DATA MINING
CLUSTERING

The k-means algorithm

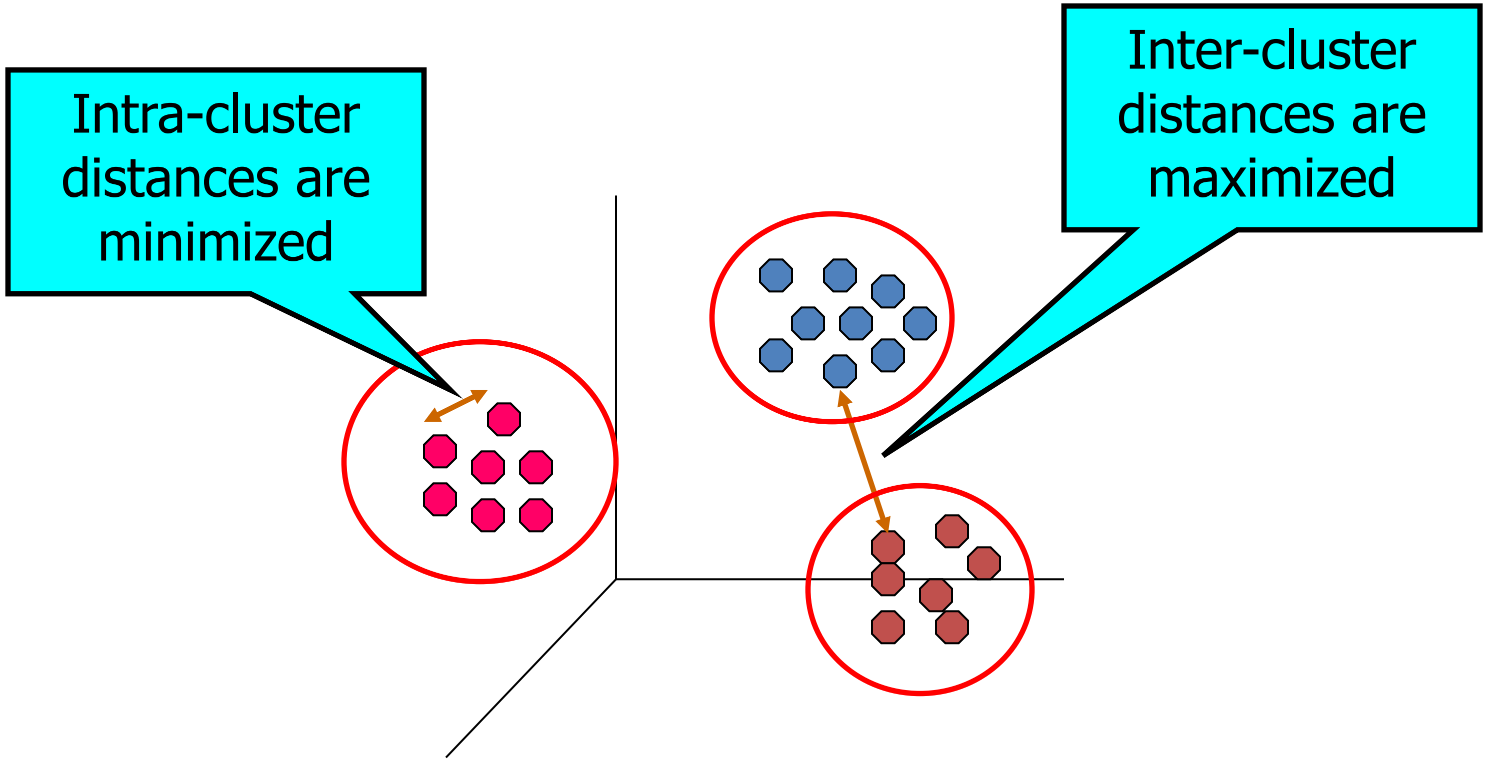
Hierarchical Clustering

The DBSCAN algorithm

Evaluation

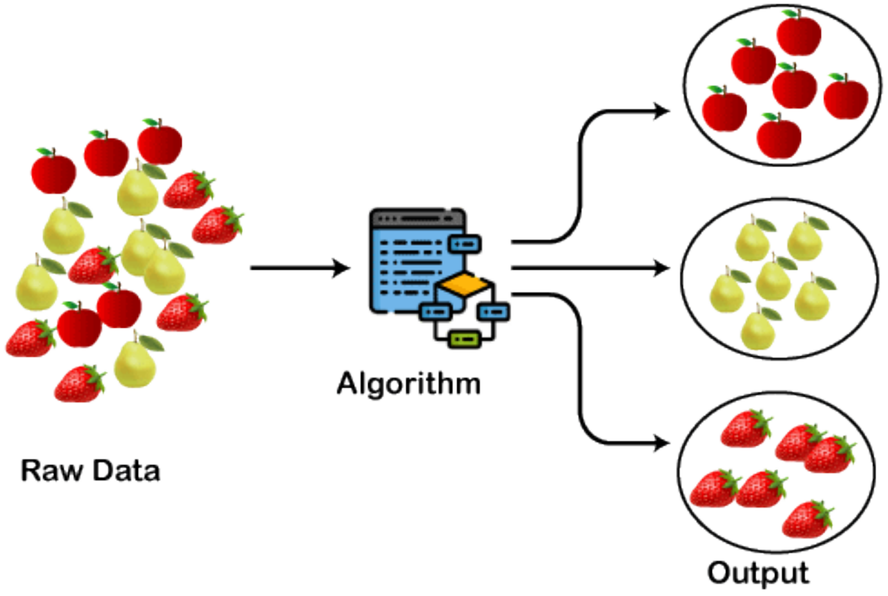
What is a Clustering?

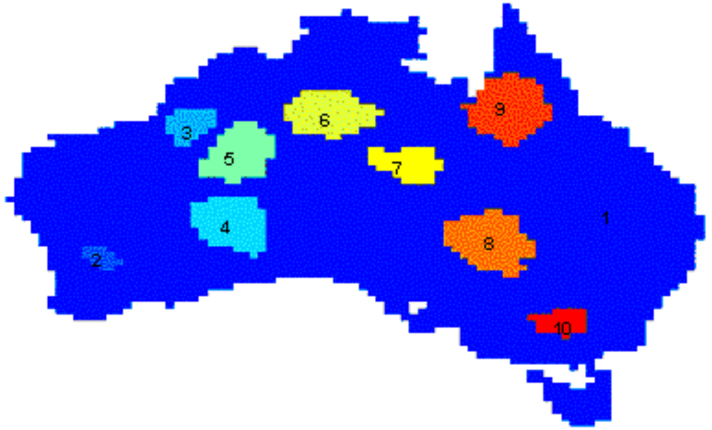
A grouping of objects such that the objects in a group (cluster) are similar (or related) to one another and different from (or unrelated to) the objects in other groups (clusters)



Why Cluster Analysis

- **Understanding**
  - Group related documents for browsing, genes and proteins that have similar functionality, stocks with similar price fluctuations, users with same behavior
- **Summarization**
  - Reduce the size of large data sets
- **Applications**
  - Recommendation systems
  - Search Personalization





Clustering precipitation 降水量 in Australia

Early applications of cluster analysis

- John Snow, London 1854

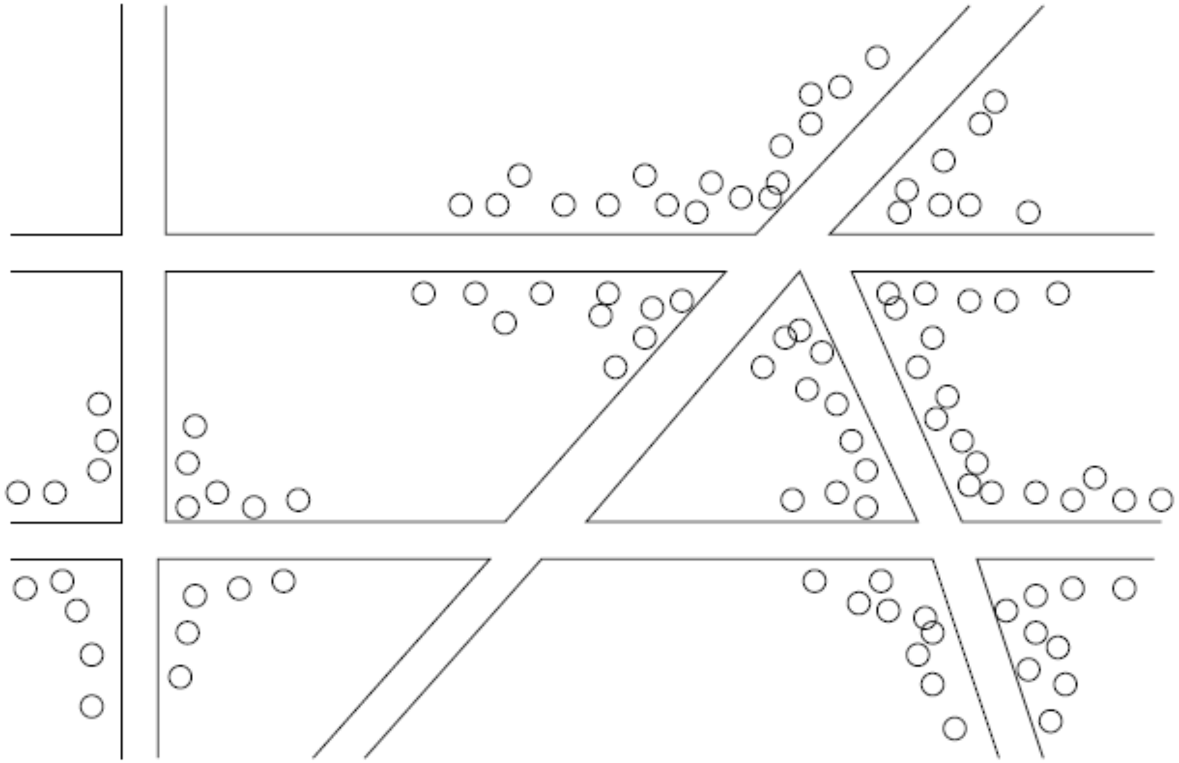


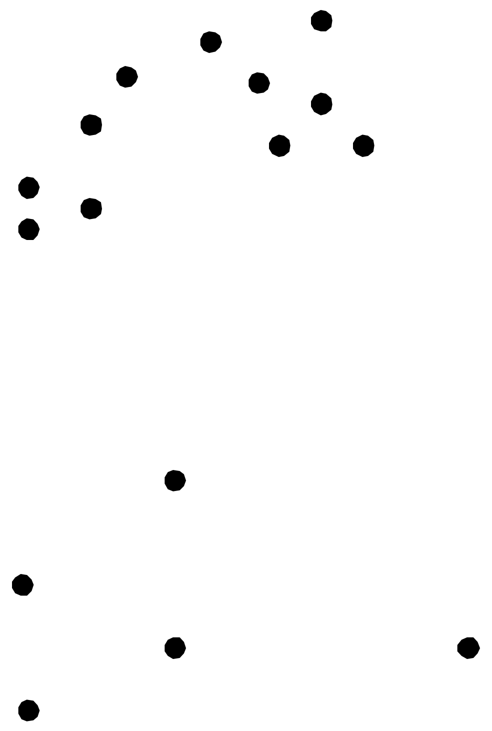
Figure 1.1: Plotting cholera cases on a map of London

霍乱

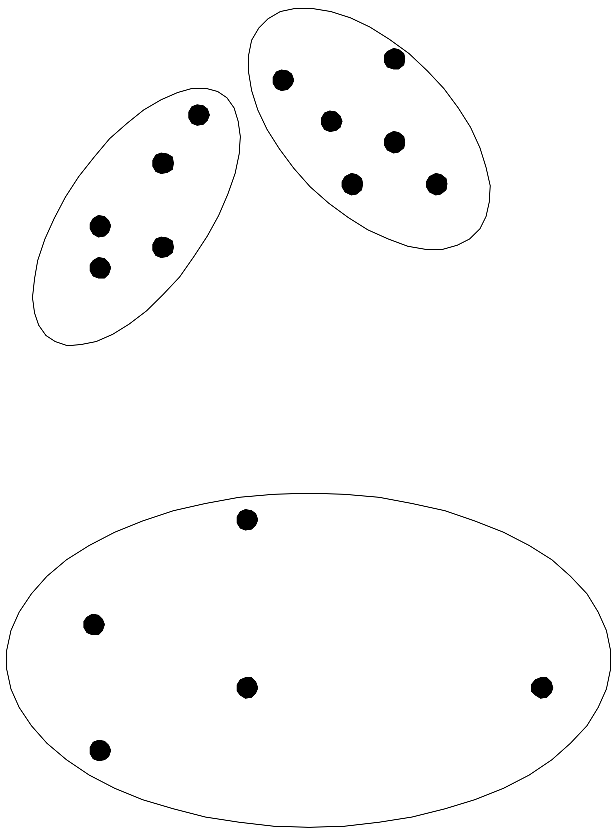
Types of Clusterings

- Important distinction between hierarchical(分级的) and partitional sets of clusters
- Partitional Clustering 划分聚类
  - A division data objects into subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering 层次聚类
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

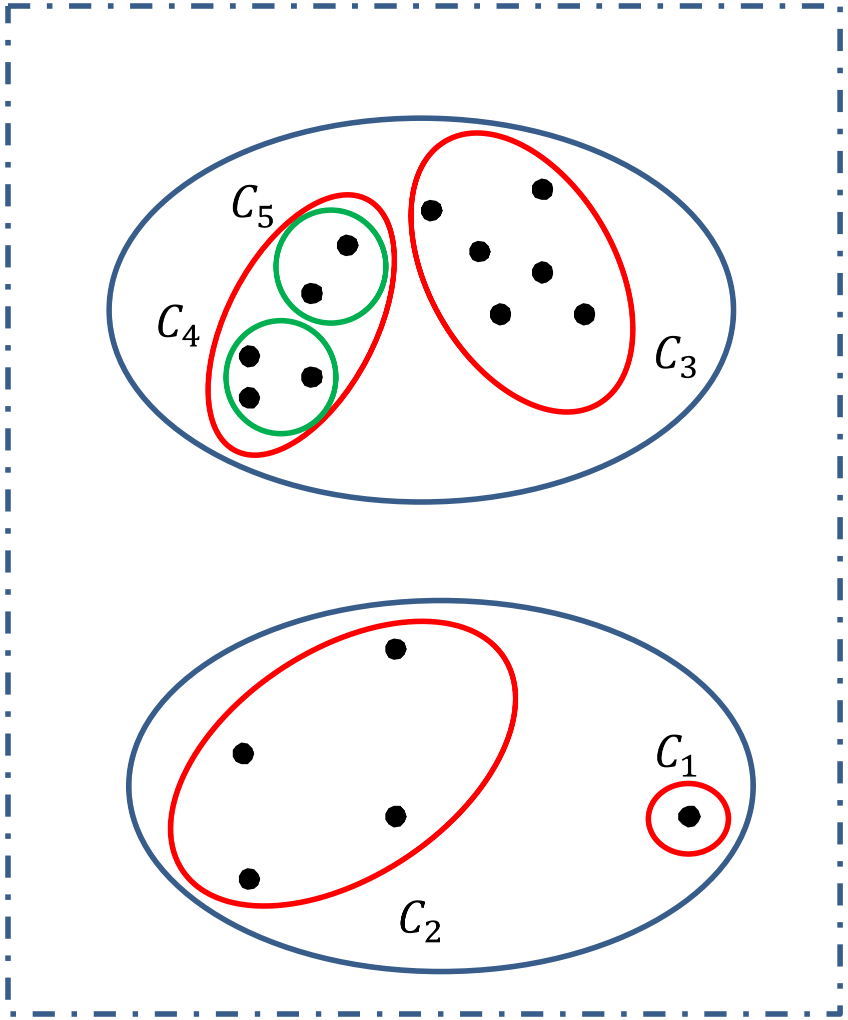


Original Points

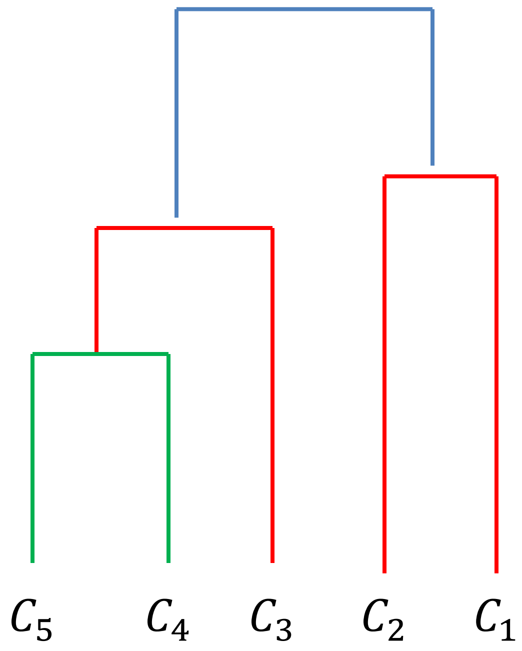


A Partitional Clustering

Hierarchical Clustering



Hierarchical Clustering



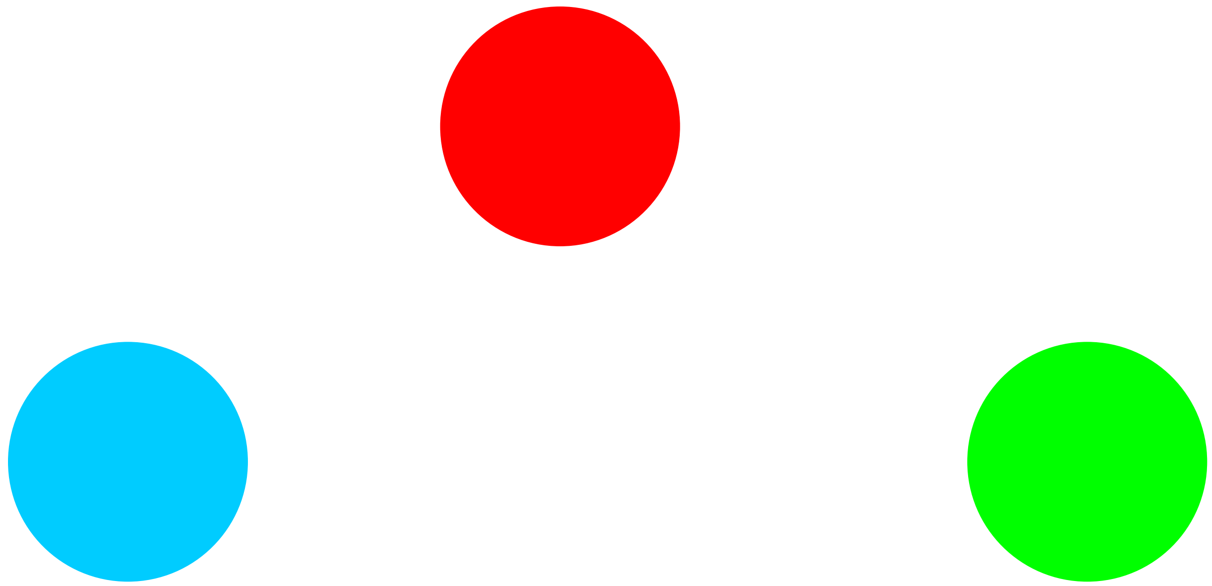
Hierarchical Clustering dendrogram

Other types of clustering

- Exclusive(排他的) (or non-overlapping) versus non-exclusive (or overlapping)
  - In non-exclusive clusterings, points may belong to multiple clusters.
    - Points that belong to multiple classes, or ‘border’ points
- Fuzzy(模糊的) (or soft) versus non-fuzzy (or hard)
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
    - Weights usually must sum to 1 (often interpreted as probabilities)
- Partial versus complete
  - In some cases, we only want to cluster some of the data

Clustering objectives

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



3 well-separated clusters

Clustering objectives

- Center-based Clusters:
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the minimizer of distances from all the points in the cluster, or a medoid, the most "representative" point of a cluster

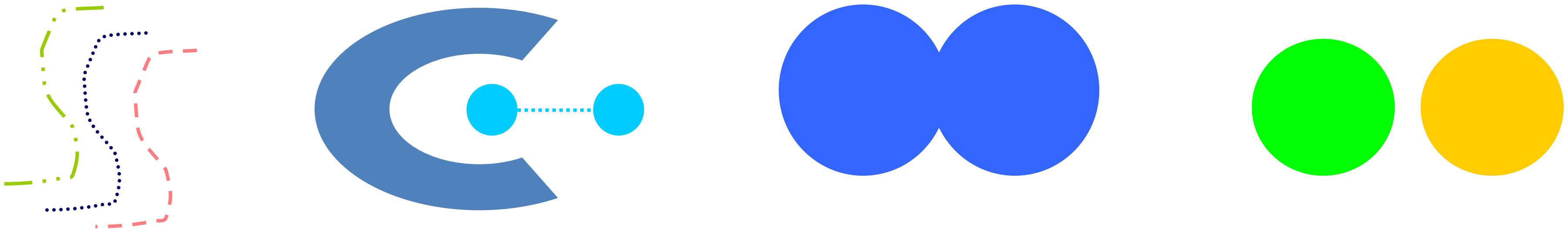
Centroid: the arithmetic mean position of all the points

Medoid: restricted to be a member of the data set

4 center-based clusters

Clustering objectives

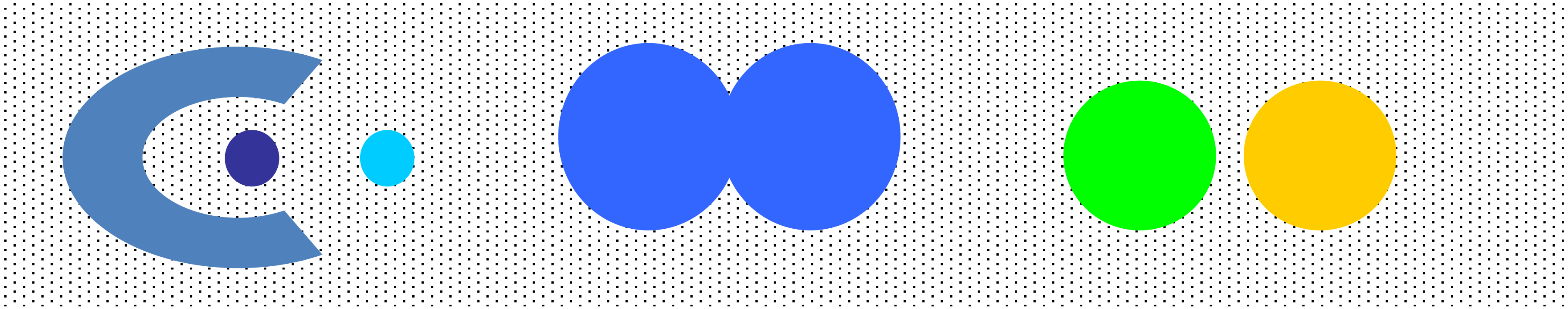
- Contiguous Clusters (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Clustering Objectives

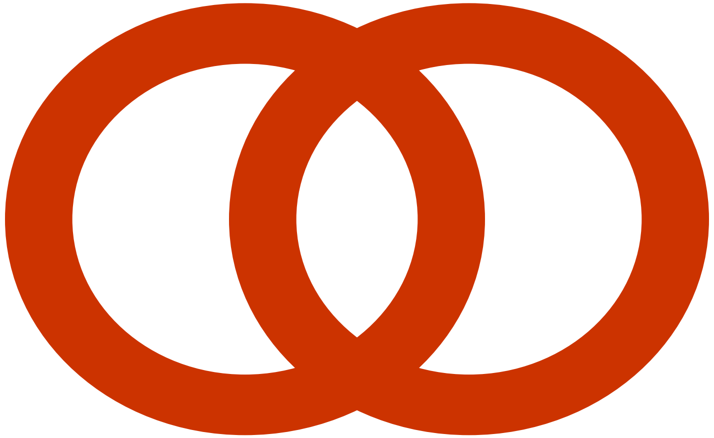
- Density-based clusters
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined(缠绕的), and when noise and outliers are present.



6 density-based clusters

Clustering objectives

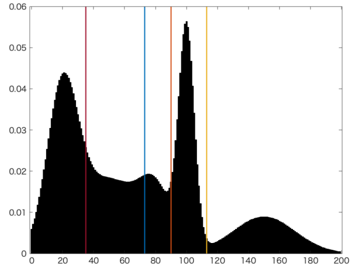
- Shared Property or Conceptual Clusters
  - Finds clusters that share some common property or represent a particular concept.



A cluster is defined as a set of points that lie on a circle

Clustering objectives

- Clustering as an optimization problem
  - Finds clusters that minimize or maximize an objective function.
  - Consider all possible ways of dividing the points into clusters and compute the `goodness' of each clustering using the objective function to find the best one.
    - Usually, finding the best is NP-hard (no polynomial algorithm).
  - Can have global or local objectives.
    - Hierarchical clustering algorithms typically have local objectives
    - Partitional algorithms typically have global objectives



  - A variation of the global objective function approach is to fit the data to a parameterized (probabilistic) model.
    - The parameters for the model are determined from the data, and they determine the clustering
    - E.g., Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.

Clustering Algorithms

- K-means and its variants
- Hierarchical clustering
- DBSCAN

K-MEANS

K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The objective is to:
  - find K centroids and
  - the assignment of points to clusters/centroids
  - so as to minimize the sum of distances of the points to their respective centroid

K-means Clustering as an optimization problem

- Problem: Given a set X of n objects and an integer K, find a grouping of the points into K clusters $C = \{C_1, C_2, \dots, C_K\}$ with centroids $\{c_1, c_2, \dots, c_K\}$ that minimizes the cost function

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

Definition for a general distance function $dist$

- Note: We need to find both the grouping into clusters and the centroids per cluster.

K-means Clustering

- Most common definition is with Euclidean distance, minimizing the Sum of Squares Error (SSE) – distance function
  - Sometimes K-means clustering is defined like that

- Problem: Given a set X of n points in a d-dimensional space and an integer K group the points into K clusters $C = \{C_1, C_2, \dots, C_K\}$ such that

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

Sum of Squares Error (SSE)

is minimized, where c_i is the mean of the points in cluster C_i

K-means Clustering 1-dimension

- NP-hard if the dimensionality of the data is at least 2 ($d \geq 2$)
  - Finding the best solution in polynomial time is infeasible.
  - For $d = 1$ the problem is solvable in polynomial time (how?)

We introduce a dynamic programming algorithm to guarantee optimality of clustering in 1-D. We define a sub-problem as finding the minimum *withinss* of clustering $x_1, \ldots, x_i$ into m clusters. We record the corresponding minimum *withinss* in entry $D[i, m]$ of an $n + 1$ by $k + 1$ matrix D. Thus $D[n, k]$ is the minimum *withinss* value to the original problem. Let j be the index of the smallest number in cluster m in an optimal solution to $D[i, m]$. It is evident that $D[j - 1, m - 1]$ must be the optimal *withinss* for the first $j - 1$ points in $m - 1$ clusters, for otherwise one would have a better solution to $D[i, m]$. This establishes the optimal substructure for dynamic programming and leads to the recurrence equation

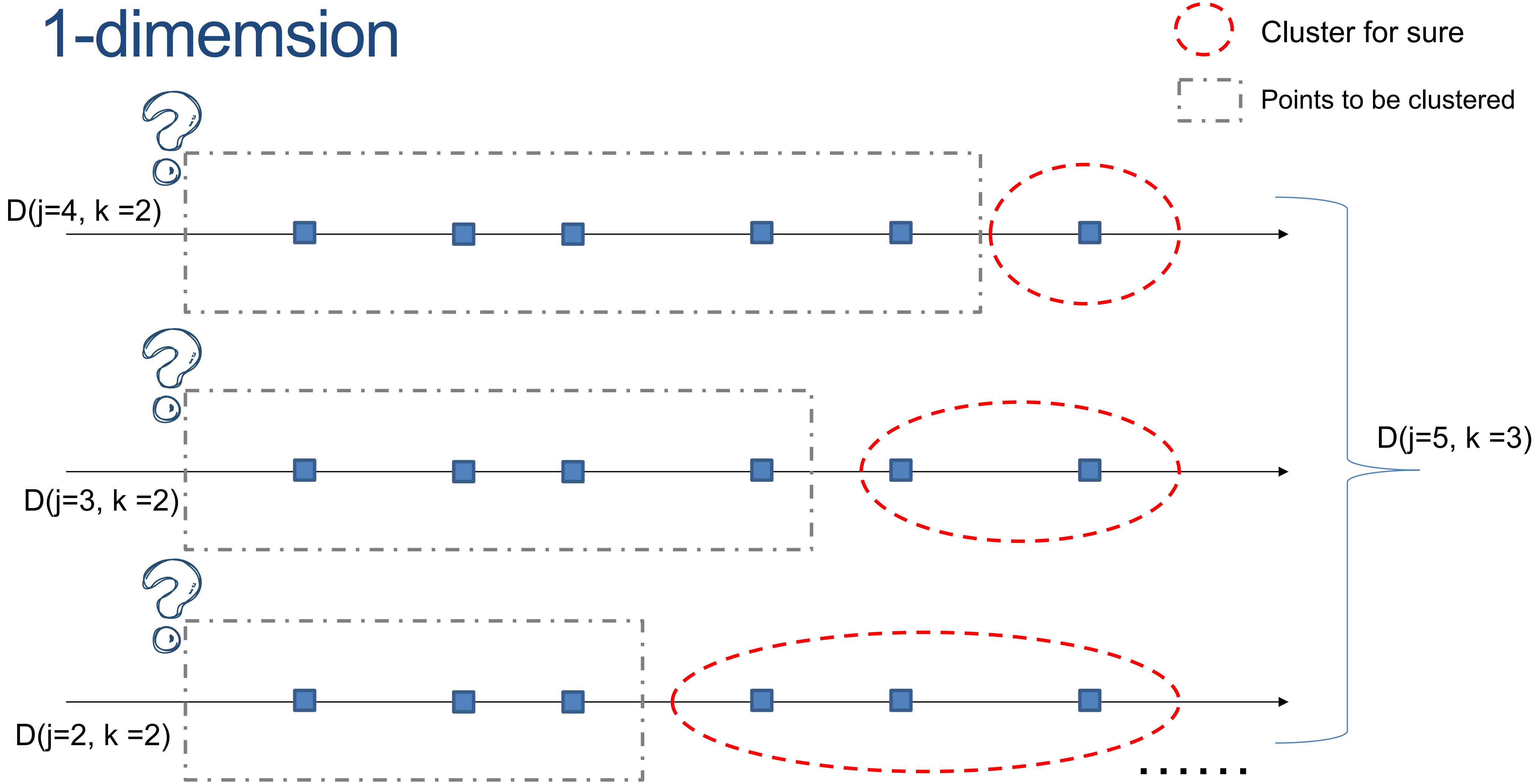
$O(n^2k)$.

$$D[i, m] = \min_{m \leq j \leq i} \{D[j - 1, m - 1] + d(x_j, \ldots, x_i)\},$$

$$1 \leq i \leq n, 1 \leq m \leq k$$

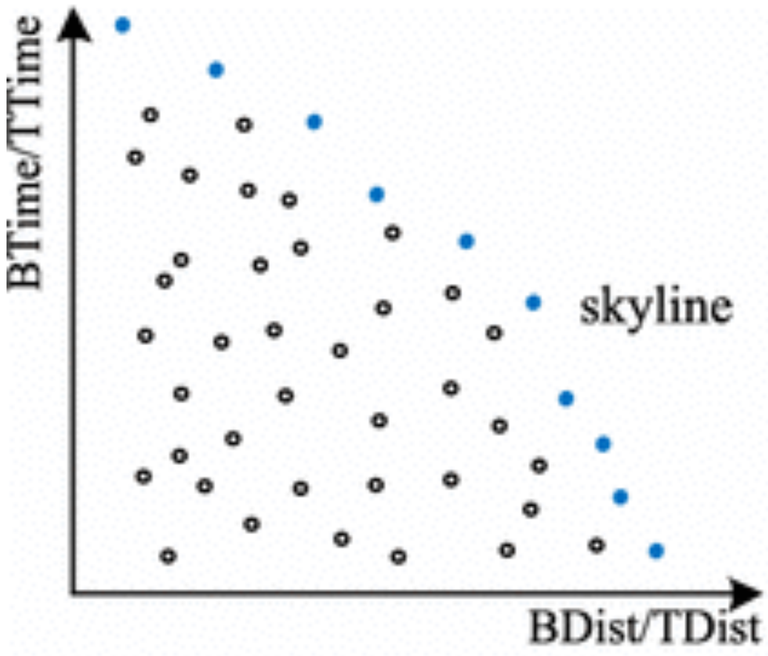
where $d(x_j, \ldots, x_i)$ is the sum of squared distances from $x_j, \ldots, x_i$ to their mean. The matrix is initialized as $D[i, m] = 0$, when $m = 0$ or $i = 0$.

1-dimemsion



Cluster for sure
Points to be clustered
D(j=4, k =2)
D(j=3, k =2)
D(j=2, k =2)
D(j=5, k =3)
......

1-dimemsion



(a)

OD pair	BDist/TDist	BTime/TTime	BStop/TDist
1	1.4	2.6	1.6
2	1.3	3.7	1.8
3	1.0	3.5	1.4
4	2.2	3.0	1.0
5	1.8	2.4	2.4
6	2.4	3.4	1.4
7	1.3	2.3	2.0
8	1.6	3.2	2.2

(b)

K-means Algorithm

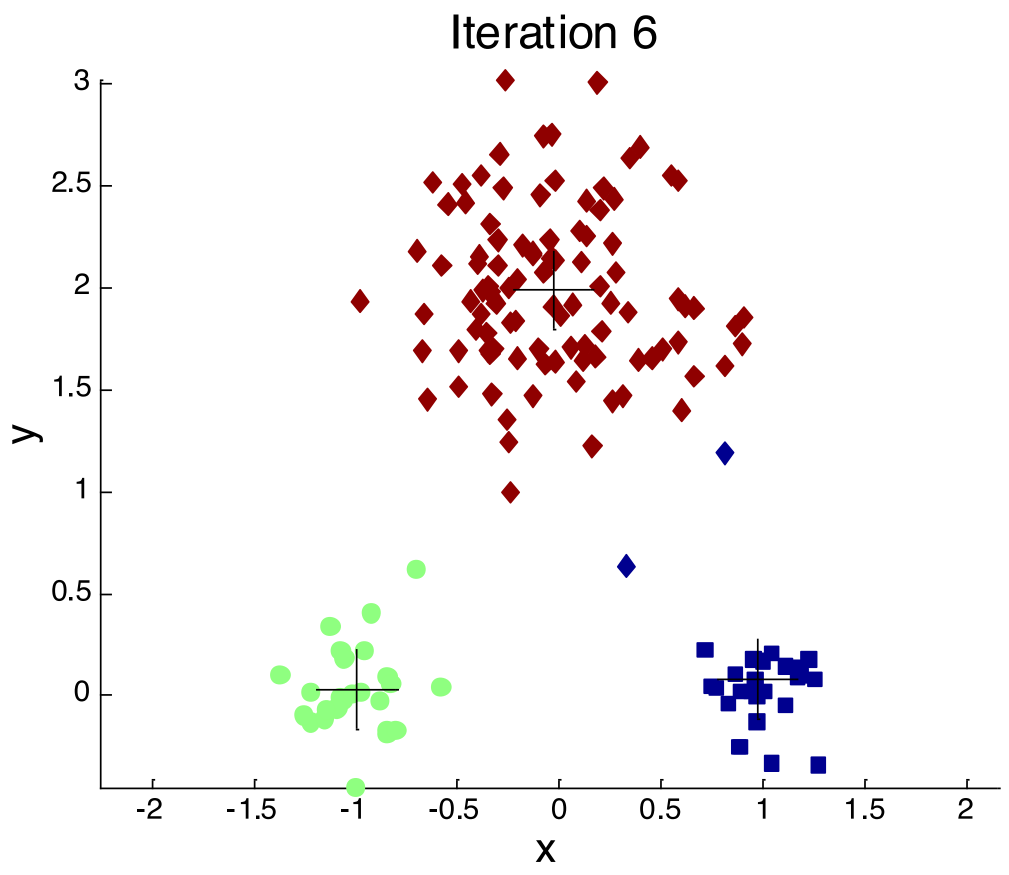
For $d \geq 2$

- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

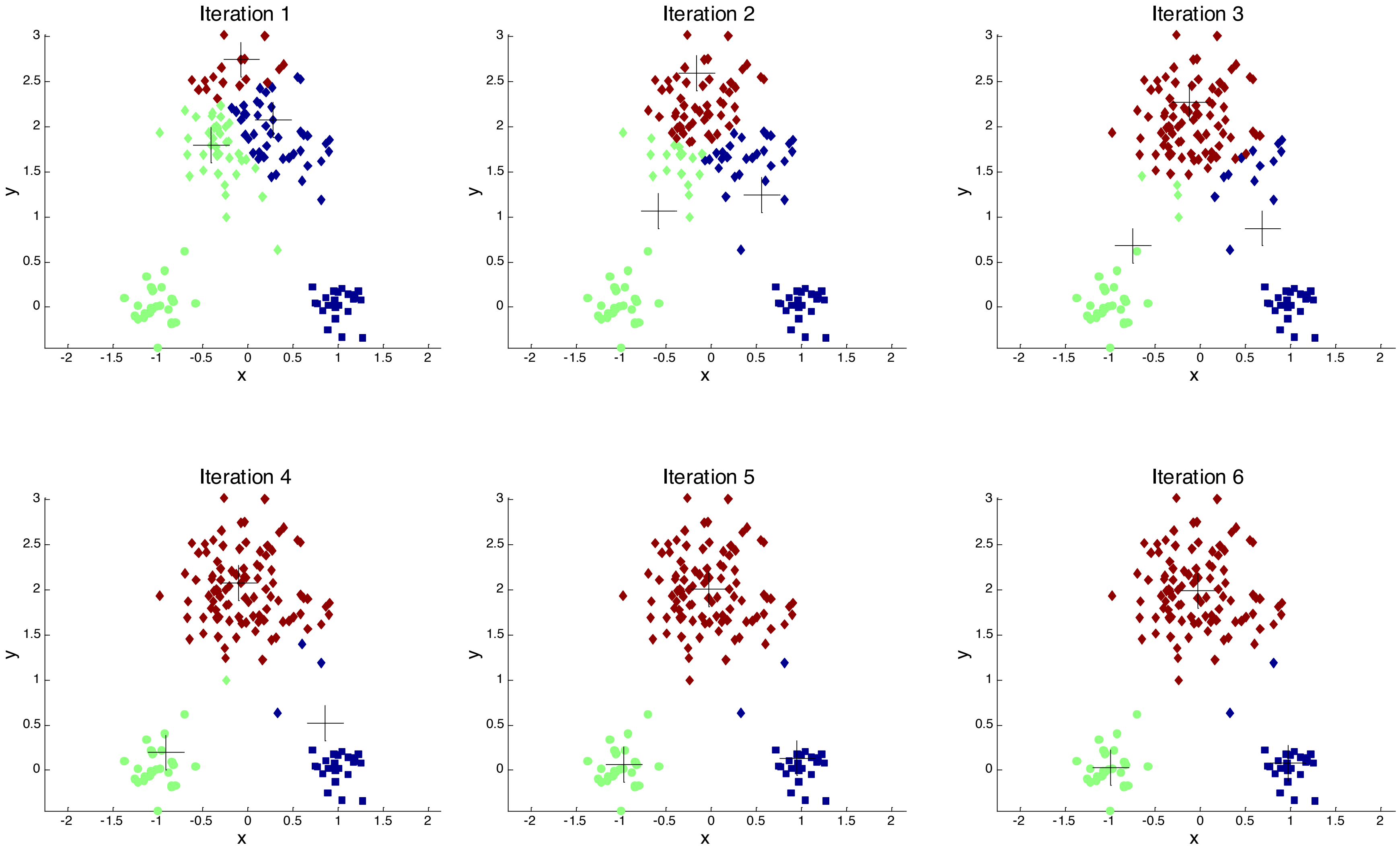
1. Select K points as the initial centroids
2. **repeat**
3. Form K clusters by assigning each point to the closest centroid
4. Compute the new centroid* of each cluster
5. **until** The centroids do not change

*The centroid of a set of points is the point that is minimizes the sum of distances from the points in the set

Example



Example


Iteration 1
Iteration 2
Iteration 3
Iteration 4
Iteration 5
Iteration 6
x
y

Example

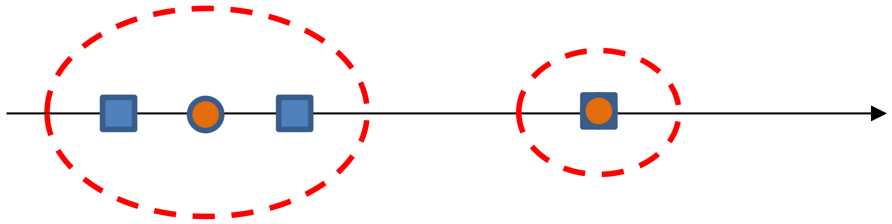
n: number of data points; k: number of clusters; d: number of dimensions

- The complexity of k-means clustering?
  - Each iteration computes the distances of all centroid-point pairs, which needs O(n * k * d). Assigning centroids and updating centroids both needs O(n).
  - If the pre-defined iteration limit is t, the total complexity is O(t*n * k * d).
- Does k-means guarantee optimality?
  - Nope.
  - Find a counter-example.

Counter-example

Data points   centroids

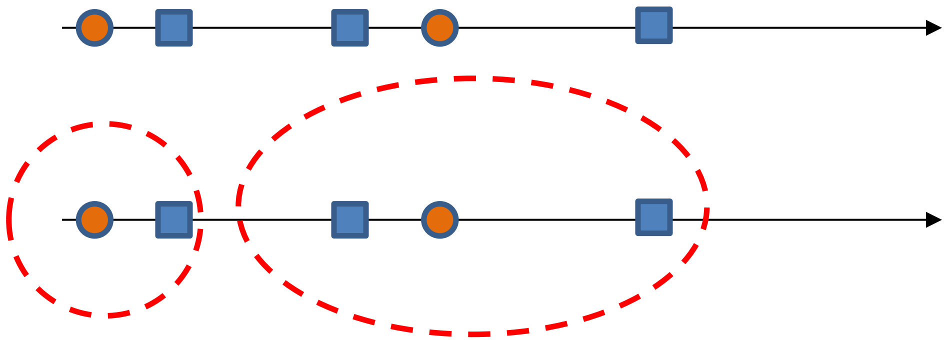
Optimum:



Iteration 0:

Initializing centroids:

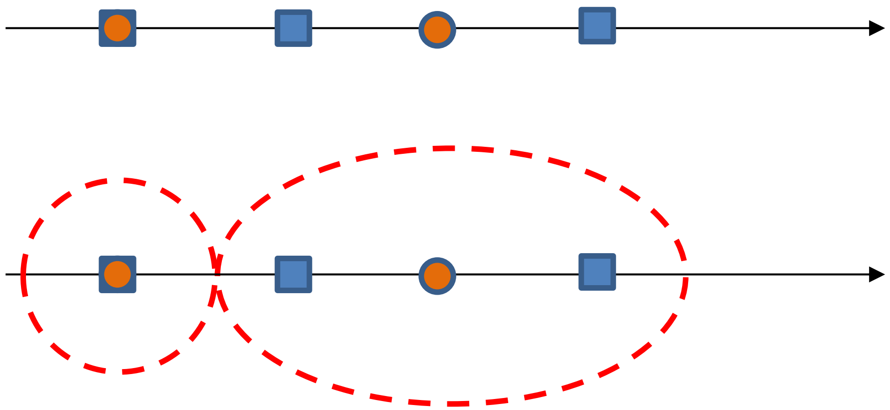
Assigning centroids:



Iteration 1:

Updating centroids:

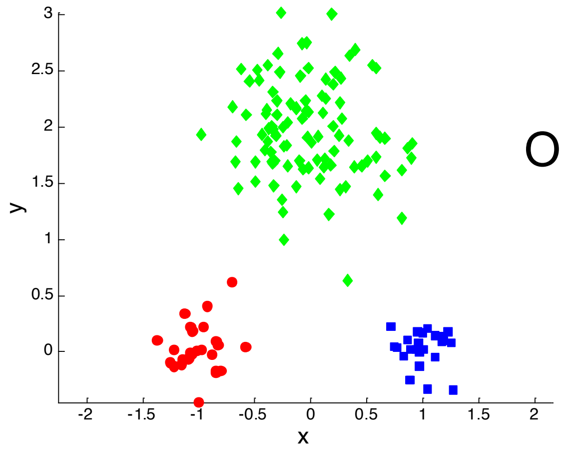
Assigning centroids:



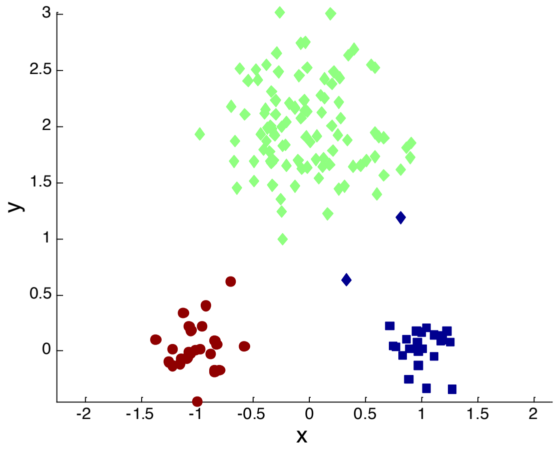
K-means Algorithm – Initialization

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.

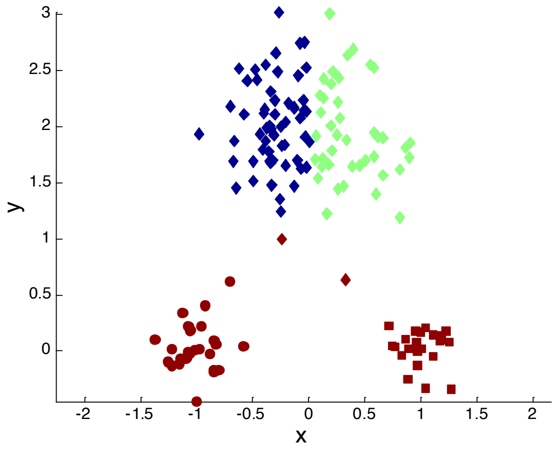
Two different K-means Clusterings



Original Points

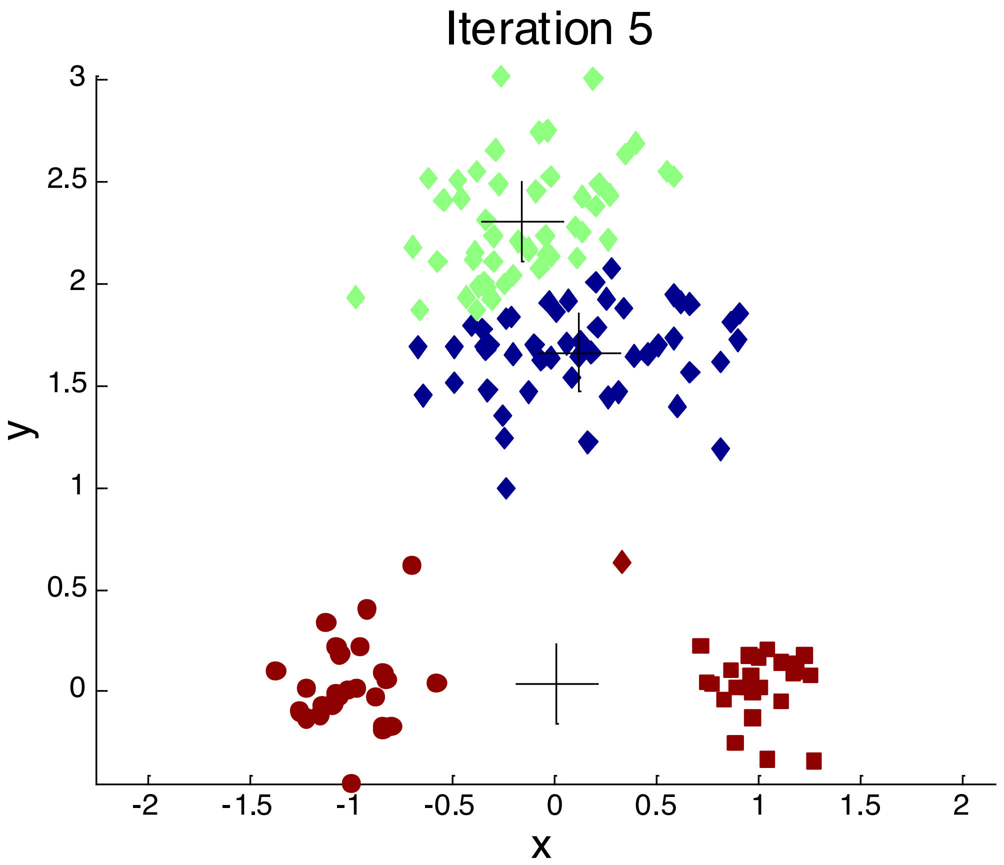


Optimal Clustering

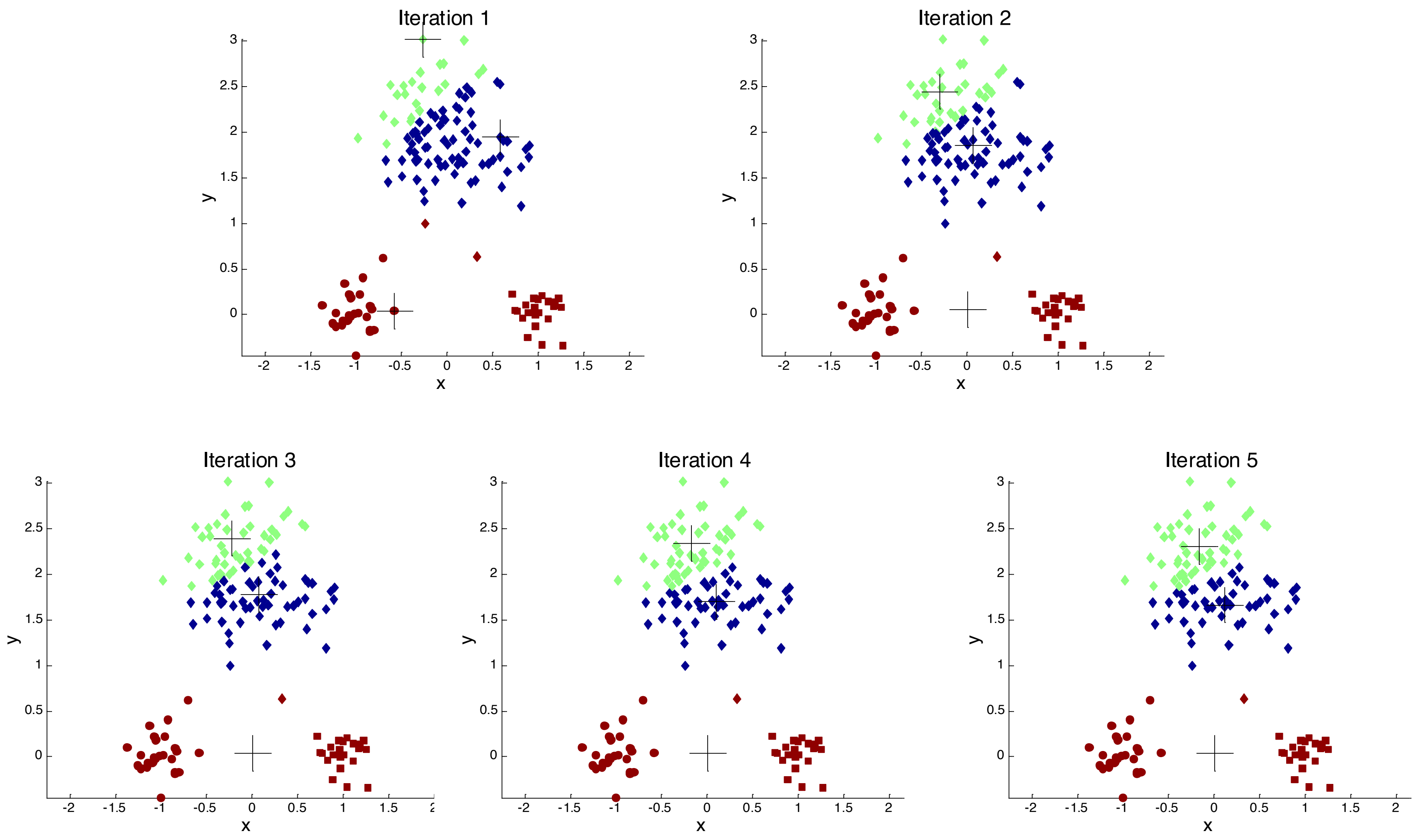


Sub-optimal Clustering

Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids …



Dealing with Initialization

- Do multiple runs and select the clustering with the smallest error
- Select original set of points by methods other than random. E.g., pick the most distant (from each other) points as cluster centers (K-means++ algorithm)

K-means Algorithm – Centroids

- ‘Closeness’ is measured by some similarity or distance function
  - E.g., Euclidean distance (SSE), cosine similarity, correlation, etc.
- The centroid depends on the distance function
  - The minimizer for the distance function
- Centroid:
  - The mean of the points in the cluster for SSE, and cosine distance
  - The median for Manhattan distance.

K-means Algorithm – Convergence

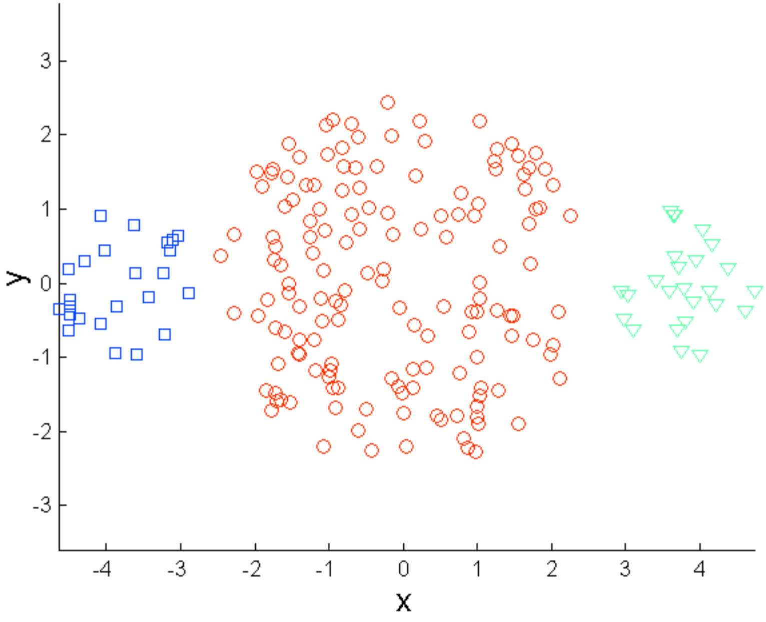
- K-means will converge for common similarity measures mentioned above.
  - Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'
- Complexity is $O(n \cdot K \cdot I \cdot d)$
  - n = number of points,
  - K = number of clusters,
  - I = number of iterations,
  - d = dimensionality
- In general, a fast and efficient algorithm

Limitations of K-means

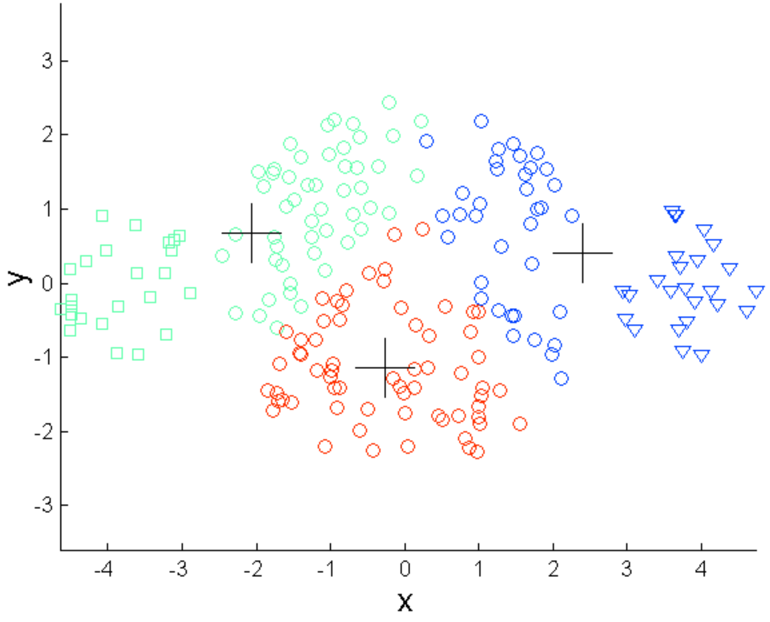
- K-means has problems when clusters are of different:
  - sizes
  - densities
  - non-globular(球状的) shapes

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

Limitations of K-means: Differing Sizes

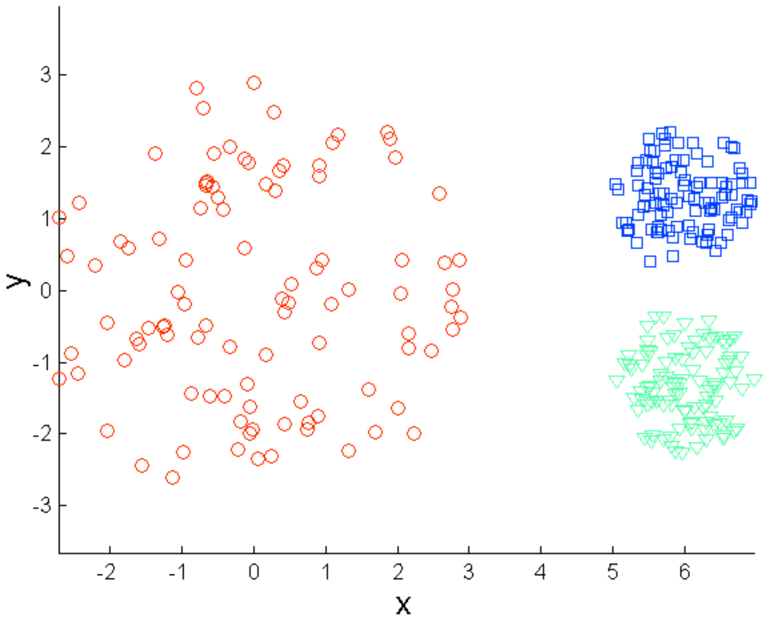


Original Points

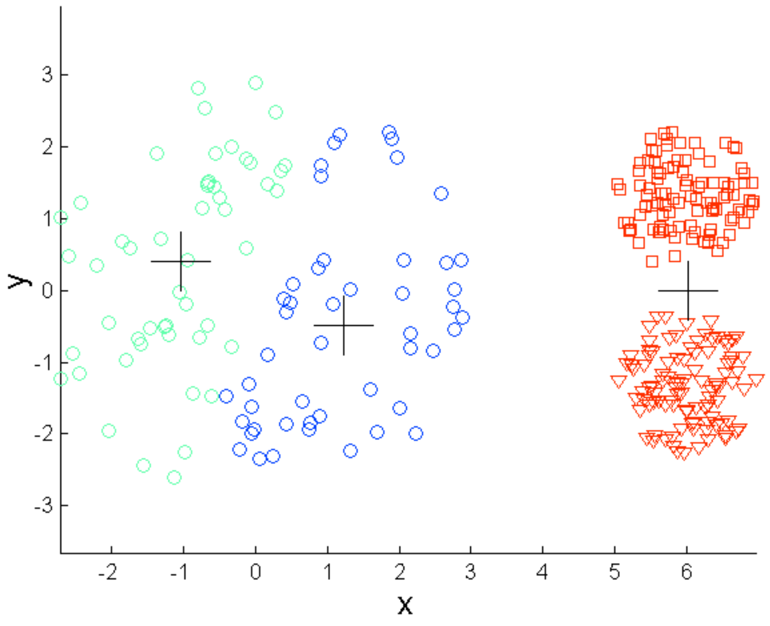


K-means (3 Clusters)

Limitations of K-means: Differing Density

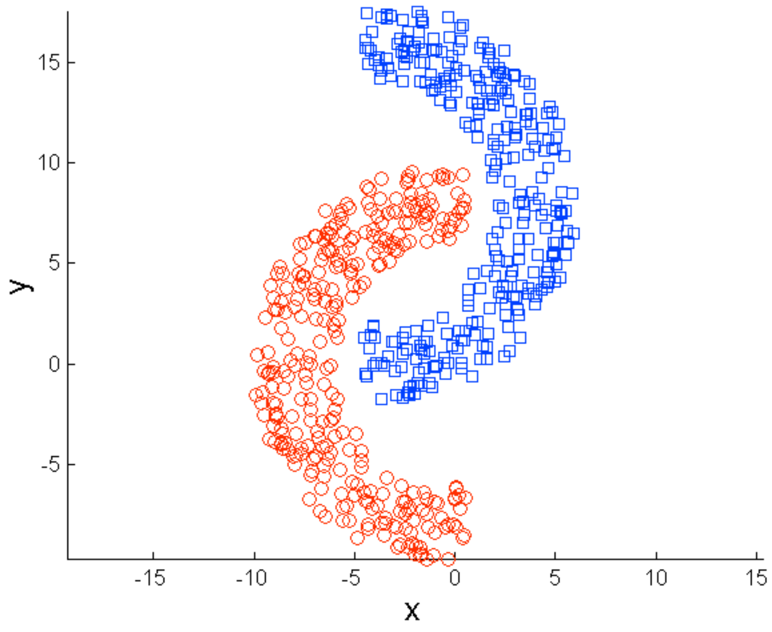


Original Points

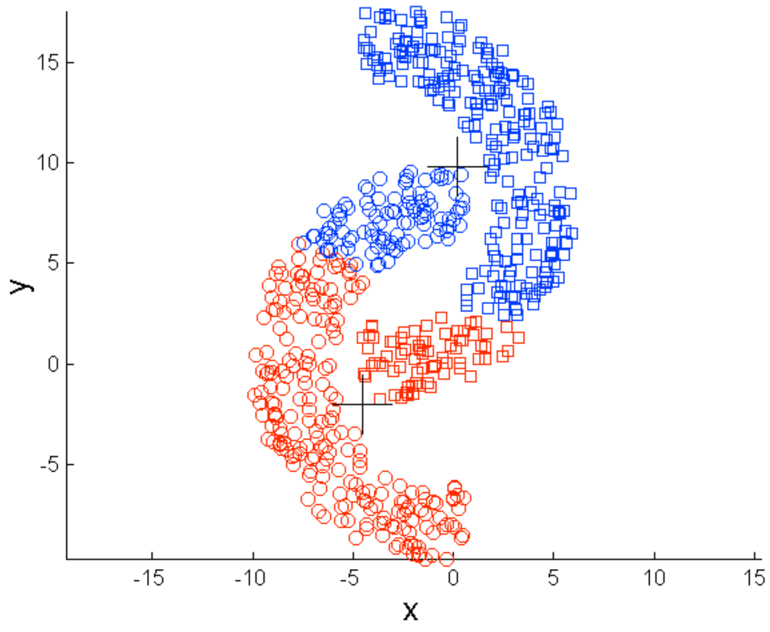


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

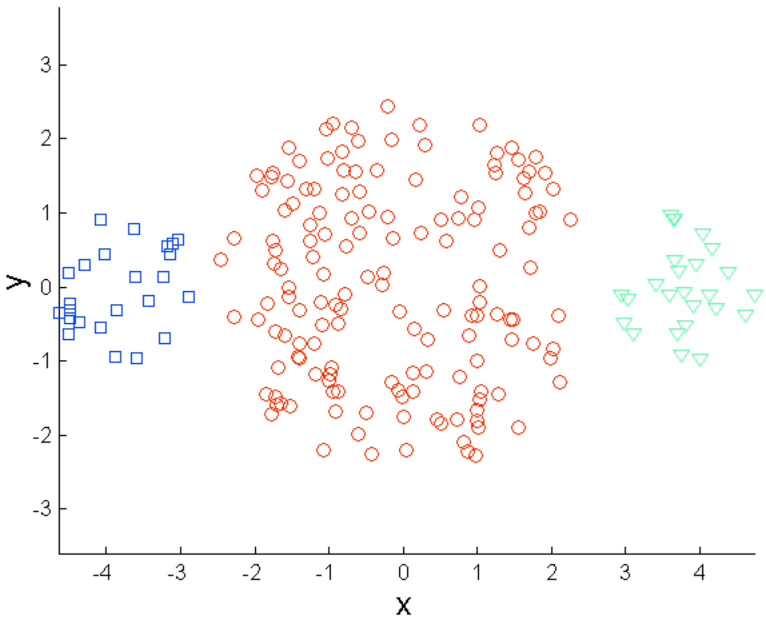


Original Points

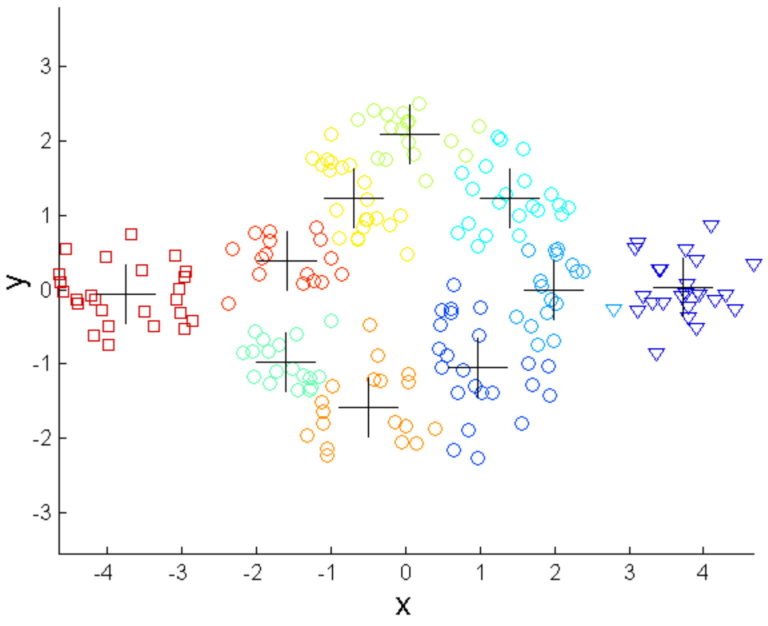


K-means (2 Clusters)

Overcoming K-means Limitations



Original Points

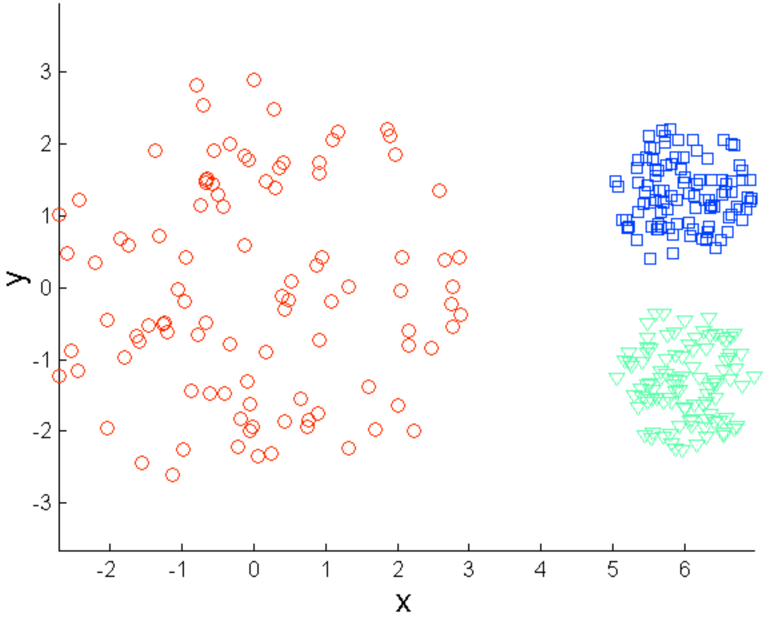


K-means Clusters

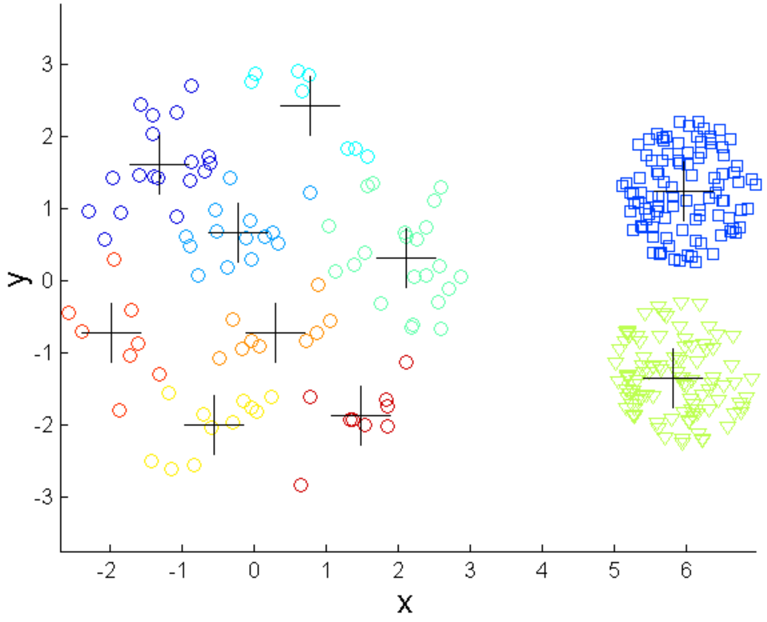
One solution is to use many clusters.

Find parts of clusters, but need to put together.

Overcoming K-means Limitations

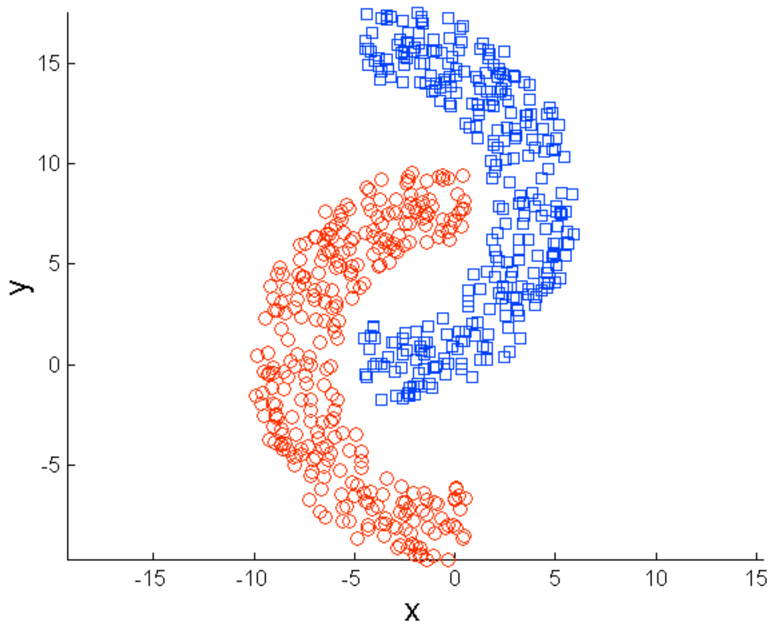


Original Points

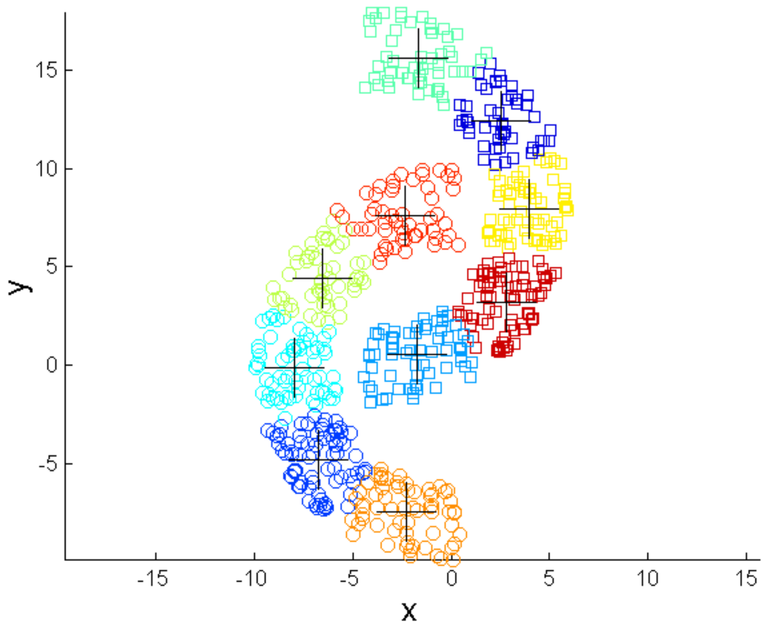


K-means Clusters

Overcoming K-means Limitations



Original Points



K-means Clusters

Variations

- K-medoids: Similar problem definition as in K-means, but the centroid of the cluster is defined to be one of the points in the cluster (the medoid).

- K-centers: Similar problem definition as in K-means, but the goal now is to minimize the maximum diameter of the clusters
    - diameter of a cluster is maximum distance between any two points in the cluster.

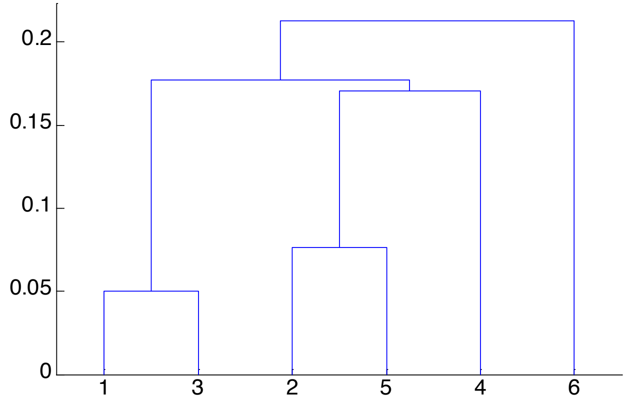
HIERARCHICAL CLUSTERING

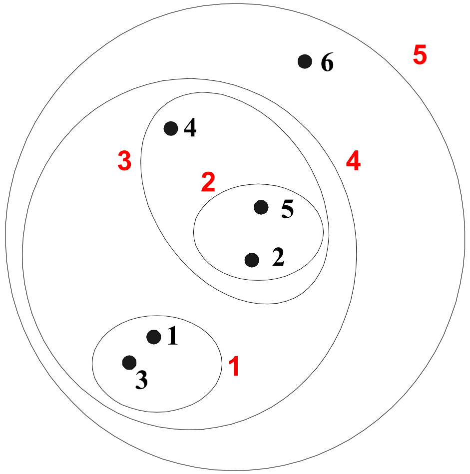
Hierarchical Clustering

- Two main types of hierarchical clustering
  - Agglomerative(聚合式):
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive(分裂式):
    - 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

Hierarchical Clustering

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





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

- Dendrograms may correspond to meaningful taxonomies(分类)
  - Example in biological sciences (e.g., animal kingdom(动物分界), phylogeny reconstruction(生物系统演化), …)

Agglomerative Clustering Algorithm

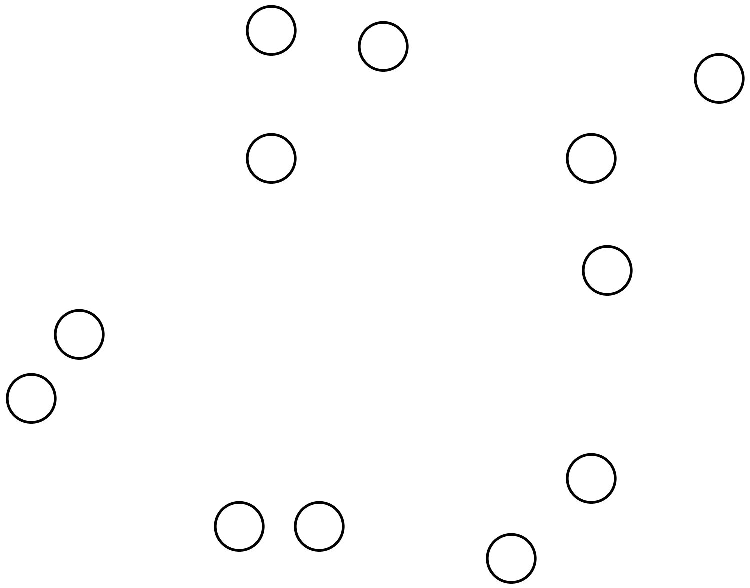
- Most popular hierarchical clustering technique
- Basic algorithm is straightforward

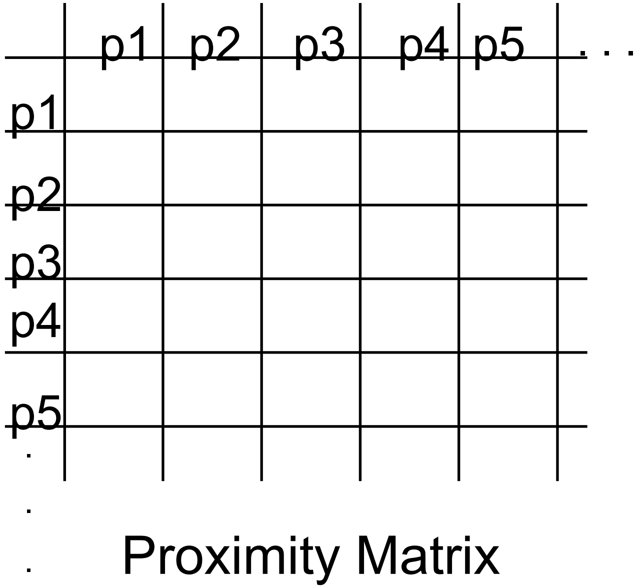
1. Compute the proximity matrix(相似性矩阵)
2. Let each data point be a cluster
3. **Repeat**
4. Merge the two closest clusters
5. Update the proximity matrix
6. **Until** only a single cluster remains

- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance between clusters distinguish the different algorithms

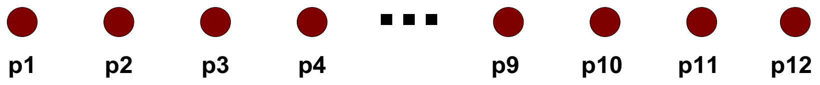
Starting Situation

- Start with single-point clusters and a proximity matrix between points



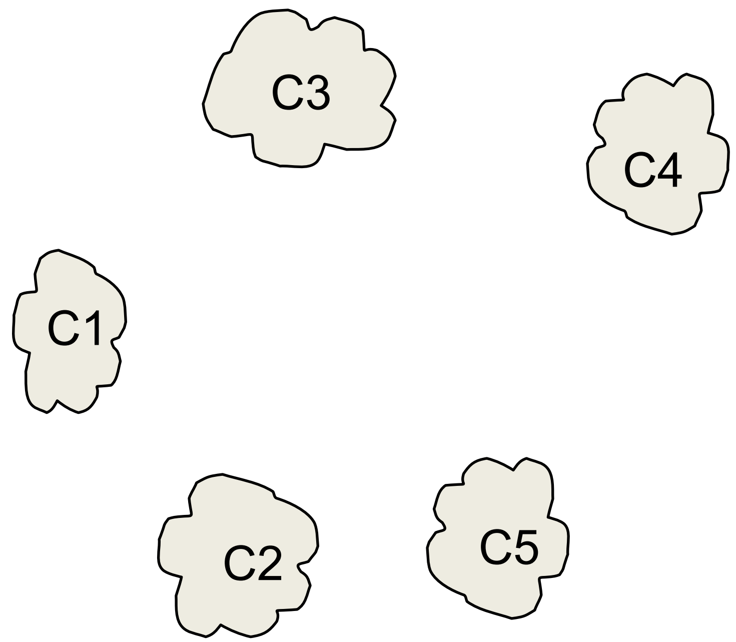


Proximity Matrix



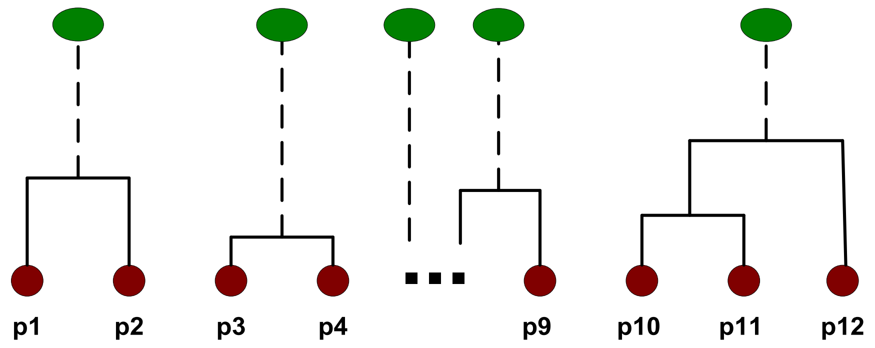
Intermediate Situation

- After some merging steps, we have some clusters and a proximity matrix between clusters



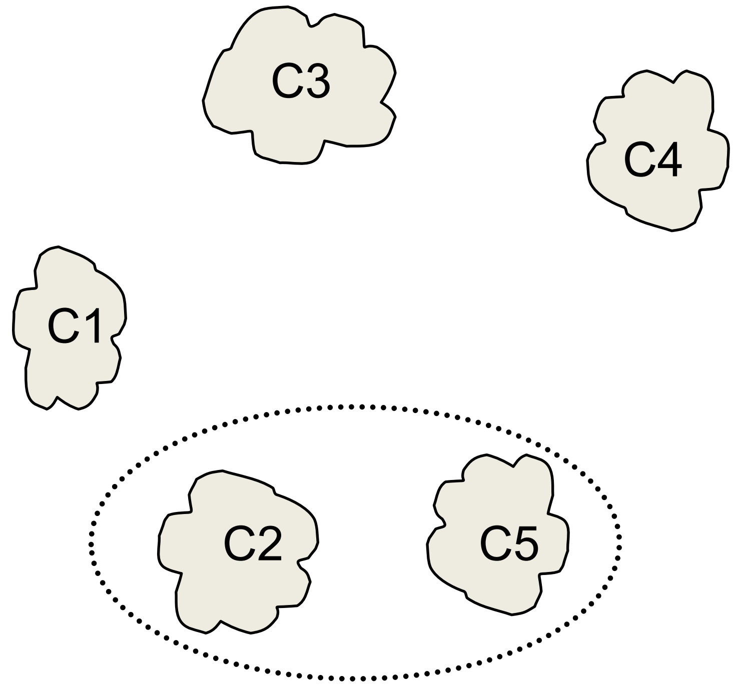
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

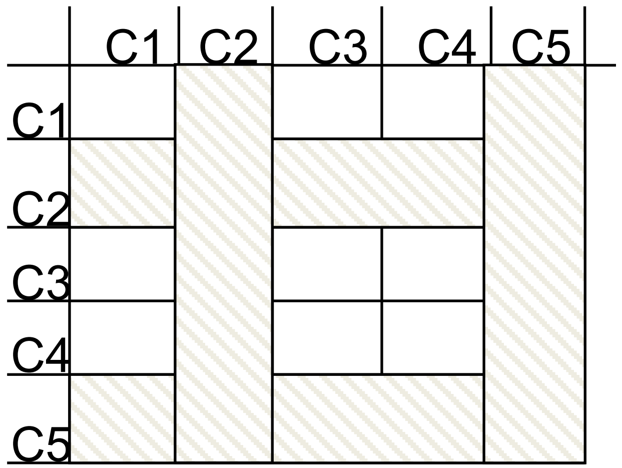
关联性矩阵



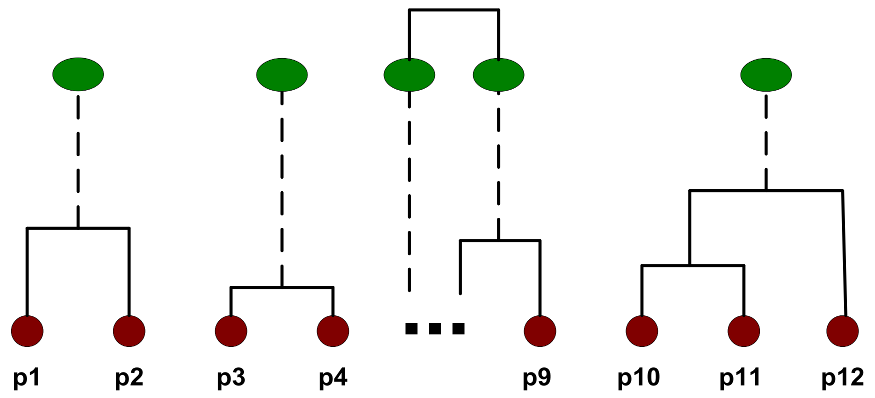
Intermediate Situation

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



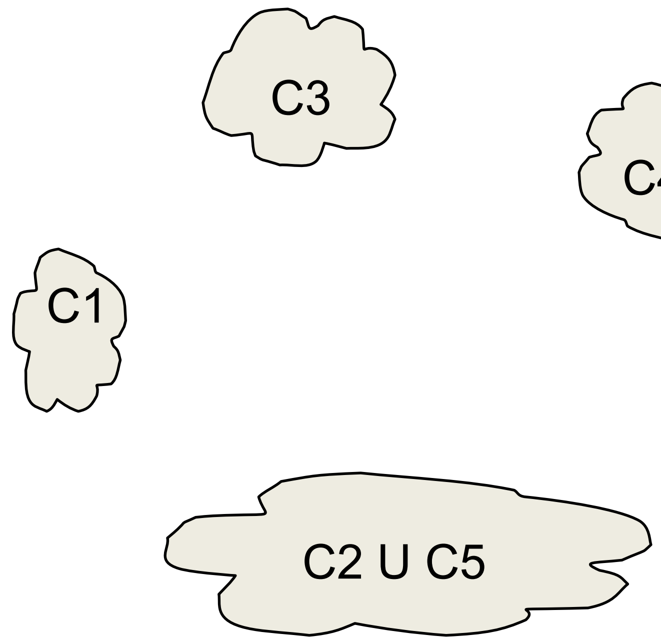


Proximity Matrix



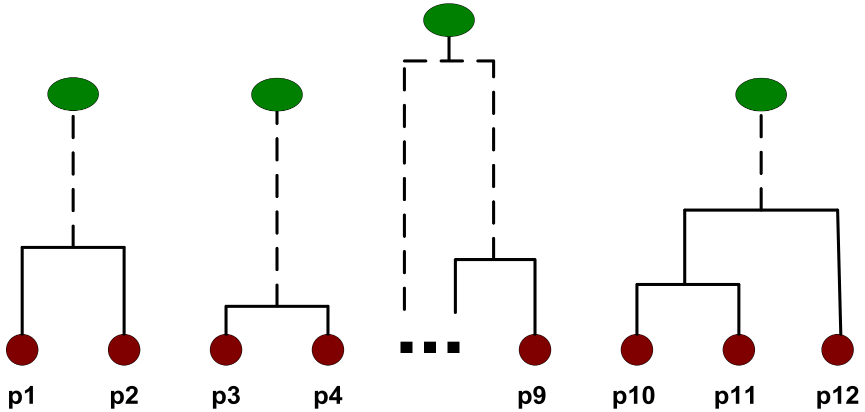
After Merging

- The question is “How do we update the proximity matrix?”

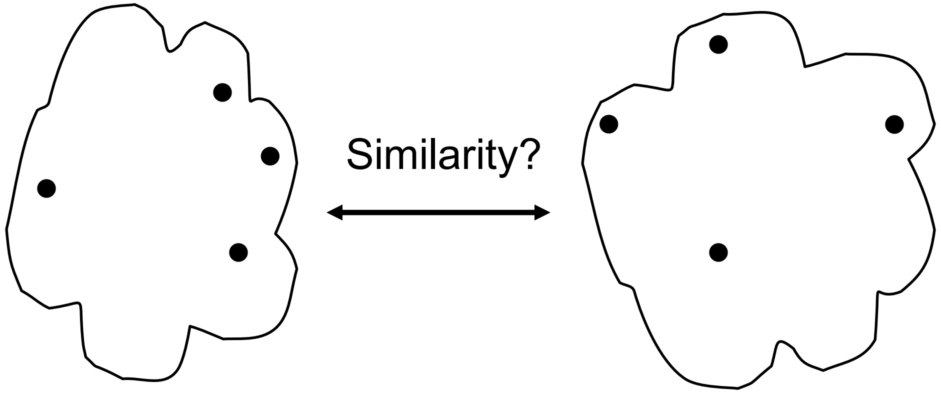


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Similarity

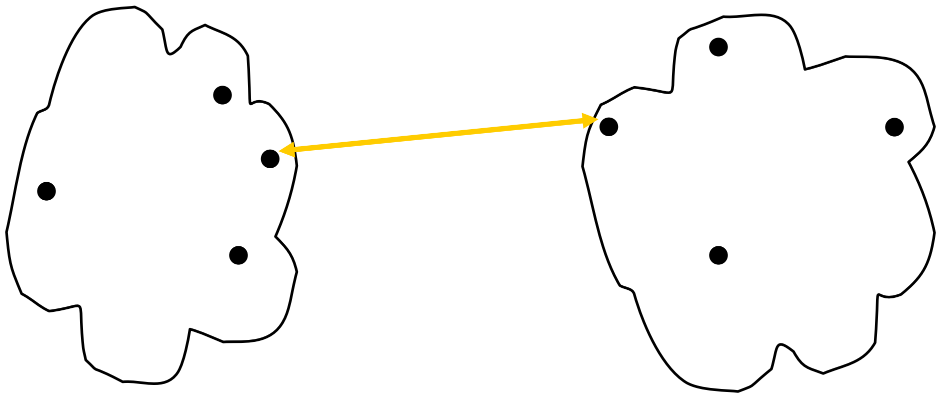


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

How to Define Inter-Cluster Similarity



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

Proximity Matrix

- MIN
- MAX
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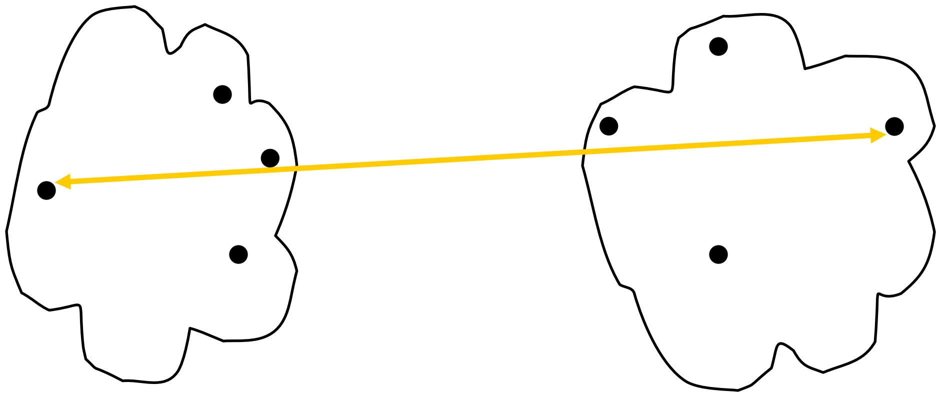
How to Define Inter-Cluster Similarity



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

Proximity Matrix

- MIN
- MAX
- Group Average
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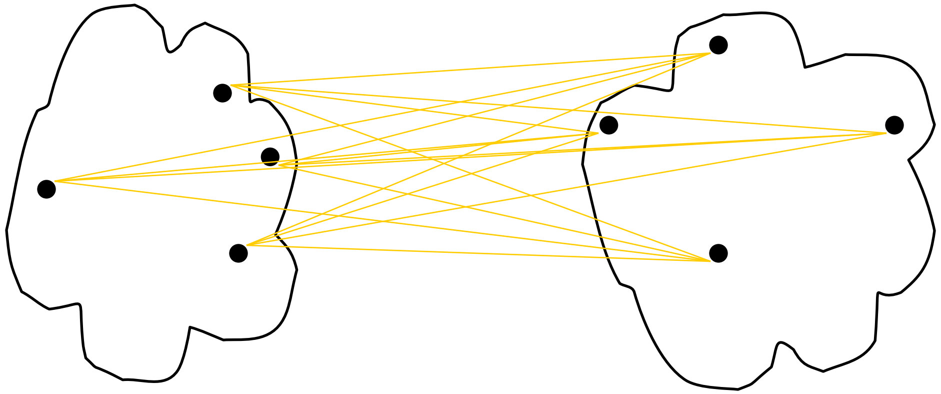
How to Define Inter-Cluster Similarity



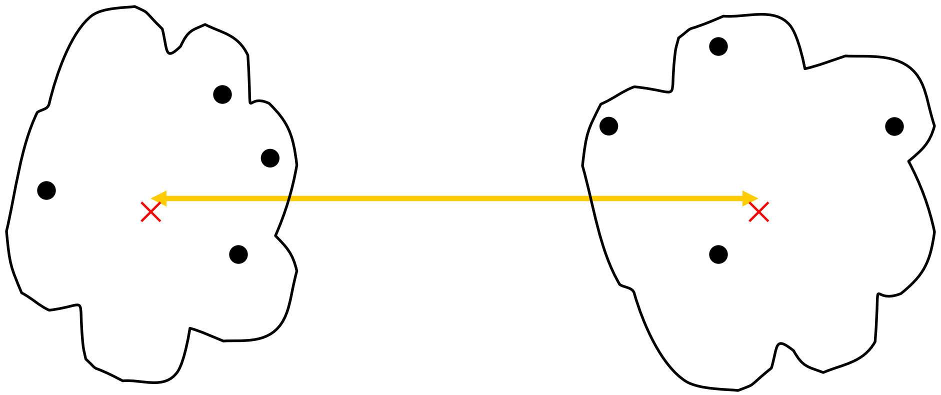
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

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

How to Define Inter-Cluster Similarity



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

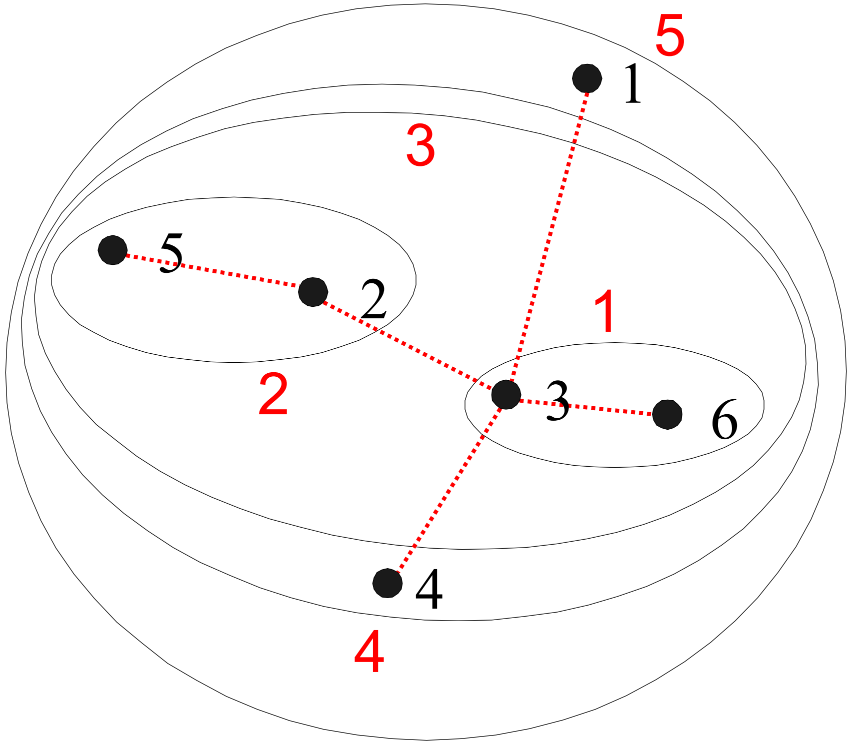
Proximity Matrix

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

Single Link – Complete Link

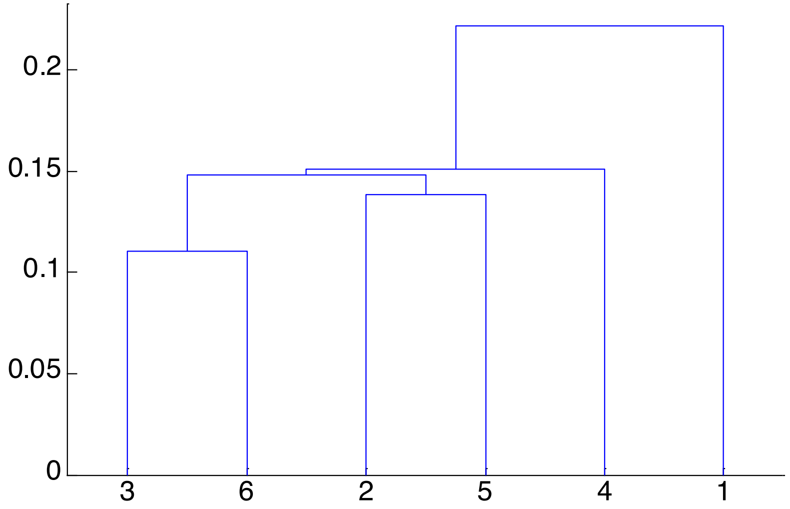
- Another way to view the processing of the hierarchical algorithm is that we create links between the elements in order of increasing distance
  - The MIN – Single Link, will merge two clusters when a single pair of elements is linked
  - The MAX – Complete Linkage will merge two clusters when all pairs of elements have been linked.

Hierarchical Clustering: MIN



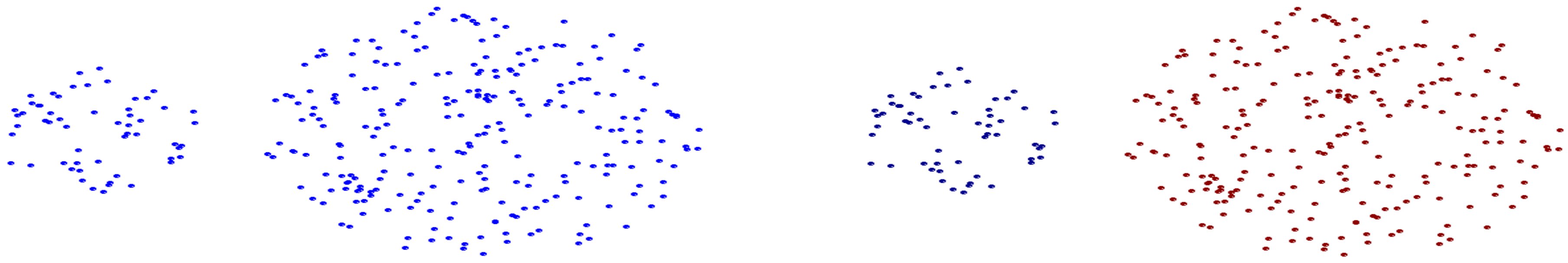
Nested Clusters

	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Dendrogram

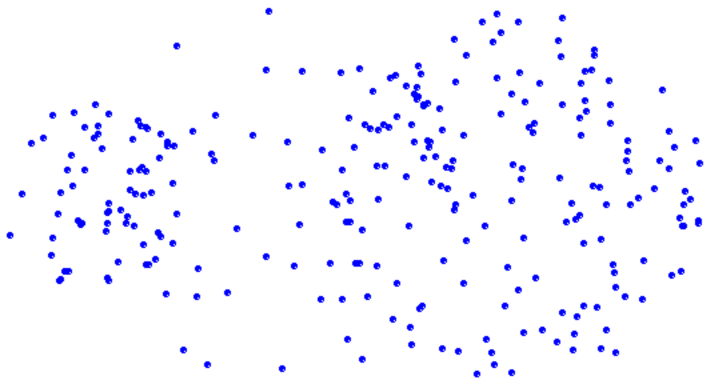
Strength of MIN



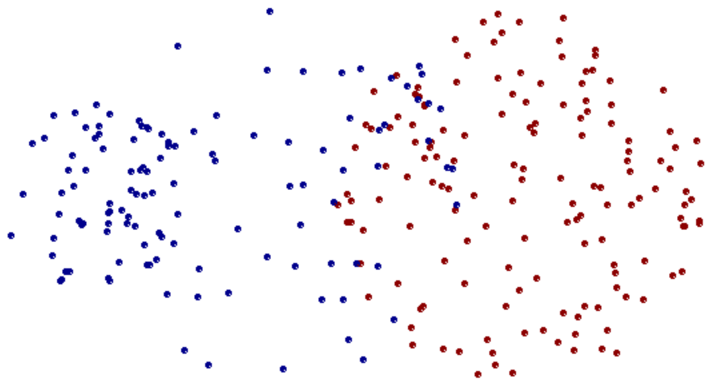
Original Points   Two Clusters

- Can handle non-elliptical(非椭圆的) shapes

Limitations of MIN



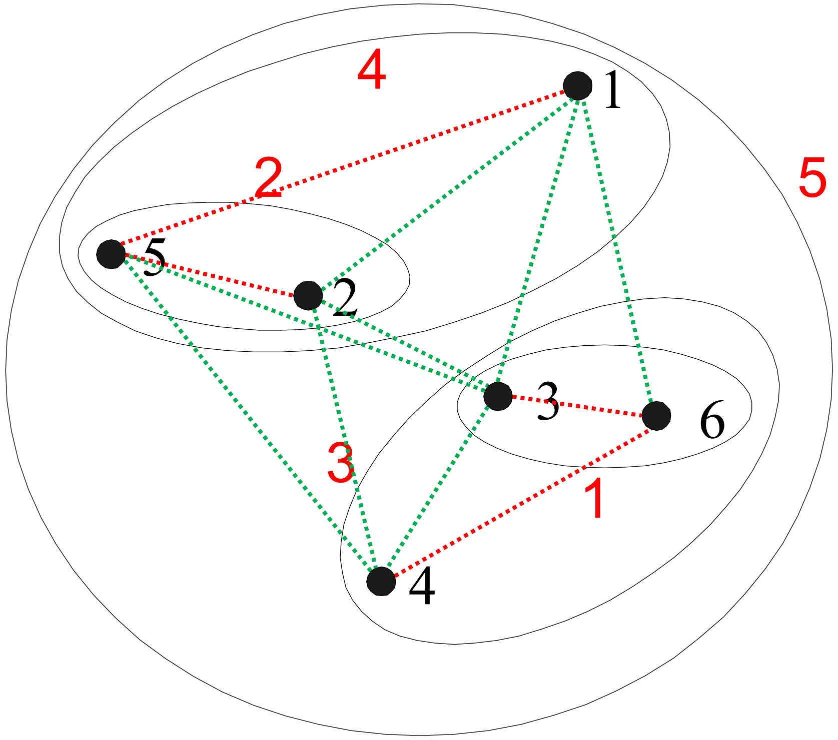
Original Points



Two Clusters

- Sensitive to noise and outliers

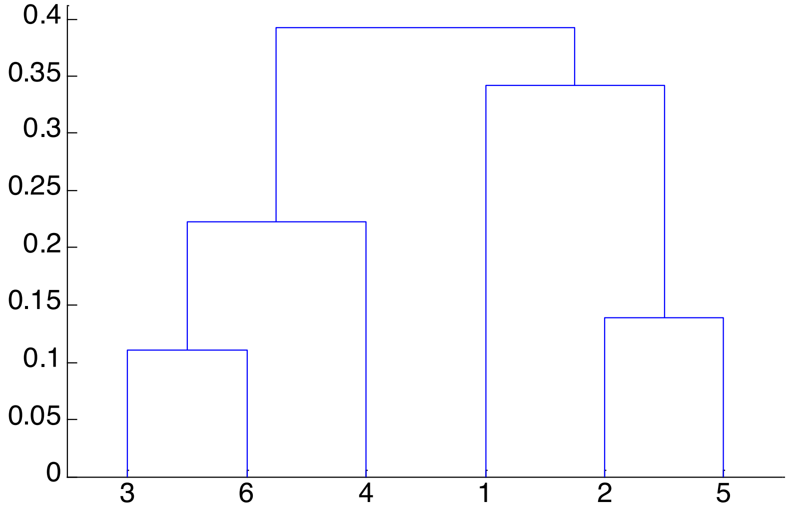
Hierarchical Clustering: MAX



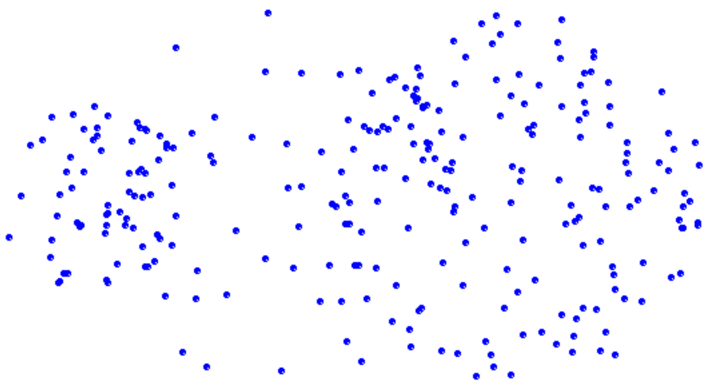
Nested Clusters

Dendrogram

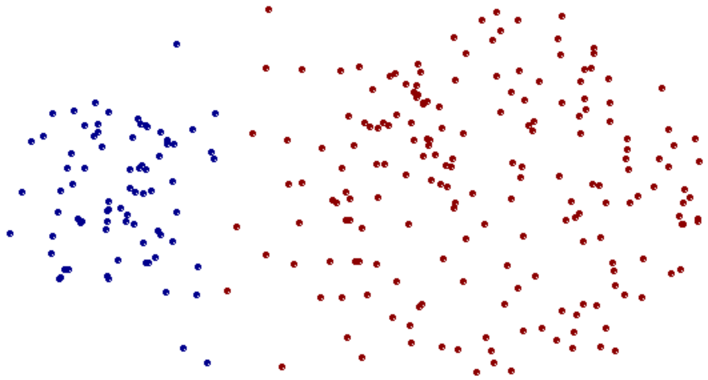
	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Strength of MAX



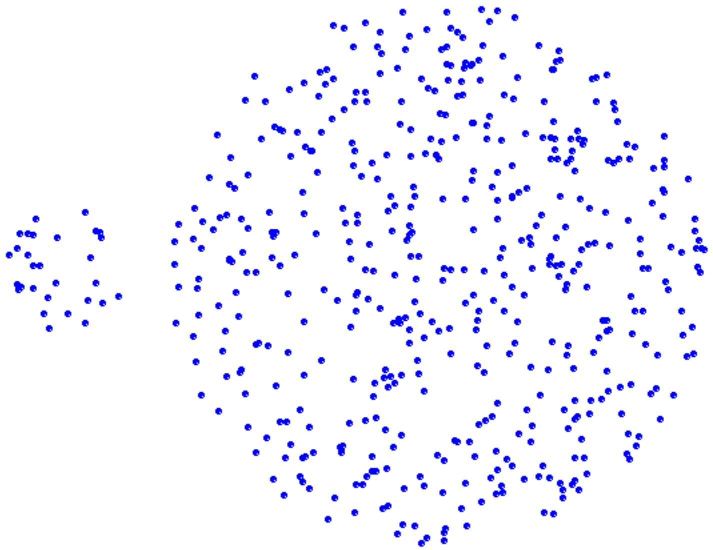
Original Points



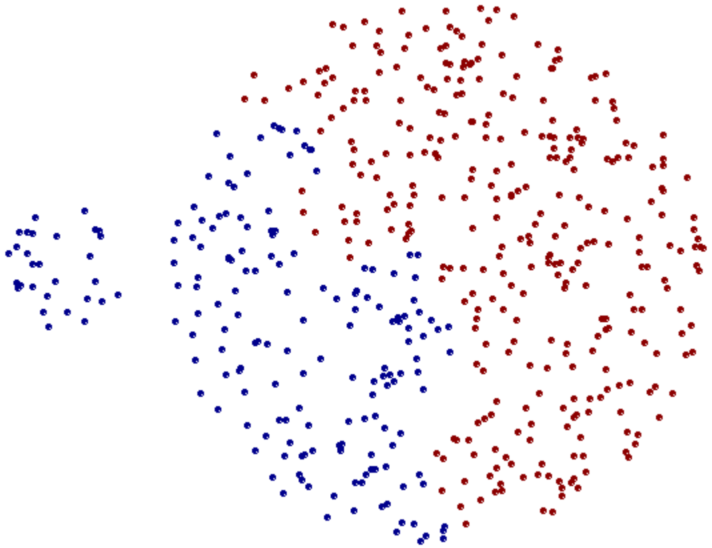
Two Clusters

- Less susceptible(受影响的) to noise and outliers

Limitations of MAX



Original Points

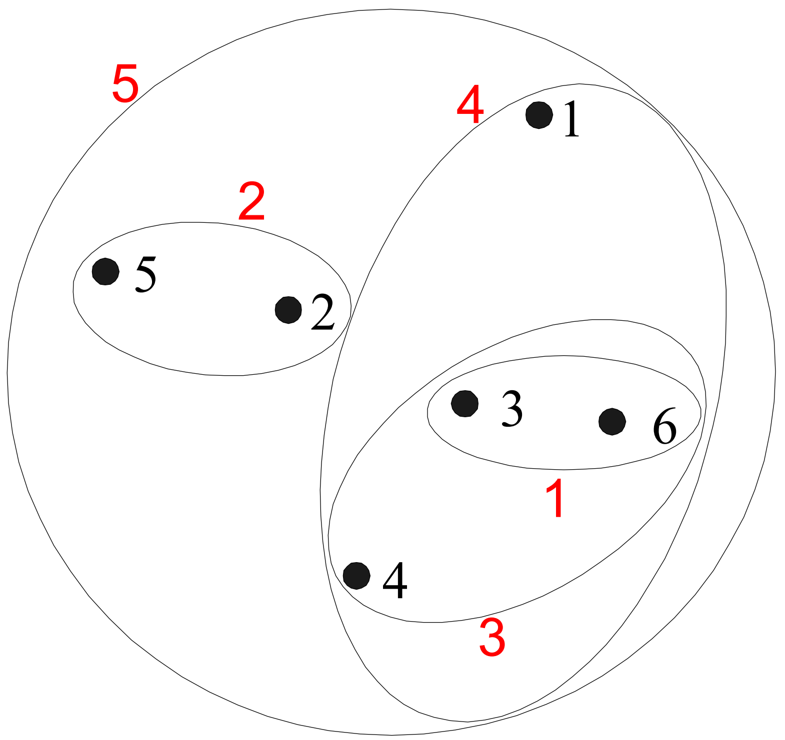


Two Clusters

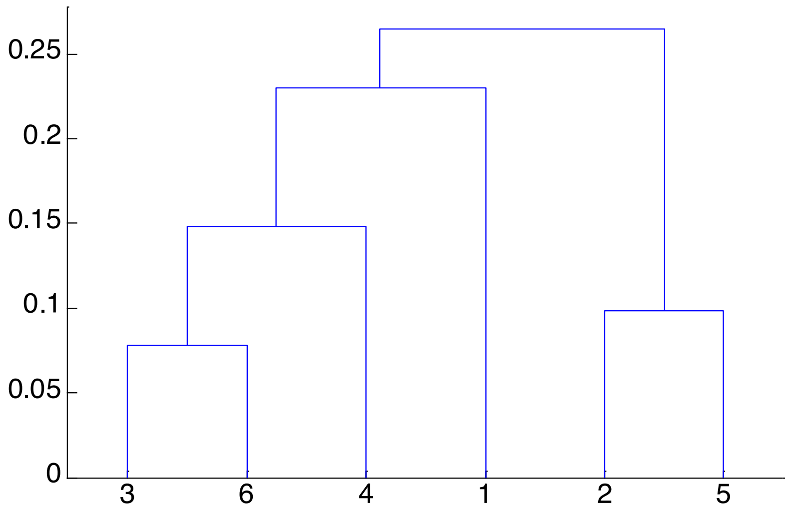
- Tends to break large clusters
- Biased towards globular球状 clusters

Hierarchical Clustering: Group Average

	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Nested Clusters



Dendrogram

Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link

- Strengths
  - Less susceptible (易受影响的) to noise and outliers

- Limitations
  - Biased towards globular clusters

Cluster Similarity: Ward's Method

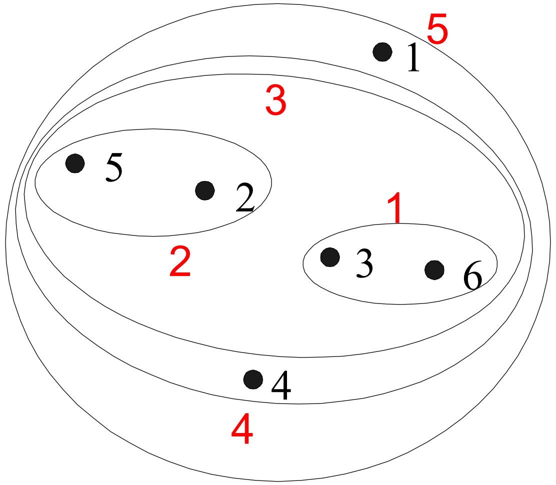
- Similarity of two clusters is based on the increase in squared error (SSE) when two clusters are merged
  - Similar to group average if distance between points is sum of squares distance

- Hierarchical analogue of K-means
  - Can be used to initialize K-means

- Less susceptible to noise and outliers

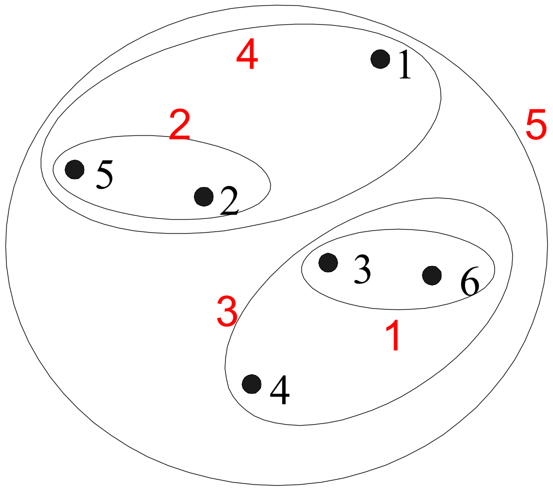
- Biased towards globular cluster

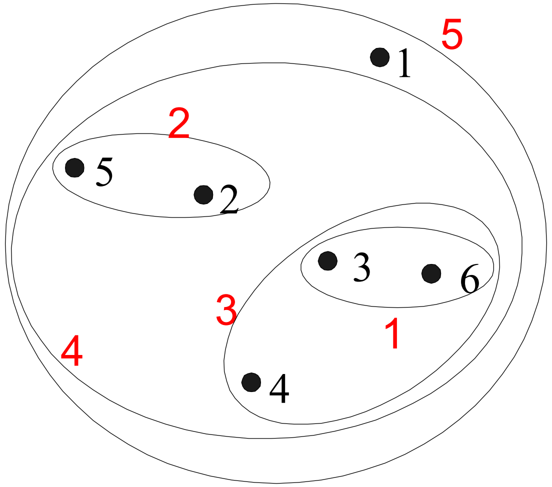
Hierarchical Clustering: Comparison



MIN

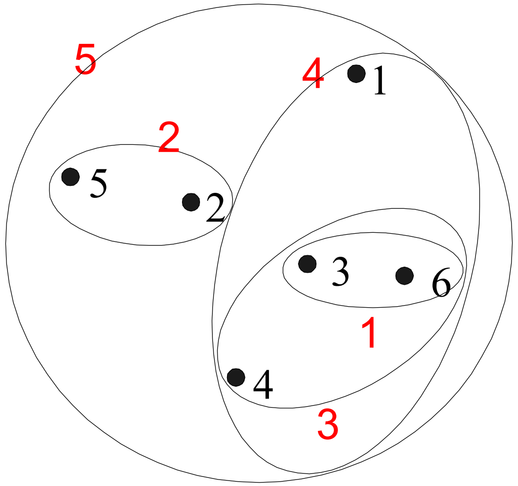
MAX





Group Average

Ward's Method



Hierarchical Clustering: Time and Space requirements

- $O(N^2)$ space since it uses the proximity matrix.
  - N is the number of points.

- $O(N^3)$ time in many cases
  - There are N steps and at each step the size, N^2, proximity matrix must be updated and searched
  - Complexity can be reduced to $O(N^2 \log(N))$ time for some approaches

Hierarchical Clustering: Problems and Limitations

- Computational complexity in time and space

- Once a decision is made to combine two clusters, it cannot be undone

- No objective function is directly minimized

- Different schemes have problems with one or more of the following:
  - Sensitivity to noise and outliers
  - Difficulty handling different sized clusters and convex shapes(凸型形状)
  - Breaking large clusters

DBSCAN

DBSCAN: Density-Based Clustering

- DBSCAN is a Density-Based Clustering algorithm

- Reminder: In density-based clustering we partition points into dense regions separated by not-so-dense regions.

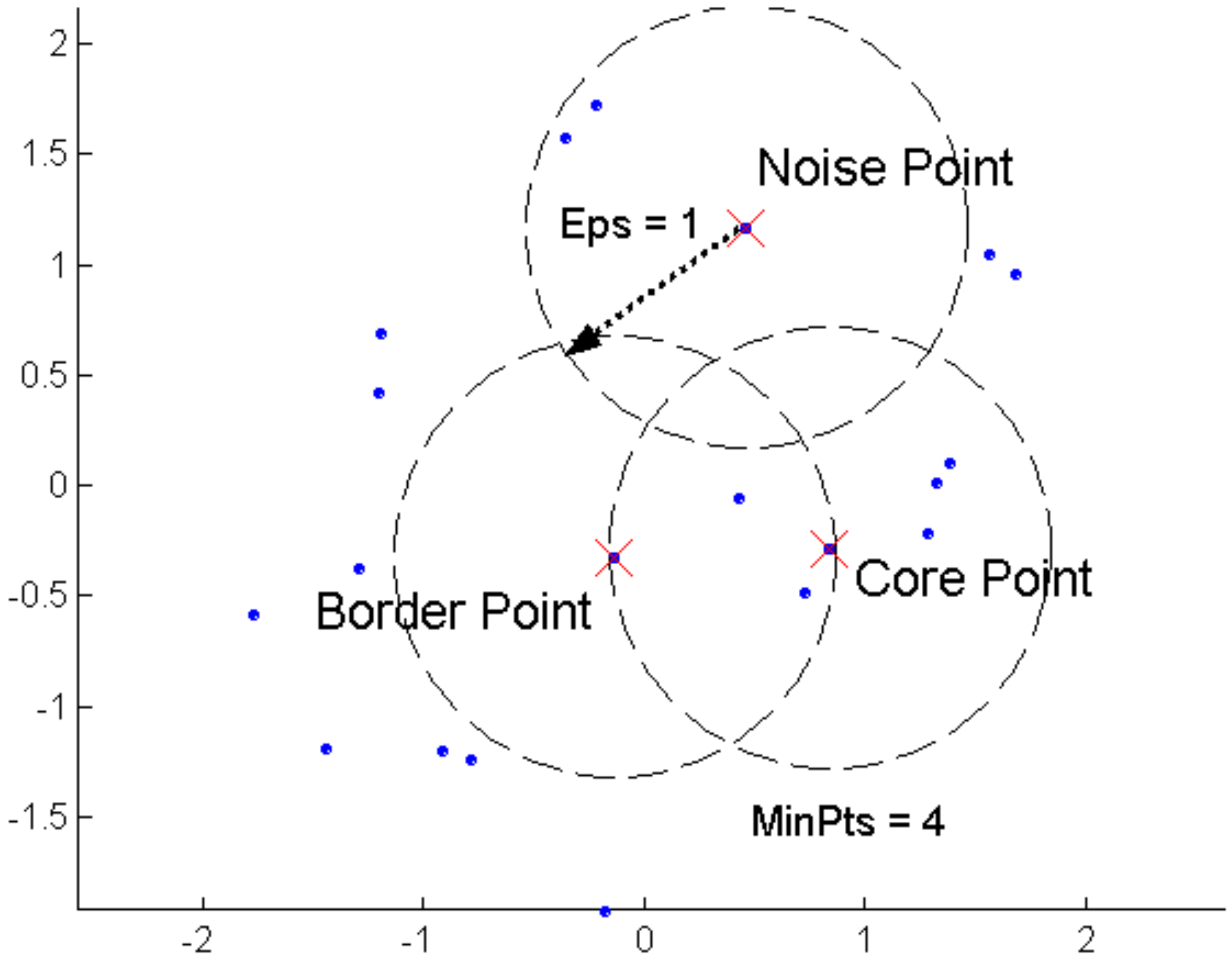
- Important Questions:
  - How do we measure density?
  - What is a dense region?

- DBSCAN:
  - Density at point p: number of points within a circle of radius Eps
  - Dense Region: A circle of radius Eps that contains at least MinPts points

DBSCAN

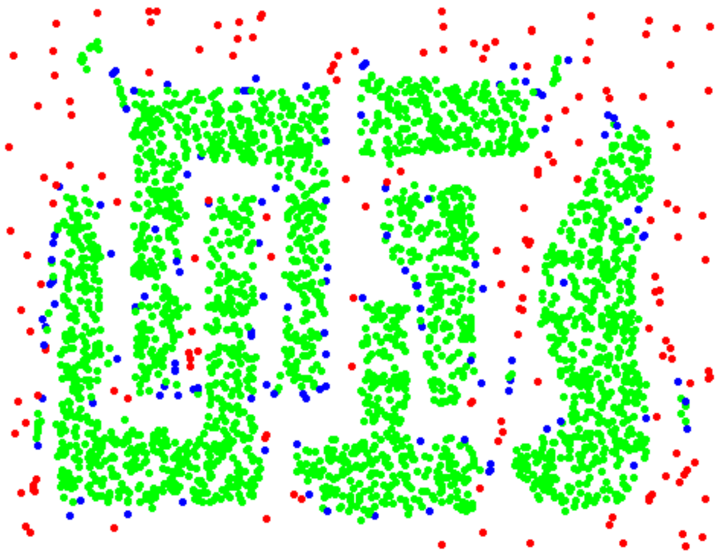
- Characterization of points
  - A point is a core point if it has more than a specified number of points (MinPts) within Eps
    - These points belong in a dense region and are at the interior内部 of a cluster
  - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.
  - A noise point is any point that is not a core point or a border point.

DBSCAN: Core, Border, and Noise Points



DBSCAN: Core, Border and Noise Points

Original Points

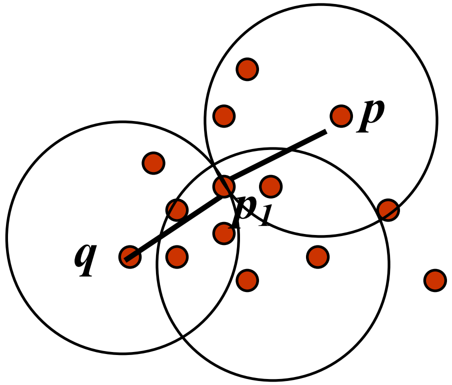


Point types: core, border and noise

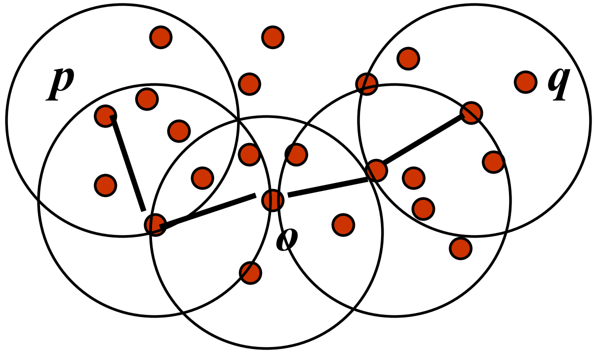
Eps = 10, MinPts = 4

Density-Connected points

- Density edge
  - We place an edge between two core points q and p if they are within distance Eps.



- Density-connected
  - A point p is density-connected to a point q if there is a path of edges from p to q

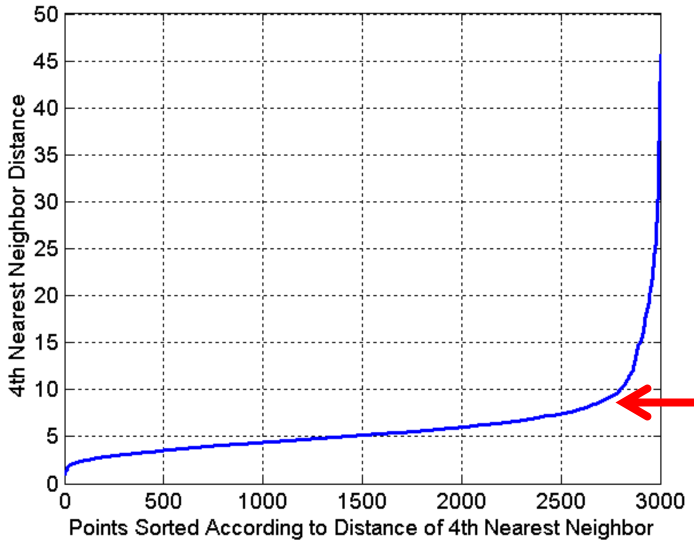


DBSCAN Algorithm

- Label points as core, border and noise
- Eliminate noise points
- For every core point p that has not been assigned to a cluster
  - Create a new cluster with the point p and all the points that are density-connected to p.
- Assign border points to the cluster of the closest core point.

DBSCAN: Determining Eps and MinPts

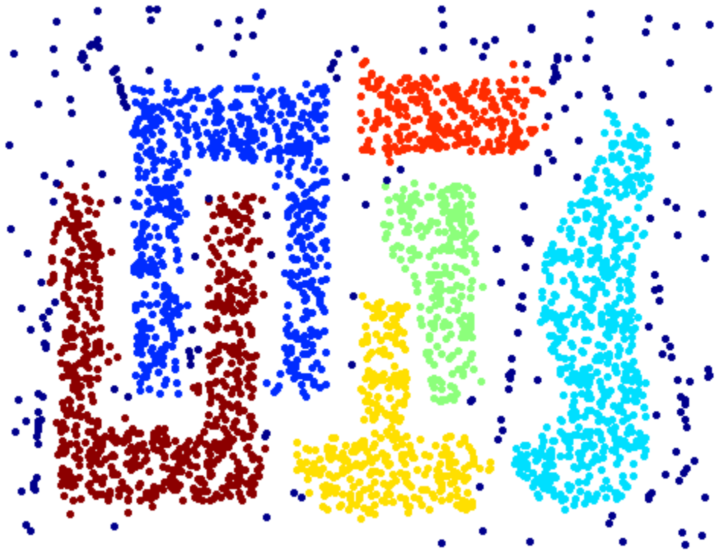
- Idea: for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor
- Find the distance d where there is a "knee"(膝) in the curve
  - Eps = d, MinPts = k



Eps ~ 7-10
MinPts = 4

When DBSCAN Works Well

Original Points



Clusters

- Resistant(不受影响的) to Noise
- Can handle clusters of different shapes and sizes

DBSCAN: Sensitive to Parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

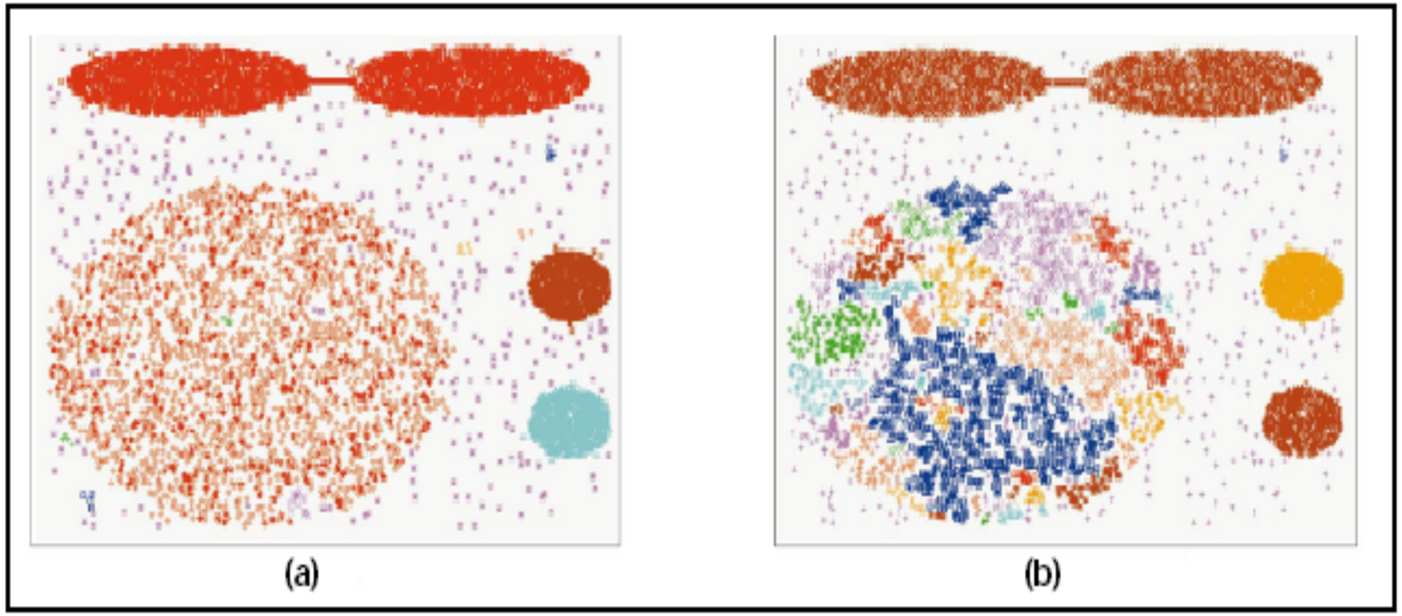
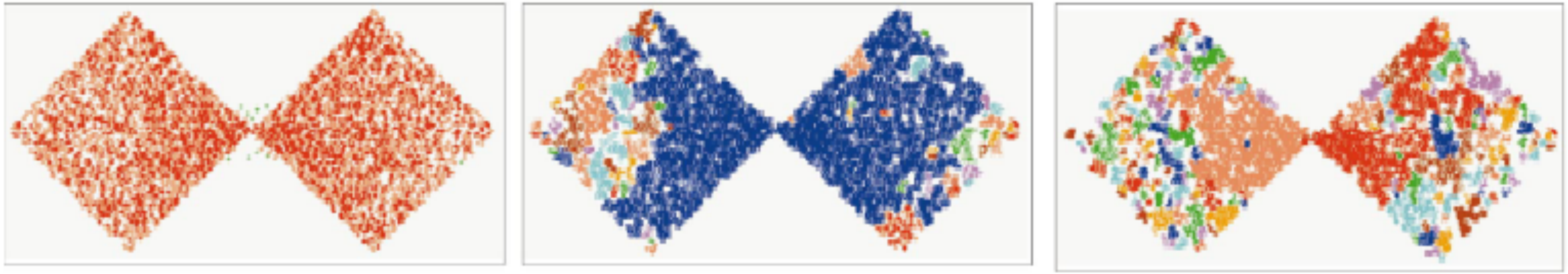
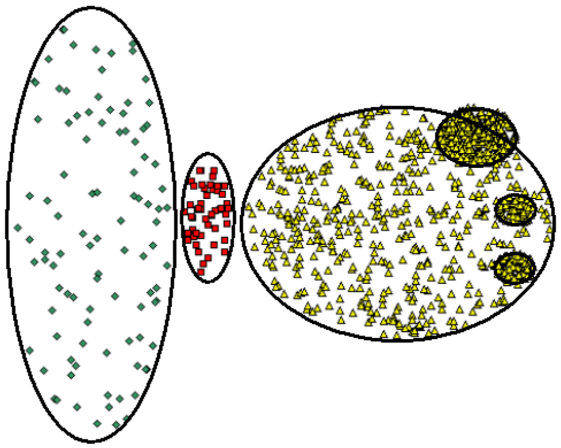


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.

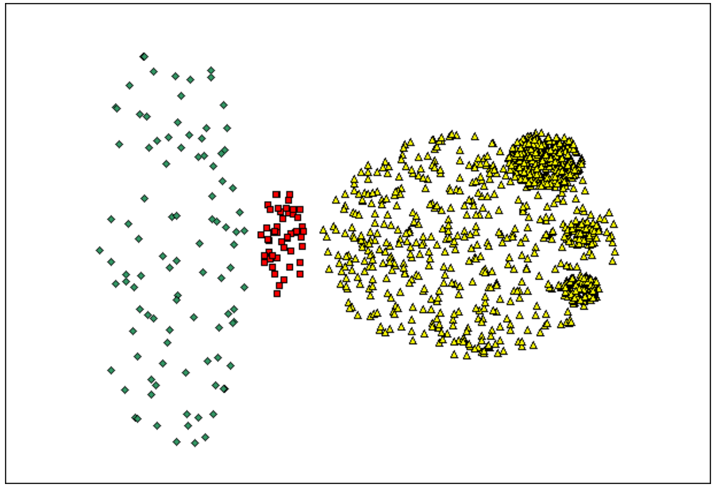


(a) (b) (c)

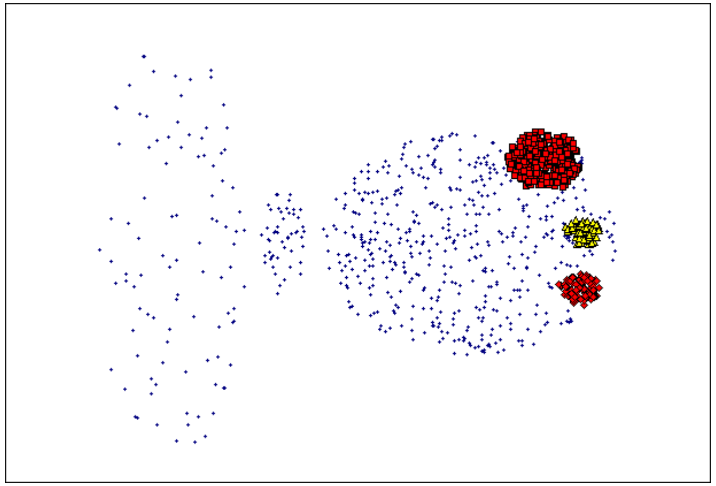
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

- Varying densities
- High-dimensional data

Other algorithms

- PAM, CLARANS: Solutions for the k-medoids problem
- BIRCH: Constructs a hierarchical tree that acts a summary of the data, and then clusters the leaves.
- MST: Clustering using the Minimum Spanning Tree.
- ROCK: clustering categorical data by neighbor and link analysis
- LIMBO, COOLCAT: Clustering categorical data using information theoretic tools.
- CURE: Hierarchical algorithm uses different representation of the cluster
- CHAMELEON: Hierarchical algorithm uses closeness and interconnectivity for merging

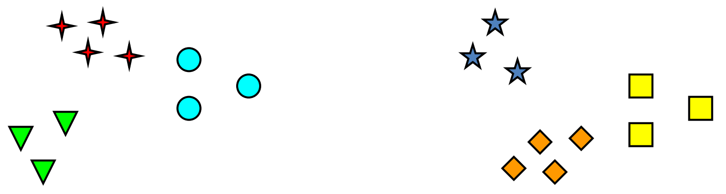
CLUSTERING EVALUATION

Clustering Evaluation

- We need to evaluate the “goodness” of the resulting clusters?
- But “clustering lies in the eye of the beholder”!
  - 一千个读者有一千个哈姆雷特

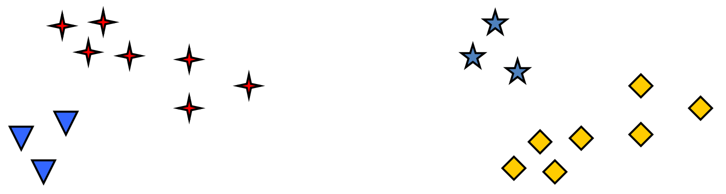
Quality of Clustering can be Ambiguous

How many clusters?



Six Clusters

Two Clusters



Four Clusters

Clustering Evaluation

- Then why do we want to evaluate them?
  - 避免找到的是噪音的模式
  - To compare clusterings, or clustering algorithms
  - To compare against a “ground truth”

Different Aspects of Cluster Validation

1. Internal Evaluation:
   1. 在不参考外部信息的情况下评估聚类分析结果与数据的拟合程度。
   2. 仅使用数据本身
   3. 确定一组数据的聚类趋势，即区分数据中是否确实存在非随机结构。
   4. 确定“正确”的簇数。
2. External Evaluation: Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.

Metrics for cluster and clustering validity

- 接下来我们将看到一些聚类有效性的指标。
- 这些指标可用于评估集群或聚类
- 在聚类有效性中，我们评估一组点，以确定它们是否正确放置在一起。

CLUSTER VALIDITY WITH INTERNAL CRITERIA

Internal Measures

- Internal Index: 用于在不参考外部信息的情况下衡量聚类结构的好坏的指标
  Example: Sum of Square Errors (SSE)
  - SSE can be used to evaluate a cluster or a clustering:
    - For a cluster of points C_i, the SSE is:

$$SSE(C_i) = \sum_{x \in C_i} (x - c_i)^2, c_i = \text{centroid of cluster } C_i$$

    - For a clustering $C = \{C_1, C_2, \ldots, C_k\}$, the SSE is:

$$SSE(C) = \sum_{i} \sum_{x \in C_i} (x - c_i)^2, c_i = \text{centroid of cluster } C_i$$

- SSE can also be used to compare clusters, or clusterings

Cohesion and Separation

- In general, we evaluate clusters and clusterings based on cohesion and separation
  - Cluster Cohesion: Measures how closely related are objects in a cluster
  - Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters

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

$$WSS = \sum_{i} \sum_{x \in C_i} (x - c_i)^2$$

We want this to be small

  - Separation is measured by the sum of square error of the centroids

$$BSS = \sum_{i} m_i (c - c_i)^2$$

We want this to be large

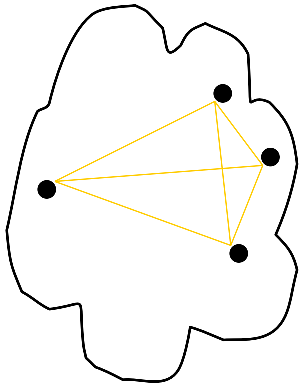
    - Where m_i is the size of cluster i , c the overall mean. It also holds that:

$$BSS = \sum_{x \in C_i} \sum_{y \in C_j} (x - y)^2$$

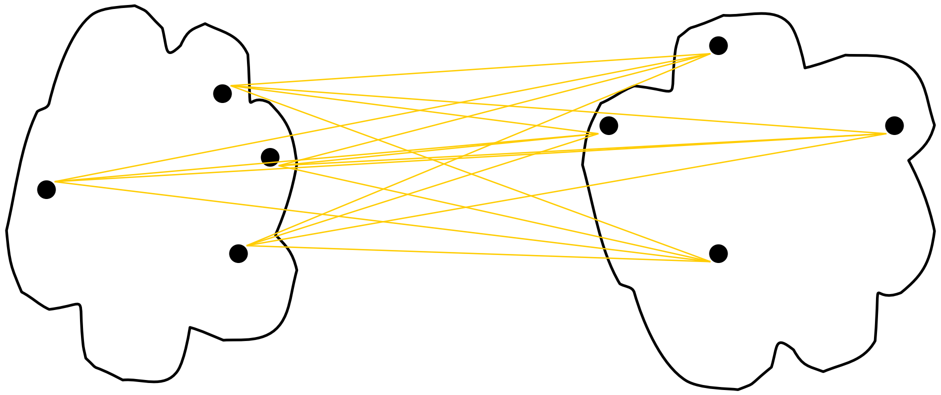
  - Interesting observation: WSS+BSS = constant

Cohesion and Separation

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



cohesion

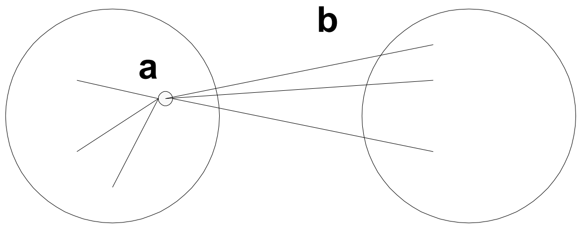


separation

Silhouette Coefficient 轮廓系数

- 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_i = average distance of i to the points in its own cluster
  - Calculate b_i = min (over clusters) of the average distance of i to points in other clusters
  - The silhouette coefficient for a point i is then given by

$$s_i = 1 - a_i/b_i$$



  - Typically, between 0 and 1, the closer to 1 the better.
  - Can be less than 0 but this is a problematic case

- Can calculate the Average Silhouette coefficient of the points for a cluster, or for a clustering

Silhouette Coefficient Example

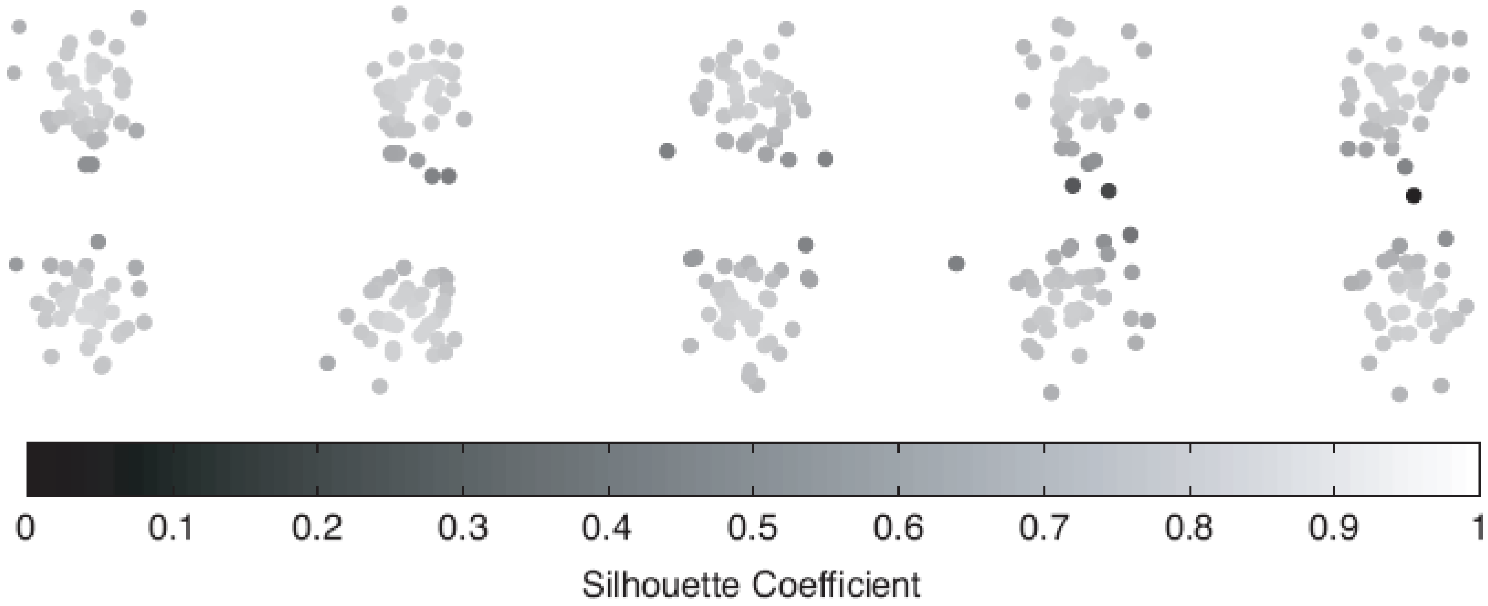
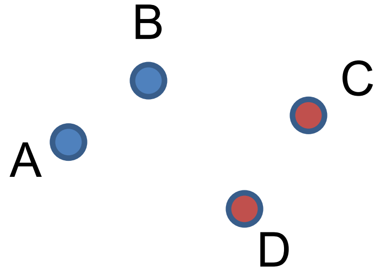


Figure 8.29. Silhouette coefficients for points in ten clusters.

Measuring Cluster Validity Via Correlation

- Two matrices
  - Similarity or Distance Matrix
    - One row and one column for each data point
    - An entry is the similarity or distance of the associated pair of points
  - "Incidence" 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



$$D = \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{bmatrix} 0 & 0.9 & 2.2 & 1.5 \\ 0.9 & 0 & 1.2 & 1.7 \\ 2.2 & 1.2 & 0 & 1.1 \\ 1.5 & 1.7 & 1.1 & 0 \end{bmatrix} \end{array} \begin{array}{c} \\ A \\ B \\ C \\ D \end{array}$$

$$I = \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ A \\ B \\ C \\ D \end{array}$$

Measuring Cluster Validity Via Correlation

- Compute the correlation between the two matrices

$$CorrCoeff(X,Y) = \frac{\sum_i (x_i - \mu_X)(y_i - \mu_Y)}{\sqrt{\sum_i (x_i - \mu_X)^2}\sqrt{\sum_i (y_i - \mu_Y)^2}}$$

  - Since the matrices are symmetric, only the correlation between n(n-1) / 2 entries needs to be calculated.

- High correlation (positive for similarity, negative for distance) indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or contiguity-based clusters.

$$S = \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{bmatrix} 0 & 0.9 & 2.2 & 1.5 \\ 0.9 & 0 & 1.2 & 1.7 \\ 2.2 & 1.2 & 0 & 1.1 \\ 1.5 & 1.7 & 1.1 & 0 \end{bmatrix} \end{array} \begin{array}{c} A \\ B \\ C \\ D \end{array}$$

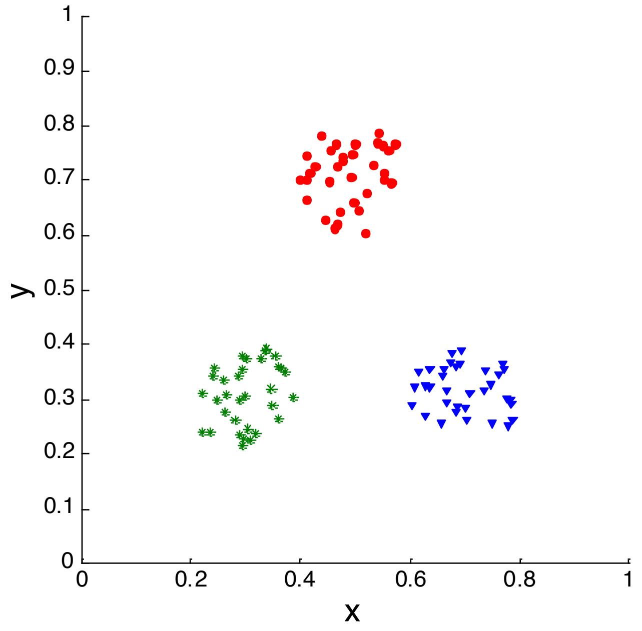
$$I = \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \end{array} \begin{array}{c} A \\ B \\ C \\ D \end{array}$$

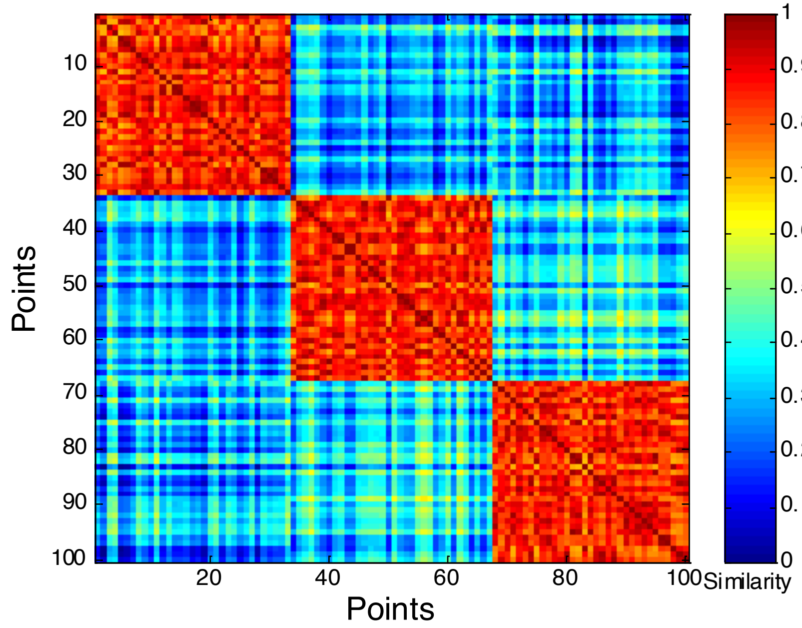
$CorrCoeff$([0.9, 2.2, 1.5, 1.2, 1.7, 1.1],
[1, 0, 0, 0, 0, 1])
= - 0.71

Using Similarity Matrix for Cluster Validation

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

Corr = -0.9235

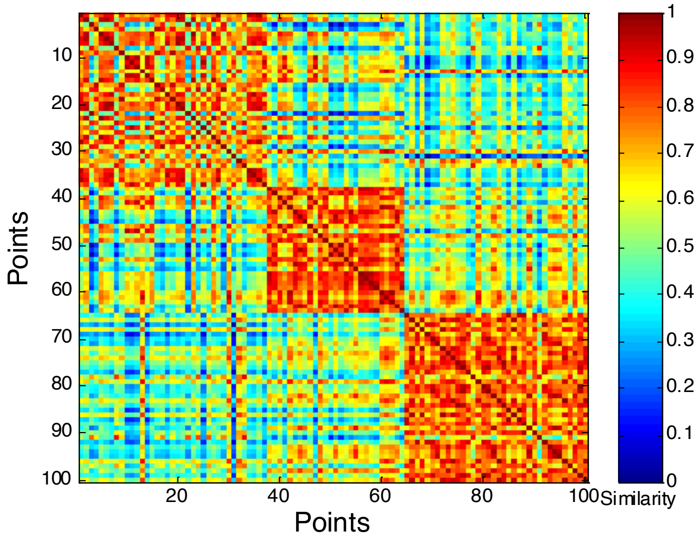


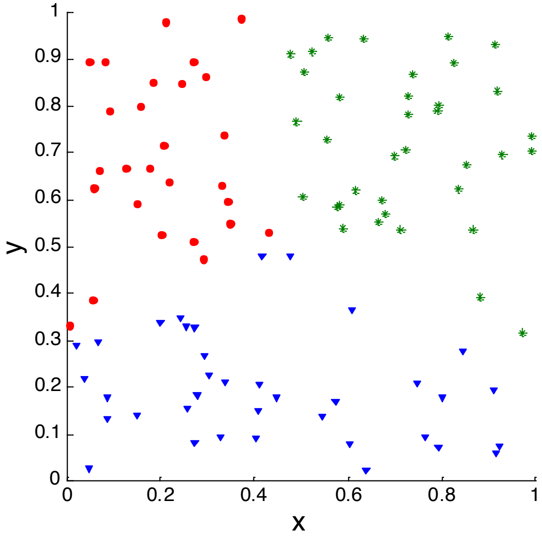


$$sim(i,j) = 1 - \frac{d_{ij} - d_{min}}{d_{max} - d_{min}}$$

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp(清晰的)

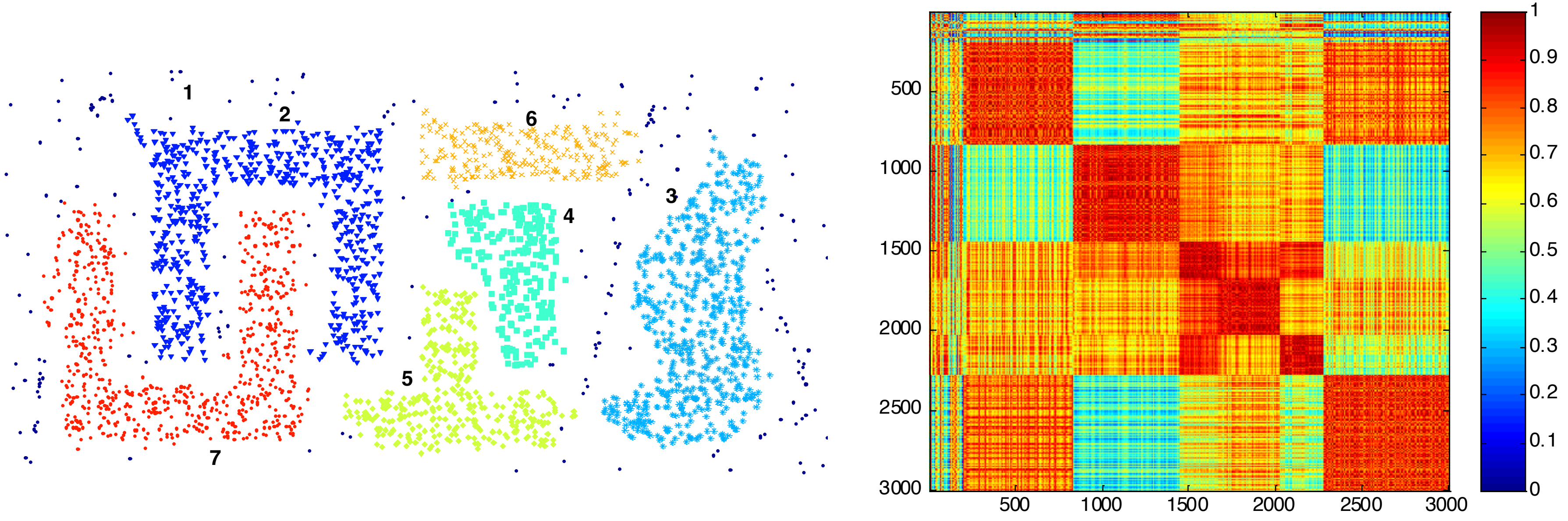




Corr = -0.5810

K-means

Using Similarity Matrix for Cluster Validation



DBSCAN

- Clusters in more complicated figures are not well separated
- This technique can only be used for small datasets since it requires a quadratic computation

Internal measures – remark

- Internal measures have the problem that the clustering algorithm did not set out to optimize this measure, so it is will not necessarily do well with respect to the measure.
  - Essentially, we check whether one criterion correlates well with another

- An internal measure can also be used as an objective function for clustering
- The algorithm that optimizes this criterion is expected to do well.

STATISTICAL FRAMEWORK FOR CLUSTER(ING) VALIDITY

Framework for Cluster Validity

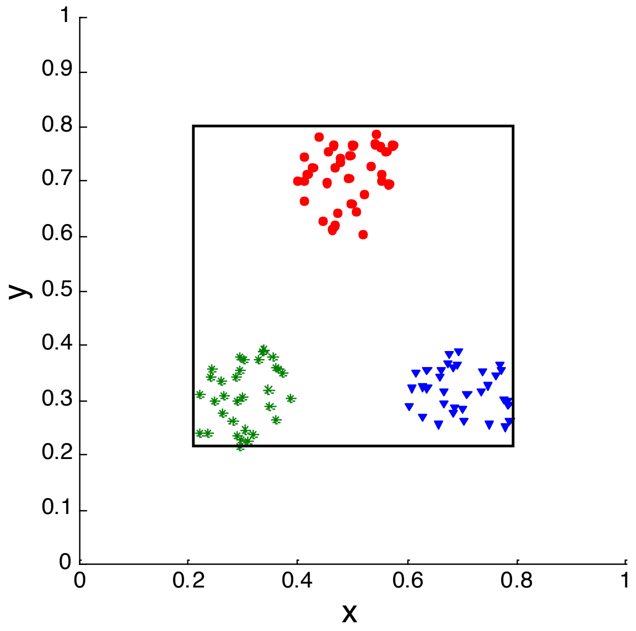
- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity
  - The more “non-random” a clustering result is, the more likely it represents valid structure in the data
  - Can compare the index value for a clustering with the values of the index that result from clustering random data, or from random clusterings.
    - If the value of the index is unlikely, then the clustering results are valid
  - Comparing against clustering of random data tells us if there is valid clustering structure in the data
  - Comparing against random clusterings tells us if the clustering algorithm is meaningful
    - Although a random clustering is a weak alternative.

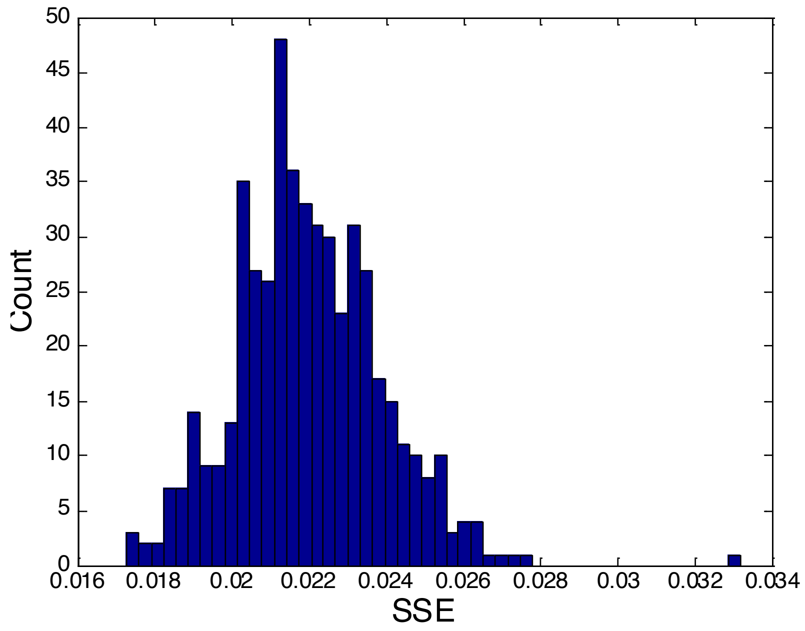
- For comparing the results of two different clusterings, a framework is less necessary, but we may want to know whether the difference between two index values is significant

Statistical Framework for SSE

- Example
  - Compare SSE of 0.005 against three clusters in random data
  - Histogram of SSE for three clusters in 500 random data sets of 100 random points distributed in the range 0.2 – 0.8 for x and y
    - Value 0.005 is very unlikely

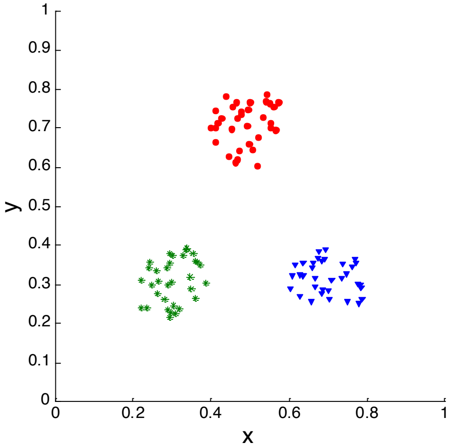
SSE = 0.005

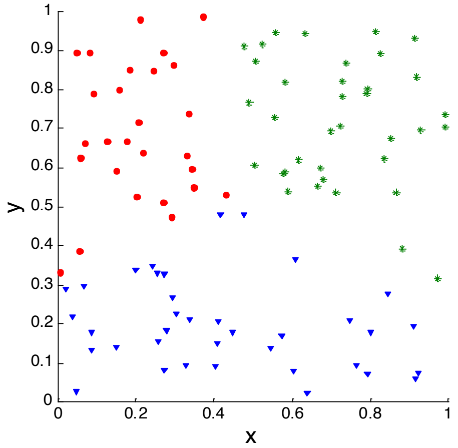


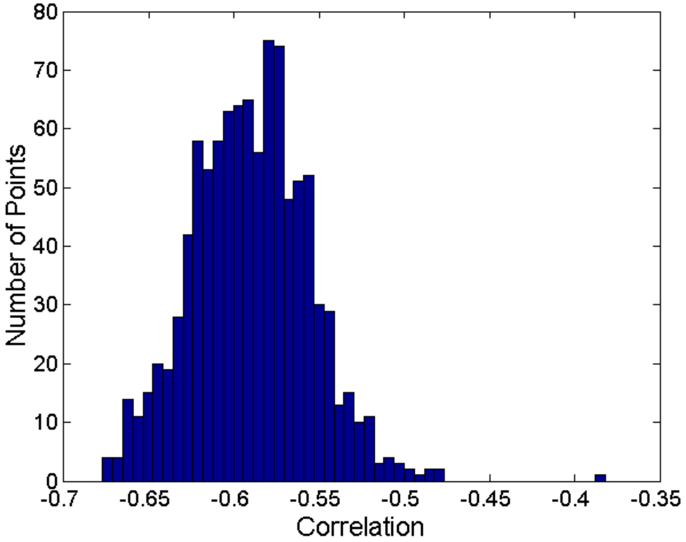


Statistical Framework for Correlation

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







Corr = -0.9235

Corr = -0.5810

Empirical p-value

- What we do is similar to a permutation test:
- We have a measurement v (e.g., the SSE value)
- We compute N measurements on random datasets
- We compute the empirical p-value as the fraction of measurements in the random data that have value less or equal than value v (or greater or equal if we want to maximize)
  - i.e., the value in the random dataset is at least as good as that in the real data

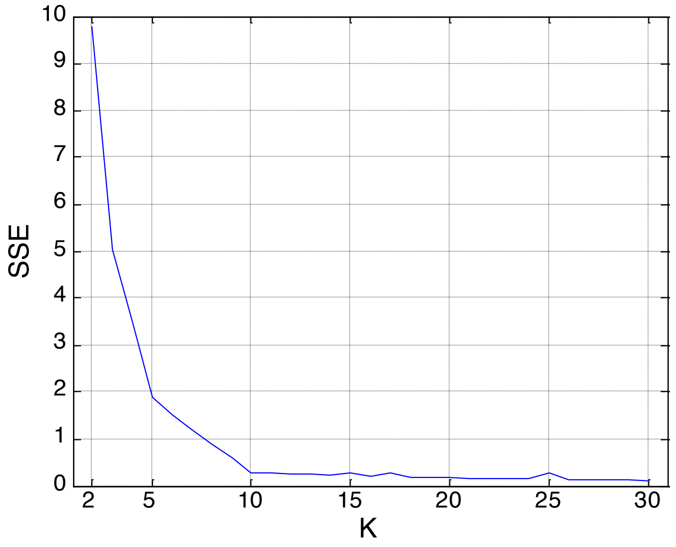
- We usually require that p-value ≤ 0.05

- Hard question: what is the right notion of a random dataset?

ESTIMATING THE “RIGHT” NUMBER OF CLUSTERS

Estimating the "right" number of clusters

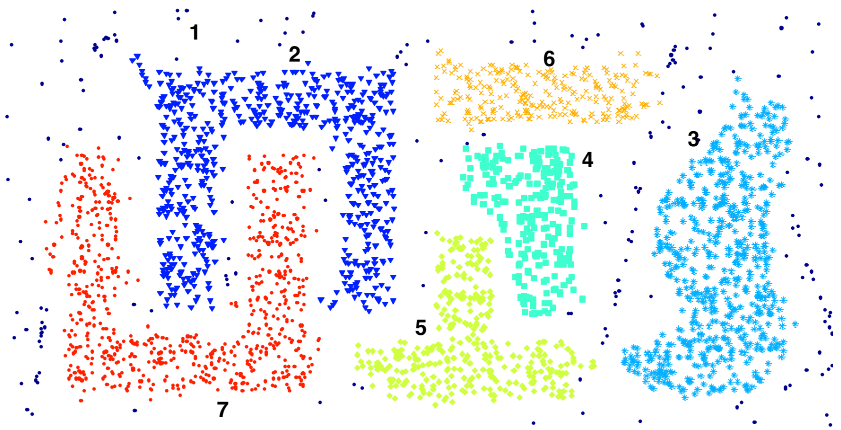
- Typical approach: find a "knee" in an internal measure curve.

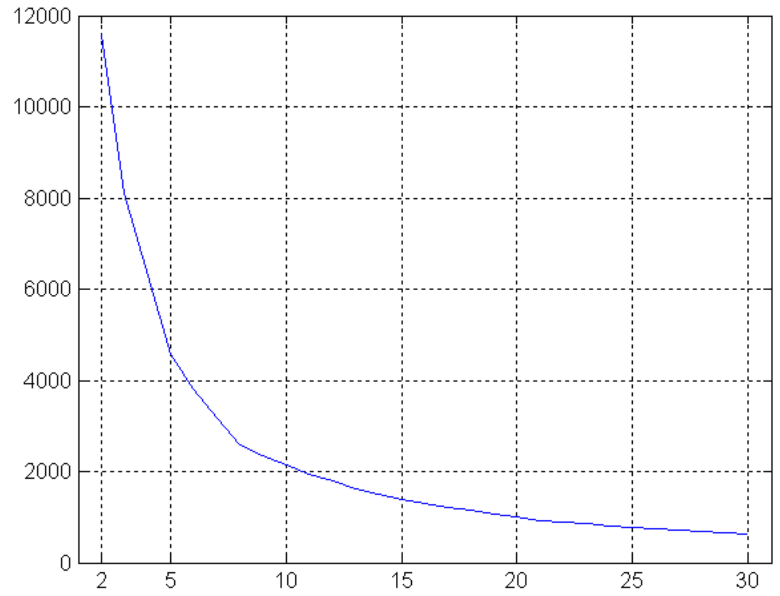


- Question: why not the k that minimizes the SSE?
  - Goal: minimize a measure, but with a "simple" clustering
- Desirable property: the clustering algorithm does not require the number of clusters to be specified (e.g., DBSCAN)

Estimating the “right” number of clusters

- SSE curve for a more complicated data set

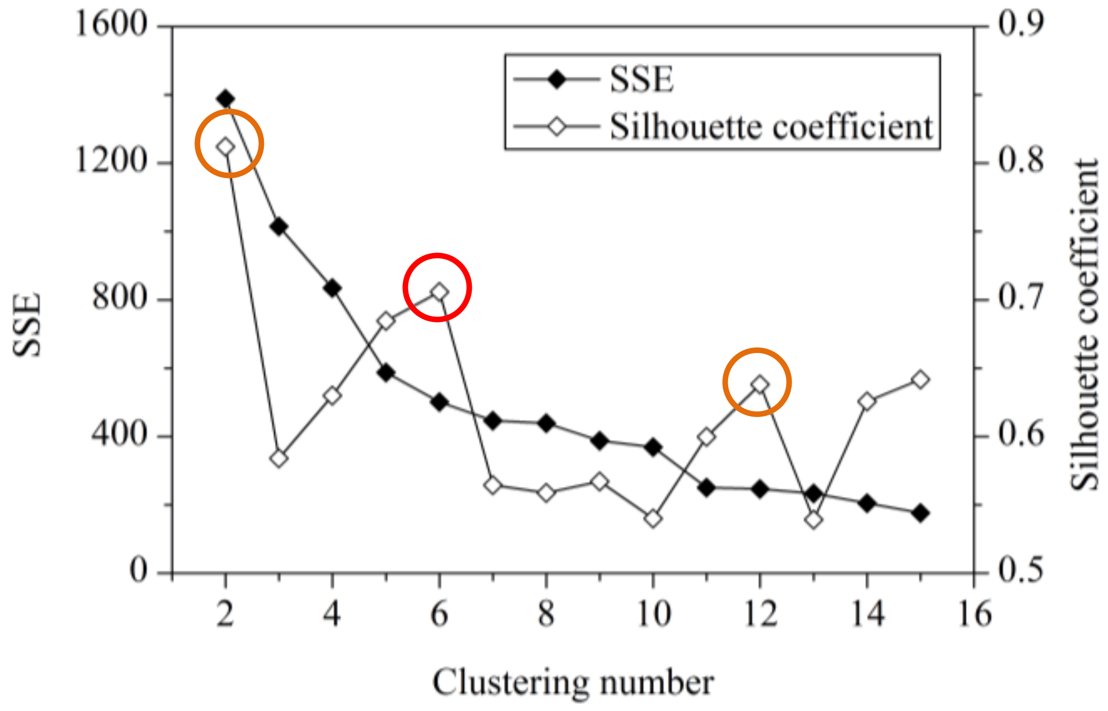




SSE of clusters found using K-means

Estimating the “right” number of clusters

- A metric that is better suited for this task is the average silhouette coefficient which does not change monotonically with the number of clusters
- In this example 6 seems to be a good number of clusters since it has high silhouette coefficient and low SSE
- 2 has the highest silhouette coefficient but highest SSE.
- 12 could be another alternative



EVALUATION WITH EXTERNAL "GROUND TRUTH"

External Measures for Clustering Validity

- Assume that the data is labeled with some class labels
  - E.g., documents are classified into topics, people classified according to their income, politicians classified according to the political party.
  - This is called the "ground truth"
- In this case we want the clusters to be homogeneous with respect to classes
  - Each cluster should contain elements of mostly one class
  - Each class should ideally be assigned to a single cluster
- This does not always make sense
  - Clustering is not the same as classification
  - …but this is what people use most of the time

Confusion/Contingency matrix

- Rows: clusters
- Columns: classes
- Entries: counts/probability of cluster-class pair
- n = number of points
- m_i = points in cluster i
- c_j = points in class j
- n_{ij}= points in cluster i coming from class j

- The confusion/contingency matrix is sometimes used for evaluation as is
  - It gives us the mapping between the clusters and ground truth classes

Confusion/Contingency matrix of clusters and classes (counts)

	Class 1	Class 2	Class 3	
Cluster 1	n_{11}	n_{12}	n_{13}	m_1
Cluster 2	n_{21}	n_{22}	n_{23}	m_2
Cluster 3	n_{31}	n_{32}	n_{33}	m_3
	c_1	c_2	c_3	n

Example

	Class 1	Class 2	Class 3	
Cluster 1	2	3	85	90
Cluster 2	90	12	8	110
Cluster 3	8	85	7	100
	100	100	100	300

Measures of cluster homogeneity

- Compute probabilities:

$$p_{ij} = \frac{n_{ij}}{m_i}$$

The probability that a randomly selected point from cluster i comes from class j.

  - Probabilities of rows sum to 1
- Purity:
  - Of a cluster i: $p_i = \max_j p_{ij}$
  - Of a clustering: $p(C) = \sum_{i=1}^{K} \frac{m_i}{n} p_i$
- Entropy:
  - Of a cluster i: $e_i = -\sum_{j=1}^{L} p_{ij} \log p_{ij}$
    - Highest when uniform, zero when single class
  - Of a clustering: $e = \sum_{i=1}^{K} \frac{m_i}{n} e_i$

	Class 1	Class 2	Class 3	
Cluster 1	p_{11}	p_{12}	p_{13}	m_1
Cluster 2	p_{21}	p_{22}	p_{23}	m_2
Cluster 3	p_{31}	p_{32}	p_{33}	m_3
	c_1	c_2	c_3	n

	Class 1	Class 2	Class 3	
Cluster 1	0.02	0.03	0.95	90
Cluster 2	0.82	0.11	0.07	110
Cluster 3	0.08	0.85	0.07	100
	100	100	100	300

Purity: (0.94, 0.81, 0.85)
– overall 0.86

Entropy: (0.33, 0.85, 0.76)
– overall 0.66

Classification-based Measures

- **Precision**:
  - Of cluster i with respect to class j:

$$Prec(i,j) = \frac{n_{ij}}{m_i} = p_{ij}$$

  - Percentage of the cluster i that comes from class j
- **Recall**:
  - Of cluster i with respect to class j:

$$Rec(i,j) = \frac{n_{ij}}{c_j}$$

  - Percentage of class j that goes to cluster i
- **F-measure**:
  - Harmonic Mean of Precision and Recall:

$$F(i,j) = \frac{2 * Prec(i,j) * Rec(i,j)}{Prec(i,j) + Rec(i,j)}$$

	Class 1	Class 2	Class 3	
Cluster 1	n_{11}	n_{12}	n_{13}	m_1
Cluster 2	n_{21}	n_{22}	n_{23}	m_2
Cluster 3	n_{31}	n_{32}	n_{33}	m_3
	c_1	c_2	c_3	n

	Class 1	Class 2	Class 3	
Cluster 1	2	3	85	90
Cluster 2	90	12	8	110
Cluster 3	8	85	7	100
	100	100	100	300

Precision-recall for cluster-class cobinations

- Precision of cluster i with respect to class j: $Prec(i,j) = \frac{n_{ij}}{m_i} = p_{ij}$
  - Percentage of the cluster i that comes from class j
- Recall of cluster i with respect to class j: $Rec(i,j) = \frac{n_{ij}}{c_j}$
  - Percentage of class j that goes to cluster i

	Class 1	Class 2	Class 3	
Cluster 1	2	3	85	90
Cluster 2	90	12	8	110
Cluster 3	8	85	7	100
	100	100	100	300

	Class 1	Class 2	Class 3
Cluster 1	0.02	0.03	0.95
Cluster 2	0.82	0.11	0.07
Cluster 3	0.08	0.85	0.07

Precision Table

	Class 1	Class 2	Class 3
Cluster 1	0.02	0.03	0.85
Cluster 2	0.90	0.12	0.08
Cluster 3	0.08	0.85	0.07

Recall Table

Precision/Recall for clusters and clusterings

- Assign to cluster i the class k_i such that $k_i = \arg\max_j n_{ij}$
- Precision:
  - Of cluster i: $Prec(i) = \frac{n_{ik_i}}{m_i}$
  - Of the clustering: $Prec(C) = \sum_i \frac{m_i}{n} Prec(i)$
- Recall:
  - Of cluster i: $Rec(i) = \frac{n_{ik_i}}{c_{k_i}}$
  - Of the clustering: $Rec(C) = \sum_i \frac{m_i}{n} Rec(i)$
- F-measure:
  - Harmonic Mean of Precision and Recall

	Class 1	Class 2	Class 3	
Cluster 1	2	3	85	90
Cluster 2	90	12	8	110
Cluster 3	8	85	7	100
	100	100	100	300

Precision: (0.94, 0.81, 0.85)
– overall 0.86
Recall: (0.85, 0.9, 0.85)
- overall 0.87

Good and bad clustering

	Class 1	Class 2	Class 3	
Cluster 1	2	3	85	90
Cluster 2	90	12	8	110
Cluster 3	8	85	7	100
	100	100	100	300

Purity: (0.94, 0.81, 0.85)
– overall 0.86
Precision: (0.94, 0.81, 0.85)
– overall 0.86
Recall: (0.85, 0.9, 0.85)
- overall 0.87

	Class 1	Class 2	Class 3	
Cluster 1	20	35	35	90
Cluster 2	30	42	38	110
Cluster 3	38	35	27	100
	100	100	100	300

Purity: (0.38, 0.38, 0.38)
– overall 0.38
Precision: (0.38, 0.38, 0.38)
– overall 0.38
Recall: (0.35, 0.42, 0.38)
– overall 0.39

Another clustering

	Class 1	Class 2	Class 3	
Cluster 1	0	0	35	35
Cluster 2	50	77	38	165
Cluster 3	38	35	27	100
	100	100	100	300

Cluster 1:

Purity: 1

Precision: 1

Recall: 0.35

External Measures of Cluster Validity: Entropy and Purity

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

entropy For each cluster, the class distribution of the data is calculated first, i.e., for cluster j we compute p_{ij}, the 'probability' that a member of cluster j belongs to class i as follows: $p_{ij} = m_{ij}/m_j$, where m_j is the number of values in cluster j and m_{ij} is the number of values of class i in cluster j. Then using this class distribution, the entropy of each cluster j is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the L is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{i=1}^{K} \frac{m_i}{m} e_j$, where m_j is the size of cluster j, K is the number of clusters, and m is the total number of data points.

purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

Final Comment on Cluster Validity

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes