Data Warehouse and Data Mining

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NTNU | Norwegian University of Science and Technology

1. Announcements and References
   - Administrative
   - References for Today's Lecture

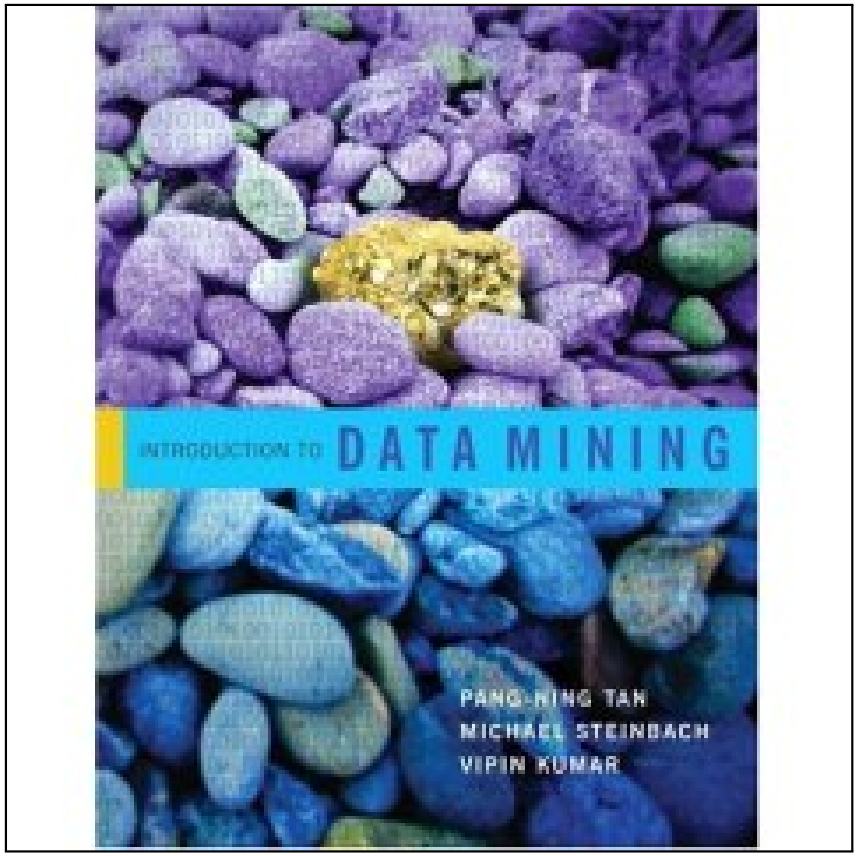
2. Clustering
   - Introduction
   - K-Means Clustering
   - Hierarchical Clustering
   - Density based Clustering
   - Evaluating Clustering and Clusters

Administrative

1. Second Assignment
   - Due by 23.February.2023.
2. Volunteers for feedback regarding course
   - Interested? Please contact me by email!

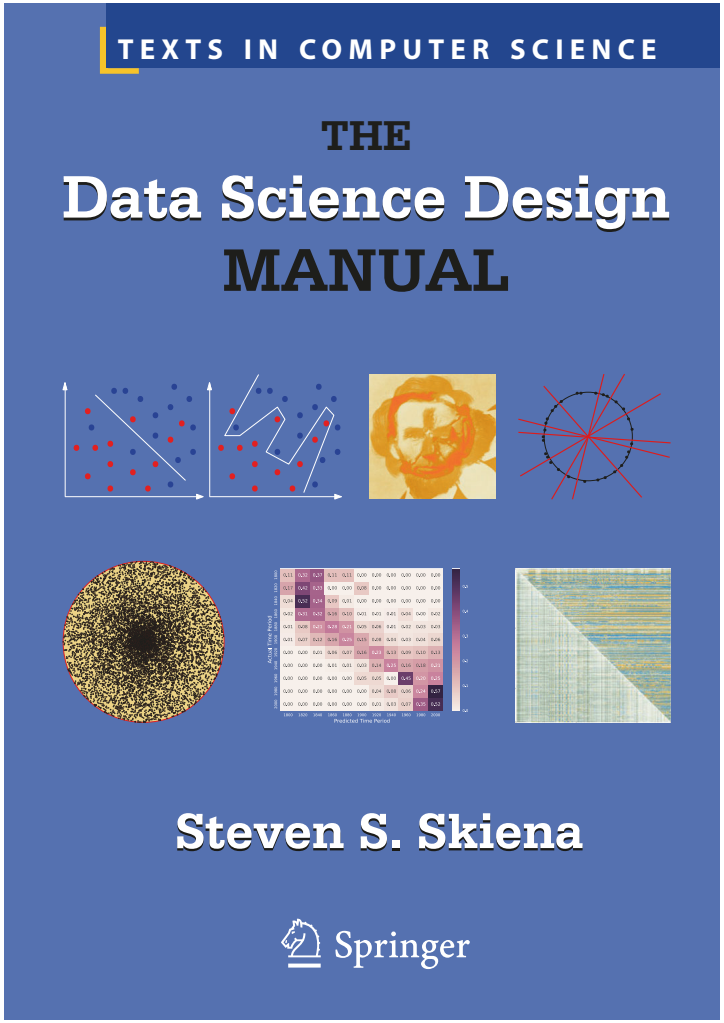
References for "Clustering"

1. Book: Tan et al. *"Introduction to Data Mining"*, 1st Edition, 2006, Pearson Education Inc.
2. Text and images for majority of slides in "Clustering" are based on the book by Tan et al.



References for "Clustering"

1. Book: Steven S. Skiena, *"The Data Science Design Manual"*, 2017, Springer.
2. All text and images for some slides in "Clustering" are based on the book by Steven S. Skiena.



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1854 Broad Street Cholera Outbreak

- On 31 August 1854, a major outbreak of cholera occurred in Soho.
- Over the next three days, 127 people on or near Broad Street died. During the next week, three quarters of the residents had fled the area. By 10 September, 500 people had died and the mortality rate was 12.8 percent in some parts of the city. By the end of the outbreak, 616 people had died.
- Snow, the physician who eventually linked the outbreak to contaminated water, later called it "the most terrible outbreak of cholera which ever occurred in this kingdom."

All from: https://en.wikipedia.org/wiki/1854_Broad_Street_cholera_outbreak.

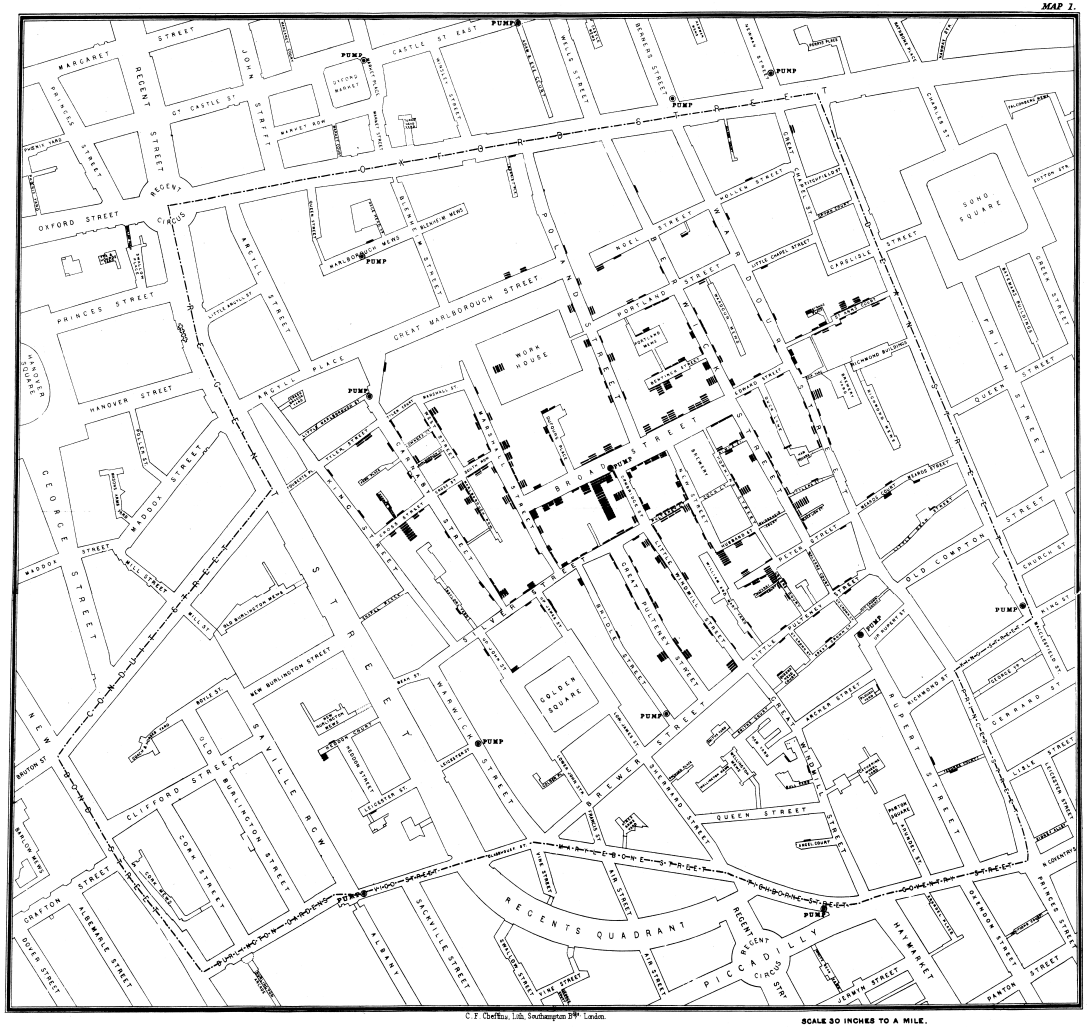
1854 Broad Street Cholera Outbreak

- By talking to local residents, Snow identified the source of the outbreak as the public water pump on Broad Street.
- Although Snow's chemical and microscope examination of a sample of the water from this Broad Street pump water did not conclusively prove its danger, his facts about the patterns of illness and death among residents in Soho persuaded the St James parish authorities to disable the well pump by removing its handle.

All from: https://en.wikipedia.org/wiki/1854_Broad_Street_cholera_outbreak.

1854 Broad Street Cholera Outbreak

- Snow later used a dot map to illustrate how cases of cholera occurred around this pump.



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1854 Broad Street Cholera Outbreak

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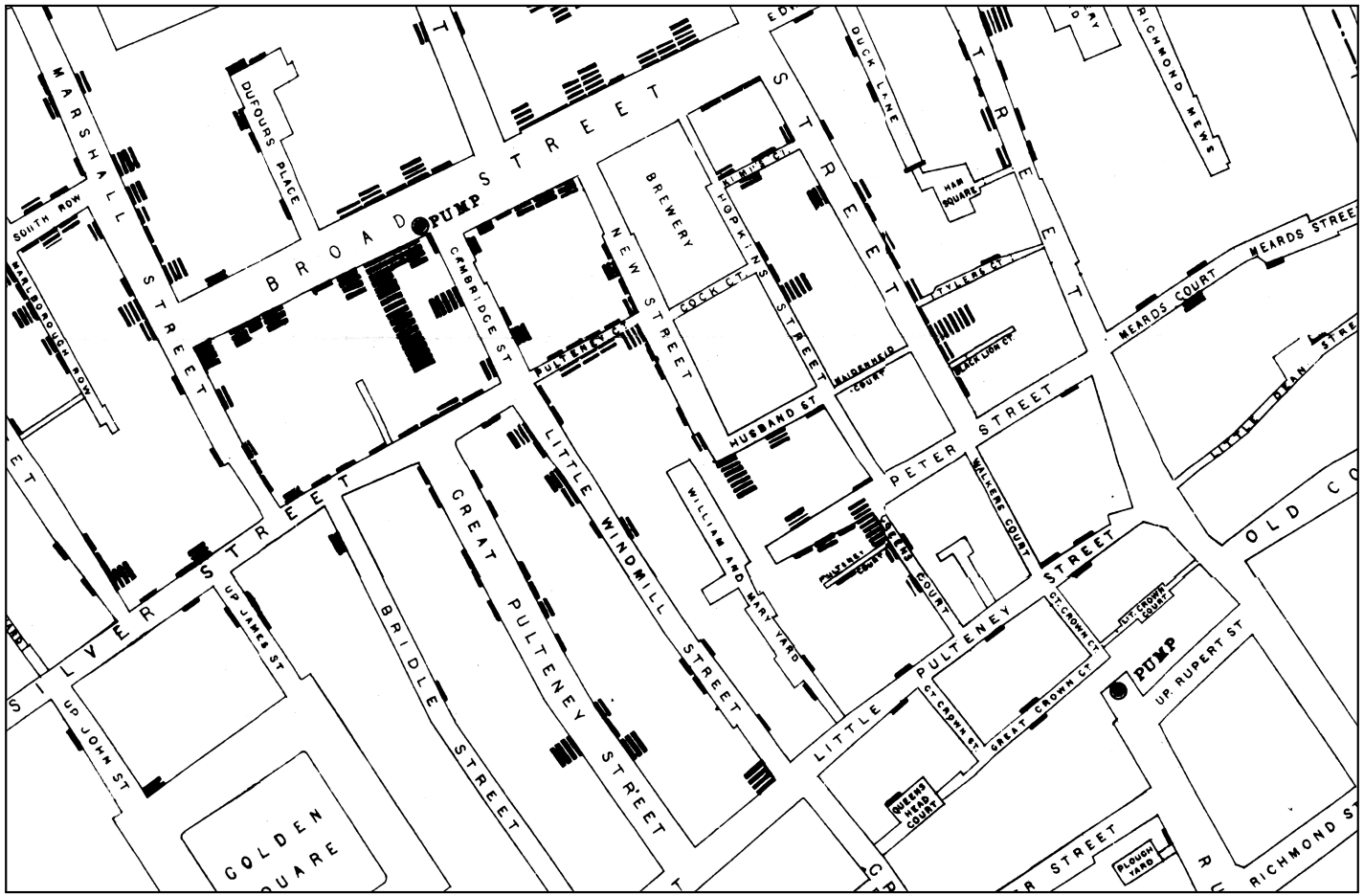
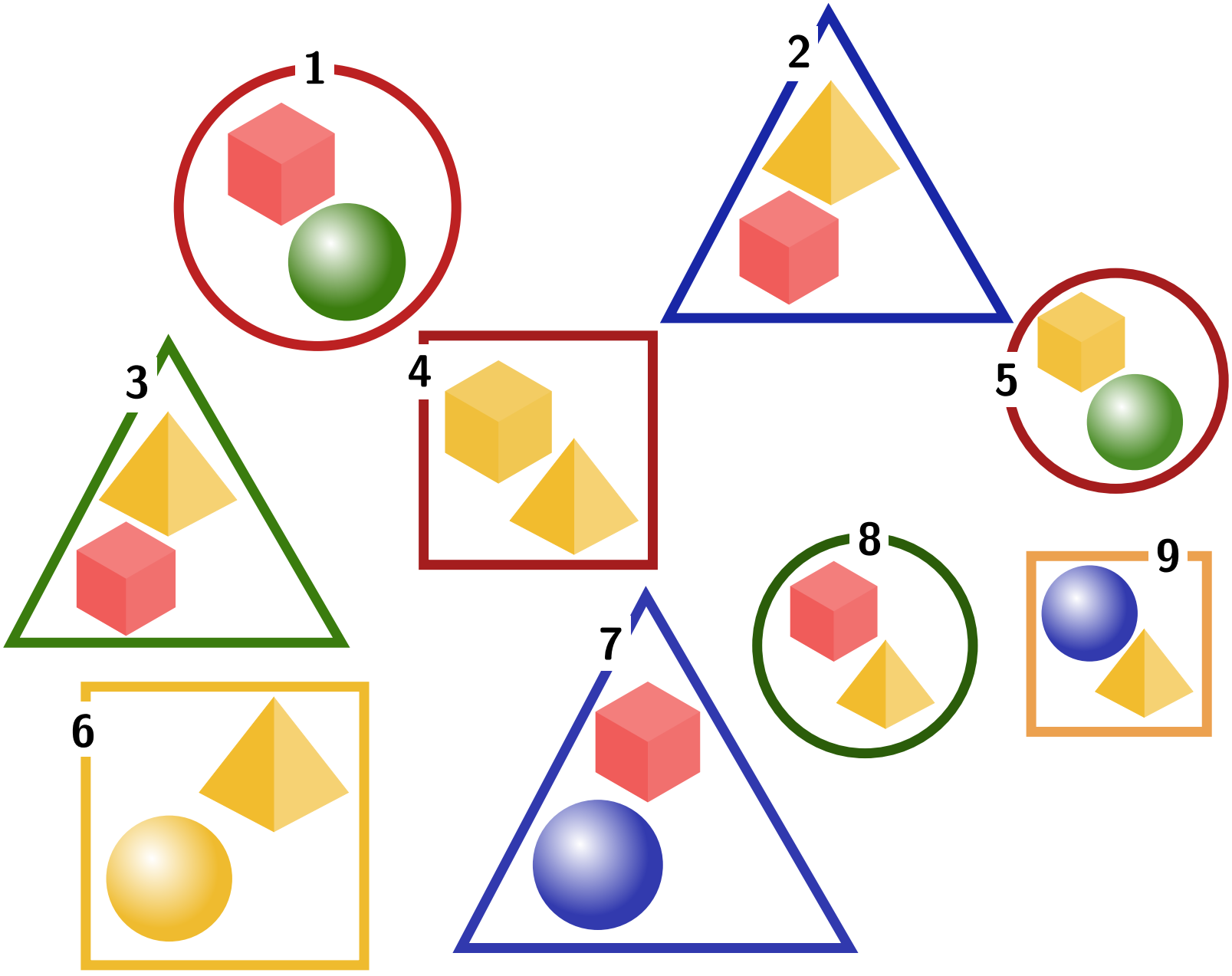


All from: https://en.wikipedia.org/wiki/1854_Broad_Street_cholera_outbreak.

Clustering — Toy Example

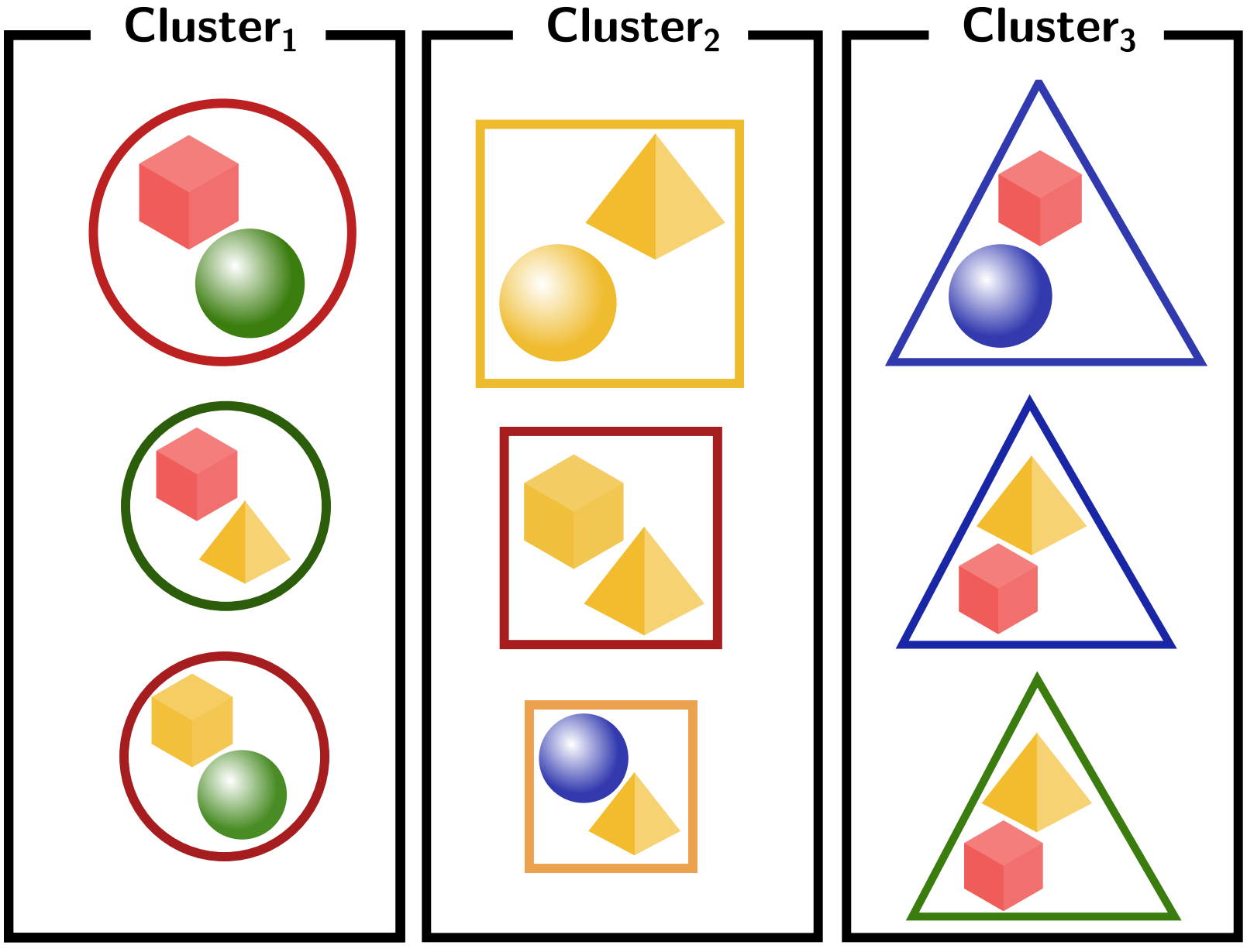


Clustering — Unsupervised Learning

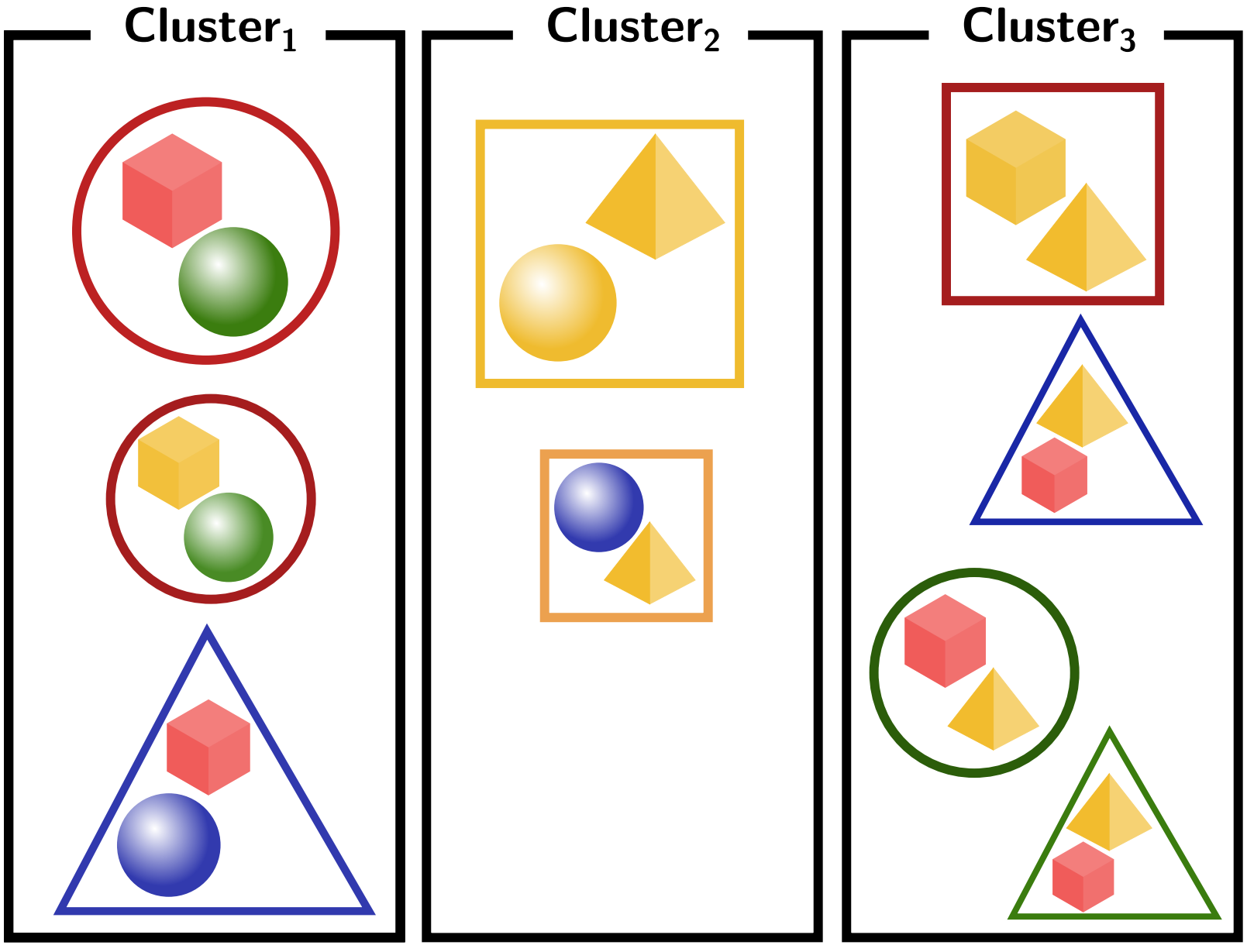
- Consider the example observations from earlier.
- Given this set of data, how can we organize this data based on its attributes so that related observations are placed together and unrelated observations are excluded?

ID	Shape	Shape Color	Object_1	Color_1	Object_2	Color_2
1	Circle	Red	Cube	Red	Sphere	Green
2	Triangle	Blue	Pyramid	Yellow	Cube	Red
3	Triangle	Green	Pyramid	Yellow	Cube	Red
4	Square	Red	Cube	Yellow	Pyramid	Yellow
5	Circle	Red	Cube	Yellow	Sphere	Green
6	Square	Yellow	Pyramid	Yellow	Sphere	Yellow
7	Triangle	Blue	Cube	Red	Sphere	Blue
8	Circle	Green	Cube	Red	Pyramid	Yellow
9	Square	Yellow	Sphere	Blue	Pyramid	Yellow

Example Clustering — Based on Shapes

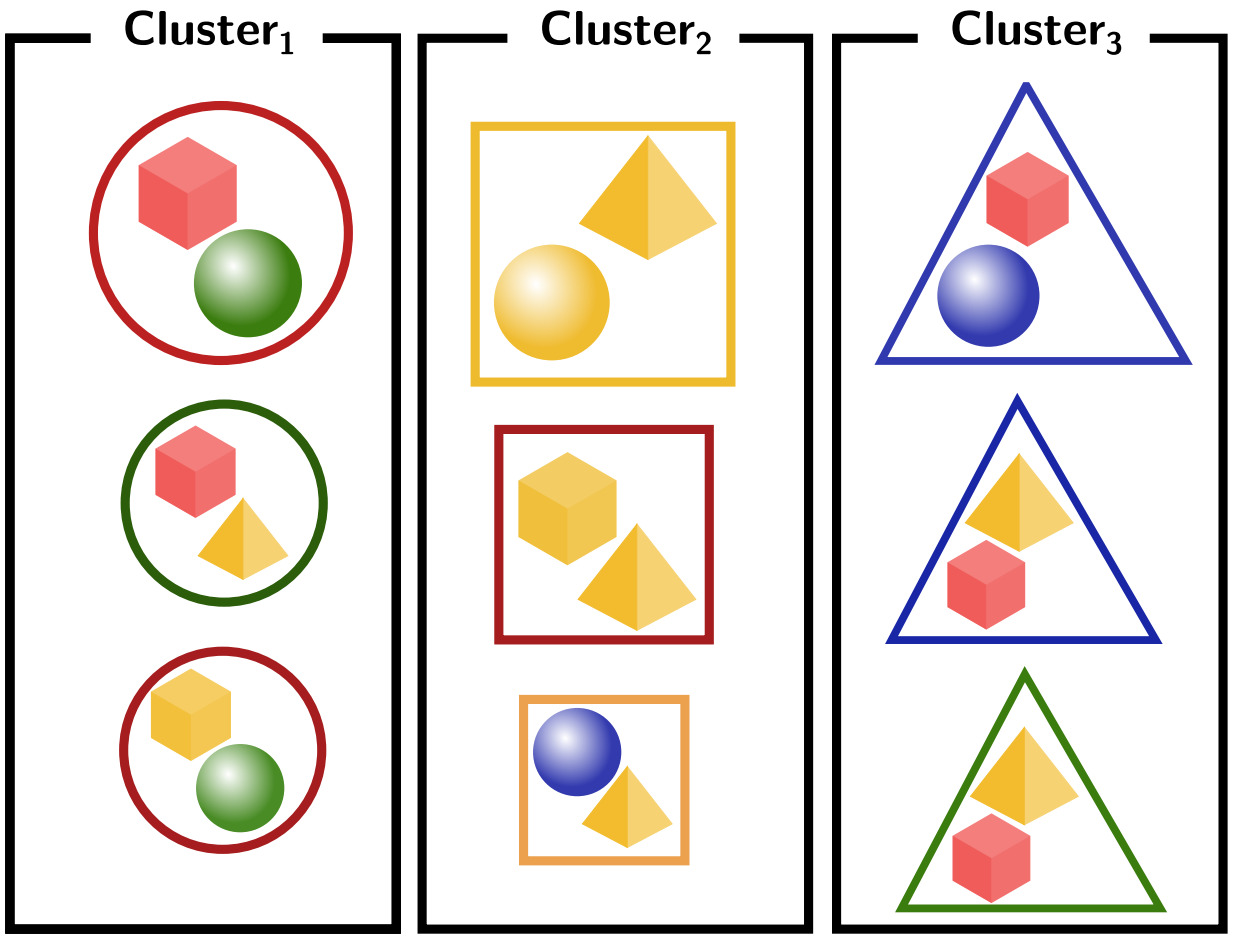


Example Clustering — Based on Objects



What is Cluster Analysis?

- Finding groups of objects 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.



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Application of Cluster Analysis

- 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.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Notion of Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

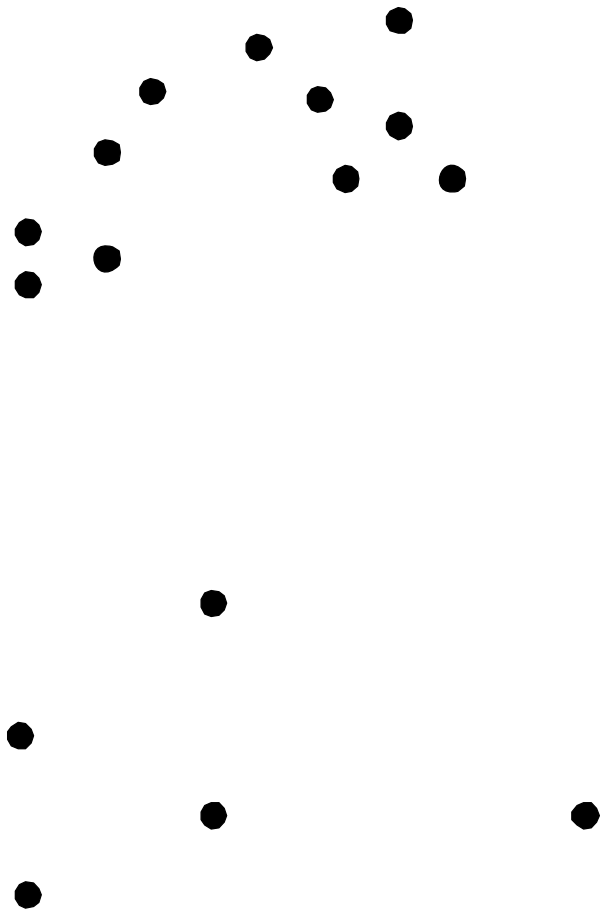
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

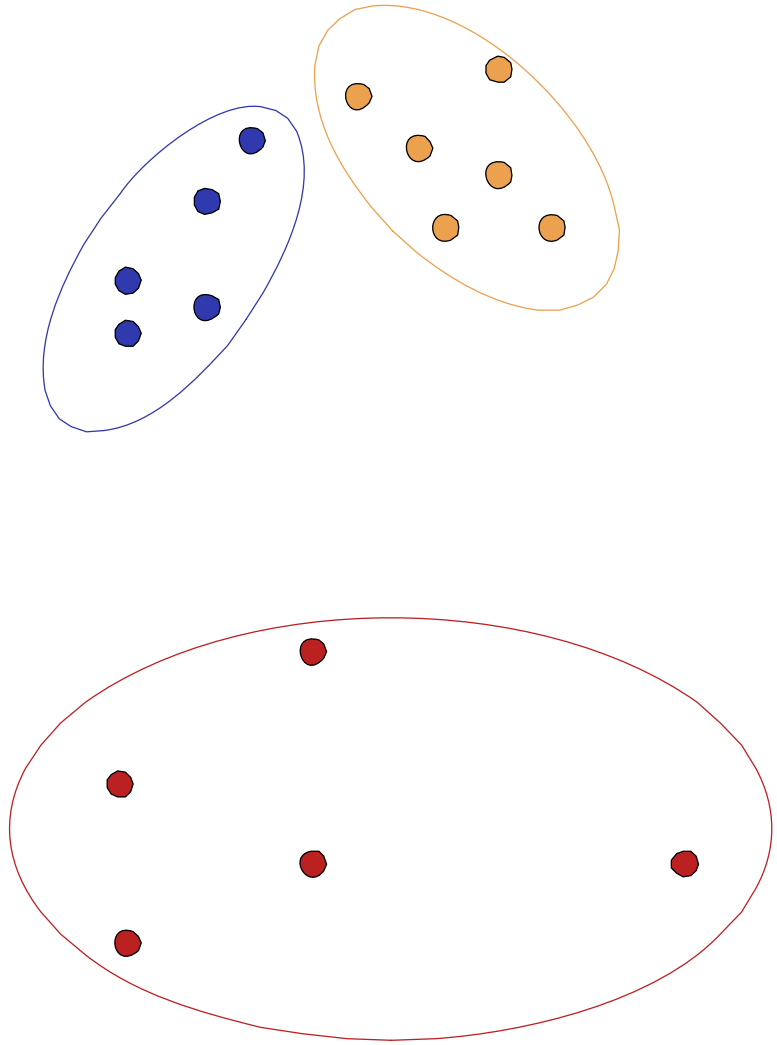
Types of Clustering

- A clustering is a set of clusters.
- Important distinction between hierarchical and partitional 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.
- Hierarchical Clustering: A set of nested clusters organized as a hierarchical tree.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Partitional Clustering



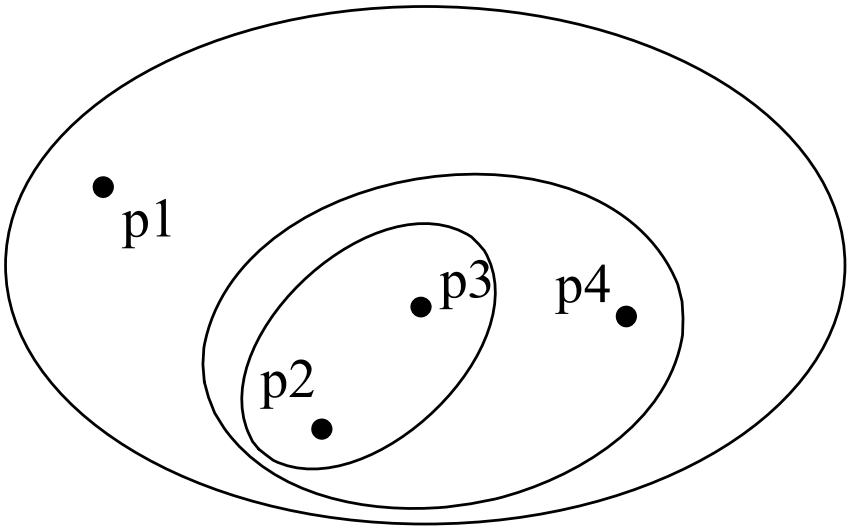


Original Points

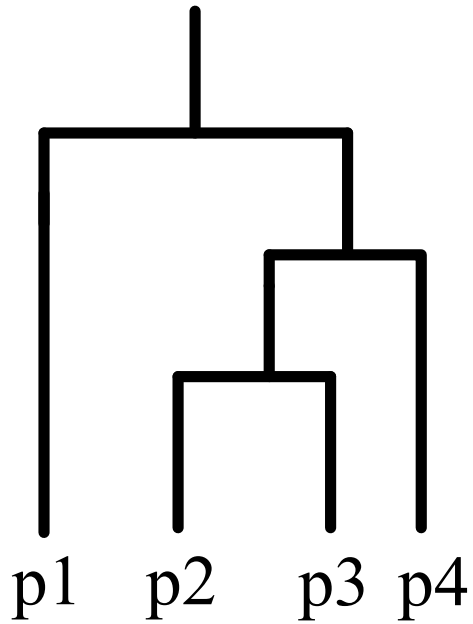
A Partitional Clustering

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering



Hierarchical Clustering



Dendrogram

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Other Types of Clustering

- Exclusive versus Non-Exclusive:
  - In non-exclusive clusterings, points may belong to multiple clusters.
  - Can belong to multiple classes or could be 'border' points.
- Fuzzy Clustering (one type of non-exclusive):
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1.
  - Weights must sum to 1.
  - Probabilistic clustering has similar characteristics.
- Partial versus Complete: In some cases, we only want to cluster some of the data.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Types of Clusters

- Well-separated clusters
- Prototype-based clusters
- Contiguity-based clusters
- Density-based clusters
- Described by an Objective Function

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Types of Clusters — Well-Seperated

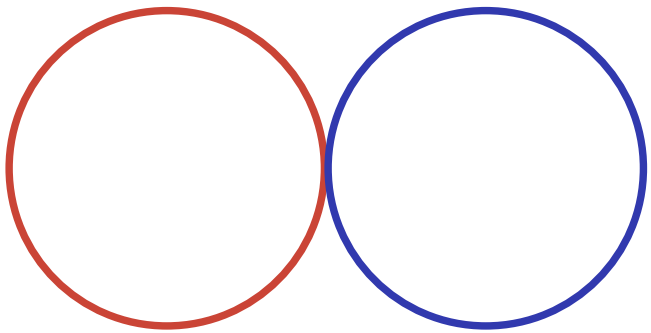
- Well-Separated Clusters: A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.

(a) Well-separated clusters. Each point is closer to all of the points in its cluster than to any point in another cluster.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Types of Clusters — Prototype-Based

- Prototype-Based:
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the prototype or "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.

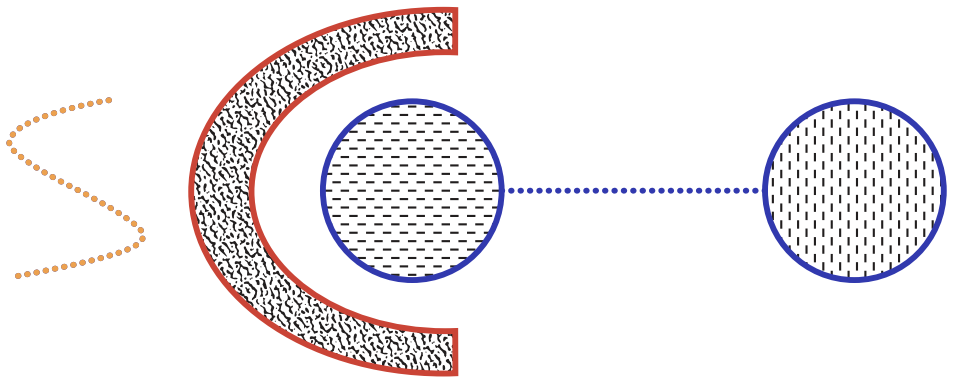


(b) Center-based clusters. Each point is closer to the center of its cluster than to the center of any other cluster.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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.

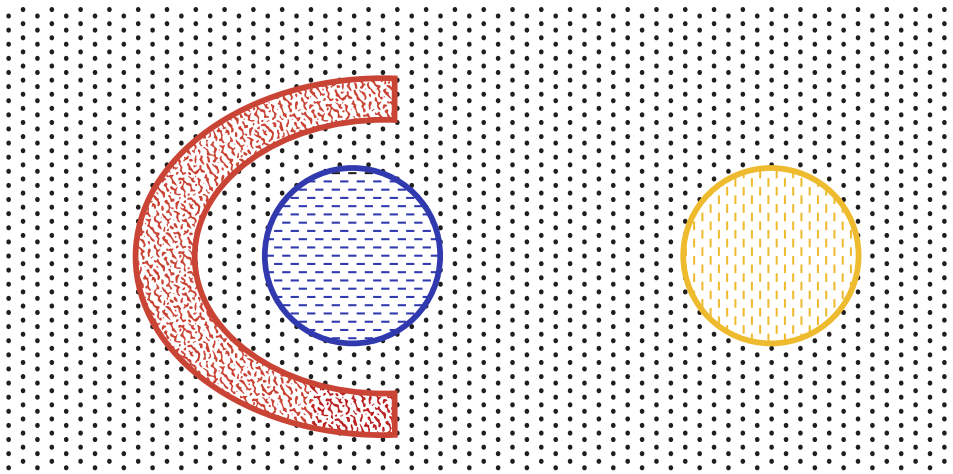


(c) Contiguity-based clusters. Each point is closer to at least one point in its cluster than to any point in another cluster.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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.

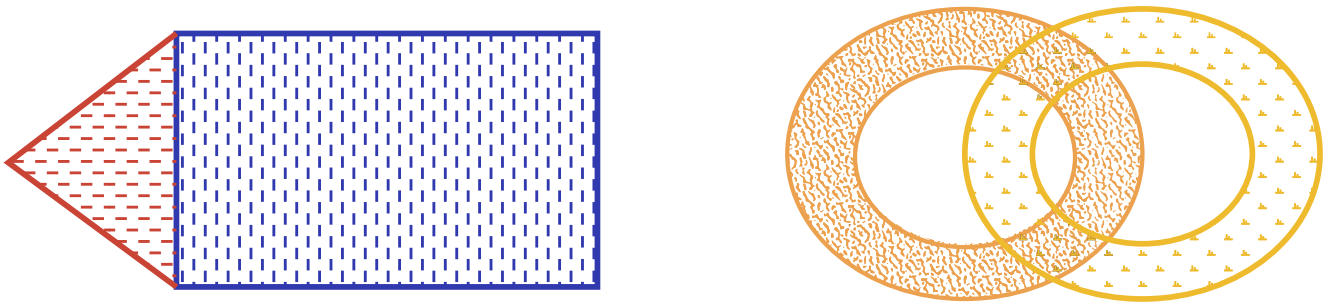


(d) Density-based clusters. Clusters are regions of high density separated by regions of low density.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Types of Clusters — Shared Property / Conceptual Clusters

- Finds clusters that share some common property or represent a particular concept.



(e) Conceptual clusters. Points in a cluster share some general property that derives from the entire set of points. (Points in the intersection of the circles belong to both.)

Figure 7.2. Different types of clusters as illustrated by sets of two-dimensional points.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Clustering Algorithms

- K-means and its variants.
- Hierarchical Clustering.
- Density-Based Clustering.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering

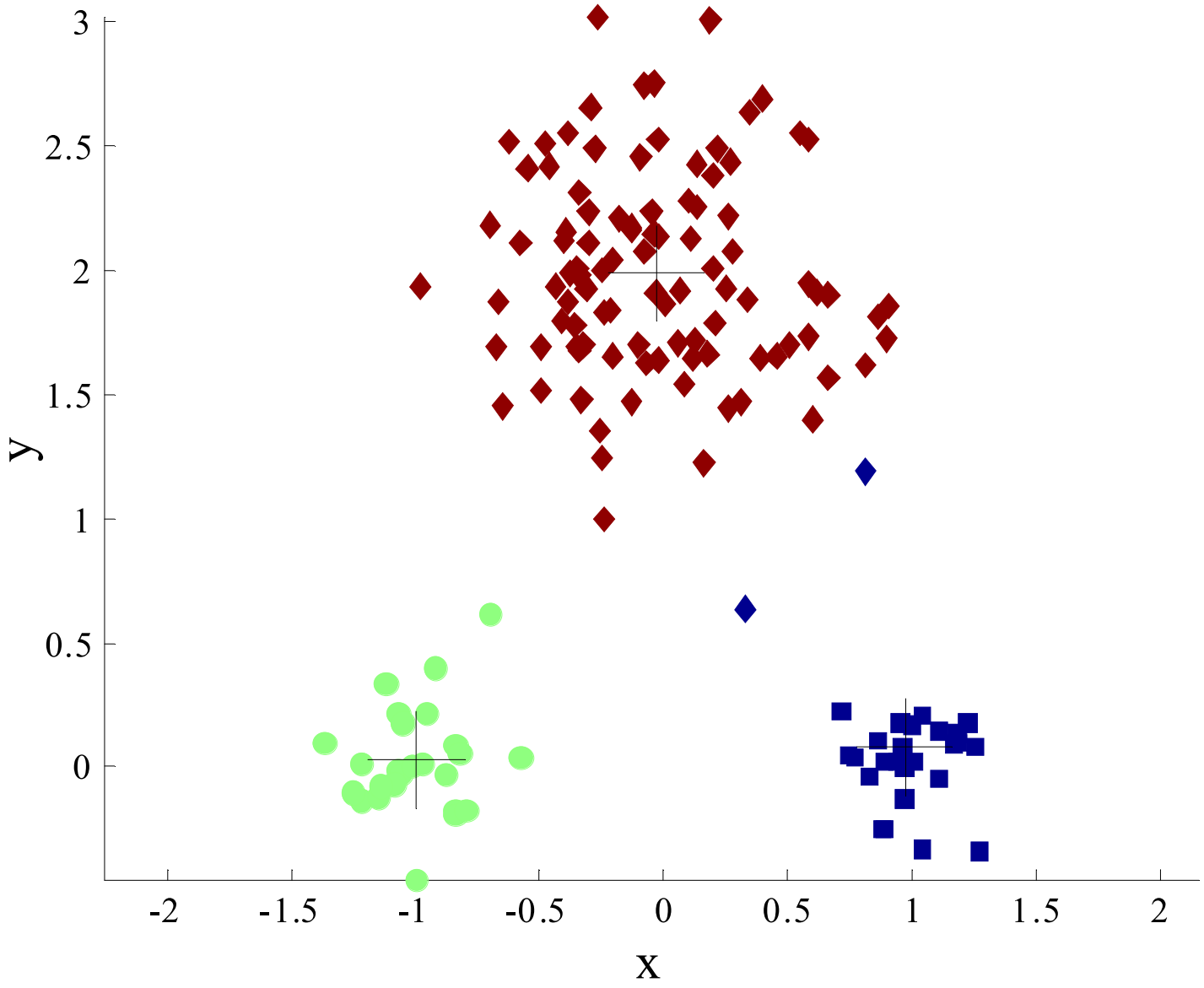
- Partitional clustering approach.
- Number of clusters, K, must be specified.
- Each cluster is associated with a centroid (center point).
- Each point is assigned to the cluster with the closest centroid.
- The basic algorithm is very simple.

Algorithm 7.1 Basic K-means algorithm.

1: Select K points as initial centroids.
2: **repeat**
3: Form K clusters by assigning each point to its closest centroid.
4: Recompute the centroid of each cluster.
5: **until** Centroids do not change.

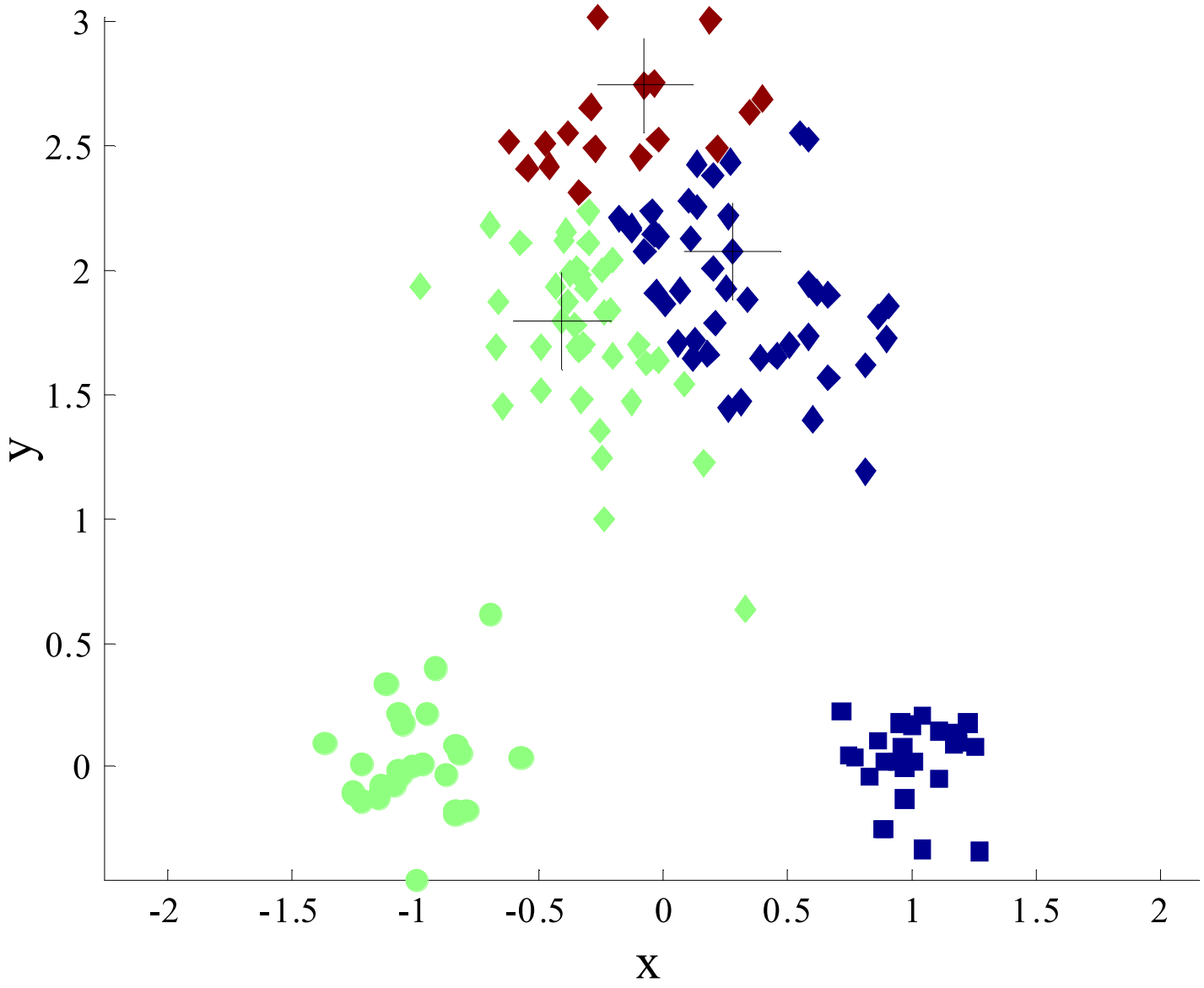
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example



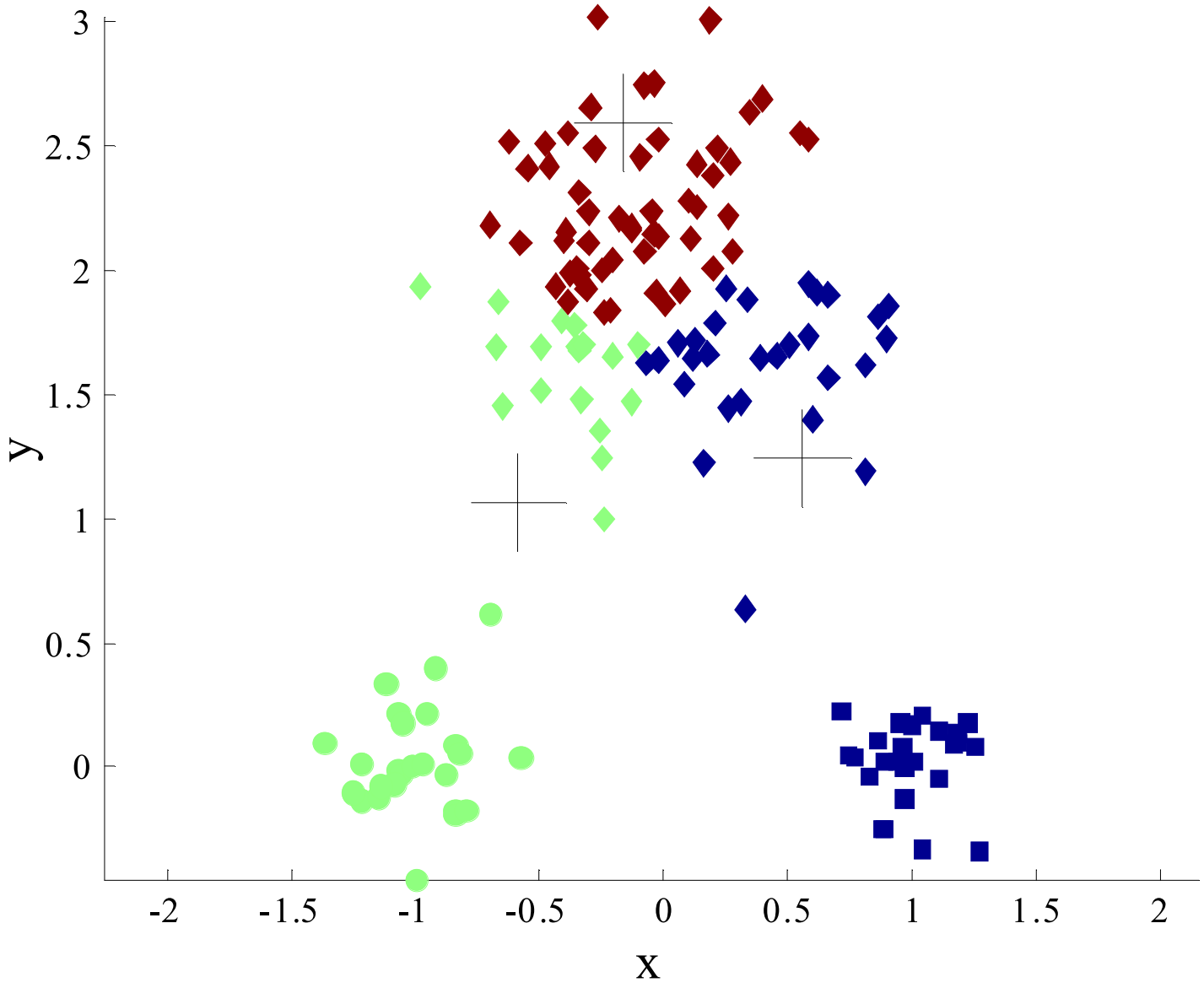
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example Iterations 1



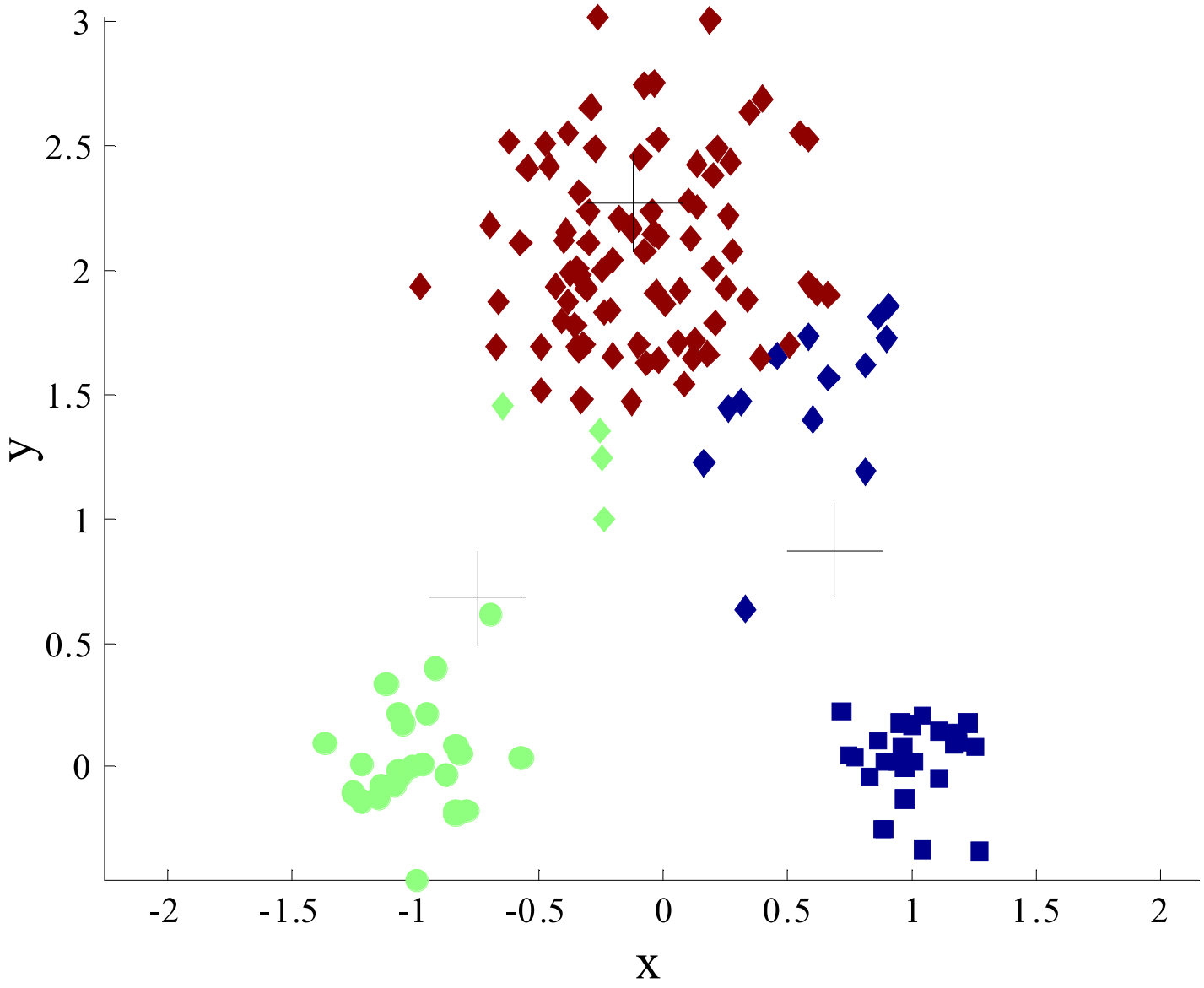
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example Iterations 2



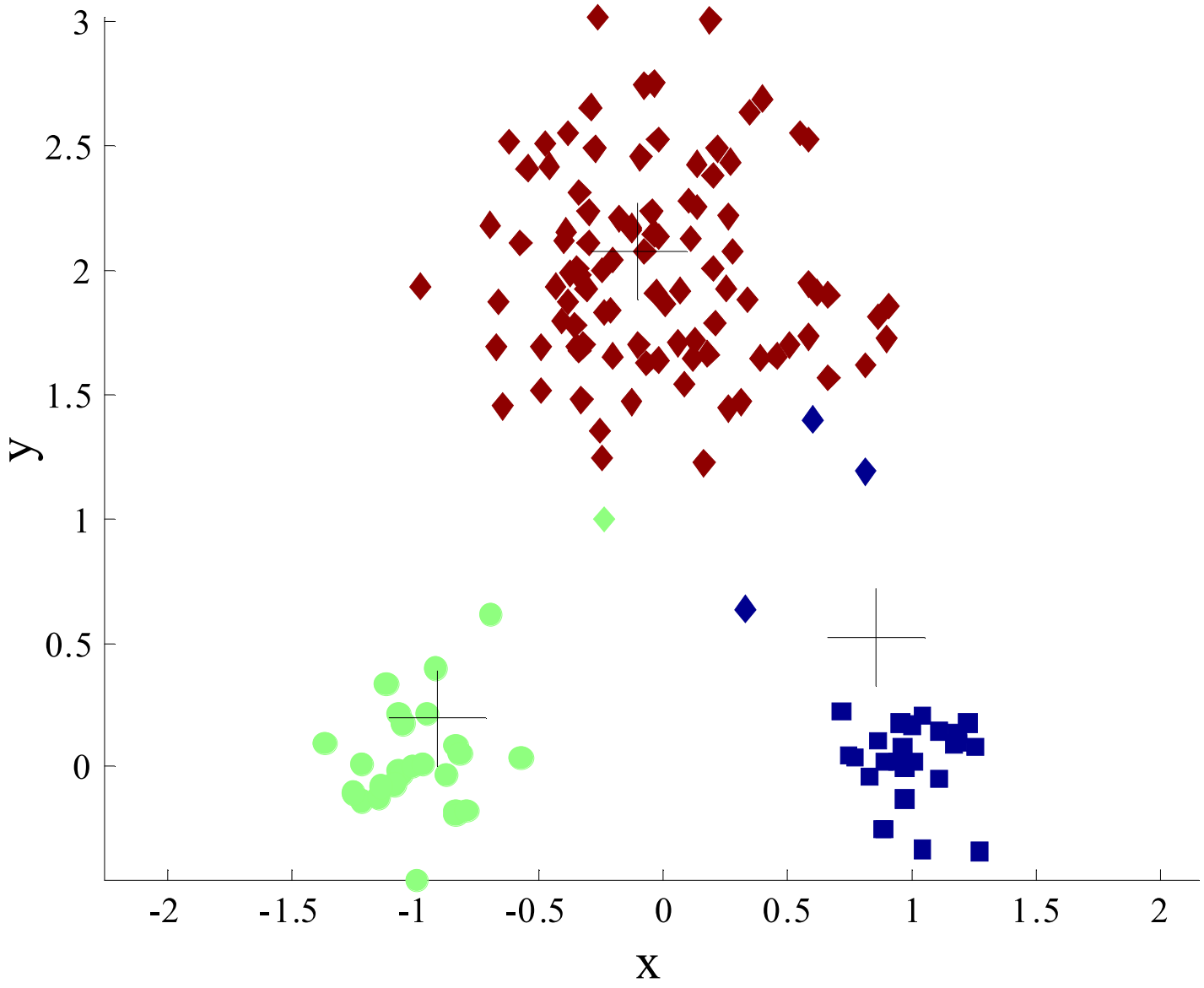
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example Iterations 3



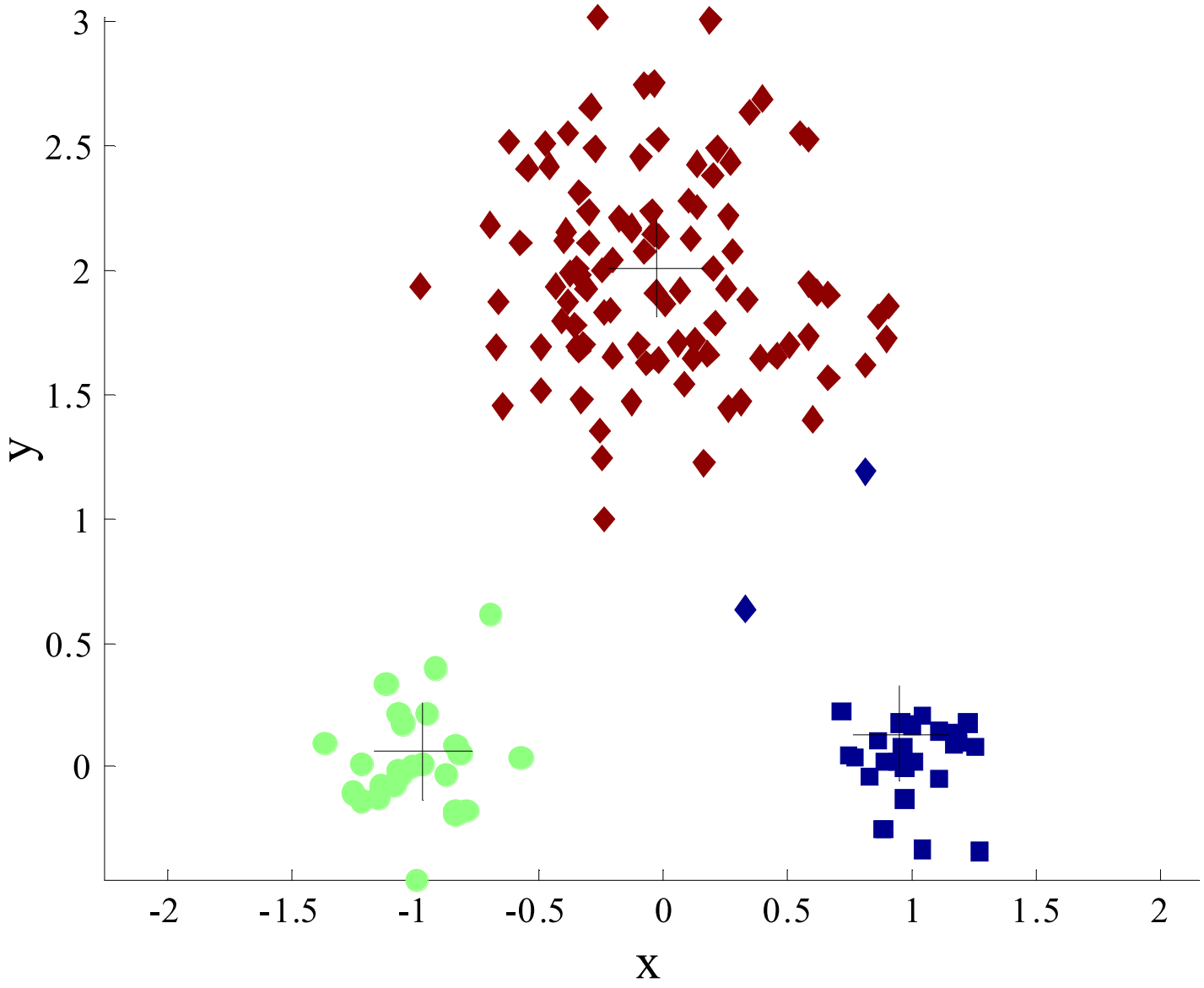
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example Iterations 4



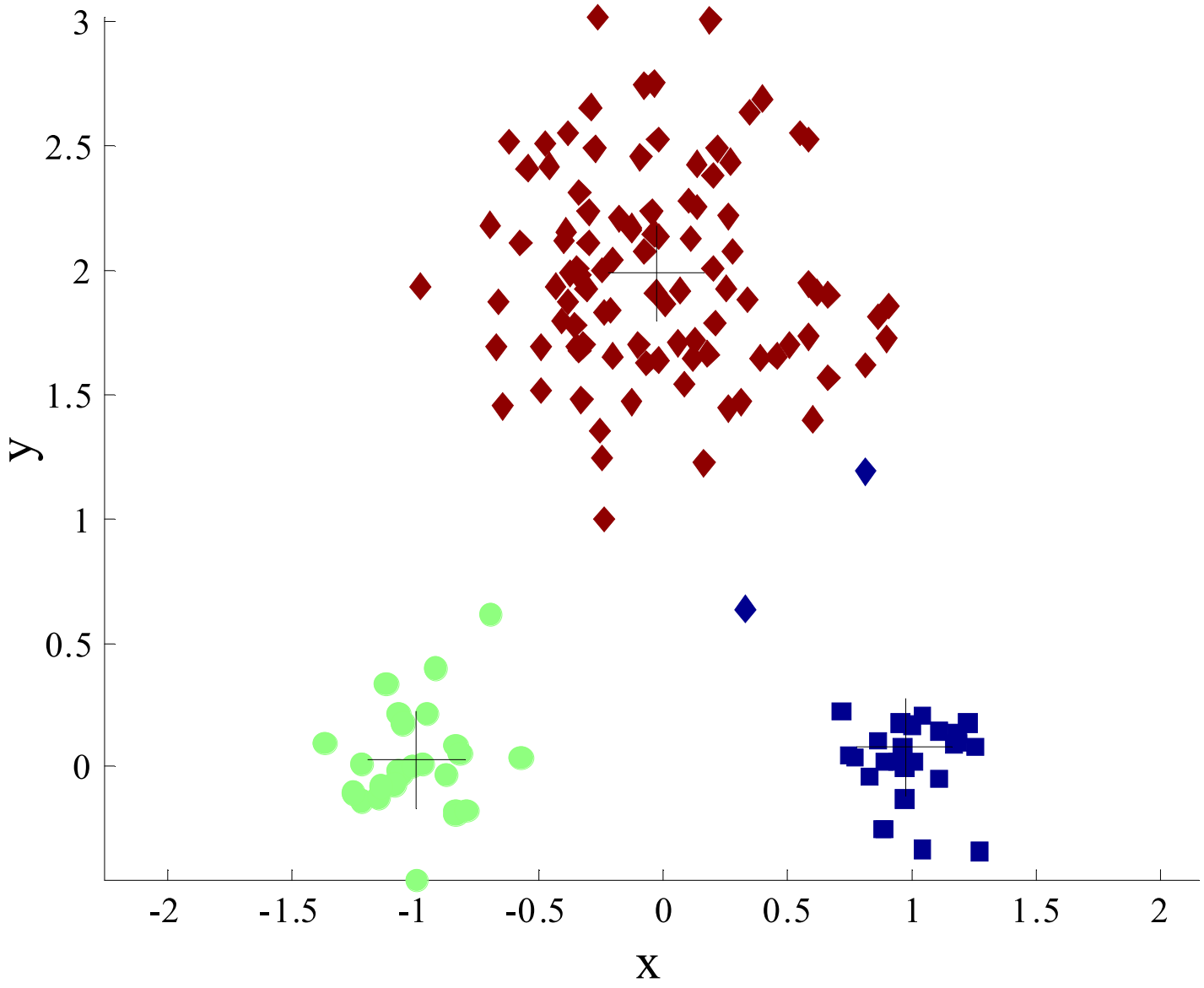
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example Iterations 5



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Example Iterations 6



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means Clustering — Details

- Simple iterative algorithm.
- Initial centroids are often chosen randomly. Therefore, clusters produced can vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster, but other definitions are possible (based on different similarity functions).
- K-means will converge for common proximity measures with appropriately defined centroid (based on different similarity functions).
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to: until relatively few points change clusters.
- Time complexity is: $\mathcal{O}(n \cdot K \cdot I \cdot d)$.
- Space complexity is: $\mathcal{O}((n + K) \cdot d)$.
  - n = number of points.
  - K = number of clusters.
  - I = number of iterations.
  - d = number of attributes.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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 center.
  - To get SSE, we square these errors and sum them.

$$\text{SSE} = \sum_{i=1}^{K} \sum_{x \in C_i} \Big(\text{dist}(m_i, x)\Big)^2. \tag{1}$$

  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i.
  - We can show that m_i corresponds to the center (mean) of the cluster:

$$c_i = \frac{1}{n_i} \sum_{x \in C_i} x. \tag{2}$$

  - where, n_i is the number of objects in the i^{th} cluster.
- One easy way to reduce SSE is to increase K, the number of clusters.
  - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Parameters — How to Select K in K-Means

- We seek from error curve: value K where the rate of decline decreases.
- Error curve should look something like an arm in typing position: it slopes down rapidly from shoulder to elbow, and then slower from the elbow to the wrist.
- Want K to be located exactly at the elbow.
- Easier to identify when compared to a similar MSE error plot for random centers, since the relative rate of error reduction for random centers should be analogous to what we see past the elbow. The slow downward drift is telling us the extra clusters are not doing anything special for us.

All from: Steven S. Skiena, "The Data Science Design Manual", 2017, Springer.

Parameters — How to Select k in K-Means

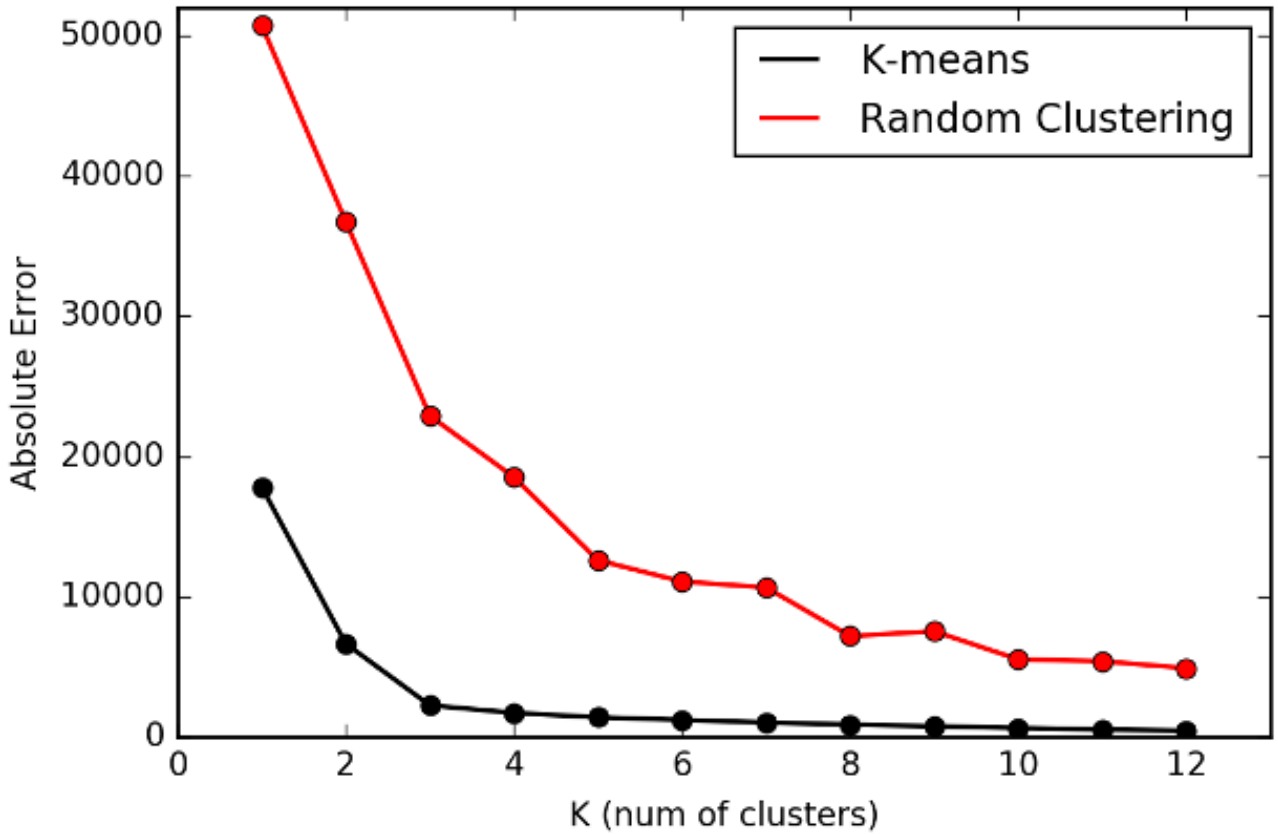
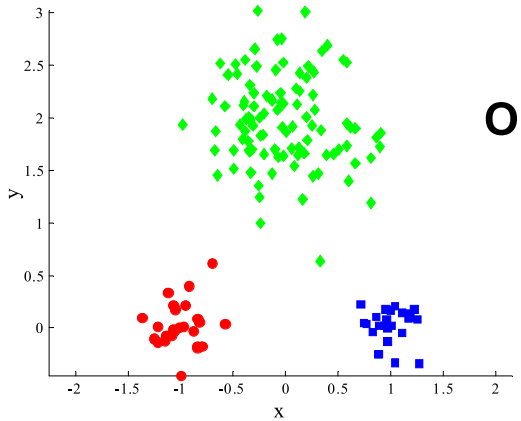


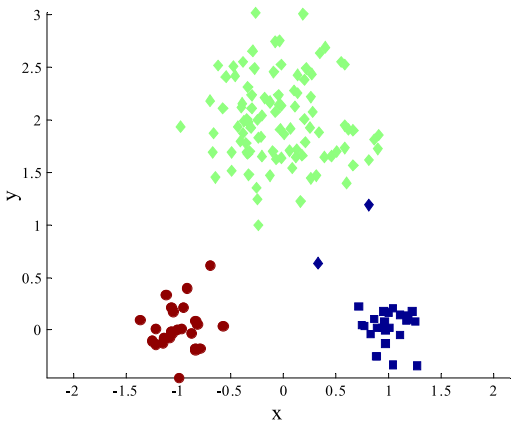
Figure 10.16: The error curve for k-means clustering on the point set of Figure 10.12, showing a bend in the elbow reflecting the three major clusters in the data. The error curve for random cluster centers is shown for comparison.

All from: Steven S. Skiena, "The Data Science Design Manual", 2017, Springer.

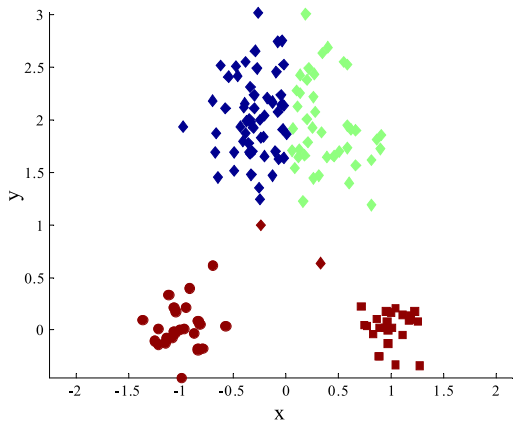
Parameters: Selecting Initial Centroids



Original Points



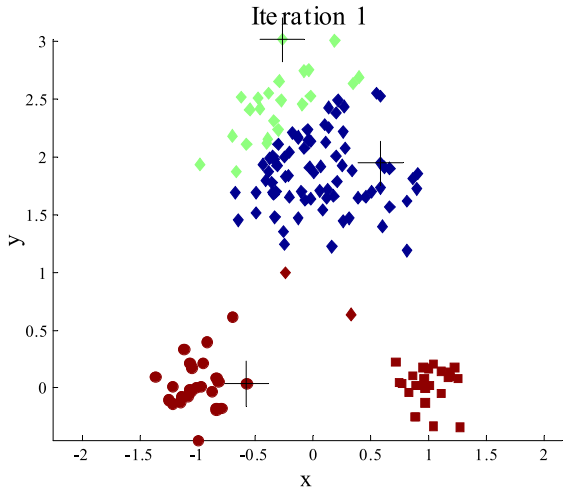
Optimal Clustering

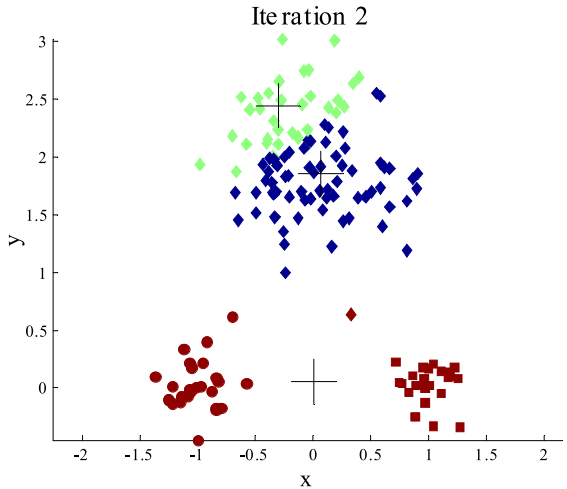


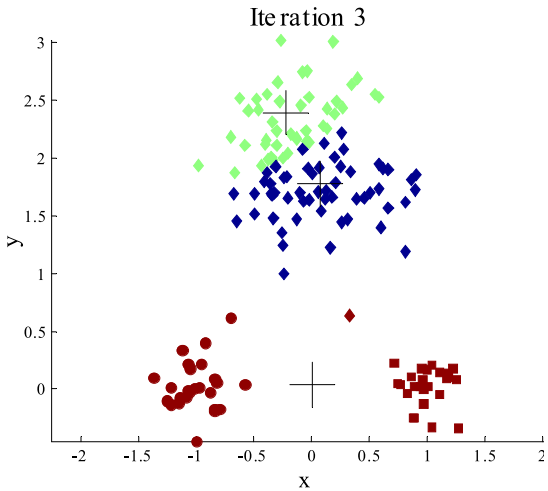
Sub-optimal Clustering

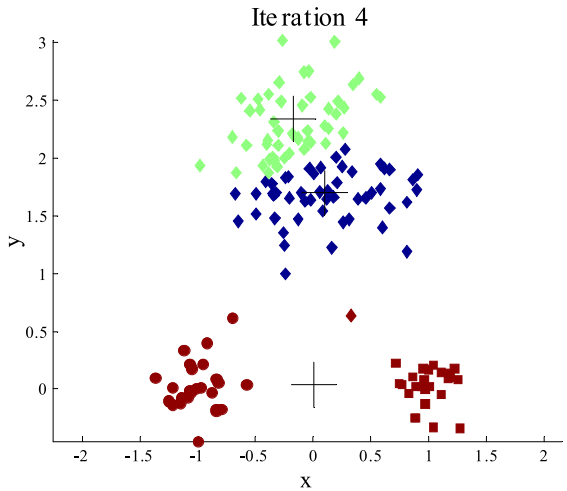
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

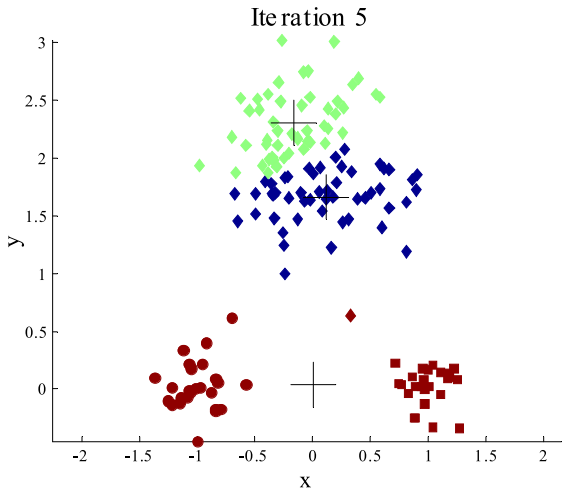
Two Different K-Means Clusterings











All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Solutions to Initial Centroids Problem

1. Multiple runs: helps, but probability is not on your side.
2. Sample and use hierarchical clustering to determine initial centroids.
3. Select more than K initial centroids and then select among these initial centroids. Select most widely separated.
4. K-Means++.
5. Bisecting K-means.
   - Not as susceptible to initialization issues.
6. Post-processing.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

K-Means++: An Approach to Selecting Initial Centroids

- This approach can be slower than random initialization, but very consistently produces better results in terms of SSE.
- Algorithm to select initial centroids C:
  1. Select an initial point at random to be the first centroid.
  2. For $k-1$ steps:
     1. For each of the N points x_i, $1 \leq i \leq N$, find the minimum squared distance to the currently selected centroids, $C_1, \ldots, C_j$, $1 \leq j < k$, i.e., $\min_j(d(C_j, x_i))^2$.
     2. Randomly select a new centroid by choosing a point with probability proportional to $\frac{\min_j(d(C_j,x_i))^2}{(\sum_i d(C_j,x_i))^2}$.
  3. End For.
- Afterwards, continue K-Means as usual.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Bisecting K-Means

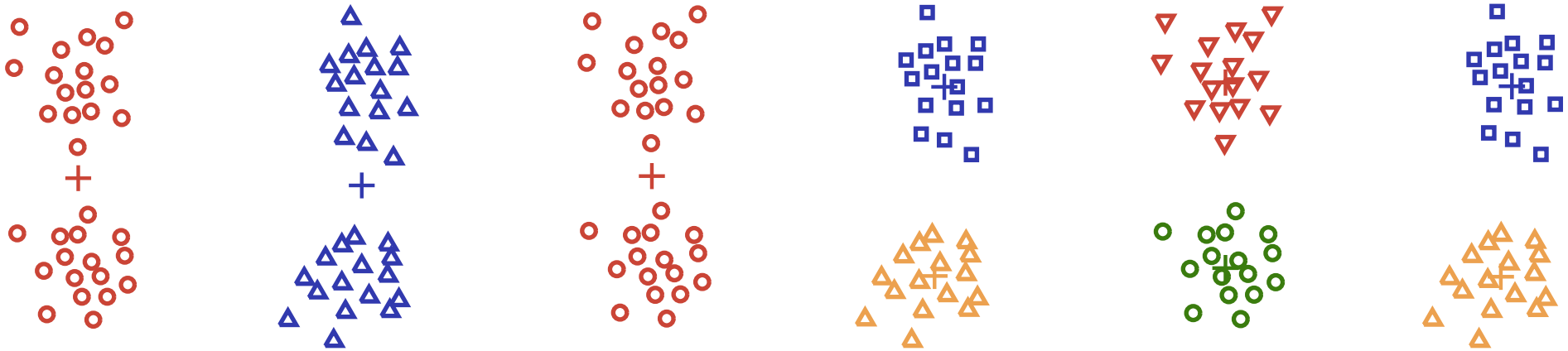
- Bisecting K-means algorithm: variant of K-means that can produce a partitional or a hierarchical clustering.
- Straightforward extension of the basic K-means algorithm:
  1. To obtain K clusters, split the set of all points into two clusters.
  2. Select one of these clusters to split, and so on,
     until K clusters have been produced.

Algorithm 7.3 Bisecting K-means algorithm.

```
1: Initialize the list of clusters to contain the cluster consisting of all points.
2: repeat
3:    Remove a cluster from the list of clusters.
4:    {Perform several "trial" bisections of the chosen cluster.}
5:    for i = 1 to number of trials do
6:       Bisect the selected cluster using basic K-means.
7:    end for
8:    Select the two clusters from the bisection with the lowest total SSE.
9:    Add these two clusters to the list of clusters.
10: until The list of clusters contains K clusters.
```

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Bisecting K-Means



(a) Iteration 1. (b) Iteration 2. (c) Iteration 3.

Figure 7.8. Bisecting K-means on the four clusters example.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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.

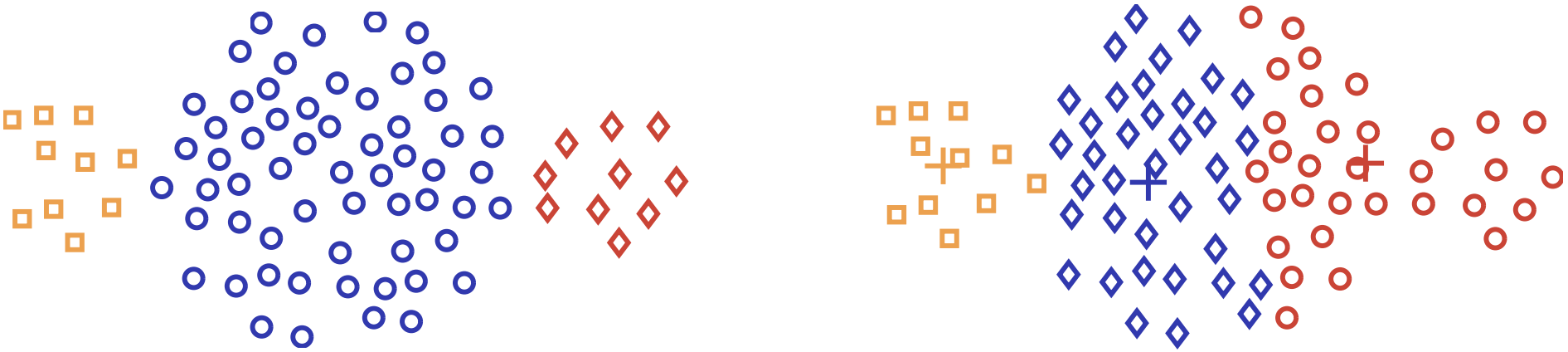
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Limitations of K-Means: Differing Sizes



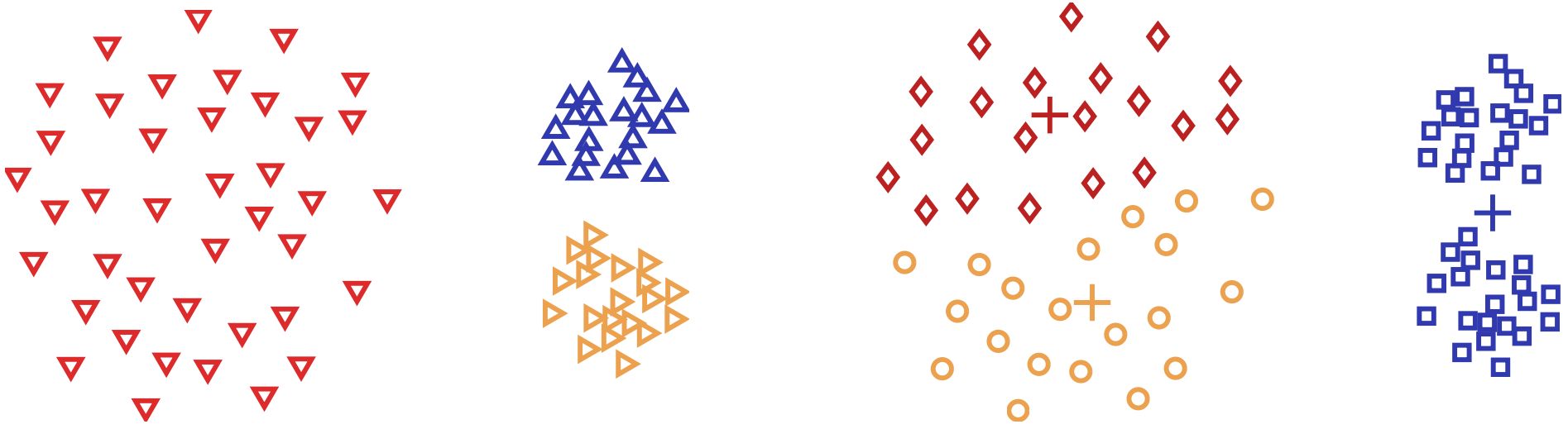
(a) Original points.

(b) Three K-means clusters.

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Limitations of K-Means: Differing Densitites



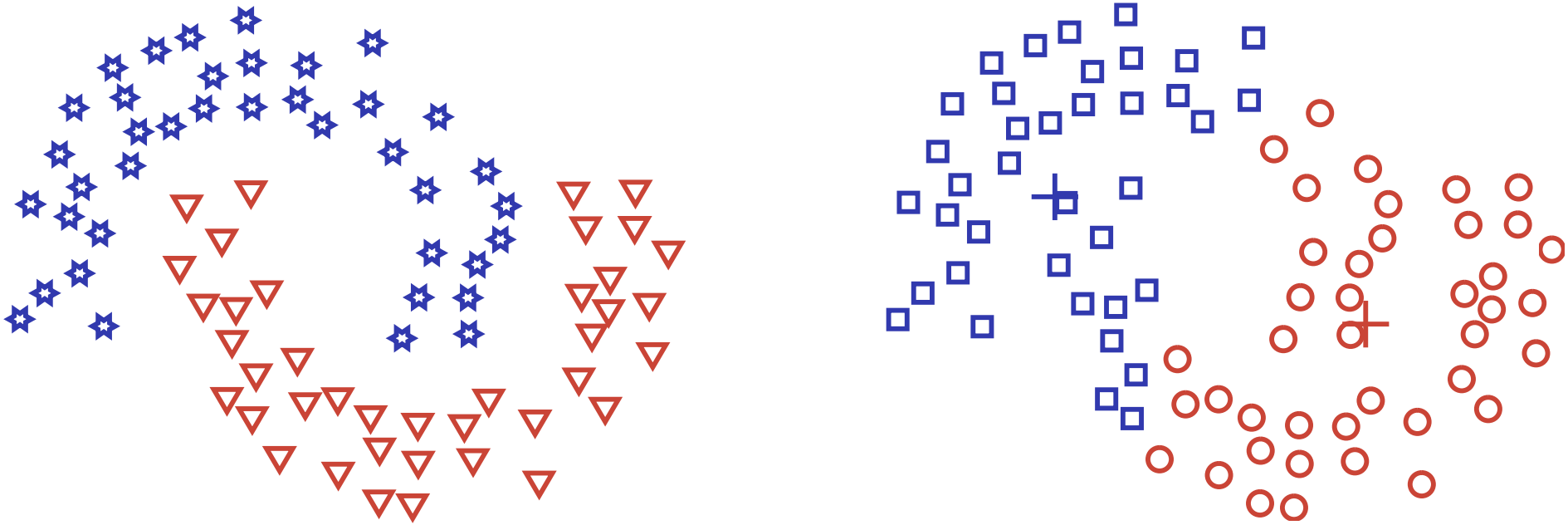
(a) Original points.

(b) Three K-means clusters.

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Limitations of K-Means: Non-Globular Clusters



(a) Original points.

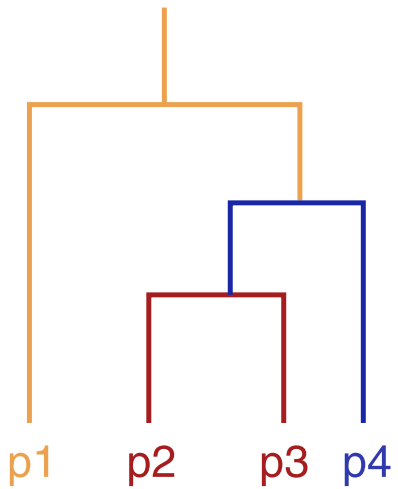
(b) Two K-means clusters.

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

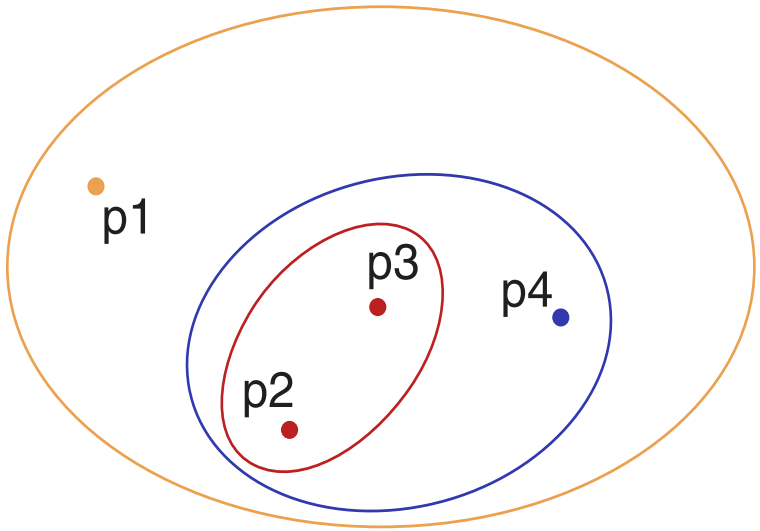
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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.



(a) Dendrogram.



(b) Nested cluster diagram.

Figure 7.13. A hierarchical clustering of four points shown as a dendrogram and as nested clusters.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

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.
- For example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...).

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering

- Two main types of hierarchical clustering:
  1. 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.
  2. 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.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

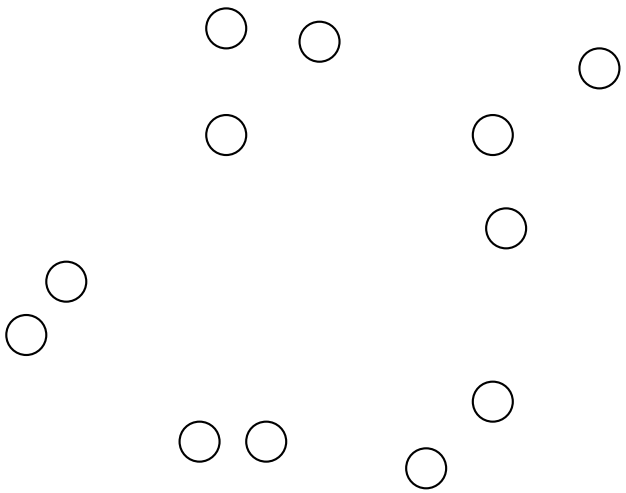
Agglomerative Clustering Algorithm

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Starting Situation

- Start with clusters of individual points and a proximity matrix.



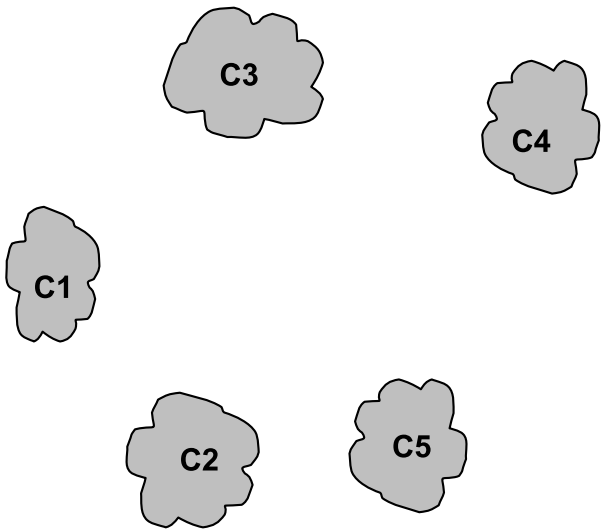
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

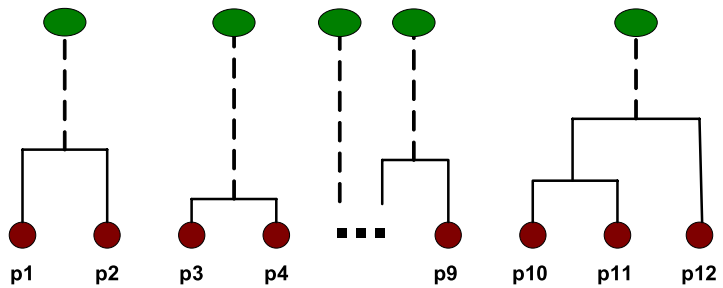
Intermediate Situation

- After some merging steps, we have some clusters.



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

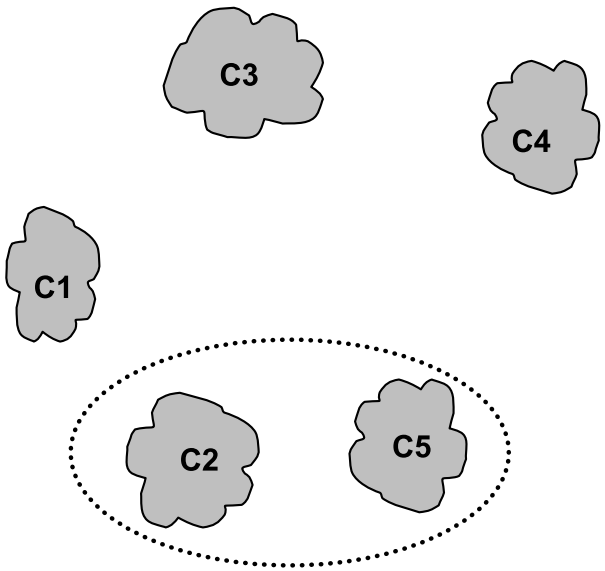
Proximity Matrix



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

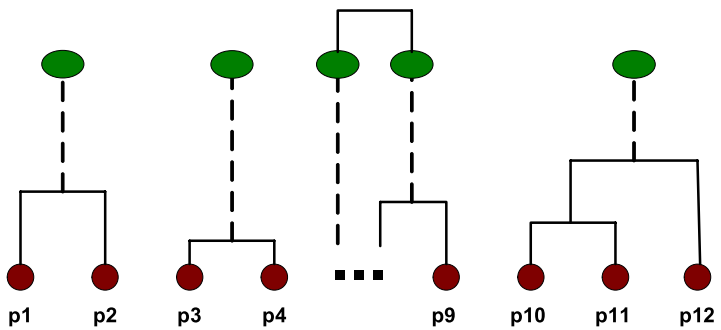
Intermediate Situation

- 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					

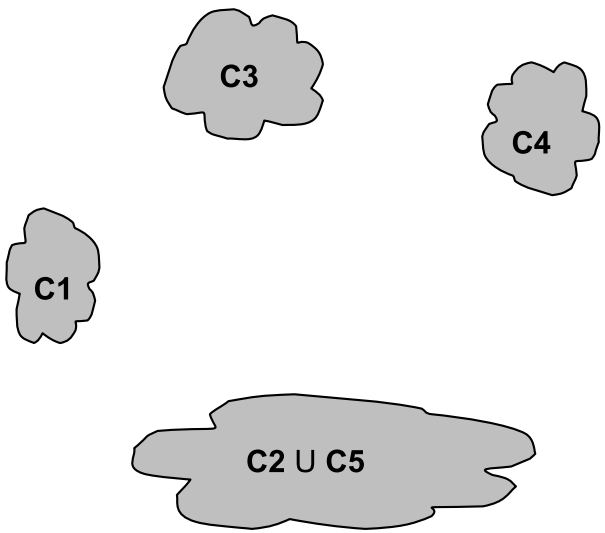
Proximity Matrix



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

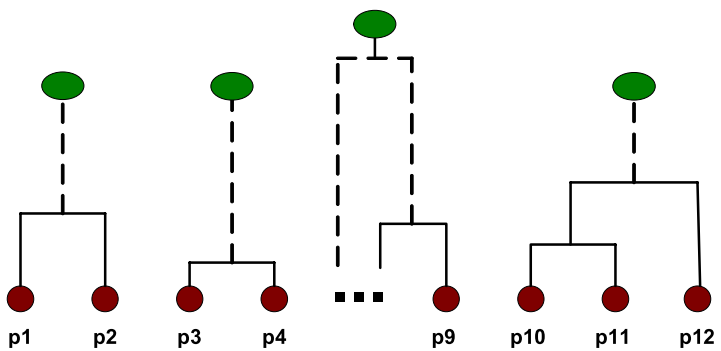
After Merging

- The question is: "How do we update the proximity matrix?".



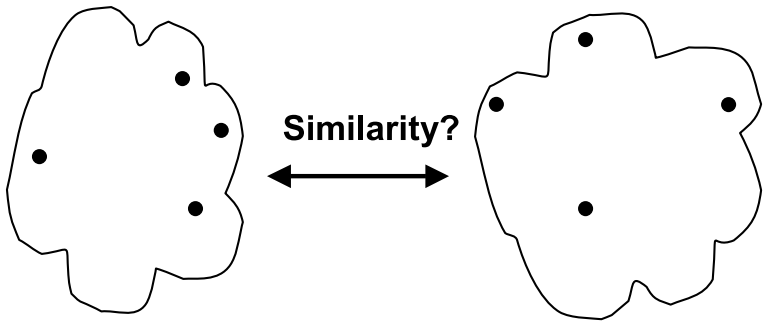
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

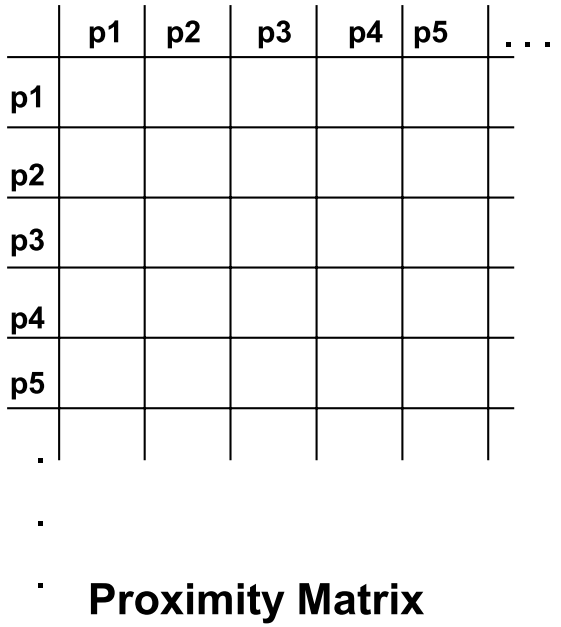
Proximity Matrix



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

How to Define Inter-Cluster Distance



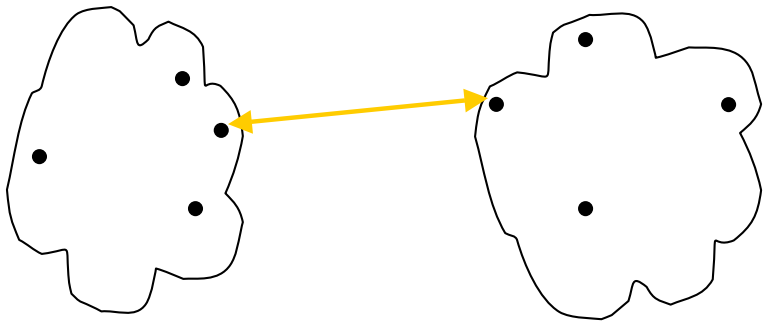


Proximity Matrix

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

How to Define Inter-Cluster Distance



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

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
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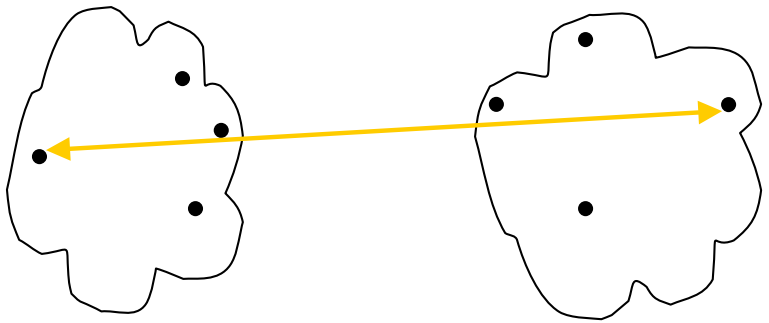
How to Define Inter-Cluster Distance



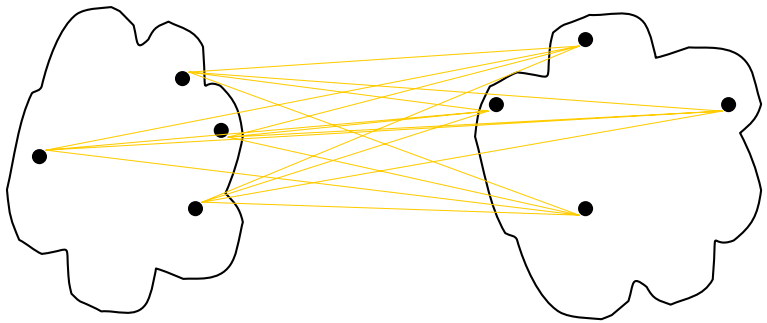
- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  - Ward's Method uses squared error

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

Proximity Matrix

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

How to Define Inter-Cluster Distance



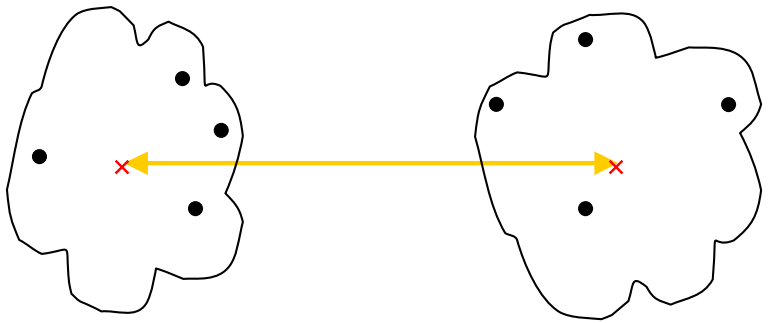
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

How to Define Inter-Cluster Distance



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

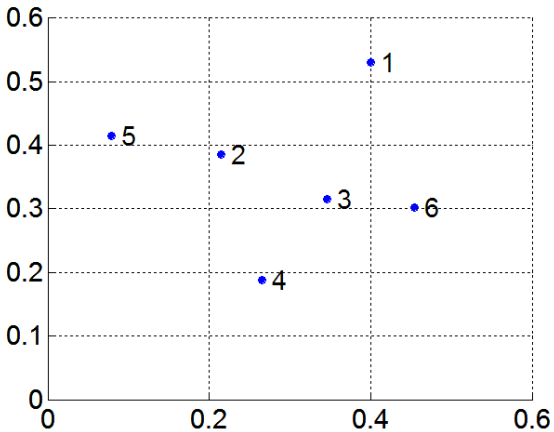
Proximity Matrix

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: MIN or Single Link

- Proximity of two clusters is based on the two closest points in the different clusters.
- Determined by one pair of points, i.e., by one link in the proximity graph.
- Example:

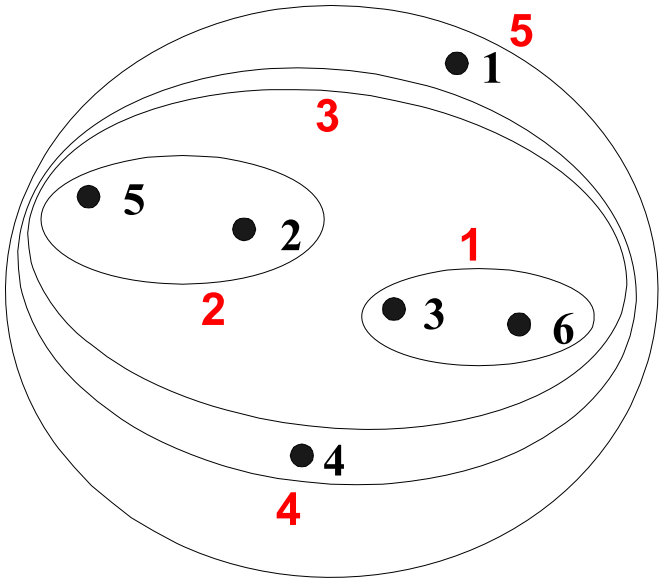


Distance Matrix:

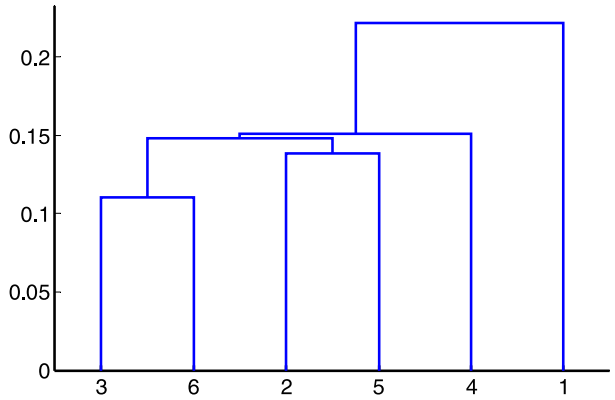
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: MIN



Nested Clusters



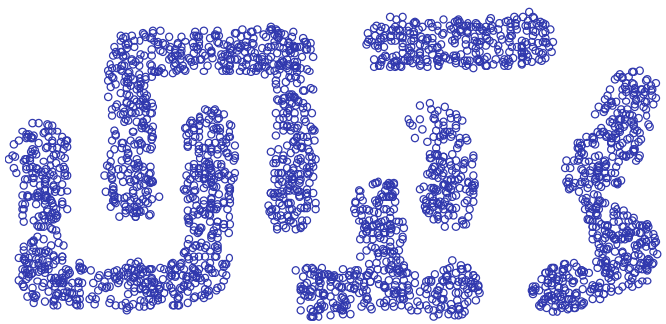
Dendrogram

$$
\begin{aligned}
dist(\{3,6\},\{2,5\}) &= \min(dist(3,2), dist(6,2), dist(3,5), dist(6,5)) \\
&= \min(0.15, 0.25, 0.28, 0.39) \\
&= 0.15.
\end{aligned}
$$

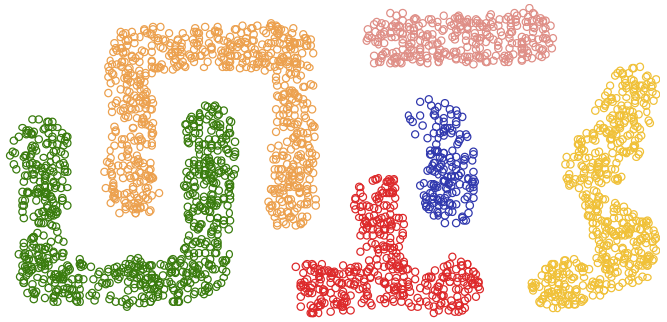
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Strengths of MIN

- Can handle non-elliptical shapes.



Original Points

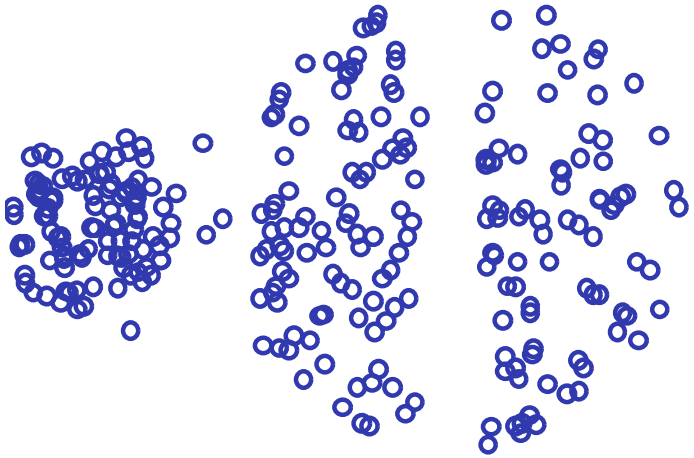


Six Clusters

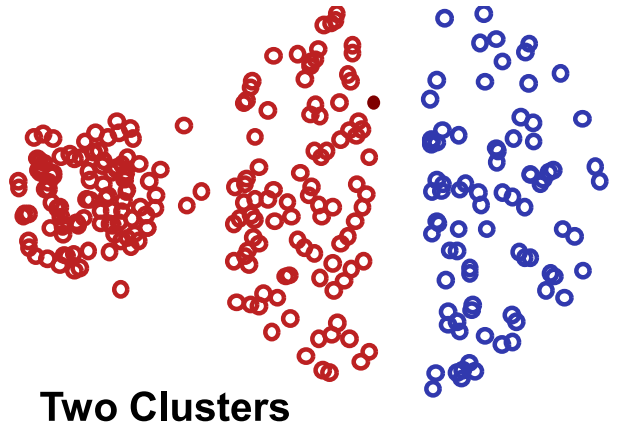
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Weakness of MIN

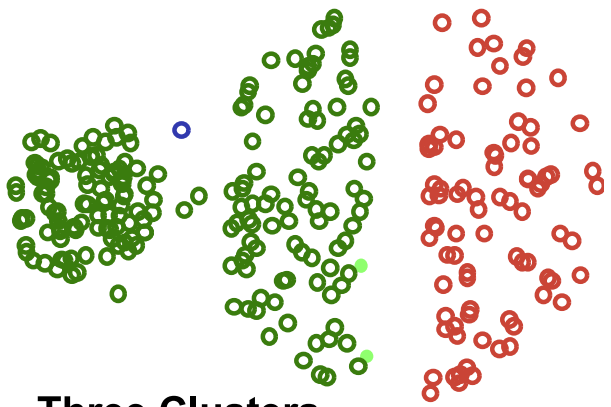
- Sensitive to noise and outliers.



Original Points



Two Clusters

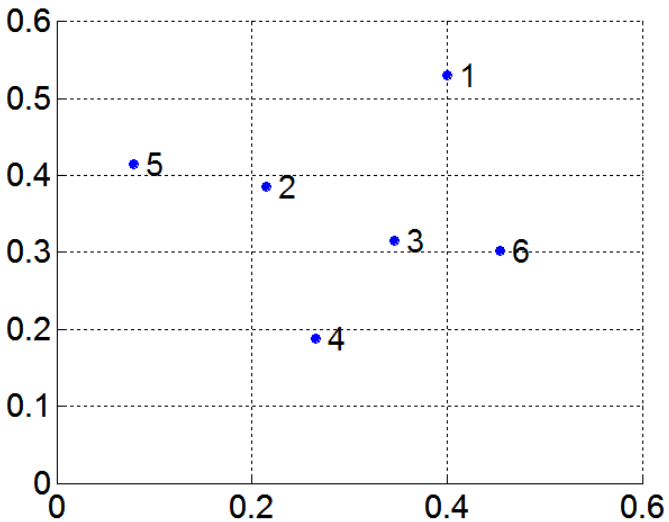


Three Clusters

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: MAX or Complete Linkage

- Proximity of two cluster is based on the two most distant points in the different clusters.
  - Determined by all pairs of points in the two clusters.

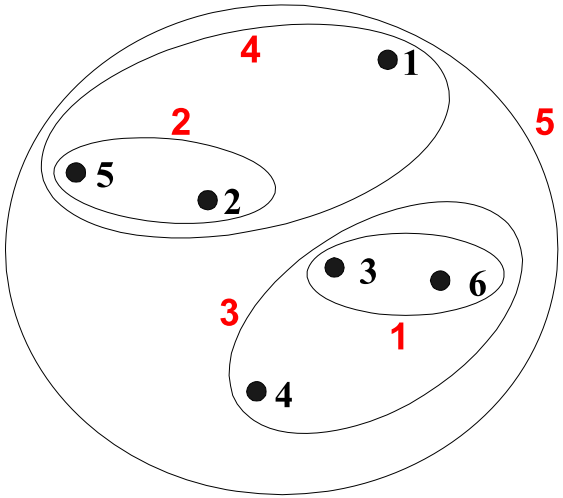


Distance Matrix:

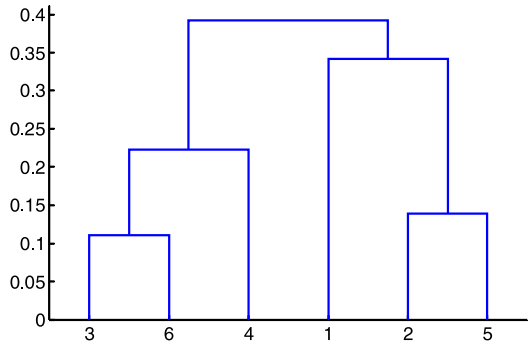
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: MAX or Complete Linkage



Nested Clusters



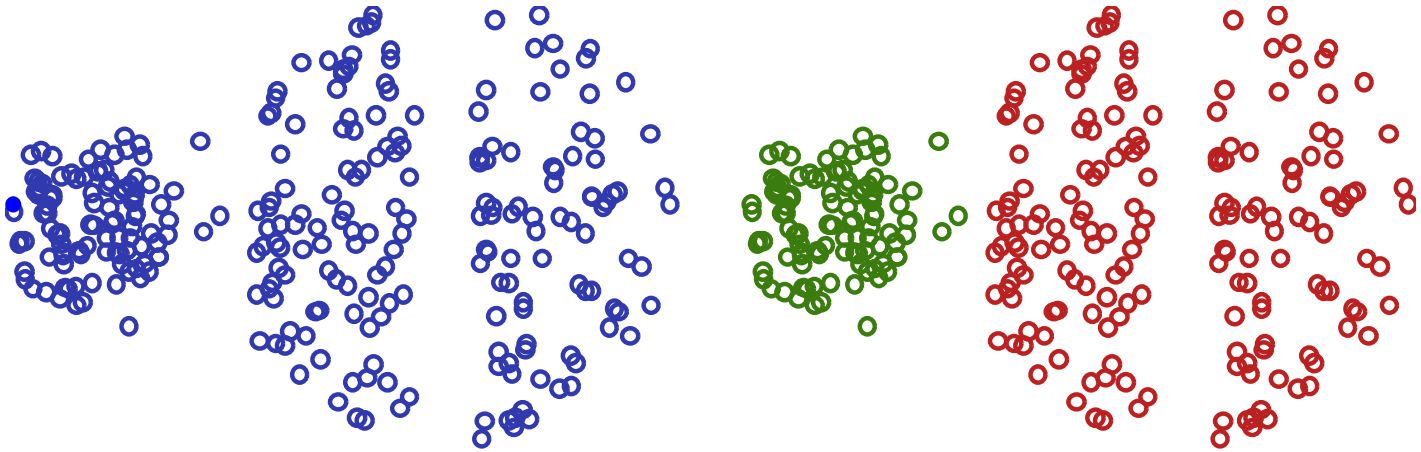
Dendrogram

$$
\begin{aligned}
dist(\{3,6\},\{4\}) &= \max(dist(3,4), dist(6,4)) \\
&= \max(0.15, 0.22) \\
&= 0.22. \\
dist(\{3,6\},\{2,5\}) &= \max(dist(3,2), dist(6,2), dist(3,5), dist(6,5)) \\
&= \max(0.15, 0.25, 0.28, 0.39) \\
&= 0.39. \\
dist(\{3,6\},\{1\}) &= \max(dist(3,1), dist(6,1)) \\
&= \max(0.22, 0.23) \\
&= 0.23.
\end{aligned}
$$

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Strengths of MAX

- Less susceptible to noise and outliers.

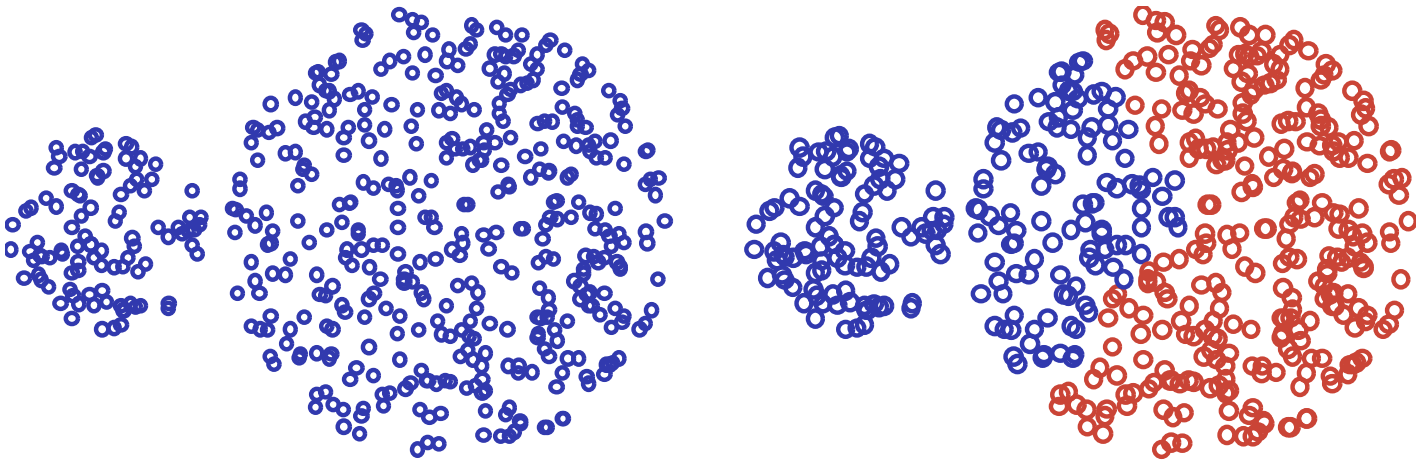


Original Points **Two Clusters**

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Limitations of MAX

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



Original Points **Two Clusters**

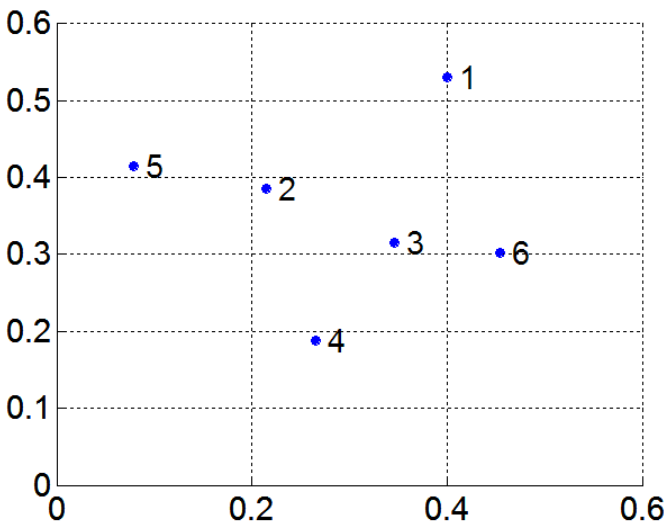
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Group Average

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

$$\text{proximity}(\text{cluster}_1, \text{cluster}_2) = \frac{\sum_{\substack{p_i \in \text{cluster}_i \\ p_j \in \text{cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{cluster}_i| \cdot |\text{cluster}_j|}. \quad (3)$$

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

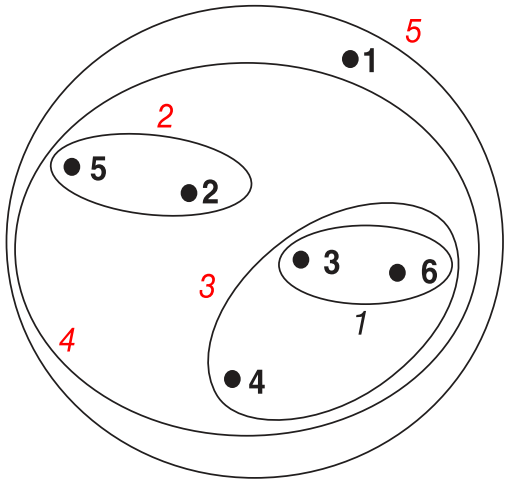


Distance Matrix:

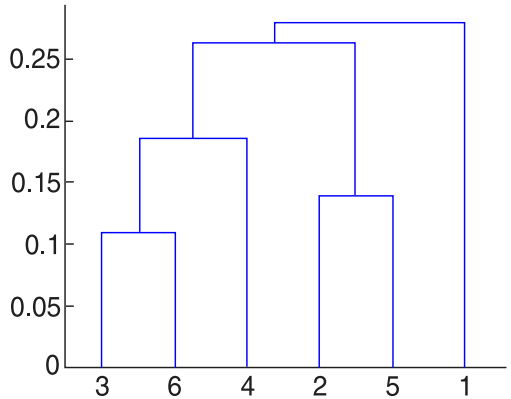
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Group Average



(a) Group average clustering.



(b) Group average dendrogram.

$$
\begin{aligned}
dist(\{3,6,4\},\{1\}) &= (0.22+0.37+0.23)/(3\times 1) \\
&= 0.28 \\
dist(\{2,5\},\{1\}) &= (0.24+0.34)/(2\times 1) \\
&= 0.29 \\
dist(\{3,6,4\},\{2,5\}) &= (0.15+0.28+0.25+0.39+0.20+0.29)/(3\times 2) \\
&= 0.26
\end{aligned}
$$

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Group Average

- Compromise between single and complete link.
- Strengths: less susceptible to noise and outliers.
- Limitations: biased towards globular clusters.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Hierarchical Clustering: Time and Space Requirements

- $\mathcal{O}(N^2)$ space since it uses the proximity matrix.
  - N is the number of points.
- $\mathcal{O}(N^3)$ 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 $\mathcal{O}(N^2 \log(N))$ time with some cleverness.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

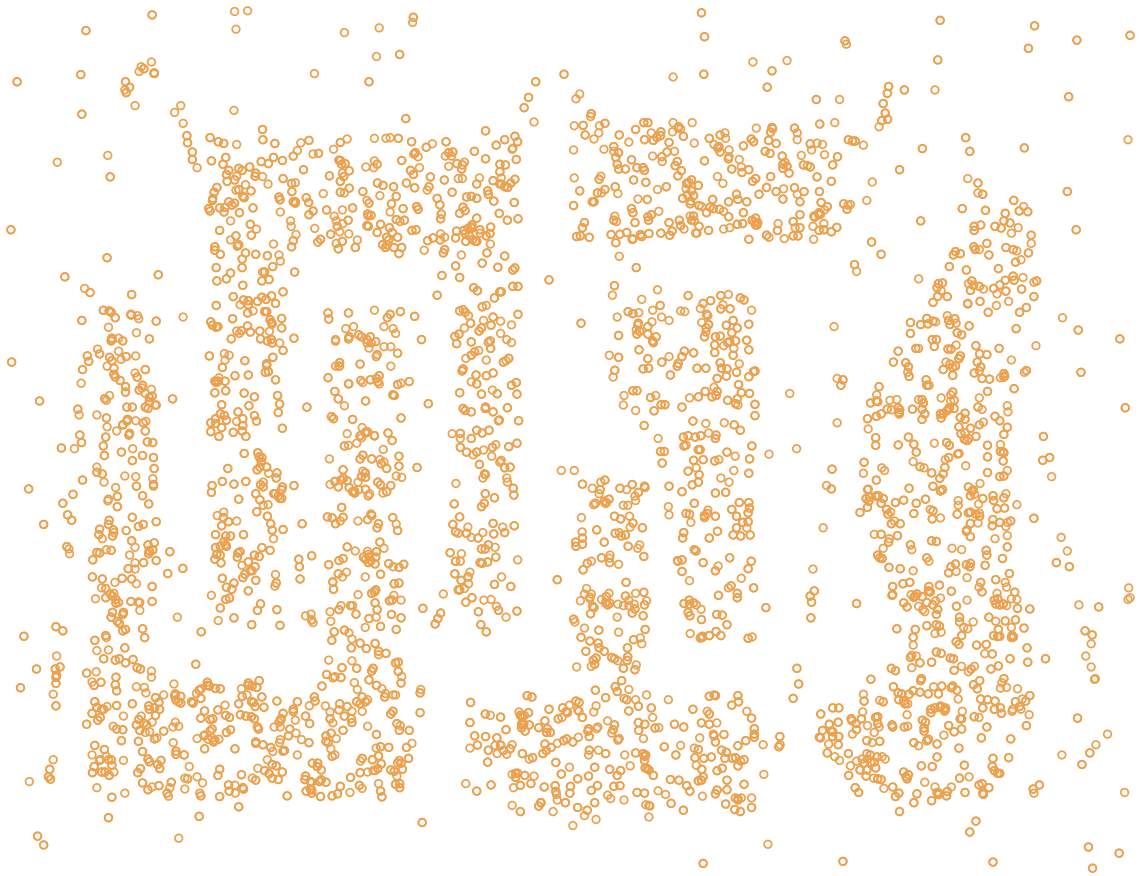
Hierarchical Clustering: Problems and Limitations

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

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Density based Clustering

- Clusters are regions of high density that are separated from one another by regions on low density.



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Density based Clustering — DBSCAN Algorithm

- 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.
    - Counts the point itself.
  - A border point is not a core point, 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.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

DBSCAN — Core, Border, and Noise Points

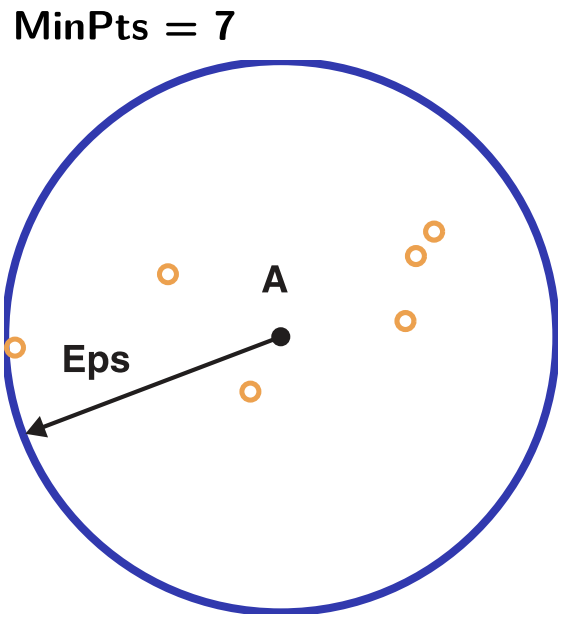


Figure 7.20. Center-based density.

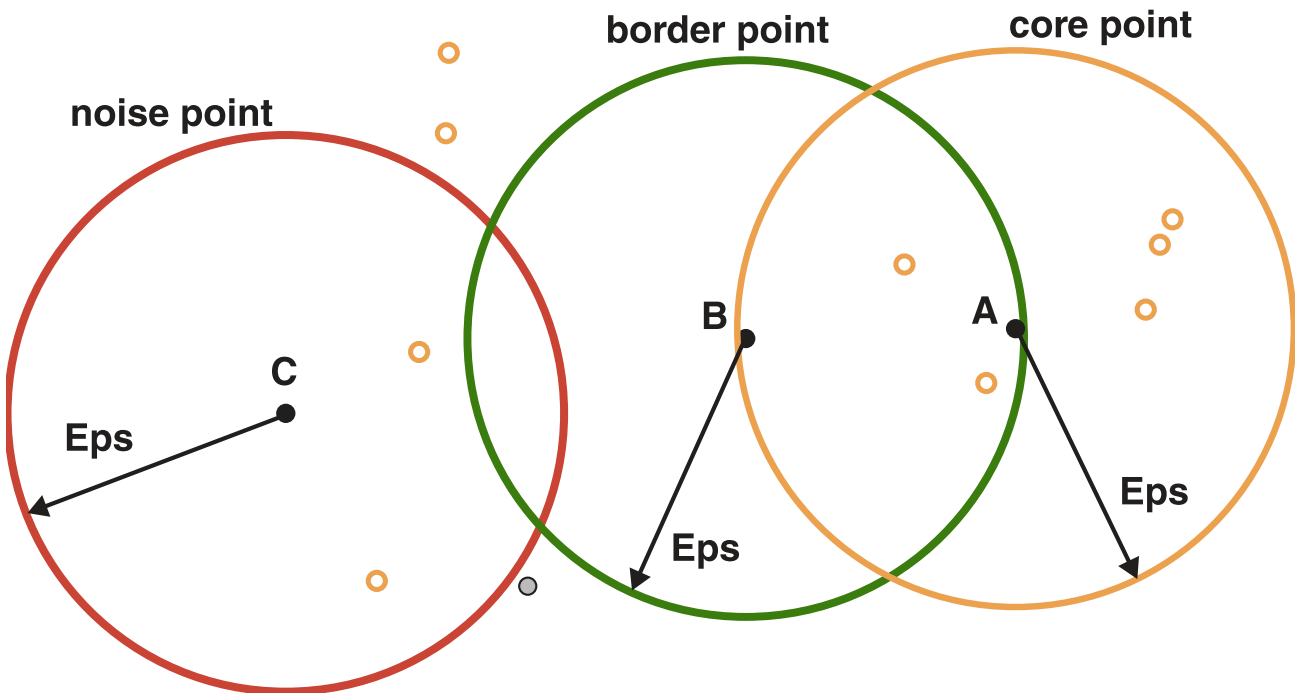
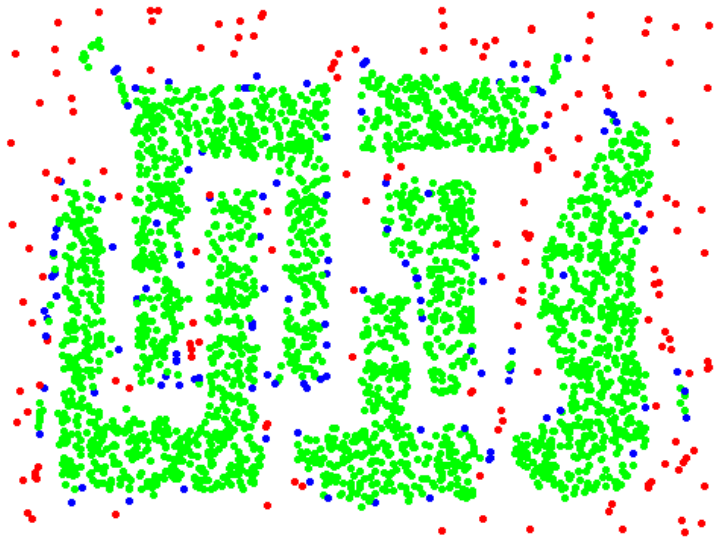


Figure 7.21. Core, border, and noise points.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

DBSCAN — Core, Border, and Noise Points

Original Points



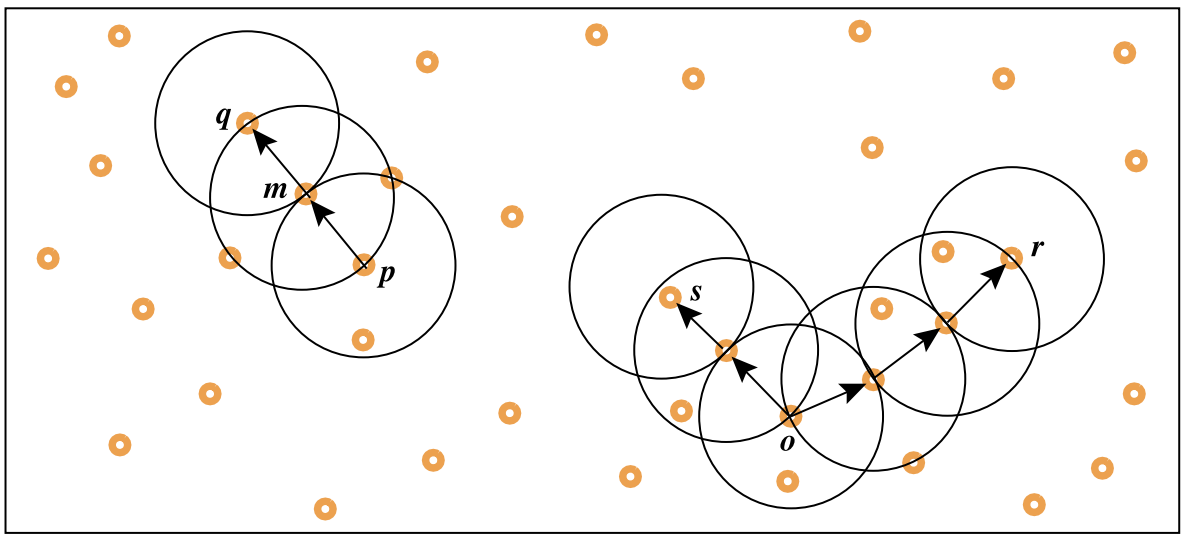
Point types: core, border and noise

Eps = 10, MinPts = 4

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

DBSCAN Algorithm

- Form clusters using core points, and assign border points to one of its neighboring clusters.
- DBSCAN Algorithm:
  1. Label all points as core, border, or noise points.
  2. Eliminate noise points.
  3. Put an edge between all core points within a distance Eps of each other.
  4. Make each group of connected core points into a separate cluster.
  5. Assign each border point to one of the clusters of its associated core points.

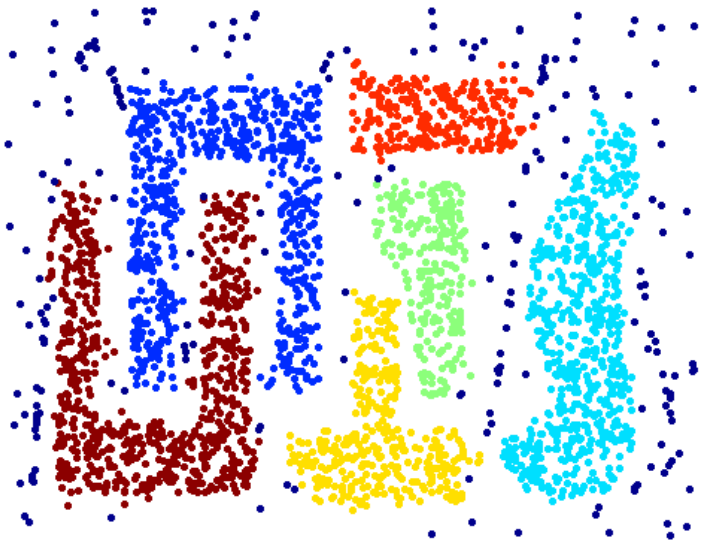


All from: 1. Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.
2. Han et al. "Data Mining Concepts and Techniques", 3rd Edition, 2012, Morgan Kaufmann Publishers.

DBSCAN— Strengths

- Resistant to noise.
- Can handle clusters of different shapes and sizes.

Original Points

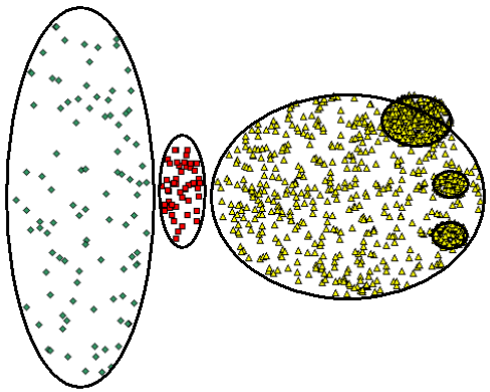


Clusters

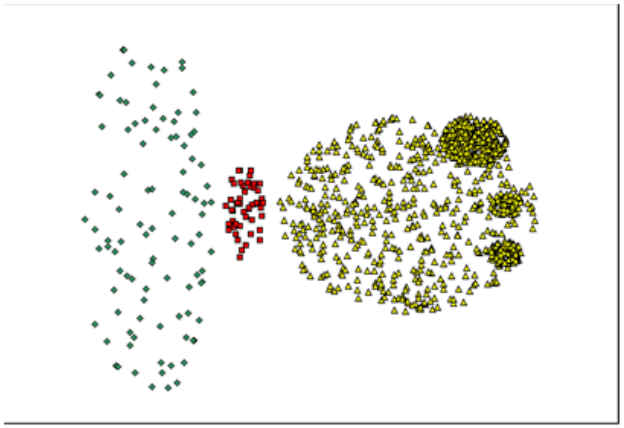
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

DBSCAN — Weakness

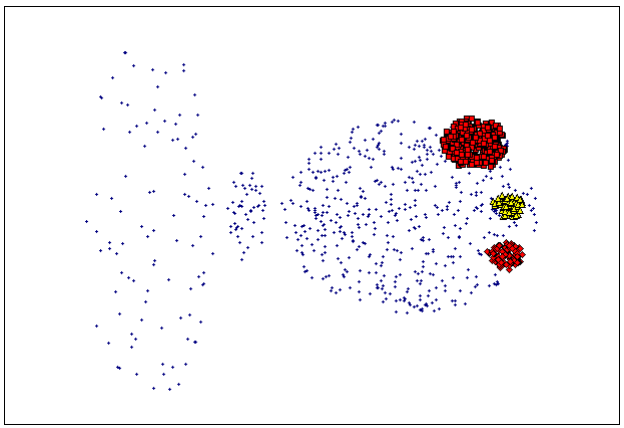
- Varying densities.
- High-dimensional data.



Original Points



(MinPts=4, Eps=9.92).



(MinPts=4, Eps=9.75)

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

DBSCAN — Determining Parameters (EPS and MinPts)

- Idea is that for points in a cluster, their k^{th} nearest neighbors are at close distance.
- Noise points have the k^{th} nearest neighbor at farther distance.
- So, plot sorted distance of every point to its k^{th} nearest neighbor.

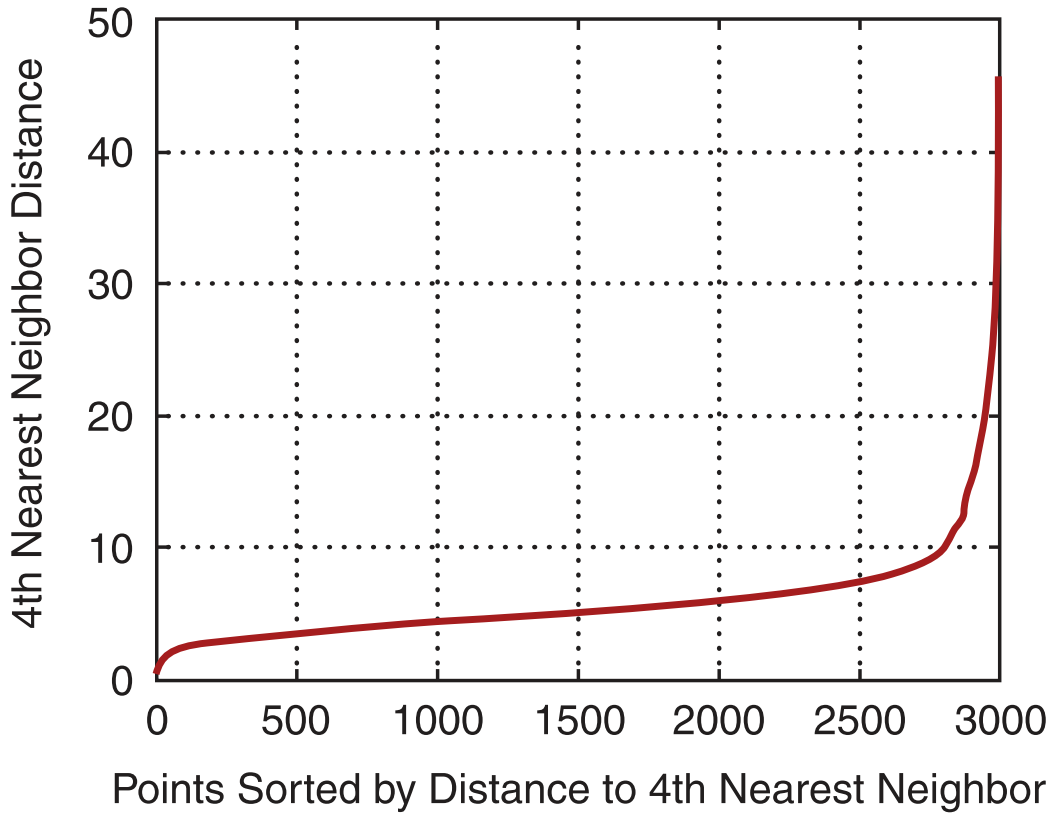


Figure 7.23. K-dist plot for sample data.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

DBSCAN — Time and Space Complexity

- Time complexity: $\mathcal{O}(m \cdot$ time to find points in the Eps-neighborhood), where m is the number of points.
- Worst case, this complexity is $\mathcal{O}(m^2)$.
- Using indexes time complexity can be as low as $\mathcal{O}(m \cdot \log(m))$.
- Space requirement is $\mathcal{O}(m)$ only a small amount of data for each point is needed (i.e., the cluster label and the identification of each point as a core, border, or noise point).

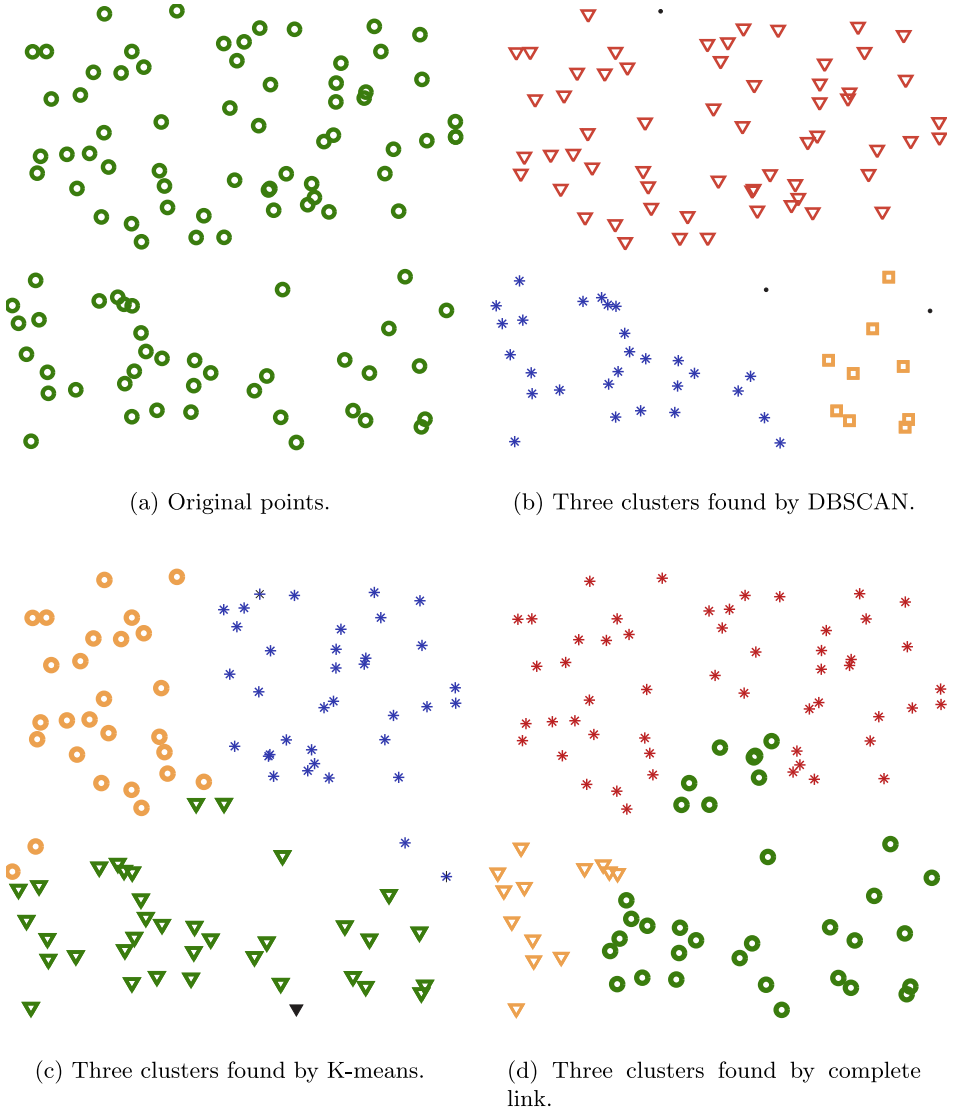
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Evaluation — 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.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Cluster that can be found in Random Data



(a) Original points.

(b) Three clusters found by DBSCAN.

(c) Three clusters found by K-means.

(d) Three clusters found by complete link.

Figure 7.26. Clustering of 100 uniformly distributed points.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Different Aspects of Cluster Validation

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data without reference to external information.
   - Use only the data.
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

- For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

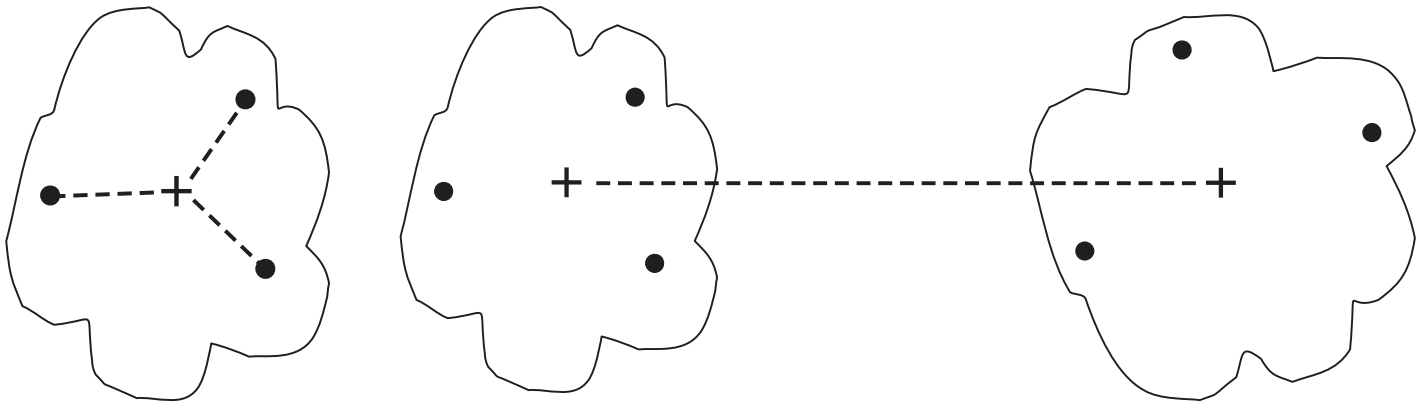
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Measures of Cluster Validity

- Numerical measures to determine cluster validity, are of three types.
- Internal Index (Unsupervised): Used to measure the goodness of a clustering structure without respect to external information.
  - Sum of Squared Error (SSE)
- External Index (Supervised): Used to measure the extent to which cluster labels match externally supplied class labels.
  - Entropy
- Relative Index: Used to compare two different clusterings or clusters.
  - Often an external or internal index is used for this function, e.g., SSE or entropy.
- Sometimes these are referred to as criteria instead of indices.
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Cohesion and Separation



(a) Cohesion. (b) Separation.

Figure 7.28. Prototype-based view of cluster cohesion and separation.

- Cluster Cohesion: Measures how closely related are objects in a cluster.
  - Example: SSE.
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Cohesion and Separation

- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE):

$$\text{SSE} = \sum_i \sum_{x \in C_i} (x - m_i)^2. \tag{4}$$

  - Separation is measured by the between cluster sum of squares.

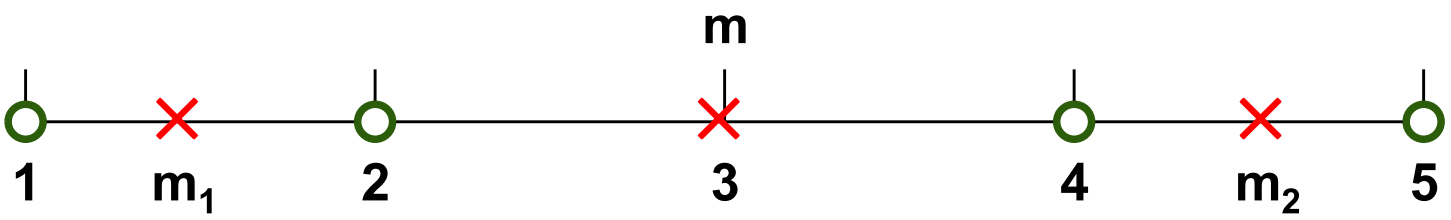
$$\text{SSB} = \sum_i |C_i| (m - m_i)^2, \tag{5}$$

  - where, $|C_i|$ is the size of cluster i.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Cohesion and Separation

- Example: SSE
  - SSB + SSE = constant.



K=1 cluster:

$$SSE = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$SSB = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

$$SSE = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

$$SSB = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

$$Total = 1 + 9 = 10$$

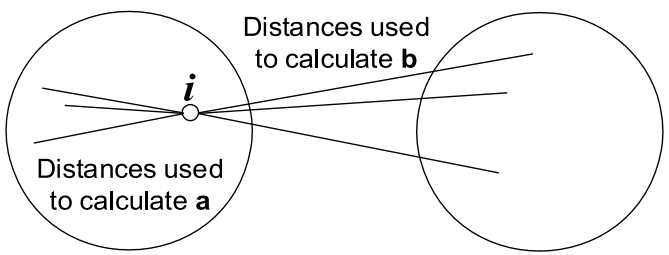
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Silhouette Coefficient

- Silhouette Coefficient: combines 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

$$s = \frac{(b - a)}{max(a, b)} \tag{6}$$

  - Value can vary between -1 and 1
  - Typically ranges between 0 and 1.
  - The closer to 1 the better.
- Can calculate the average silhouette coefficient for a cluster or a clustering.



All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Silhouette Coefficient

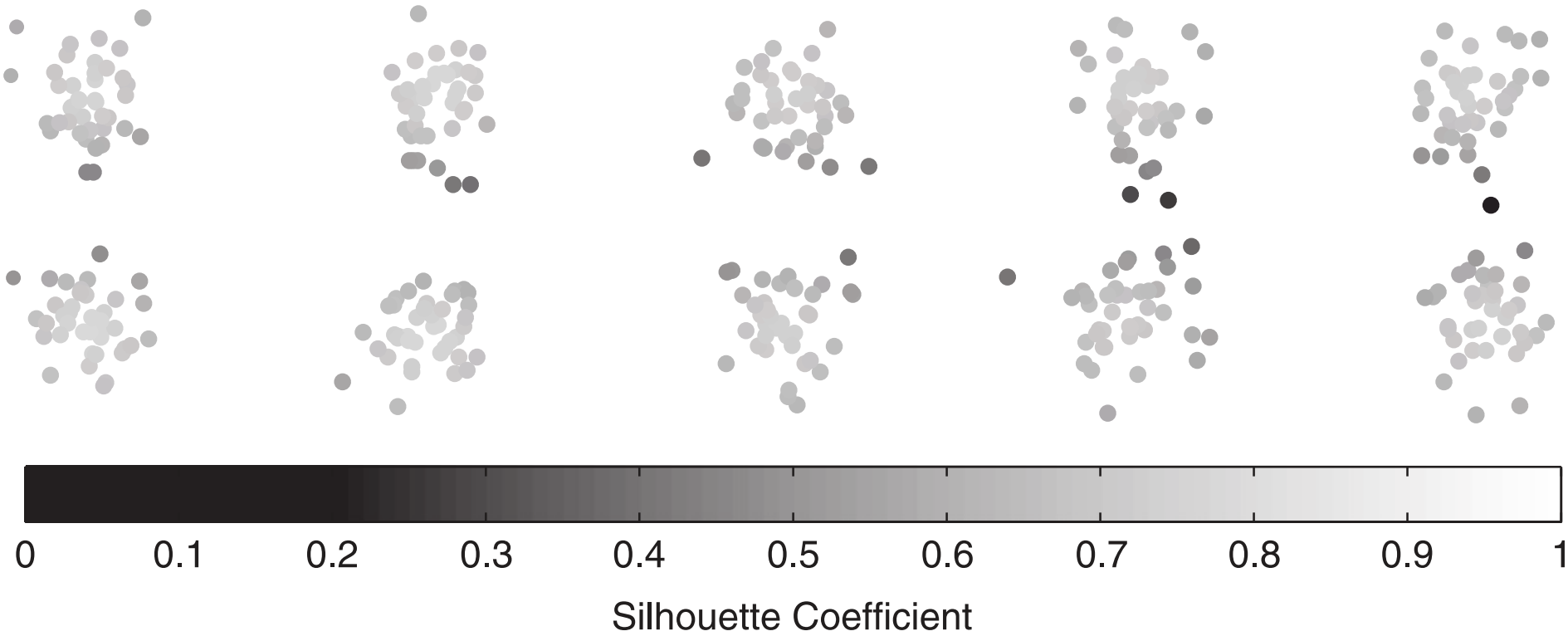


Figure 7.29. Silhouette coefficients for points in ten clusters.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Correlation

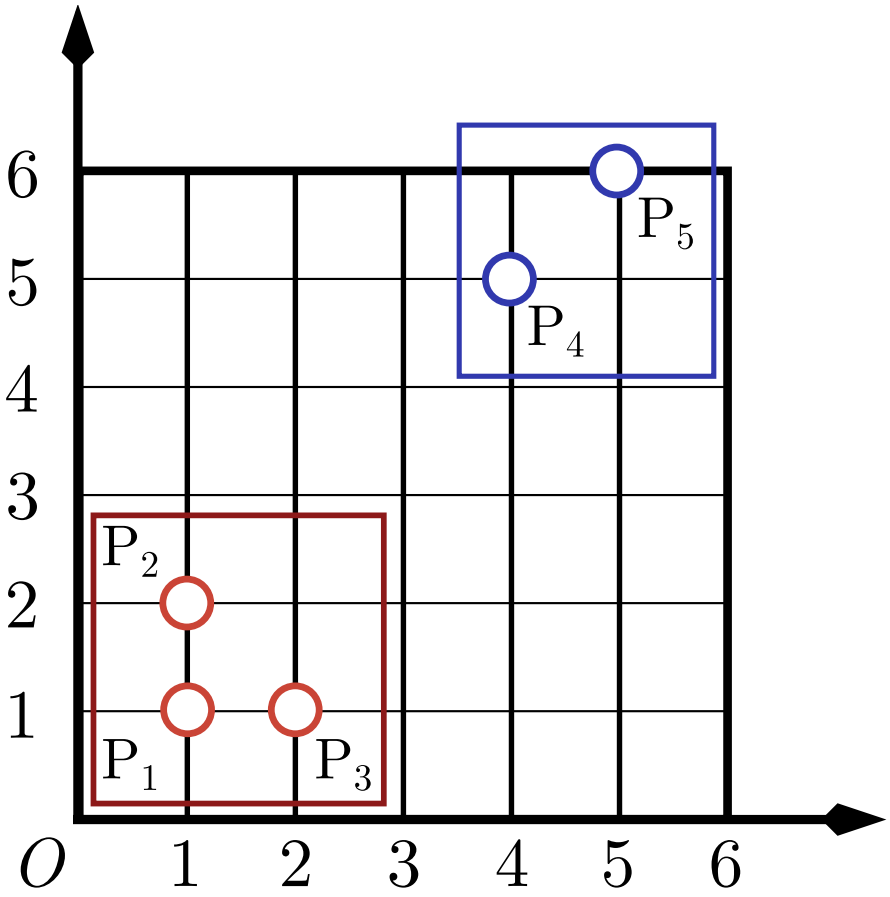
- Two matrices:
  1. Proximity Matrix
     - A similarity matrix can also be obtained by transforming / normalizing the distances using the formula:

$$s = 1 - \frac{d - d_{min}}{d_{max} - d_{min}} \tag{7}$$

  2. Ideal Similarity Matrix
     - One row and one column for each data point.
     - An entry is 1 if the associated pair of points belong to the same cluster.
     - An entry is 0 if the associated pair of points belongs to different clusters.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Correlation



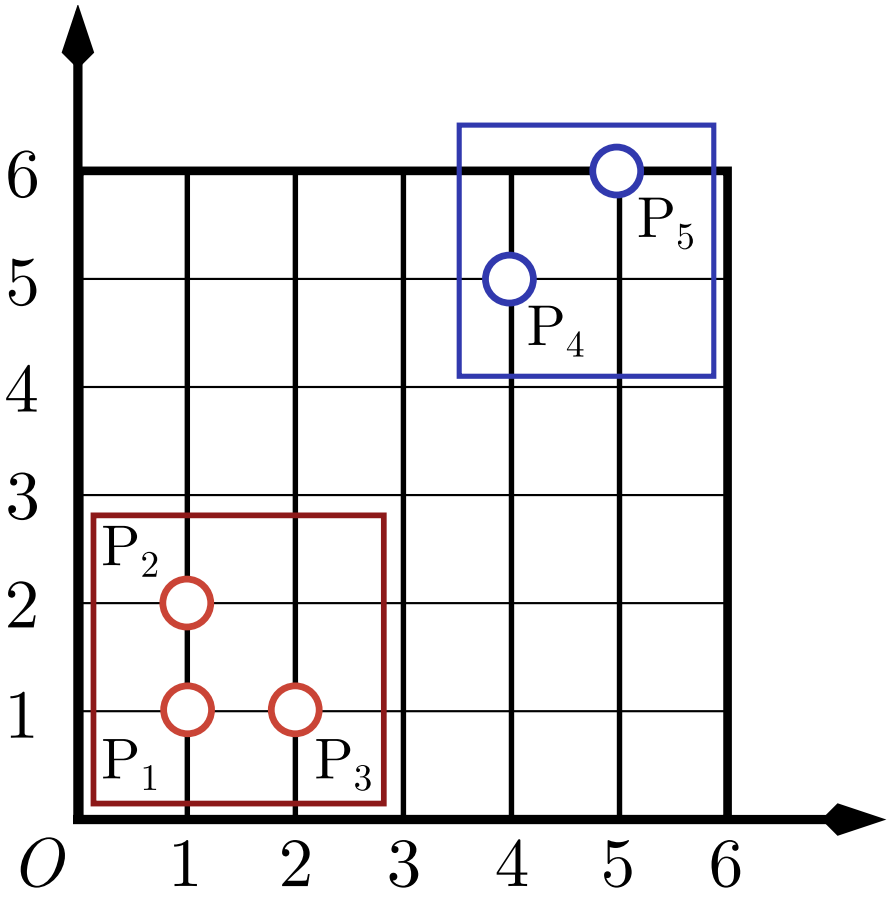
P	X	Y
1	1	1
2	1	2
3	2	1
4	4	5
5	5	6

	1	2	3	4	5
1	1	1	1	0	0
2	1	1	1	0	0
3	1	1	1	0	0
4	0	0	0	1	1
5	0	0	0	1	1

Ideal Similarity Matrix

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Correlation



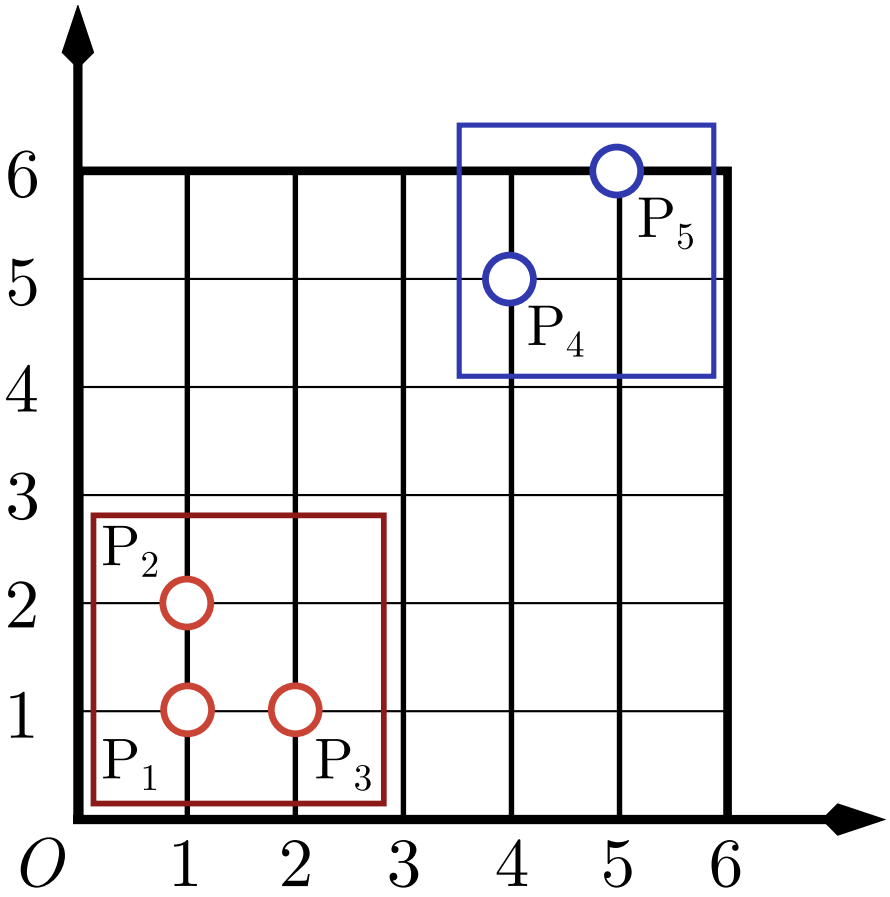
P	X	Y
1	1	1
2	1	2
3	2	1
4	4	5
5	5	6

	1	2	3	4	5
1	0	1	1	5	6.4
2	1	0	1.4	4.2	5.7
3	1	1.4	0	4.5	5.8
4	5	4.2	4.5	0	1.4
5	6.4	5.7	5.8	1.4	0

Proximity Matrix

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Correlation



P	X	Y
1	1	1
2	1	2
3	2	1
4	4	5
5	5	6

	1	2	3	4	5
1	1	0.8	0.8	0.2	0
2	0.8	1	0.8	0.3	0.1
3	0.8	0.8	1	0.3	0.1
4	0.2	0.3	0.3	1	0.8
5	0	0.1	0.1	0.8	1

Similarity Matrix

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

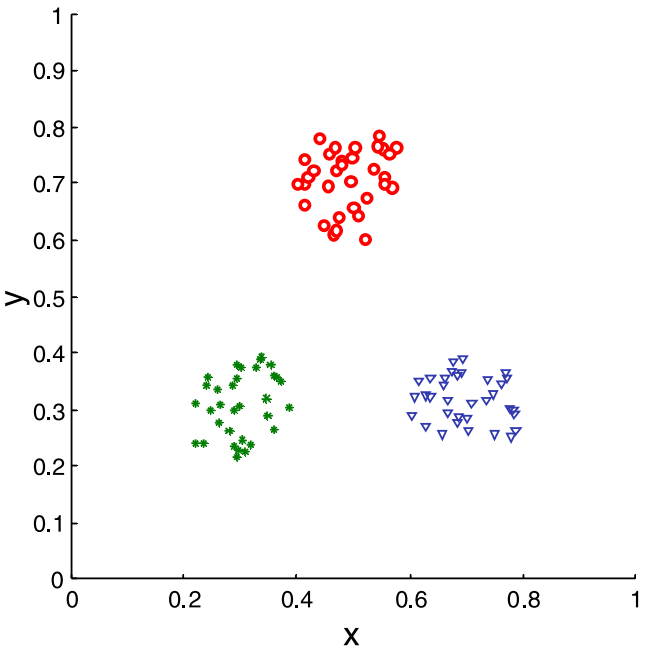
Unsupervised Cluster Evaluation: Correlation

- Compute the correlation between the two matrices.
  - Since the matrices are symmetric, only the correlation between $\frac{n \cdot (n-1)}{2}$ entries needs to be calculated.
- High magnitude of correlation indicates that points that belong to the same cluster are close to each other.
  - Correlation may be positive or negative depending on whether the similarity matrix is a similarity or dissimilarity matrix.
- Not a good measure for some density or contiguity based clusters.

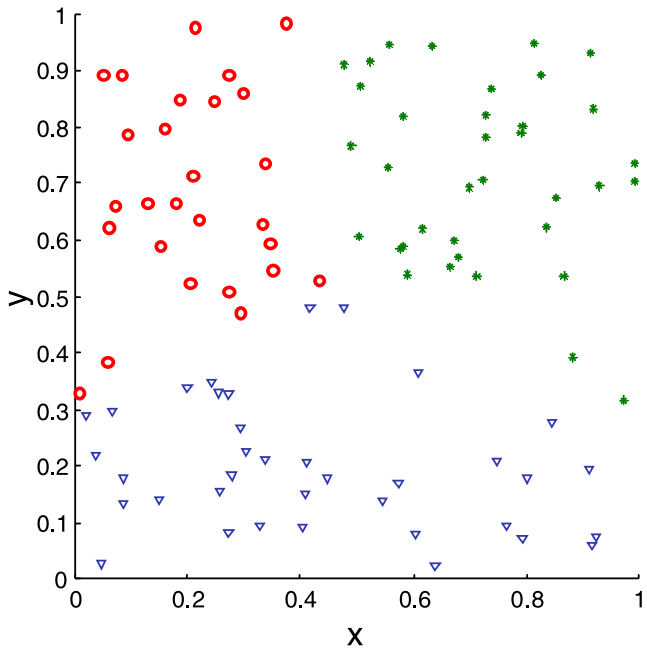
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Correlation

- Correlation of ideal similarity and proximity matrices for the K-means clusterings of the following two data sets.



Corr = -0.9235

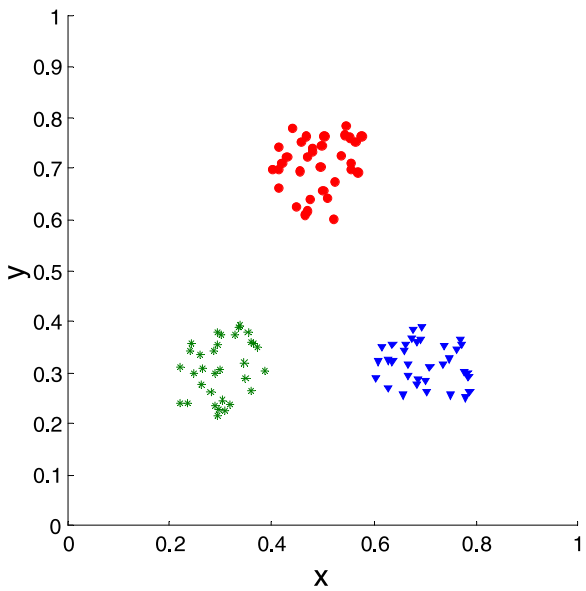


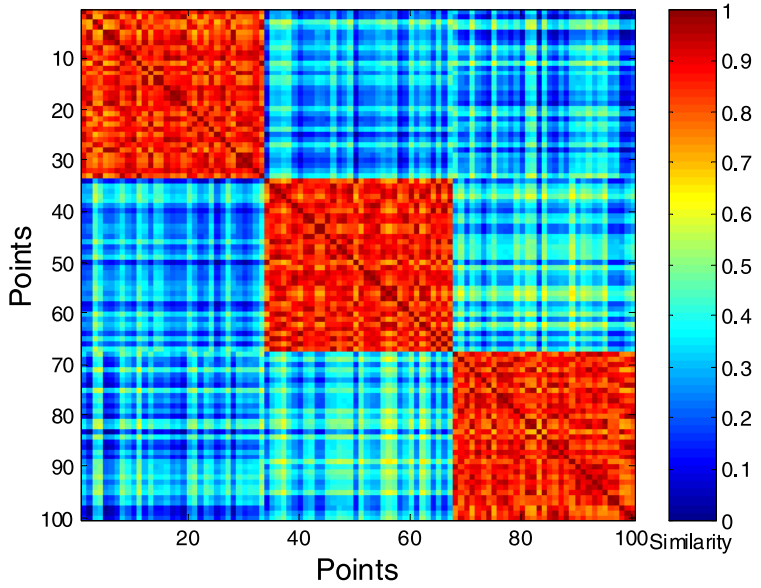
Corr = -0.5810

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Similarity Matrix

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

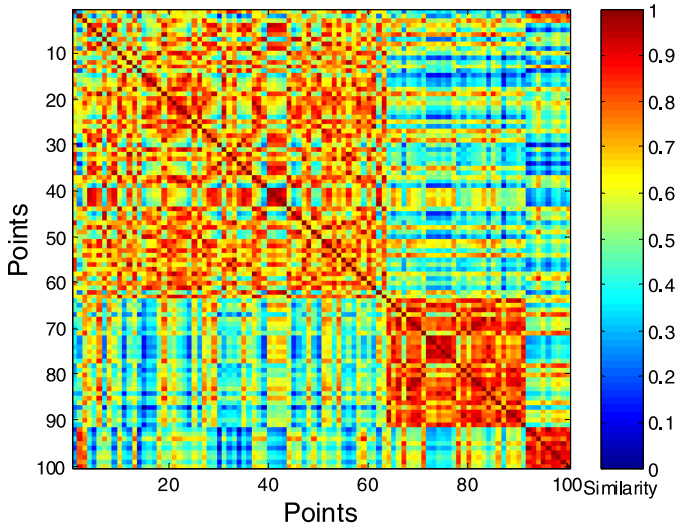


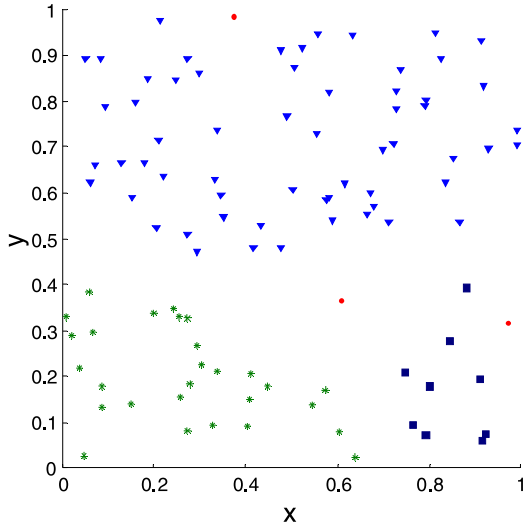


All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Similarity Matrix

- Clusters in random data are not so crisp.



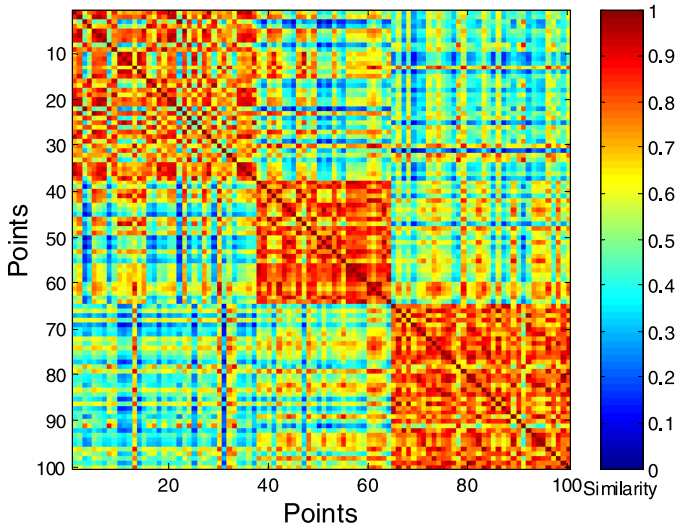


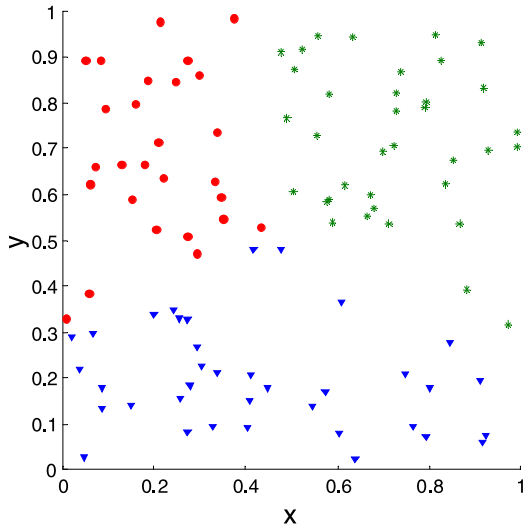
DBSCAN

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Similarity Matrix

- Clusters in random data are not so crisp.



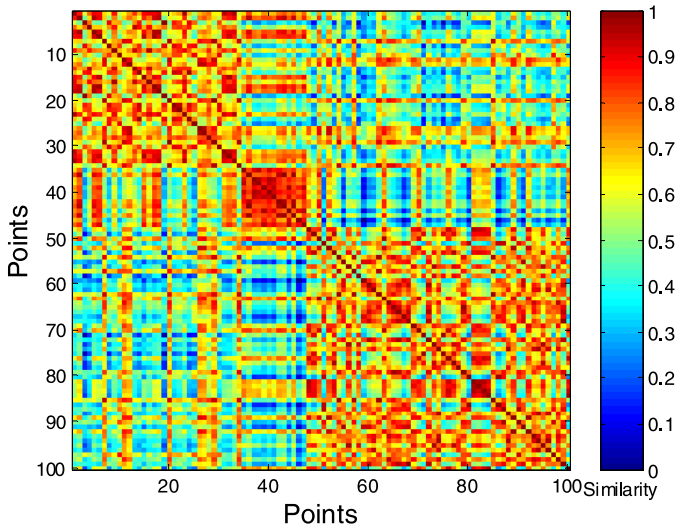


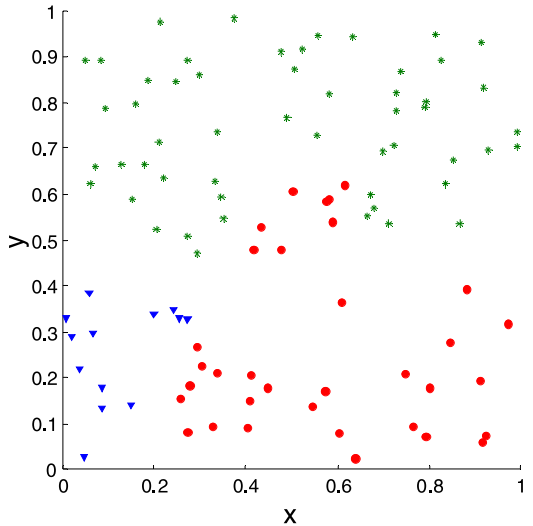
K-means

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Similarity Matrix

- Clusters in random data are not so crisp.

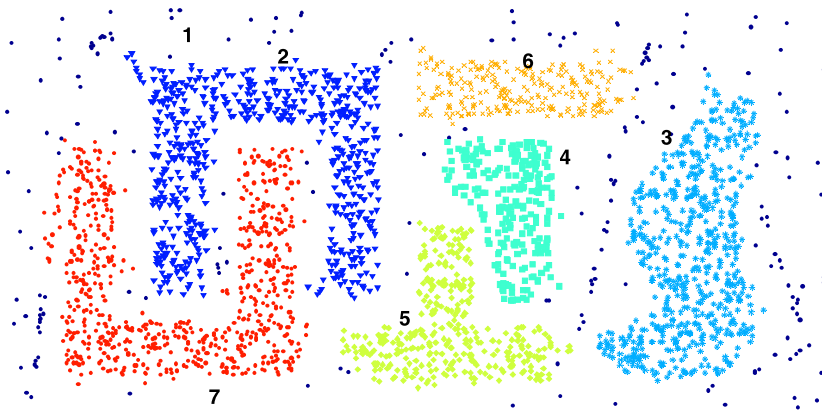


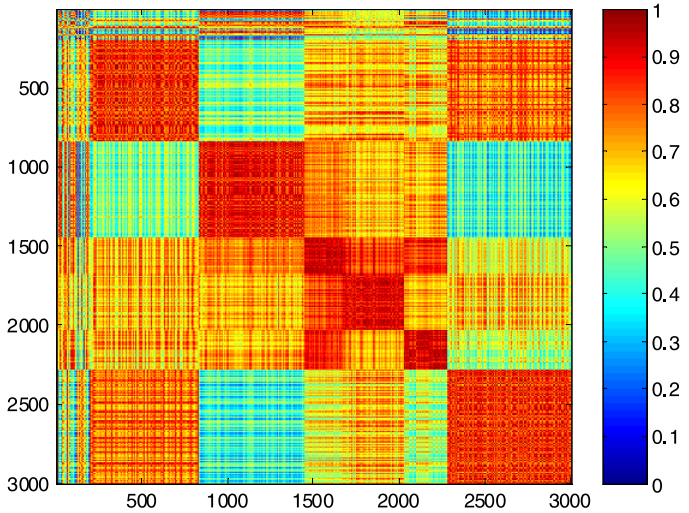


Complete Link

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Similarity Matrix





DBSCAN

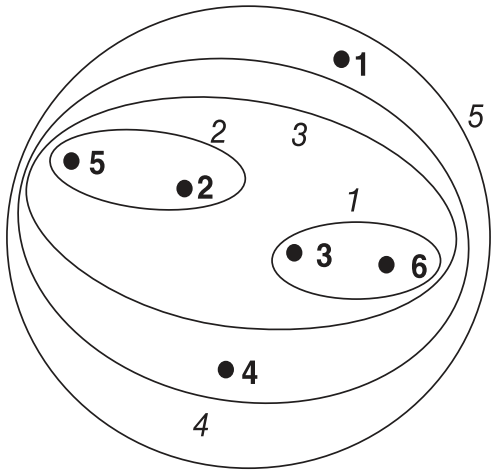
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Cophenetic Correlation

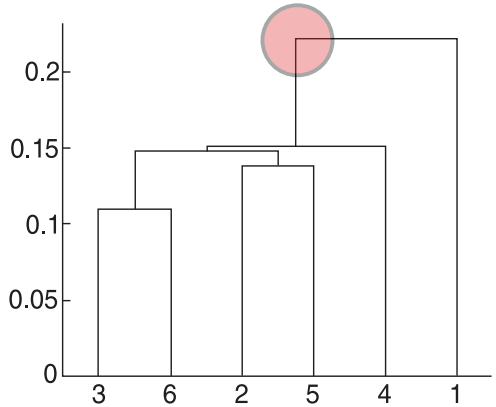
- Cophenetic Distance between two objects is the proximity at which an agglomerative hierarchical clustering technique puts the objects in the same cluster for the first time.
- Cophenetic distance matrix, the entries are the cophenetic distances between each pair of objects.
- Cophenetic Correlation Coefficient (CPCC) is the correlation between the entries of this matrix and the original dissimilarity matrix.
- It is a standard measure of how well a hierarchical clustering fits the data.
- Common use is to evaluate which type of hierarchical clustering is best for a particular type of data.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Unsupervised Cluster Evaluation: Cophenetic Correlation



(a) Single link clustering.



(b) Single link dendrogram.

Figure 7.16. Single link clustering of the six points shown in Figure 7.15.

Table 7.7. Cophenetic distance matrix for single link and data in Table 2.14 on page 90.

Point	P1	P2	P3	P4	P5	P6
P1	0	0.222	0.222	0.222	0.222	0.222
P2	0.222	0	0.148	0.151	0.139	0.148
P3	0.222	0.148	0	0.151	0.148	0.110
P4	0.222	0.151	0.151	0	0.151	0.151
P5	0.222	0.139	0.148	0.151	0	0.148
P6	0.222	0.148	0.110	0.151	0.148	0

Technique	CPCC
Single Link	0.44
Complete Link	0.63
Group Average	0.66
Ward's	0.64

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Clustering Tendency — Hopkins Statistic

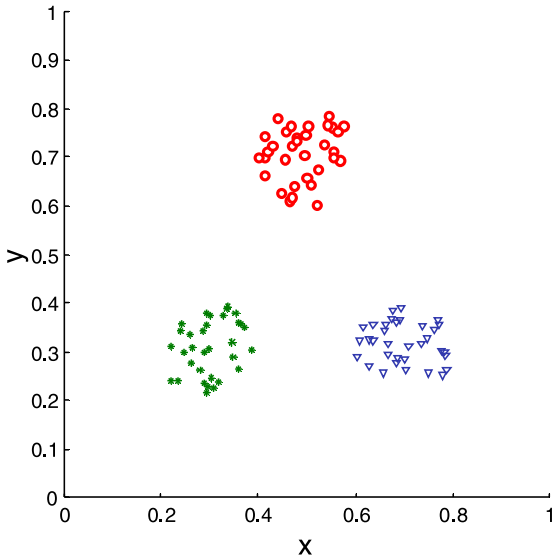
1. Generate p points that are randomly distributed across the data space.
2. Sample p actual data points.
3. For both sets of points, we find the distance to the nearest neighbor in the original data set.
4. Let the u_i be the nearest neighbor distances of the artificially generated points, while the w_i are the nearest neighbor distances of the sample of points from the original data set.
5. The Hopkins statistic H is then defined by:

$$H = \frac{\sum_{i=1}^{p} w_i}{\sum_{i=1}^{p} u_i + \sum_{i=1}^{p} w_i} \tag{8}$$

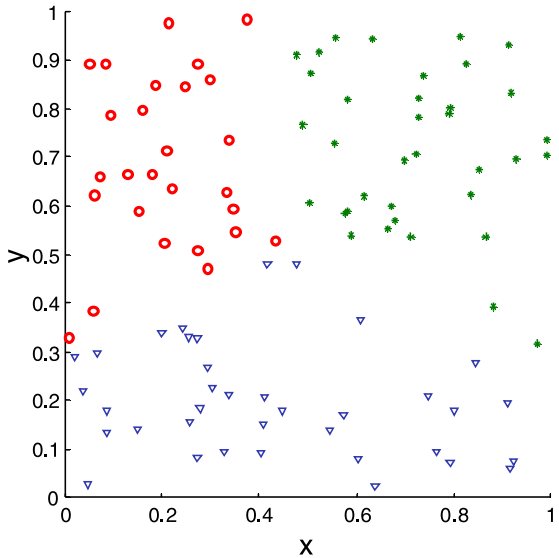
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Clustering Tendency — Hopkins Statistic

- $H \approx 0.5$: randomly generated points and the sample of data points have roughly the same nearest neighbor distances.
- $H \approx 1.0$: data that is regularly distributed in the data space.
- $H \approx 0.0$: data that is highly clustered.



Average Value of H = 0.95



Average Value of H = 0.56

Figure: Statistic accompanying the figures are wrong in the book.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Clustering Tendency — Hopkins Statistic

$$HS_i = \frac{\sum_{y_j \in \mathbf{R}_i} (\delta_{\min}(\mathbf{y}_j))^d}{\sum_{y_j \in \mathbf{R}_i} (\delta_{\min}(\mathbf{y}_j))^d + \sum_{x_j \in \mathbf{D}_i} (\delta_{\min}(\mathbf{x}_j))^d} \tag{9}$$

- This statistic compares the nearest-neighbor distribution of randomly generated points to the same distribution for random subsets of points from **D**.
- $\delta_{\min}(x_j) < \delta_{\min}(y_j)$: HS_i tends to 1.0: data is well clustered.
- $\delta_{\min}(x_j) \approx \delta_{\min}(y_j)$: HS_i tends to 0.5: data is essentially random.
- $\delta_{\min}(x_j) > \delta_{\min}(y_j)$: HS_i tends to 0.0: indicates point repulsion, with no clustering.

All from: Zaki and Meira, "Data Mining and Machine Learning: Fundamental Concepts and Algorithms", 2nd Edition, 2020, Cambridge University Press.

Clustering Tendency — Hopkins Statistic

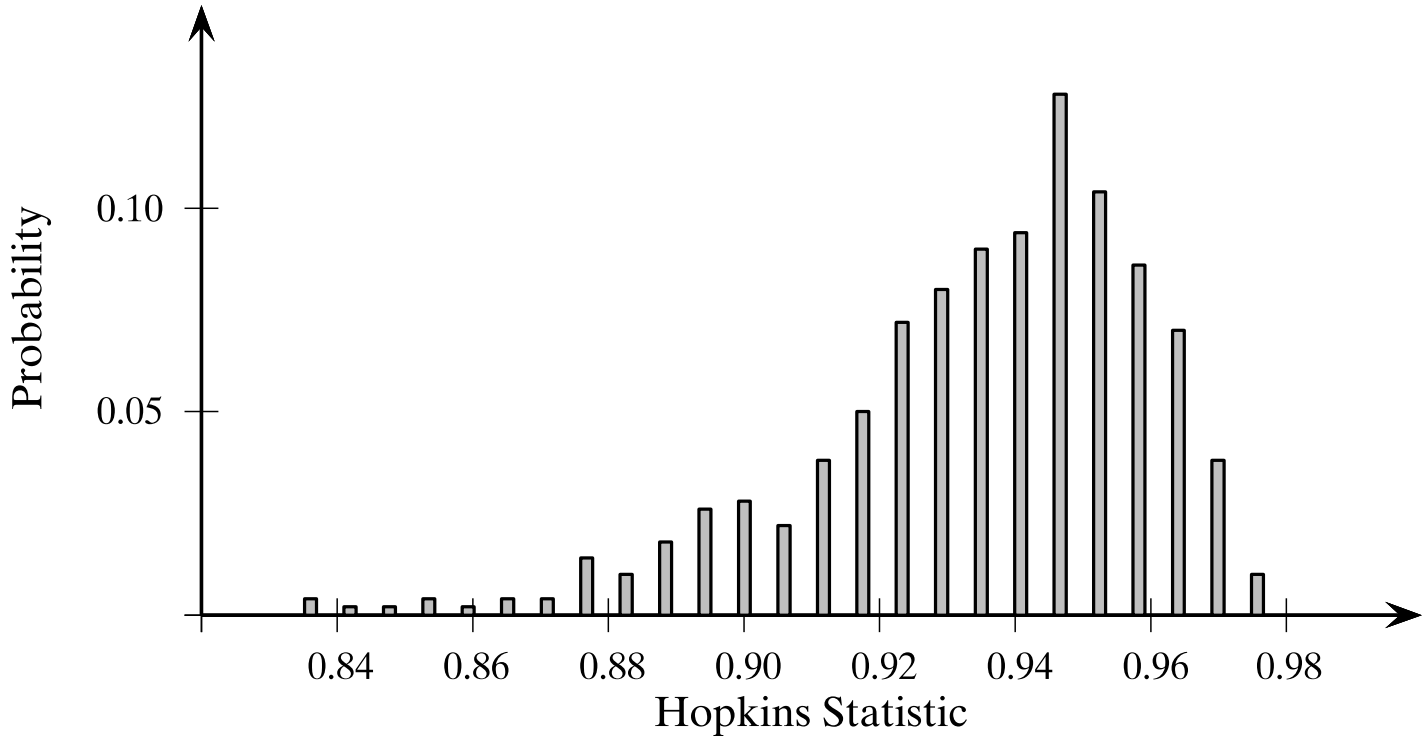


Figure 17.9. Iris dataset: Hopkins statistic distribution.

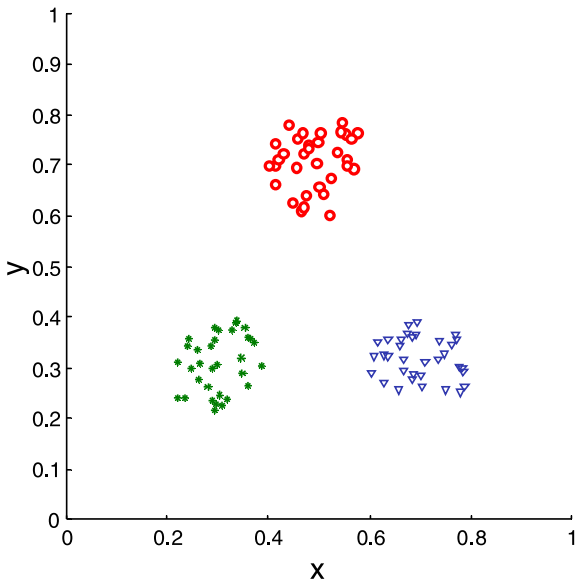
Framework for Cluster Validity

- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity.
  - The more "atypical" a clustering result is, the more likely it represents valid structure in the data.
  - Can compare the values of an index that result from random data or clusterings to those of a clustering result.
  - If the value of the index is unlikely, then the cluster results are valid.
- For comparing the results of two different sets of cluster analyses, a framework is less necessary.
  - However, there is the question of whether the difference between two index values is significant.

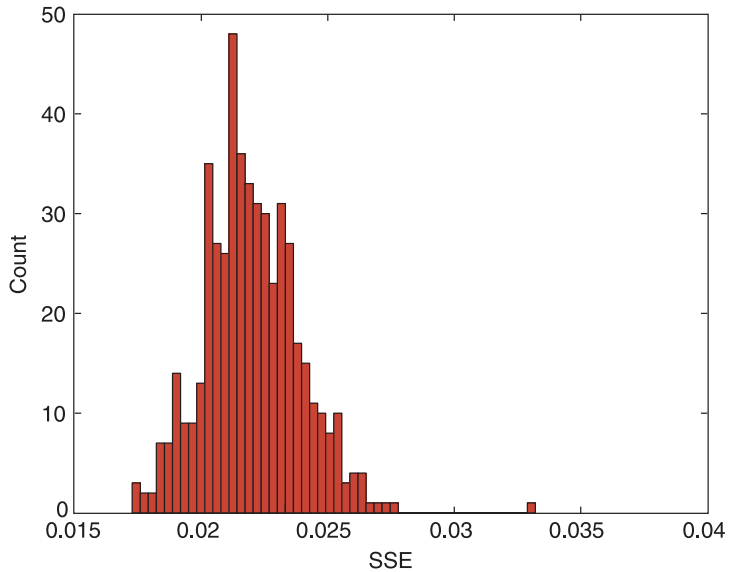
All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Statistical Framework for SSE

- Example: Compare SSE of three cohesive clusters against three clusters in random data.



SSE = 0.005



Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.

Supervised Cluster Evaluation

- We will cover supervised evaluation metrics (e.g., Precision, Recall, Entropy) in classification.

All from: Tan et al. "Introduction to Data Mining", 1st Edition, 2006, Pearson Education Inc.