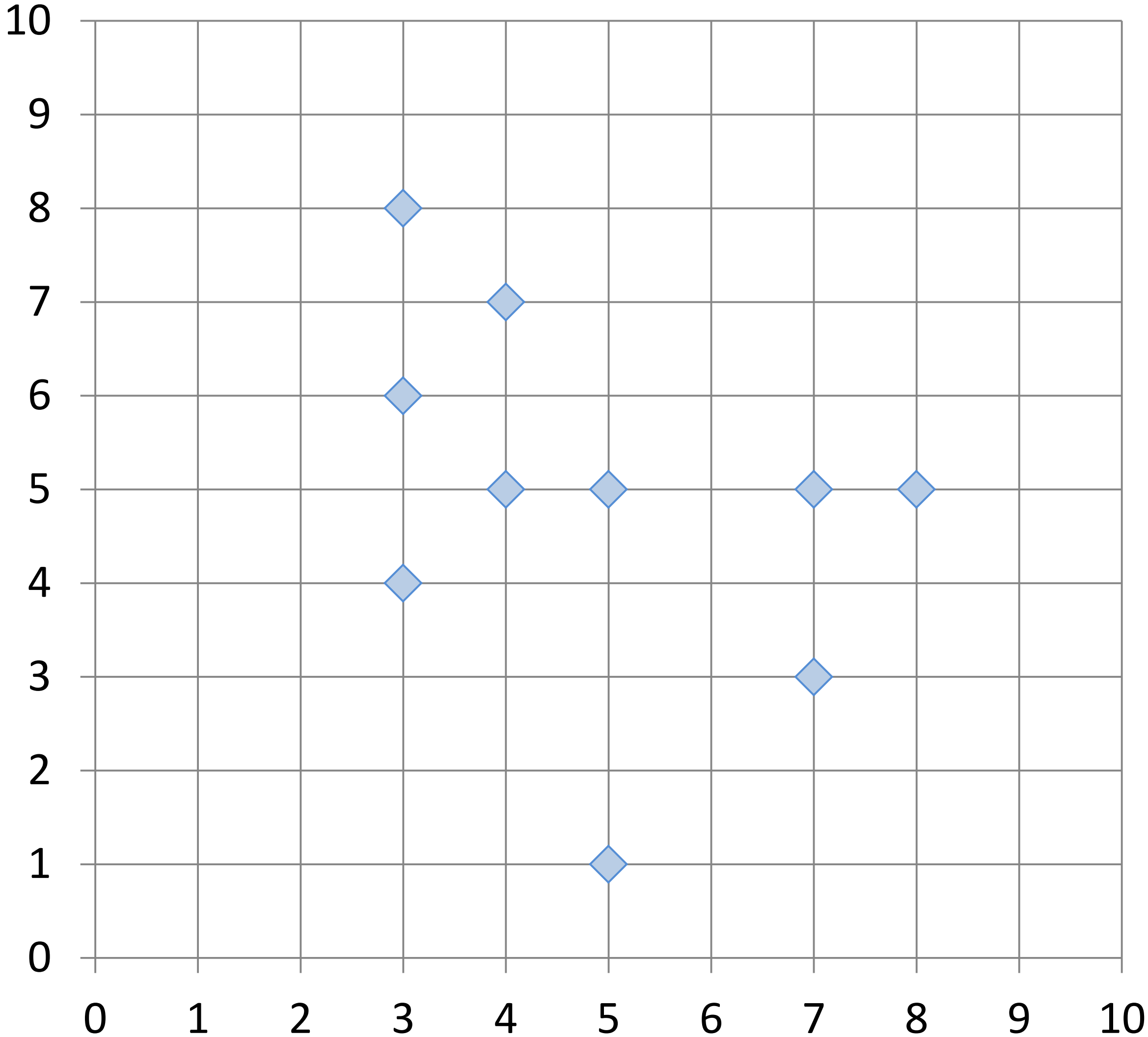
The *K-Means* Clustering Method

- Example



Source: Han & Kamber (2006)

K-Means Clustering Step by Step



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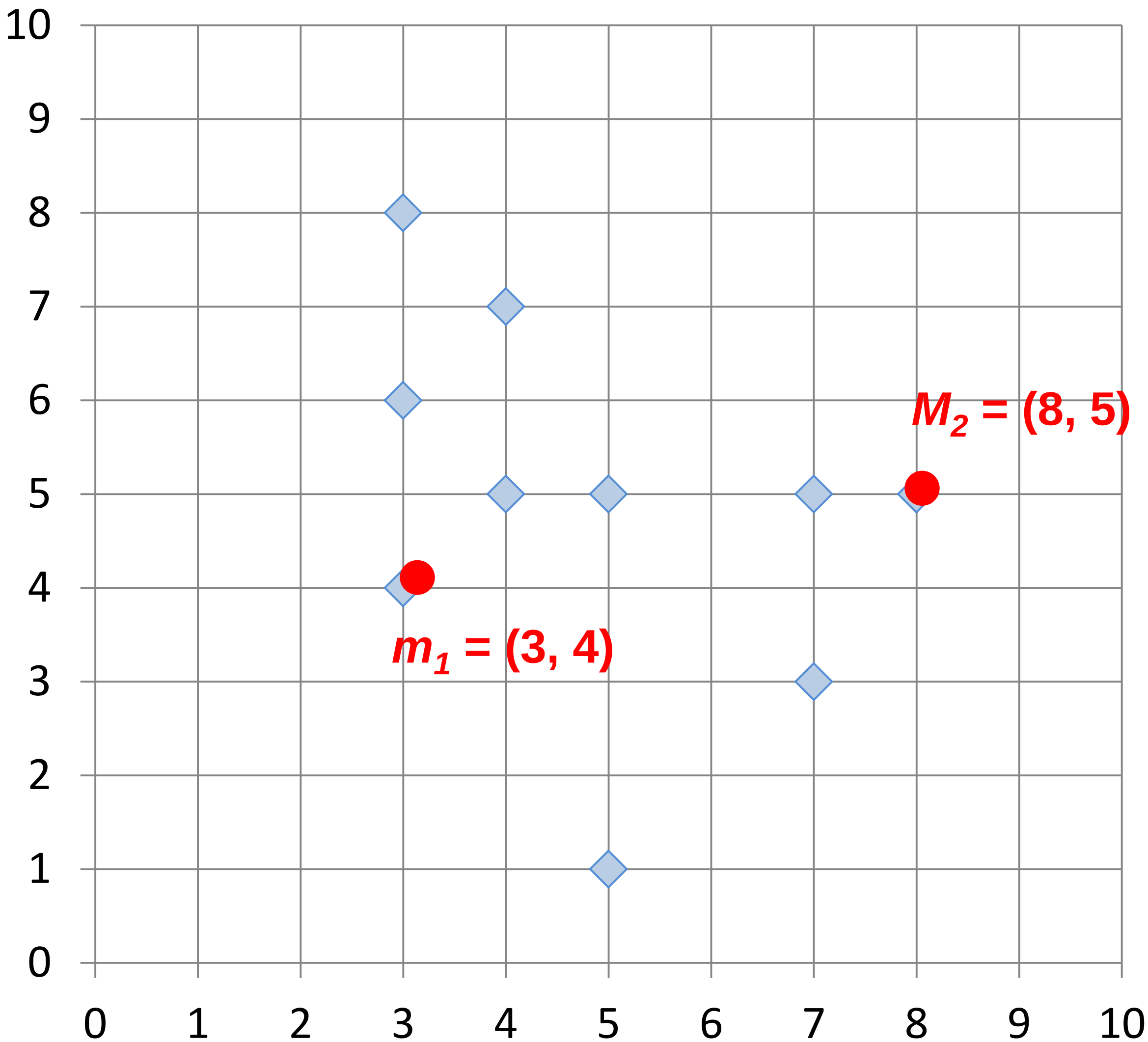
p03	c	(3, 8)
p04	d	(4, 5)
p05	e	(4, 7)
p06	f	(5, 1)
p07	g	(5, 5)
p08	h	(7, 3)
p09	i	(7, 5)
p10	j	(8, 5)

K-Means Clustering

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



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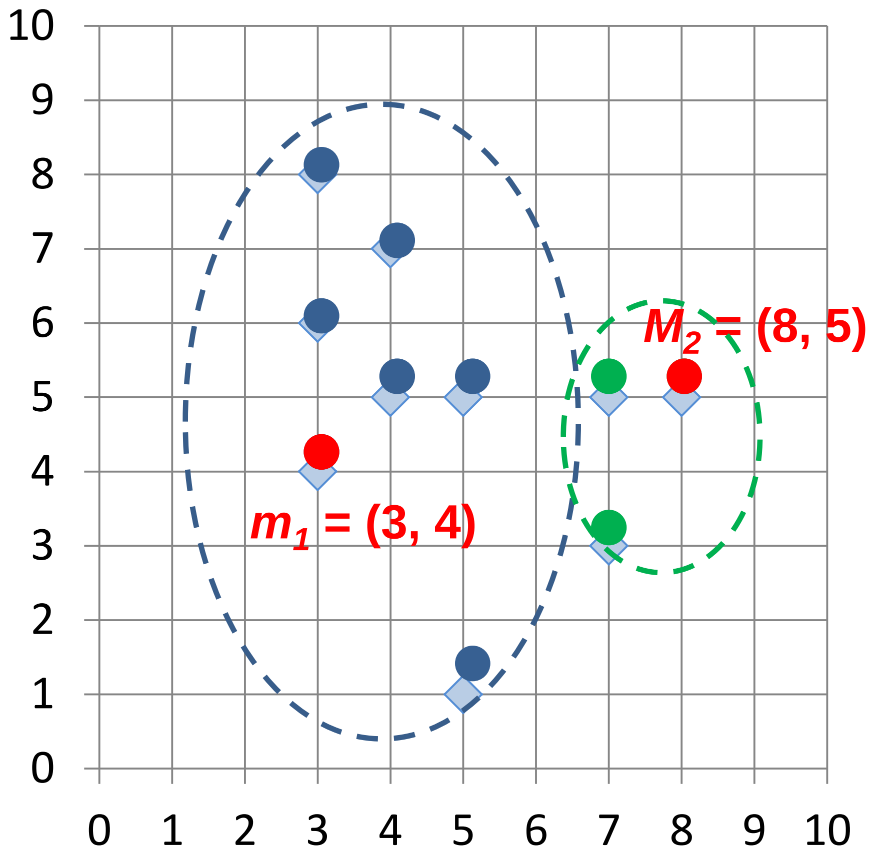
p05	e	(4, 7)
p06	f	(5, 1)
p07	g	(5, 5)
p08	h	(7, 3)
p09	i	(7, 5)
p10	j	(8, 5)
Initial	m1	(3, 4)
Initial	m2	(8, 5)

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
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

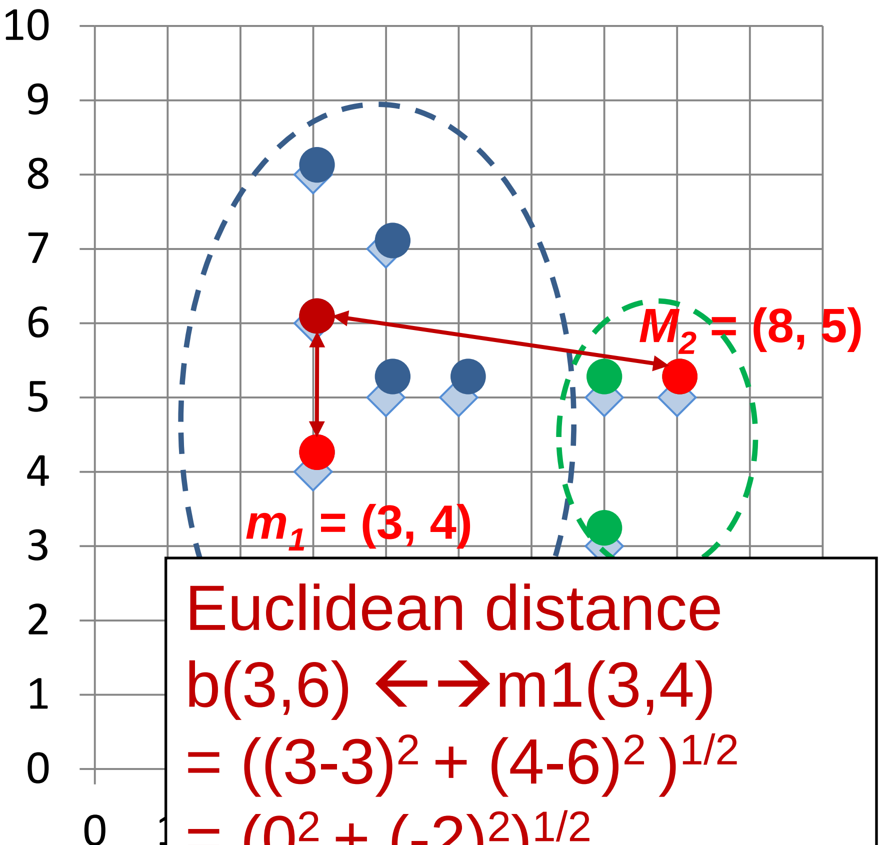
Initial m1 (3, 4)

Initial m2 (8, 5)

K-Means Clustering

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

Step 3: Assign each objects to most similar center



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

K-

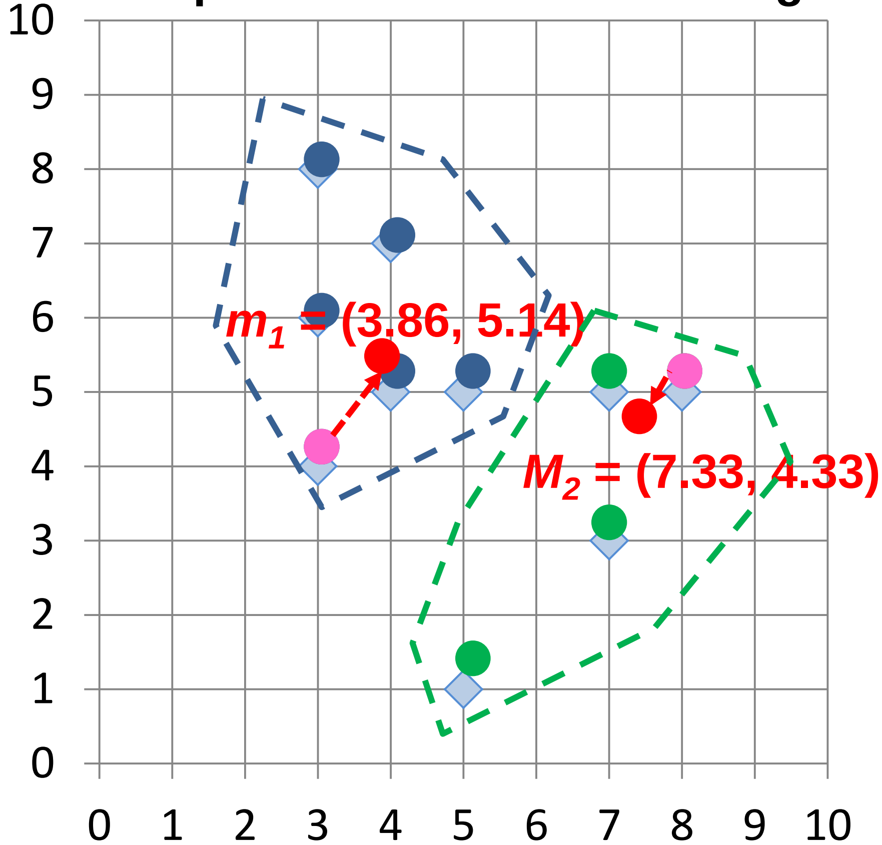
Point	P	P(x,y)	m1 distance	m2 distance	Cluster
p01	a	(3, 4)	0.00	5.10	Cluster1
p02	b	(3, 6)	2.00	5.10	Cluster1
p03	c	(3, 8)	4.00	5.83	Cluster1
p04	d	(4, 5)	1.41	4.00	Cluster1
p05					ster1
p06					ster1
p07					ster1
p08					ster2
p09					ster2
p10					ster2

Euclidean distance
b(3,6) ←→ 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,
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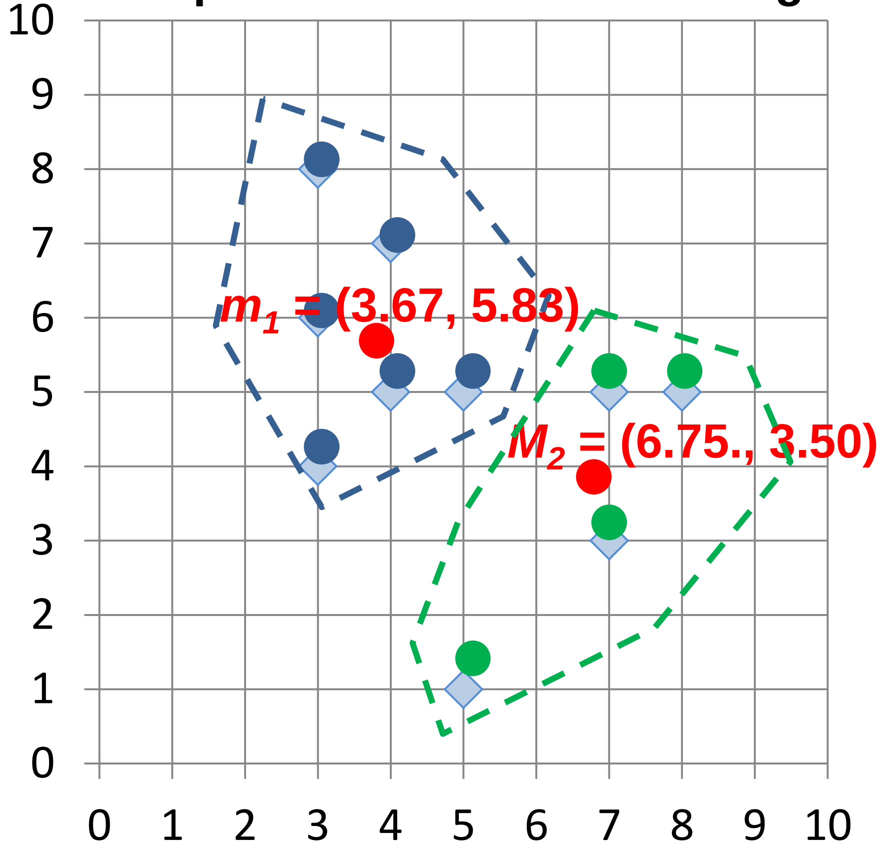


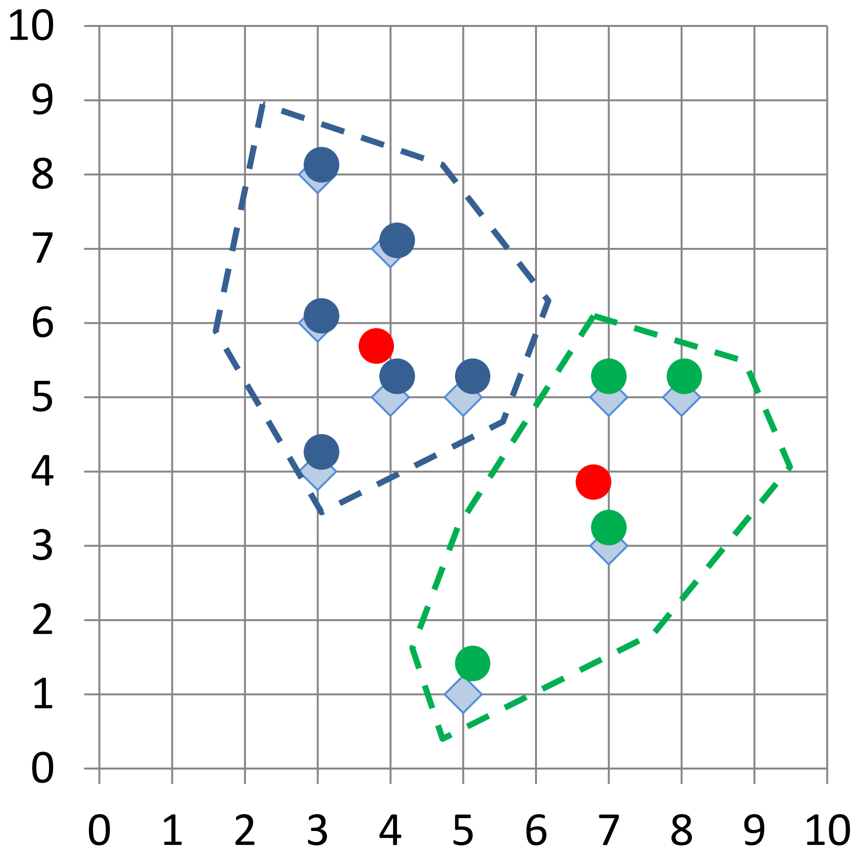
Point	P	P(x,y)	m1 distance	m2 distance	Cluster
p01	a	(3, 4)	1.95	3.78	Cluster1
p02	b	(3, 6)	0.69	4.51	Cluster1
p03	c	(3, 8)	2.27	5.86	Cluster1
p04	d	(4, 5)	0.89	3.13	Cluster1
p05	e	(4, 7)	1.22	4.45	Cluster1
p06	f	(5, 1)	5.01	3.05	Cluster2
p07	g	(5, 5)	1.57	2.30	Cluster1
p08	h	(7, 3)	4.37	0.56	Cluster2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

m1 (3.67, 5.83)

m2 (6.75, 3.50)

***K-Means* Clustering**

stop when no more new assignment



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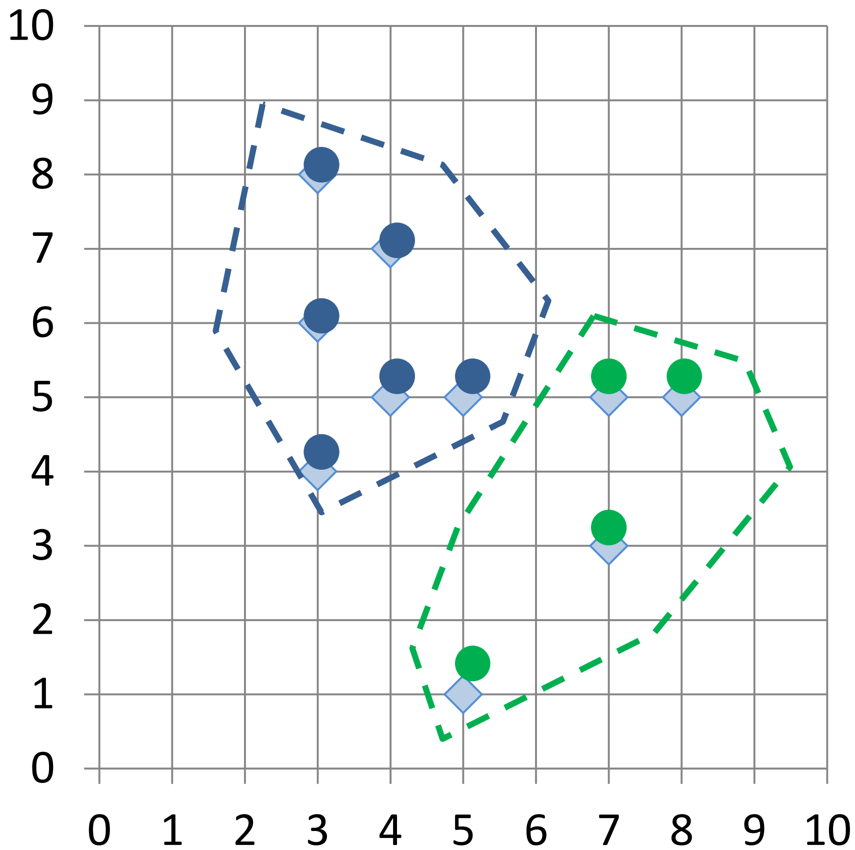
m1 (3.67, 5.83)

m2 (6.75, 3.50)

K-Means Clustering

K-Means Clustering (*K*=2, two clusters)

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

Summary

- Cluster Analysis
- *K-Means* Clustering

References

- Jiawei Han and Micheline Kamber, Data Mining: Concepts and Techniques, Second Edition, 2006, Elsevier
- Efraim Turban, Ramesh Sharda, Dursun Delen, Decision Support and Business Intelligence Systems, Ninth Edition, 2011, Pearson.