



National Technical University of Athens
Master of Science in Data Science and Machine Learning
Academic year 2023-2024 | 1st semester

Machine Learning

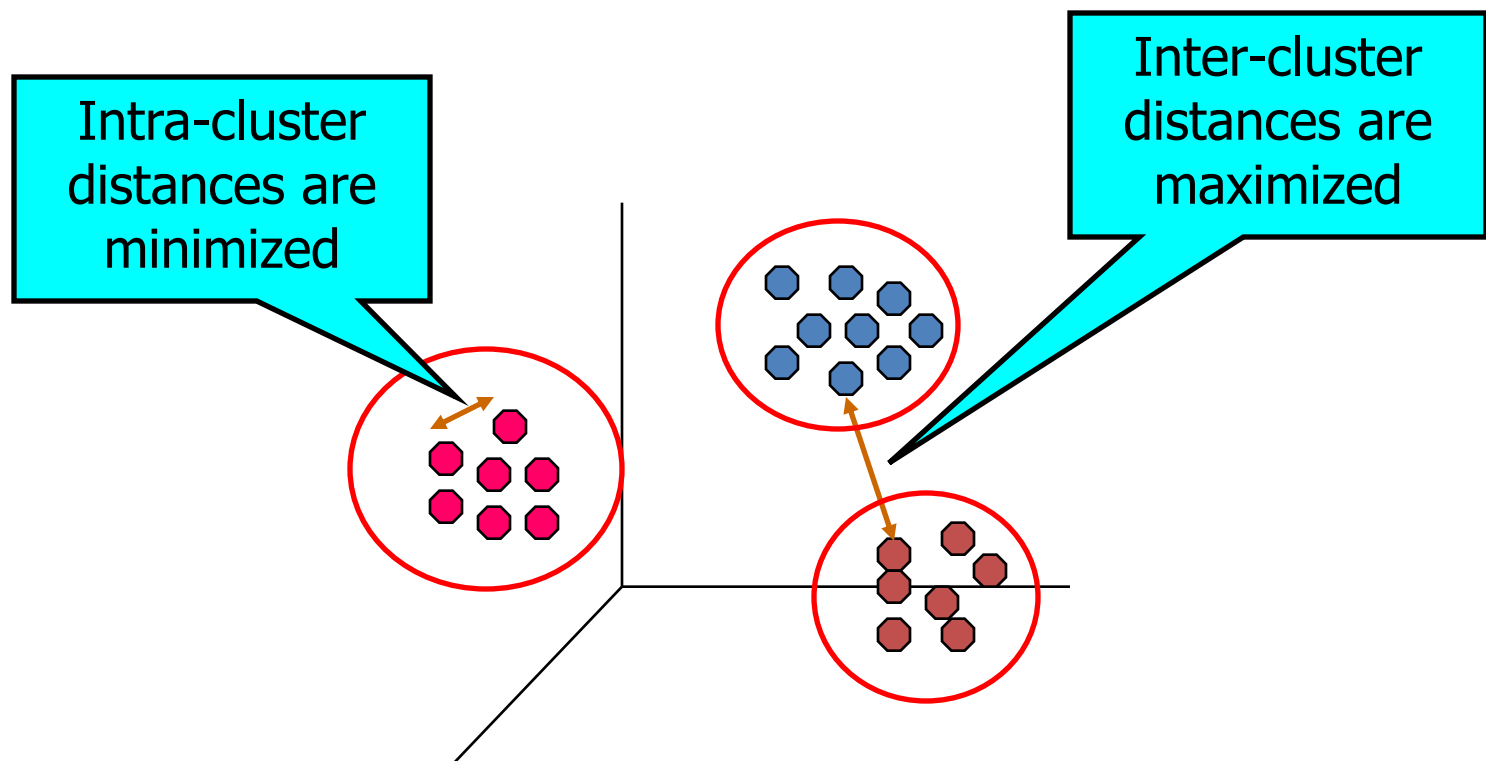
Unsupervised Learning (Clustering)

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What is a Clustering?

- In general 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



Applications of Cluster Analysis

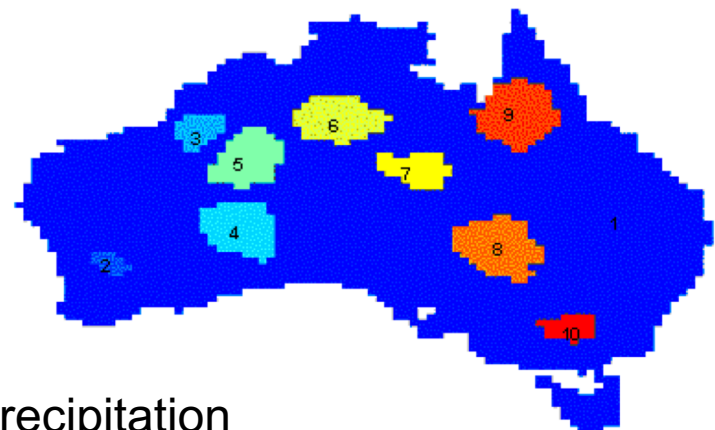
- **Understanding**

- 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

	<i>Discovered Clusters</i>	<i>Industry Group</i>
1	Applied-Matl-DOWN,Bay-Network-DOWN,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-DOWN,Tellabs-Inc-DOWN, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP	Oil-UP



Clustering precipitation
in Australia

Early applications of cluster analysis

- John Snow, London 1854

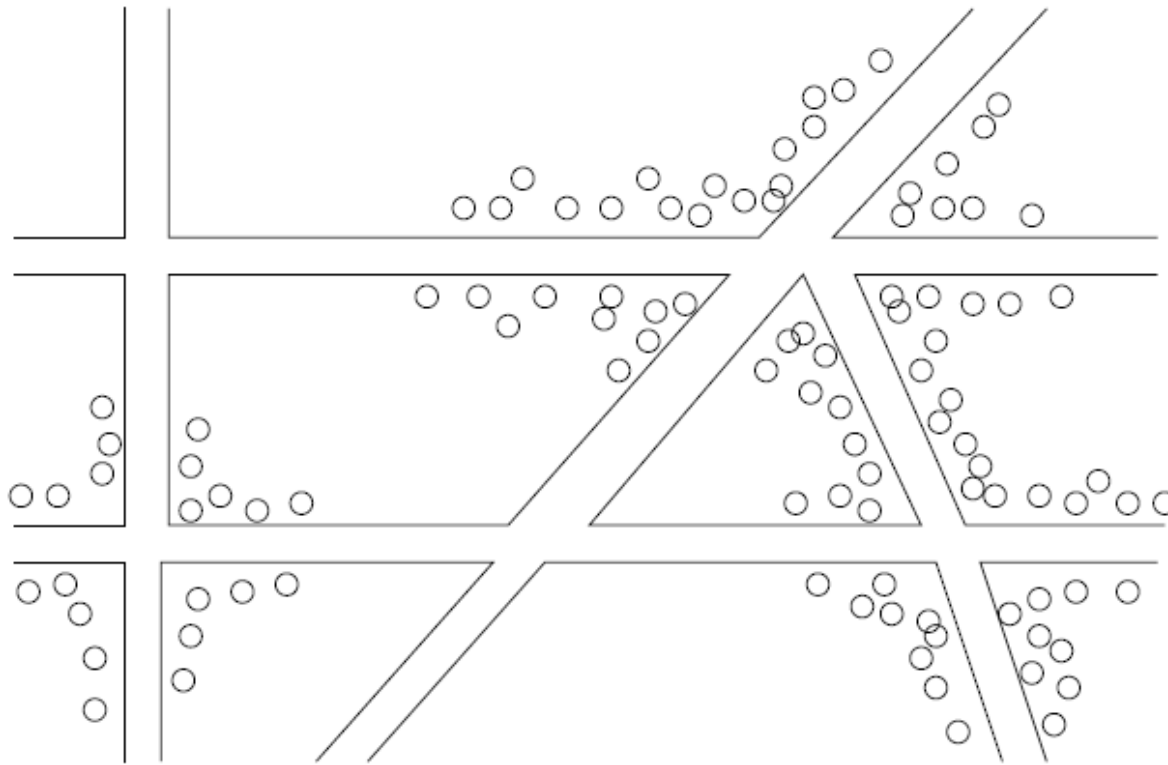
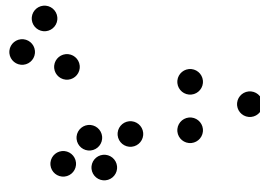
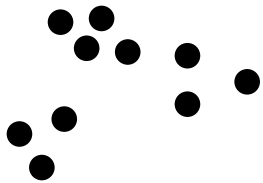
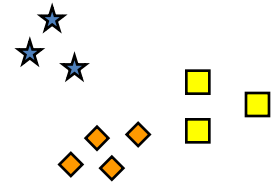
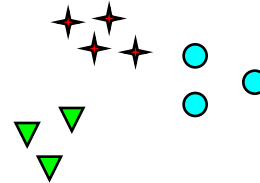


Figure 1.1: Plotting cholera cases on a map of London

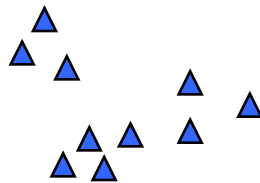
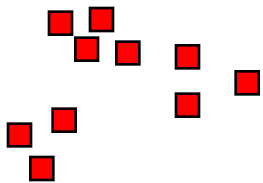
Notion of a Cluster can be Ambiguous



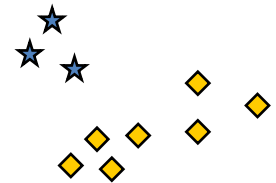
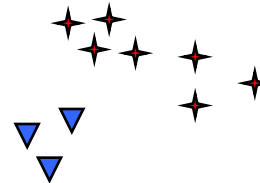
How many clusters?



Six Clusters



Two Clusters

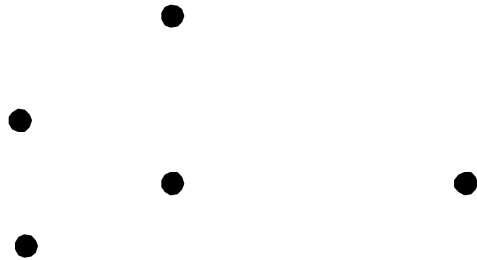
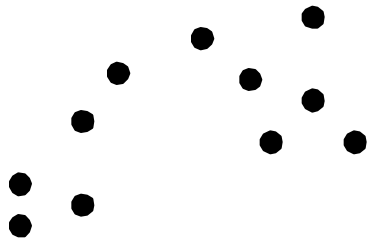


Four Clusters

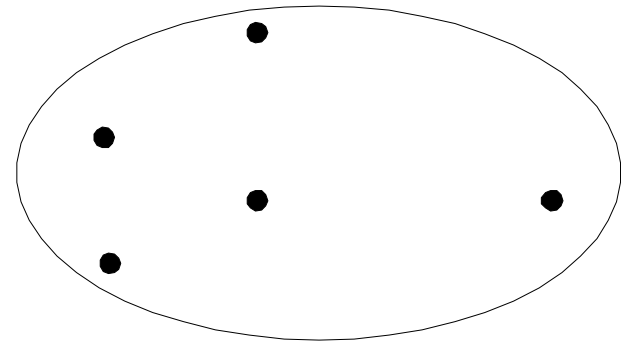
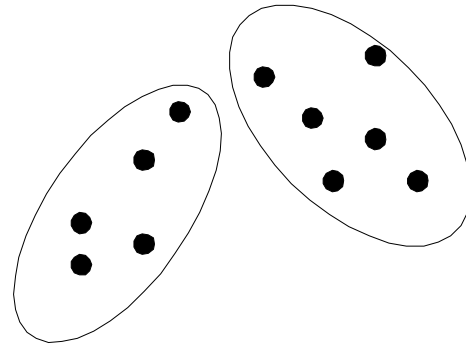
Types of Clusterings

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

Partitional Clustering

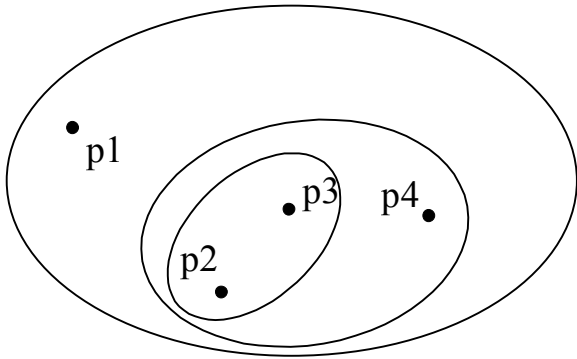


Original Points

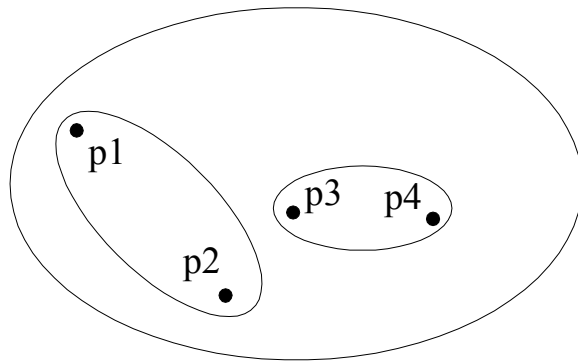


A Partitional Clustering

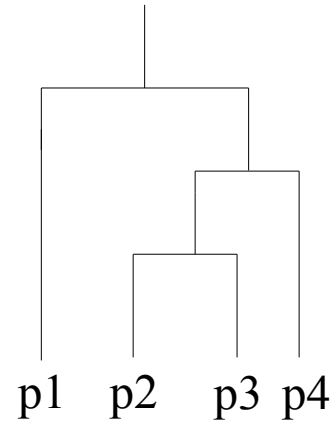
Hierarchical Clustering



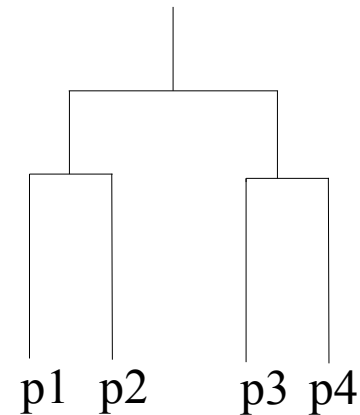
Traditional Hierarchical Clustering



Non-traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Dendrogram

Other types of clustering

- **Exclusive** (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** (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

Types of Clusters: Objective Function

- Clustering as an **optimization problem**
 - Finds clusters that minimize or maximize an **objective function**.
 - Enumerate all possible ways of dividing the points into clusters and evaluate the '**goodness**' of each potential set of clusters by using the given objective function. (NP Hard)
 - 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 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 **minimize the sum of distances** of the points to their respective **centroid**

K-means Clustering

- **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

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

is **minimized**, where c_i is the **centroid** of the points in cluster C_i

K-means Clustering

- Most common definition is with euclidean distance, minimizing the **Sum of Squares Error (SSE)** function
 - Sometimes K-means 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

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

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

Sum of Squares Error (SSE)

Complexity of the k-means problem

- 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
- A simple iterative algorithm works quite well in practice

K-means Algorithm

- 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 all points to the closest centroid.

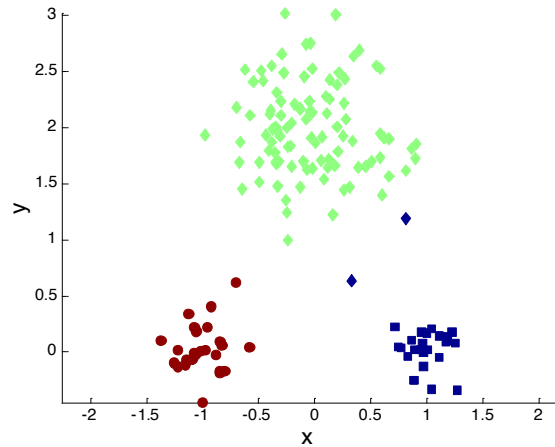
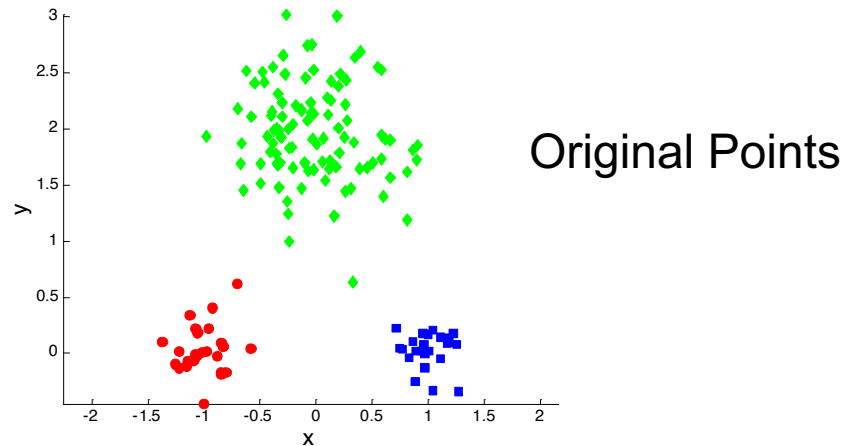
4: Recompute the centroid of each cluster.

5: **until** The centroids don't change

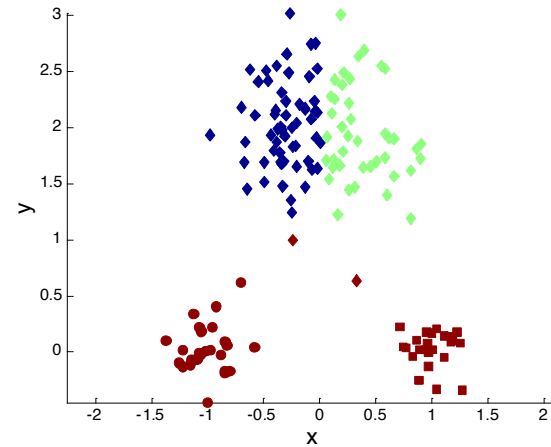
K-means Algorithm – Initialization

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

Two different K-means Clusterings

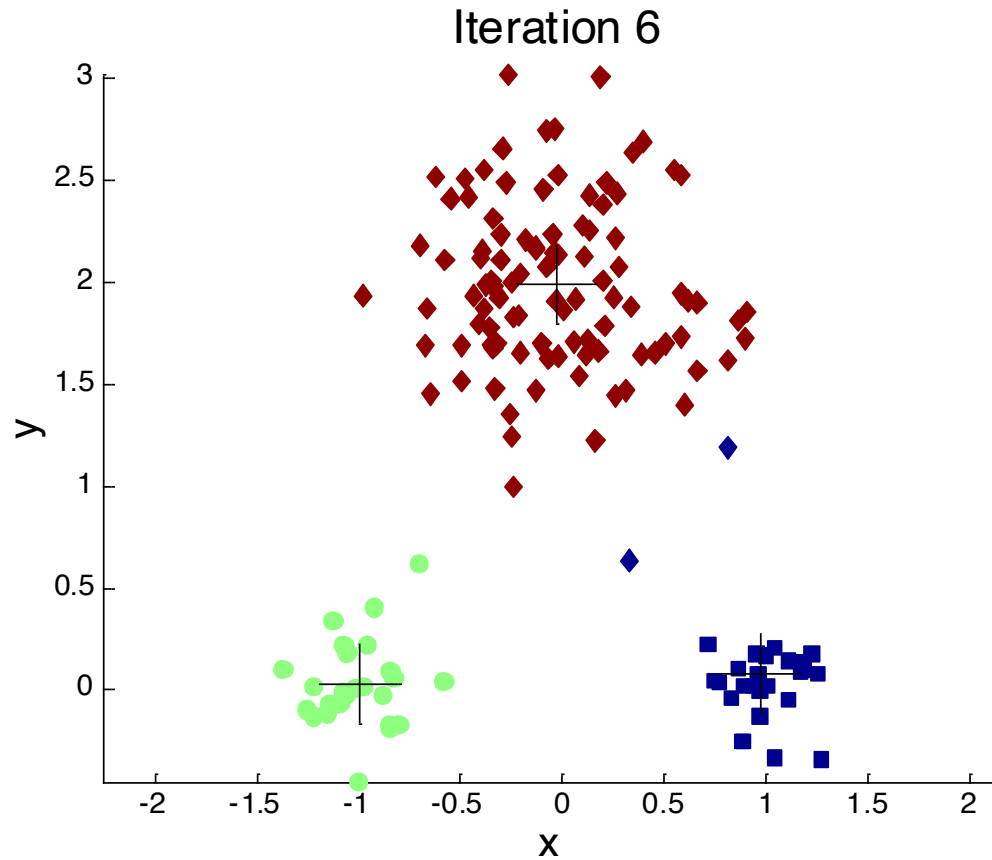


Optimal Clustering

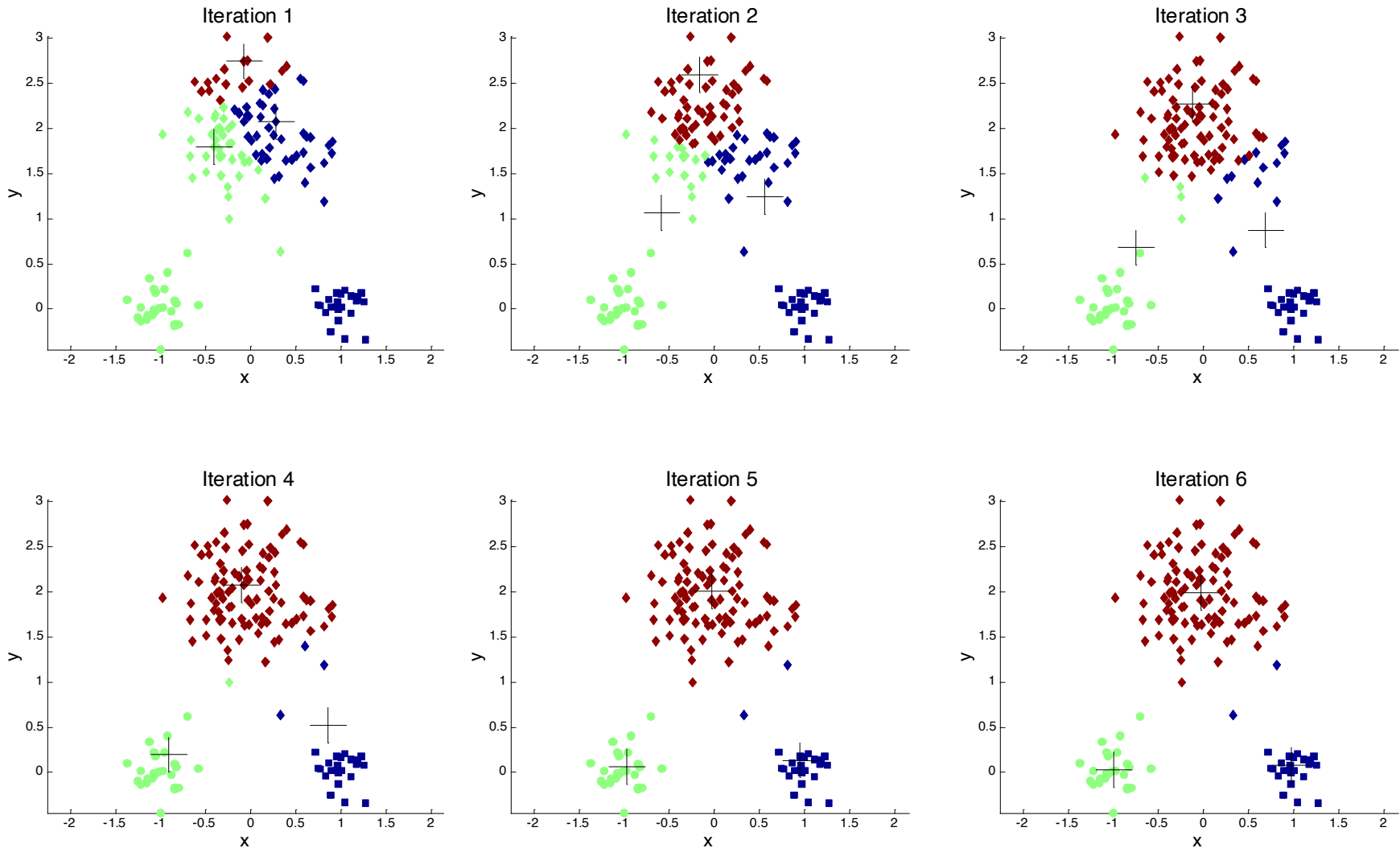


Sub-optimal Clustering

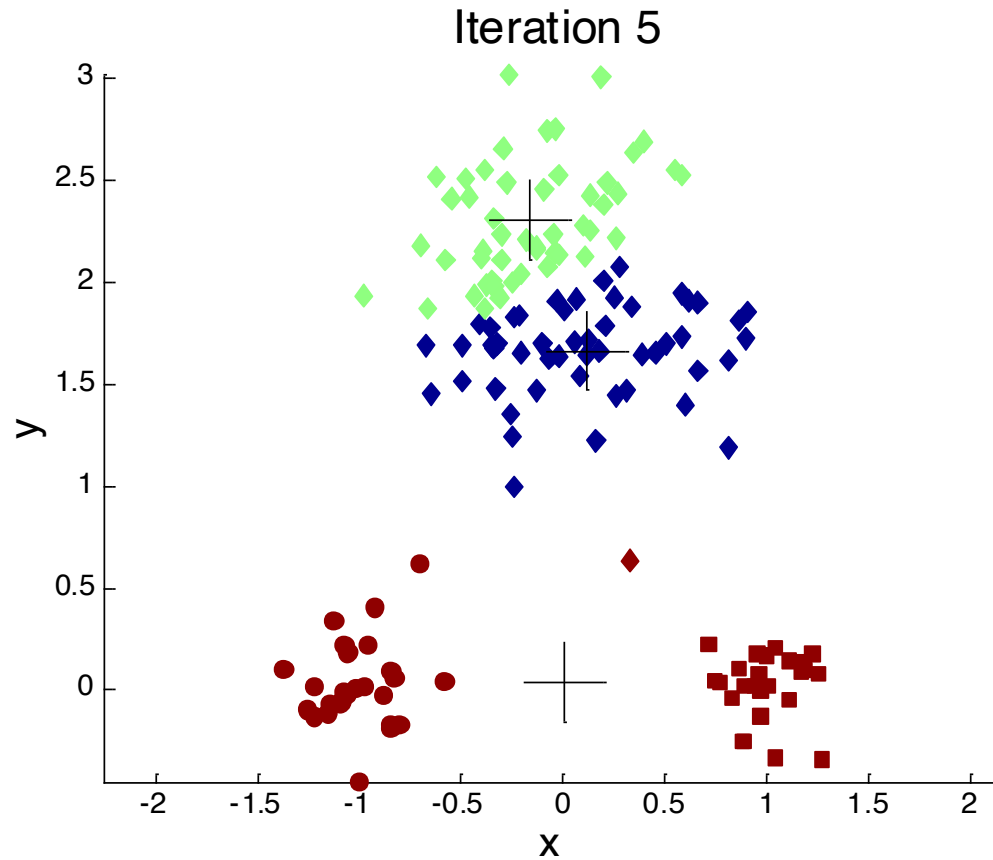
Importance of Choosing Initial Centroids



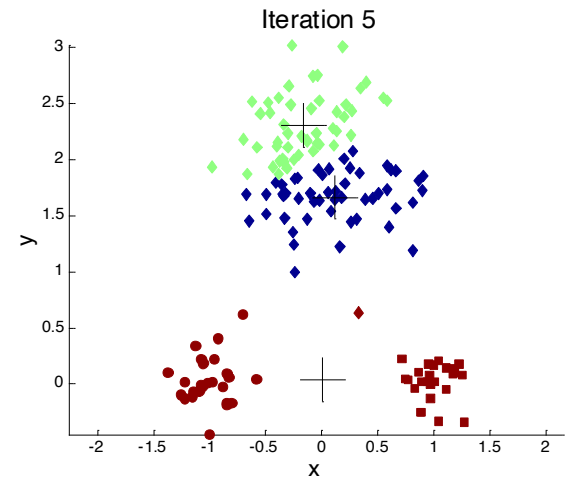
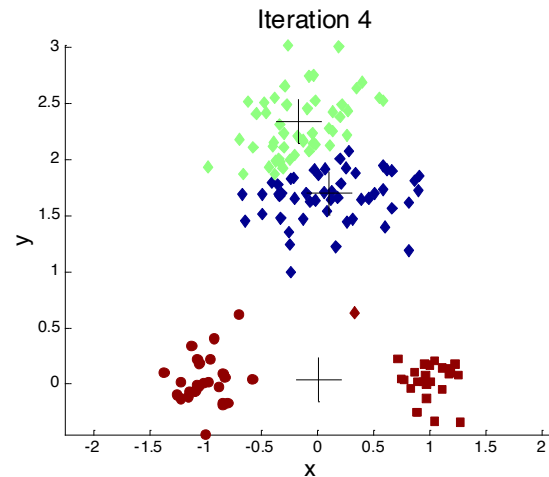
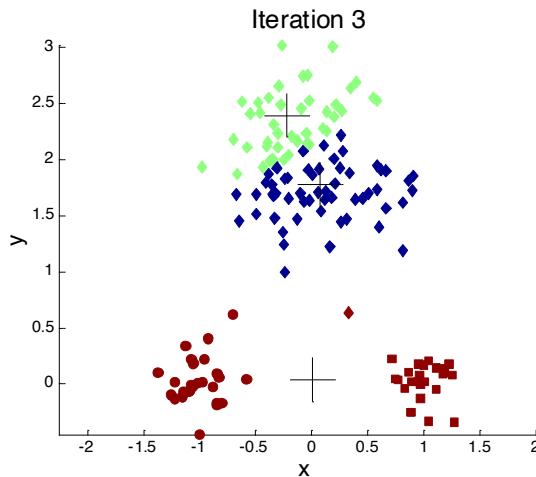
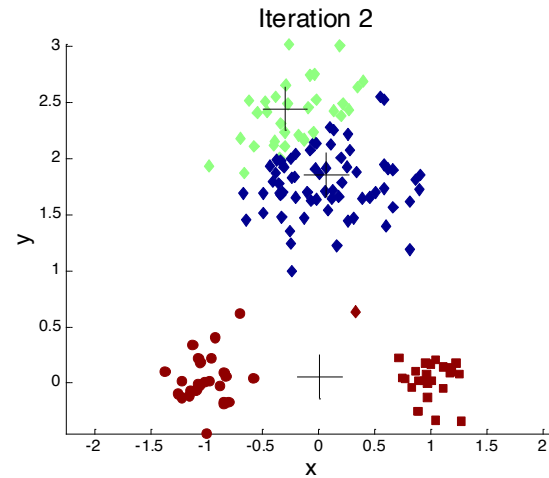
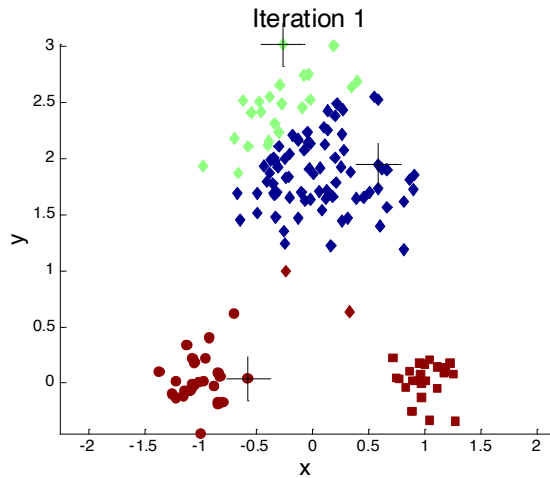
Importance of Choosing Initial Centroids



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

- The **centroid** depends on the distance function
 - The **minimizer** for the distance function
- ‘**Closeness**’ is measured by Euclidean distance (SSE), cosine similarity, correlation, etc.
- **Centroid**:
 - The **mean** of the points in the cluster for SSE, and cosine similarity
 - The **median** for Manhattan distance.
- Finding the centroid is not always easy
 - It can be an NP-hard problem for some distance functions
 - E.g., median form multiple dimensions

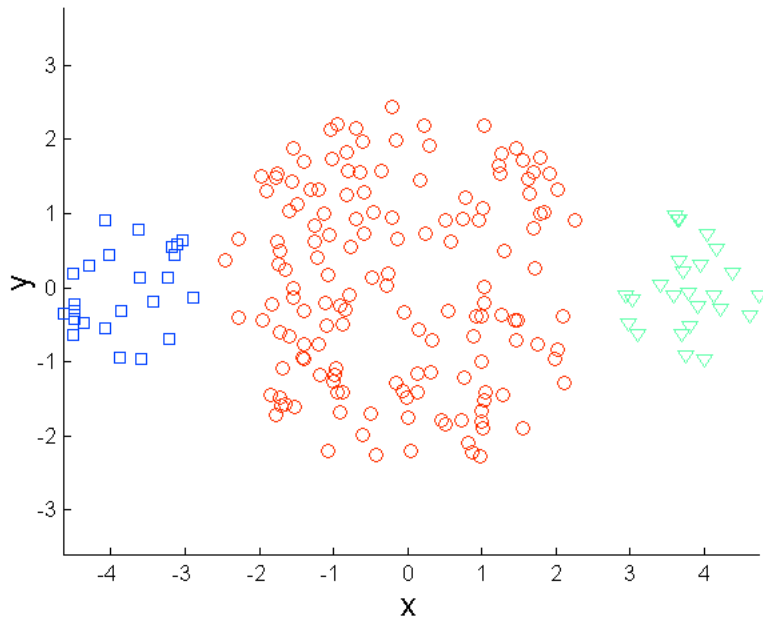
K-means Algorithm – Convergence

- 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 $O(n * K * I * d)$
 - n = number of points, K = number of clusters, I = number of iterations, d = dimensionality
- In general a fast and efficient algorithm

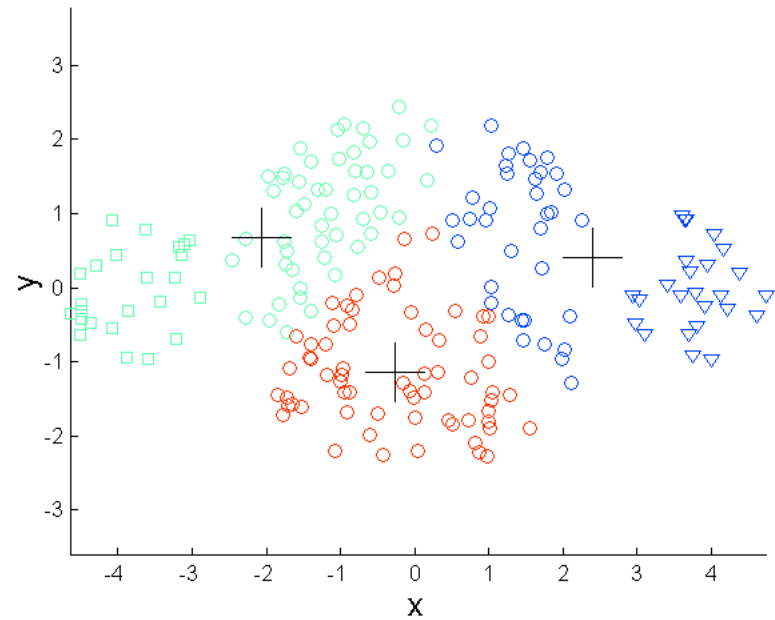
Limitations of K-means

- K-means has problems when clusters are of different
 - Sizes
 - Densities
 - Non-globular shapes
- K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

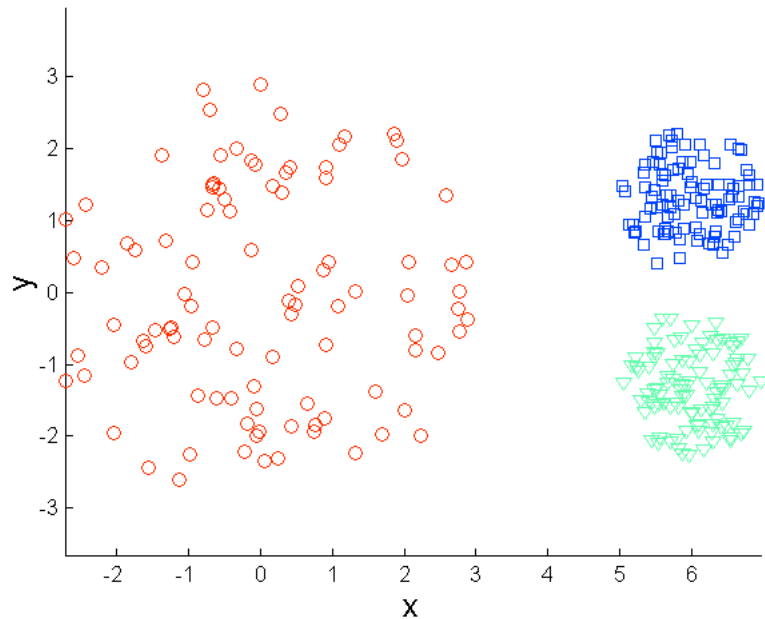


Original Points

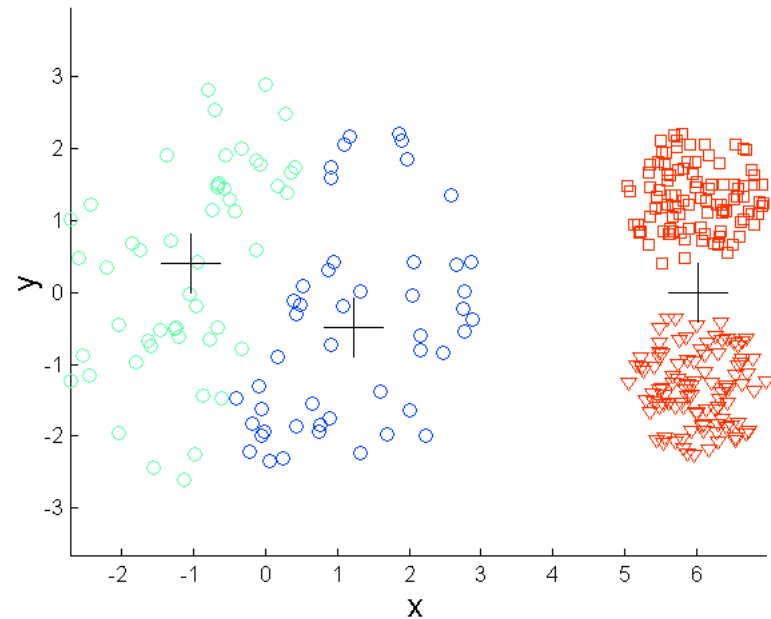


K-means (3 Clusters)

Limitations of K-means: Differing Density

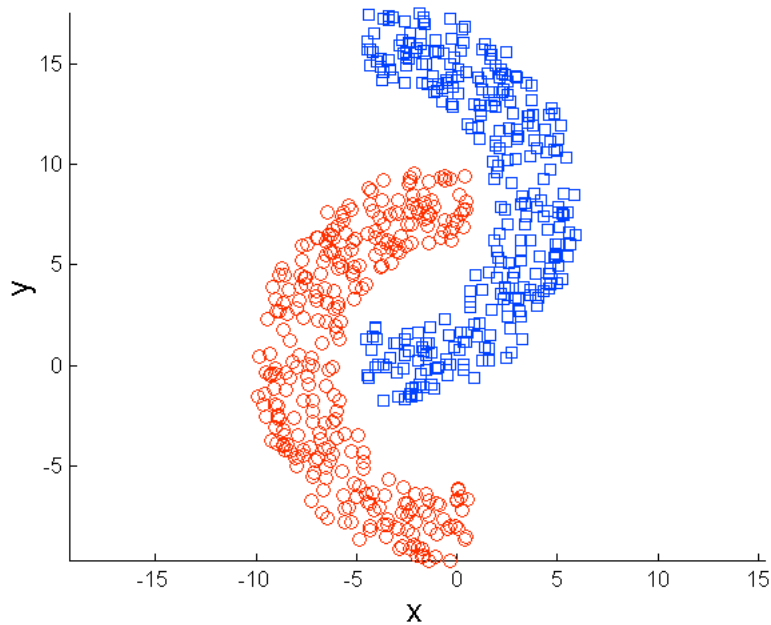


Original Points

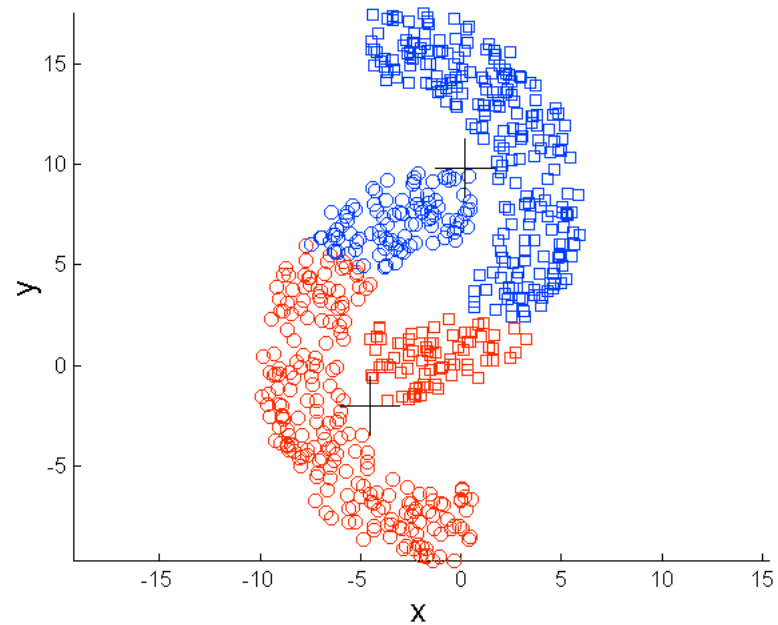


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

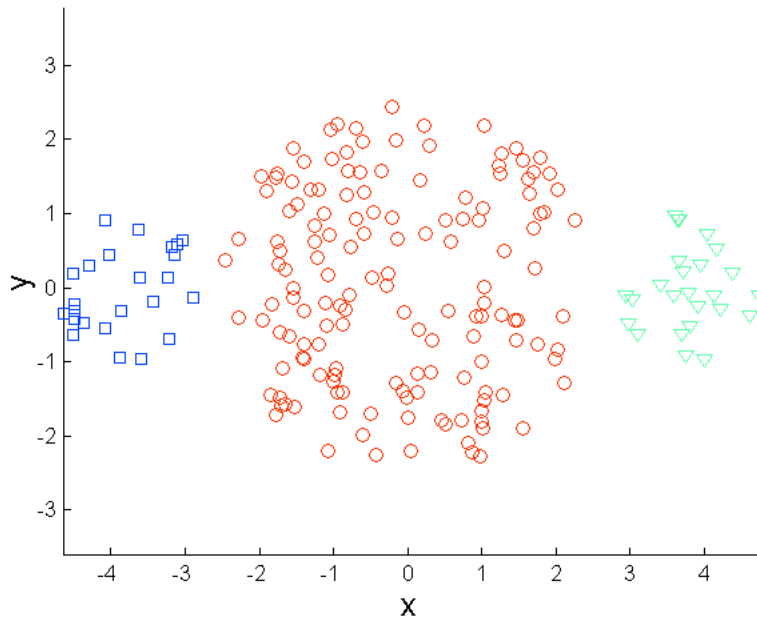


Original Points

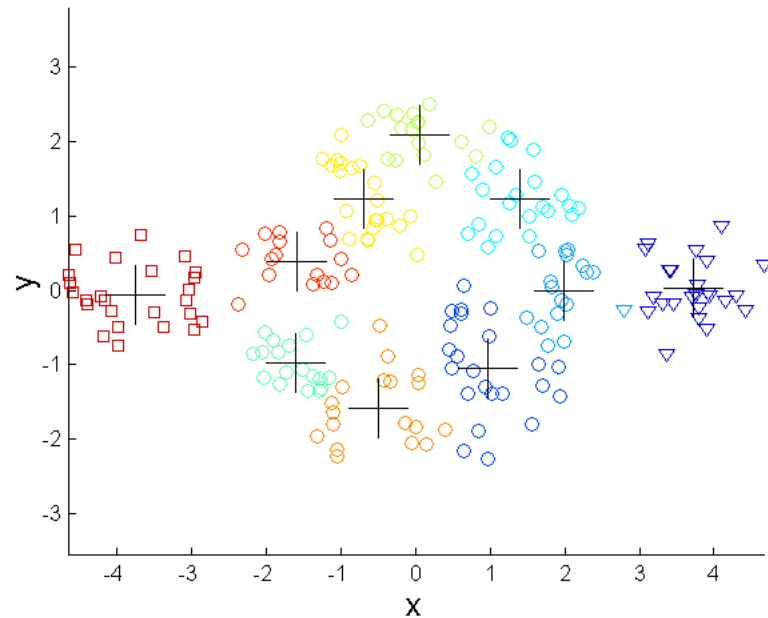


K-means (2 Clusters)

Overcoming K-means Limitations



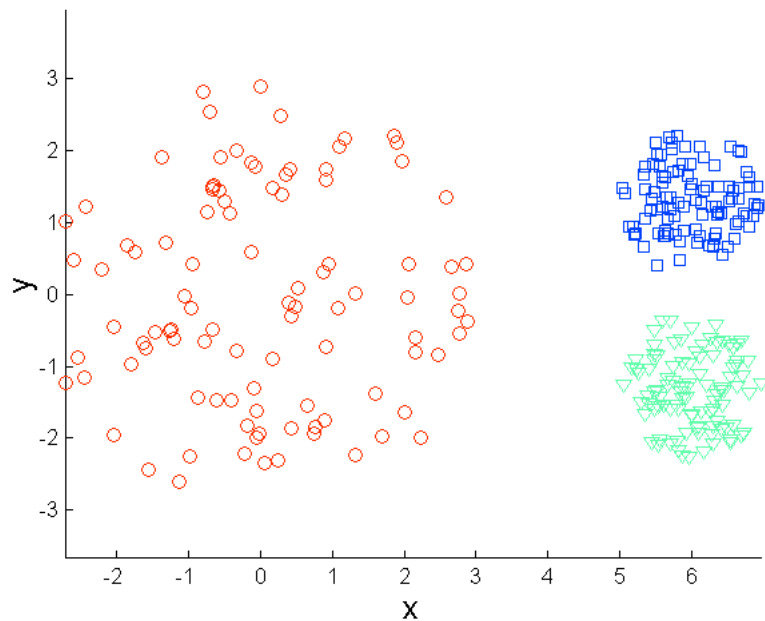
Original Points



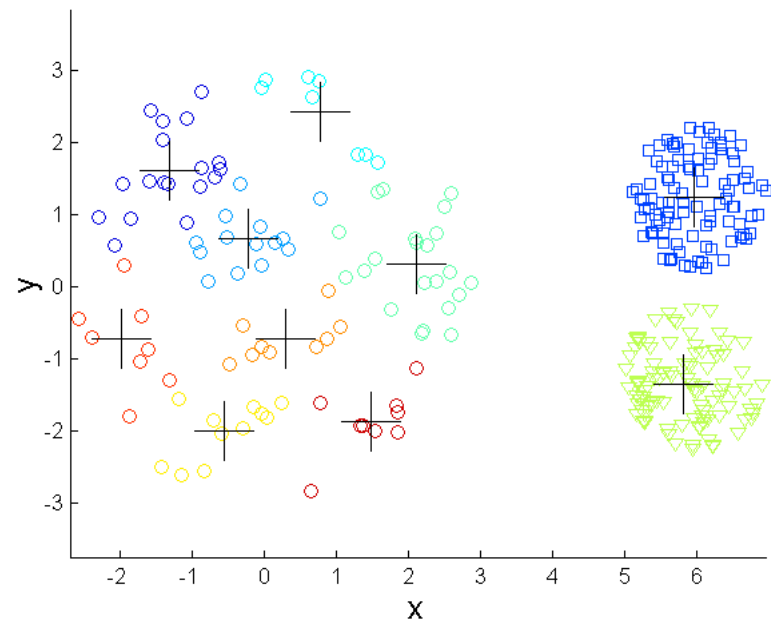
K-means Clusters

One solution is to use many clusters.
Find parts of clusters, but need to put together.

Overcoming K-means Limitations

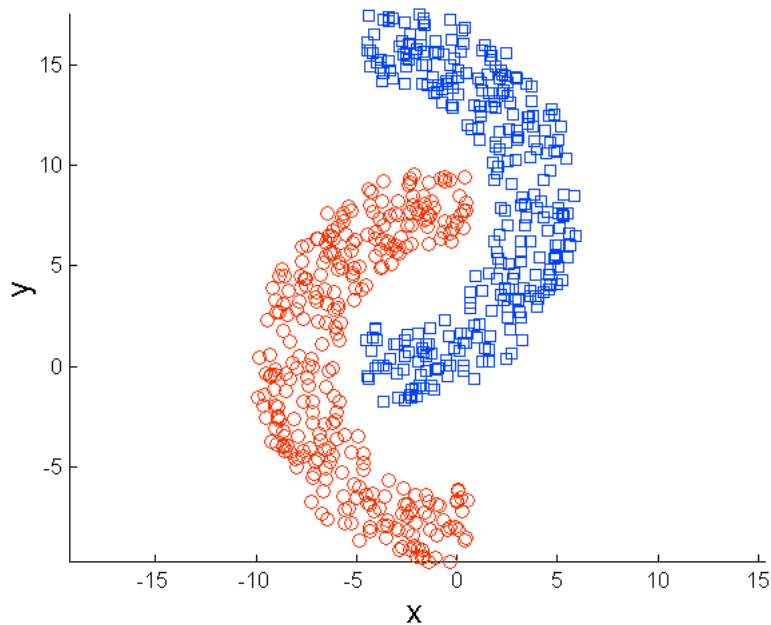


Original Points

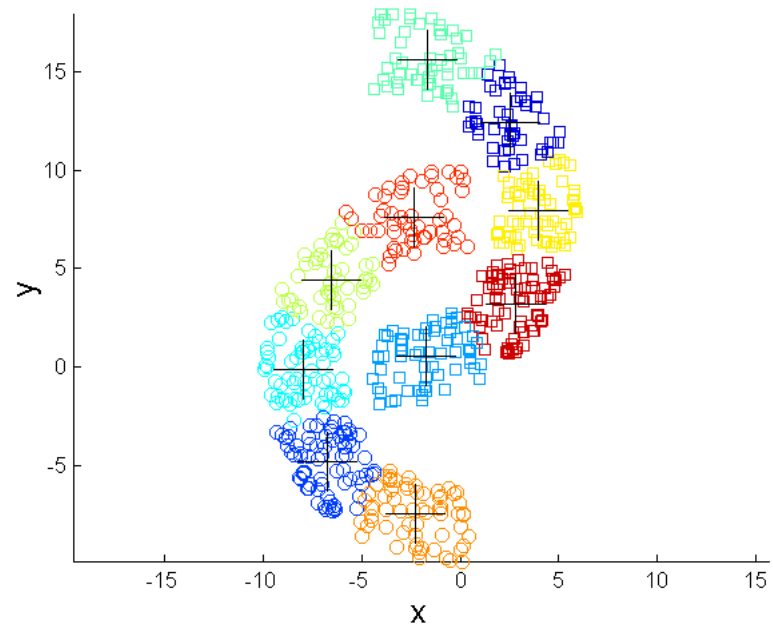


K-means Clusters

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).

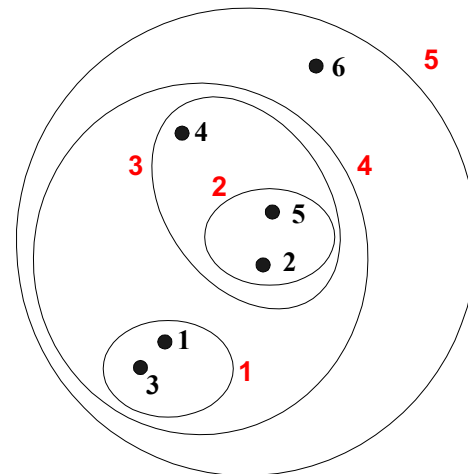
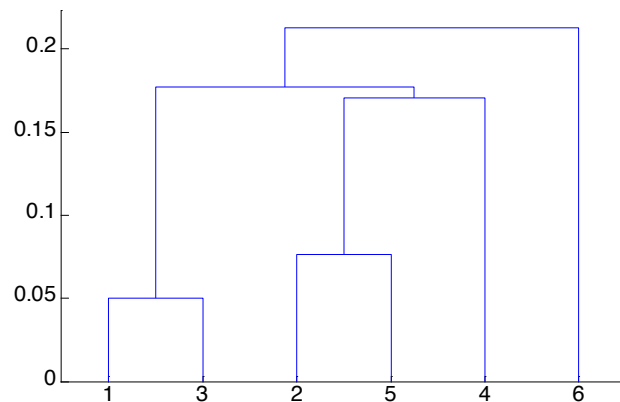
HIERARCHICAL CLUSTERING

Hierarchical Clustering

- Two main types of hierarchical clustering
 - Agglomerative:
 - Start with the points as individual clusters
 - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - Divisive:
 - Start with one, all-inclusive cluster
 - At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
 - Merge or split one cluster at a time

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



Strengths of Hierarchical Clustering

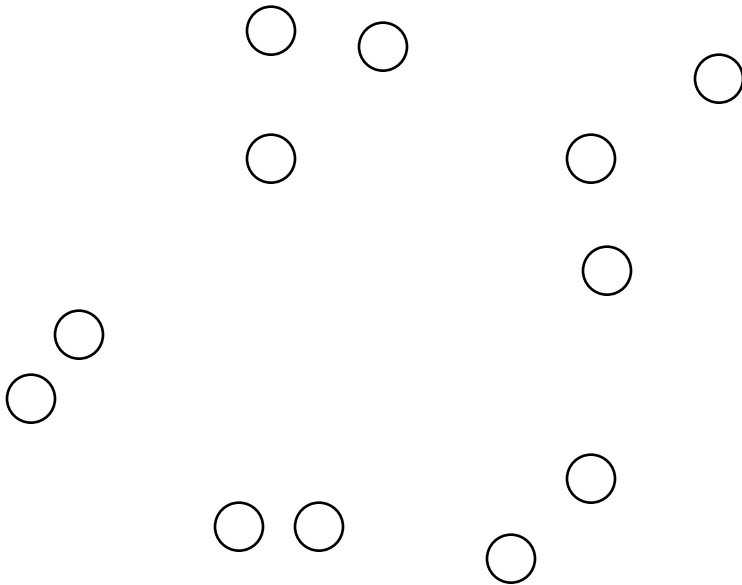
- Do not have to assume any particular number of clusters
 - Any desired number of clusters can be obtained by 'cutting' the dendrogram at the proper level
- They may correspond to meaningful taxonomies
 - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

Agglomerative Clustering Algorithm

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

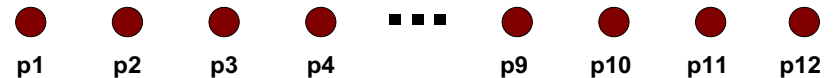
Starting Situation

- Start with clusters of individual points and a proximity matrix



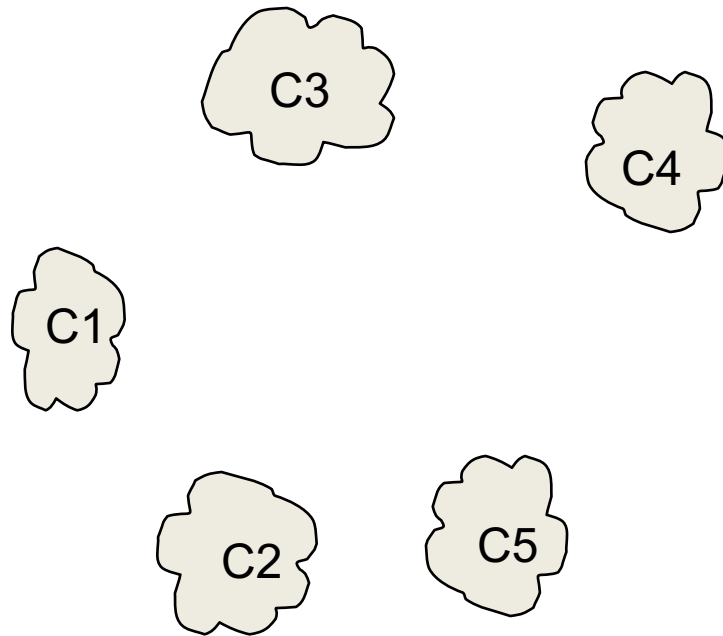
	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



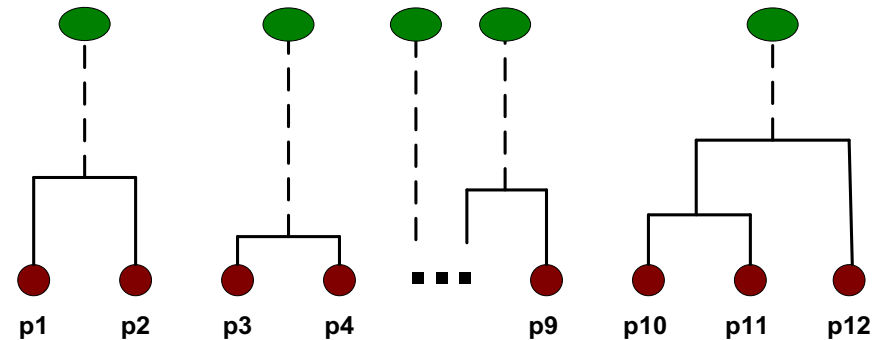
Intermediate Situation

- After some merging steps, we have some clusters



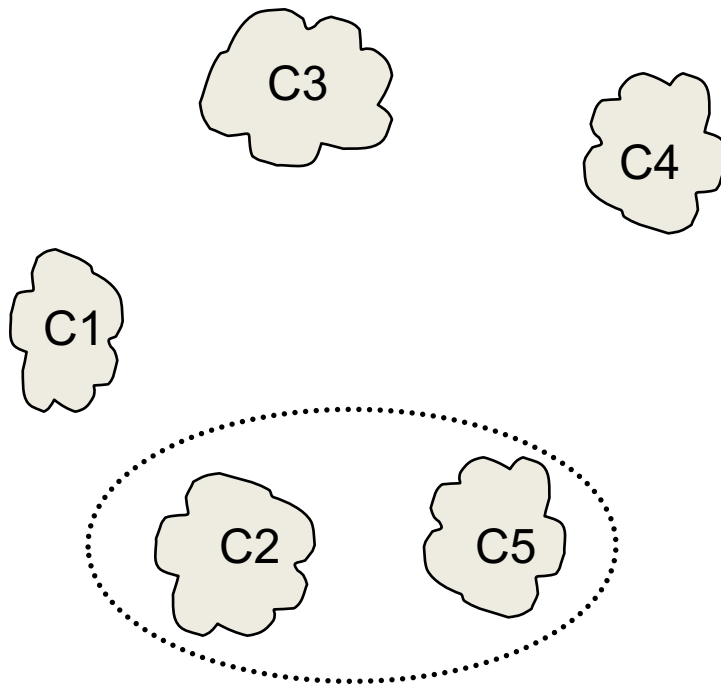
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



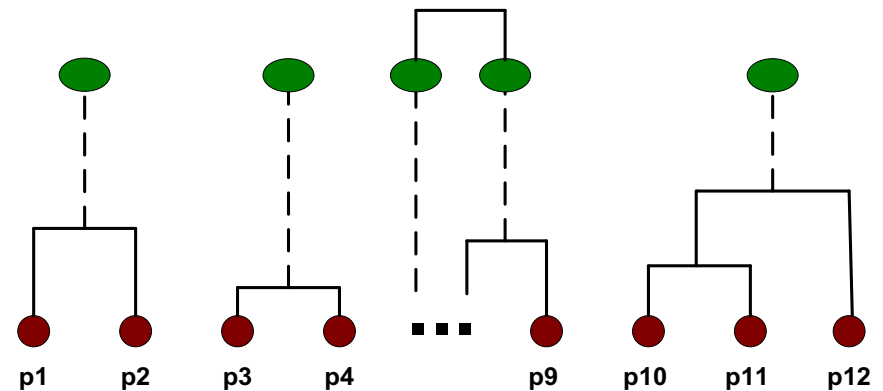
Intermediate Situation

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



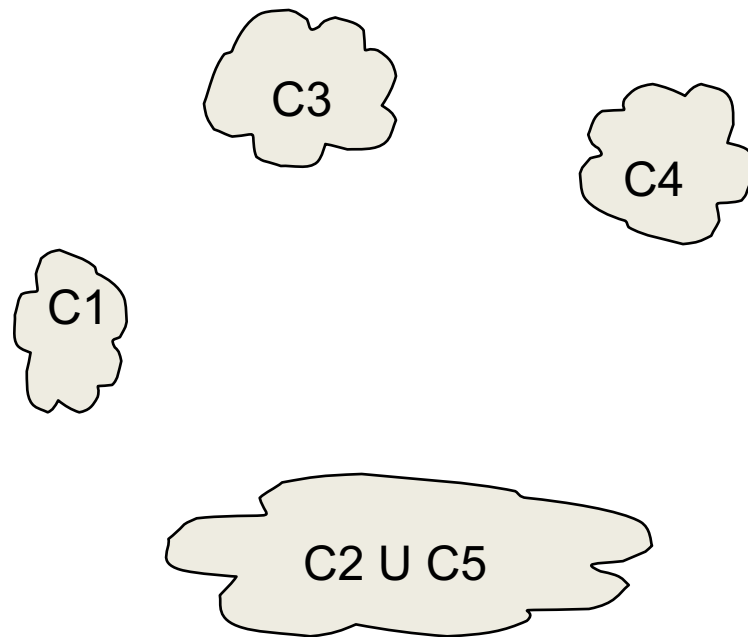
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



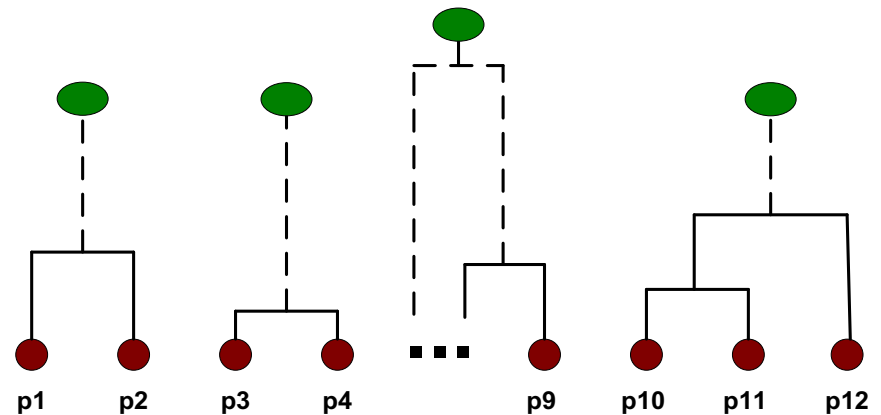
After Merging

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

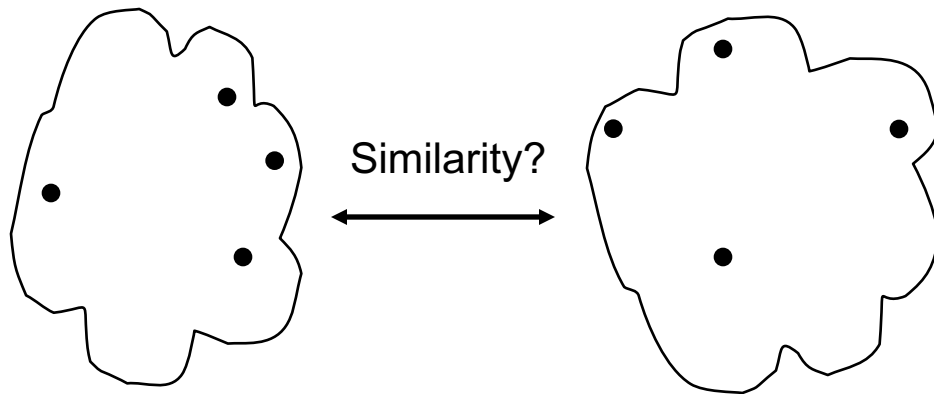


		C2 U C5			
		C1	C5	C3	C4
C1			?		
C2 U C5		?	?	?	?
C3			?		
C4			?		

Proximity Matrix



How to Define Inter-Cluster Similarity

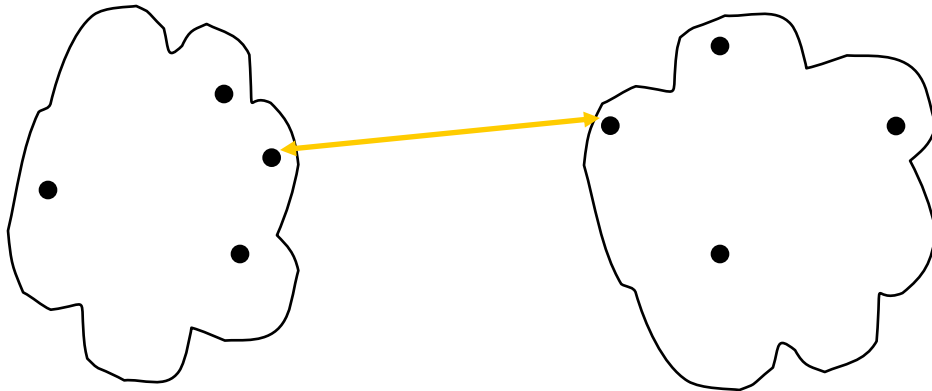


- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

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

Proximity Matrix

How to Define Inter-Cluster Similarity

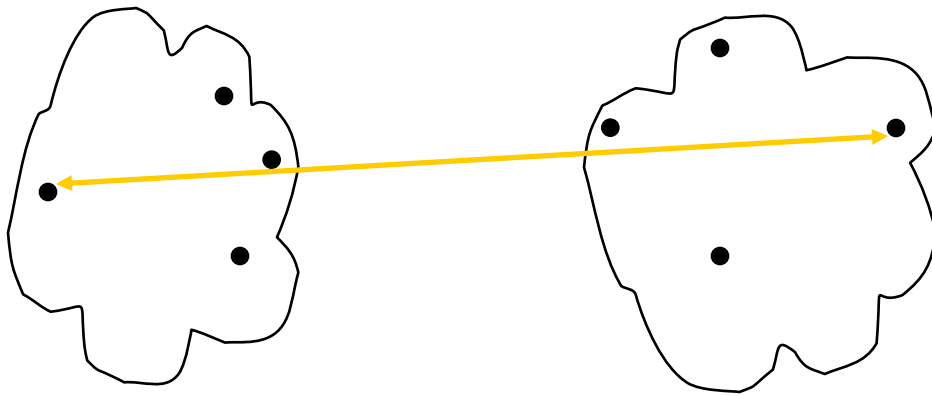


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	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
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Proximity Matrix

How to Define Inter-Cluster Similarity

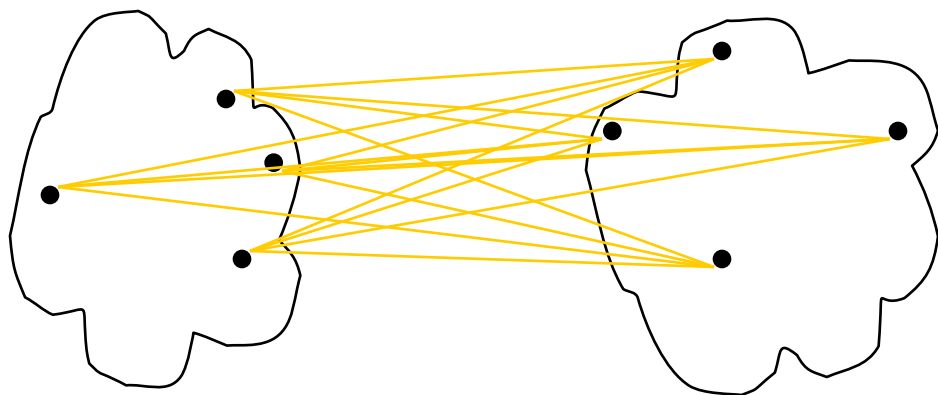


- MIN
- MAX
- Group Average
- Distance Between Centroids
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	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

How to Define Inter-Cluster Similarity

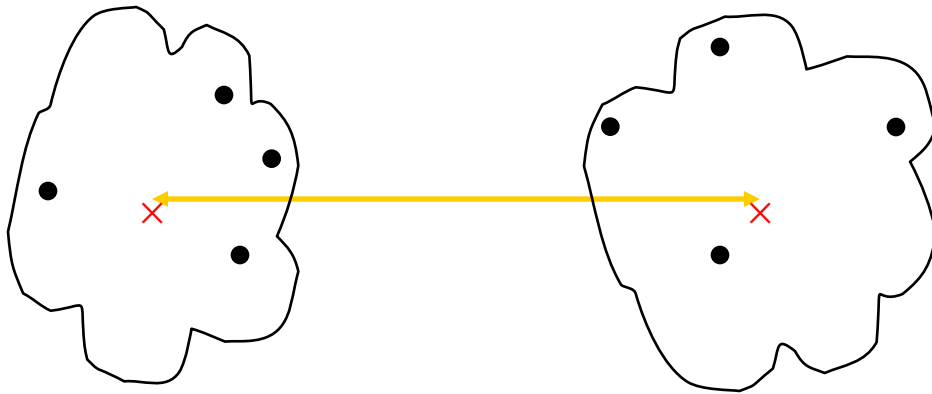


- MIN
- MAX
- **Group Average**
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

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

Proximity Matrix

How to Define Inter-Cluster Similarity

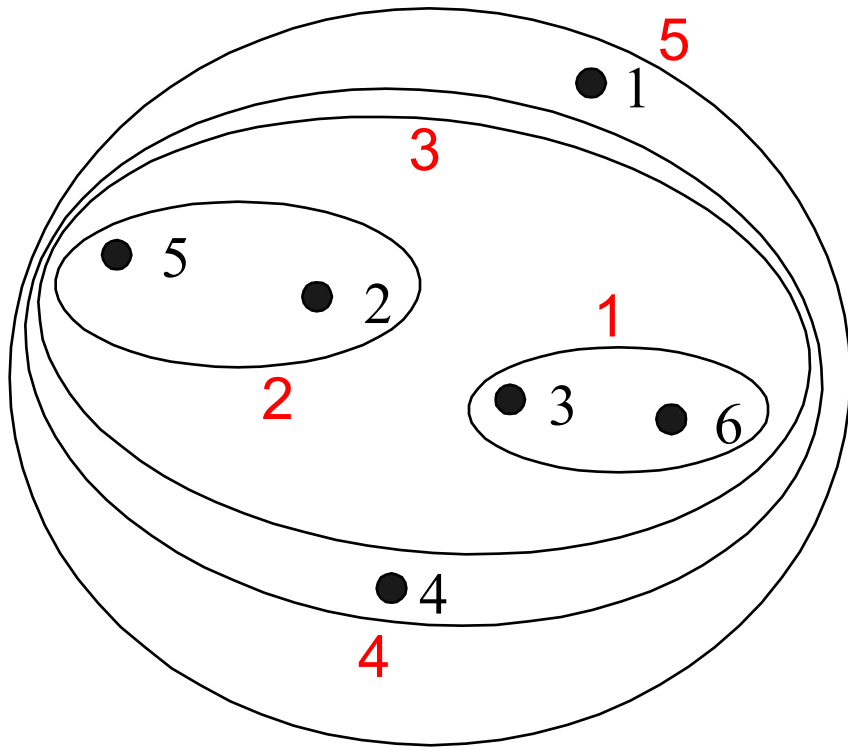


- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

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

Proximity Matrix

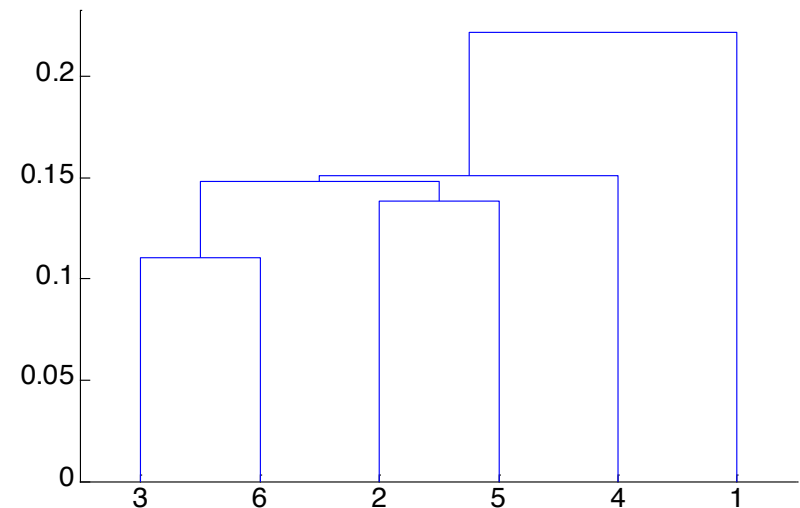
Hierarchical Clustering: MIN



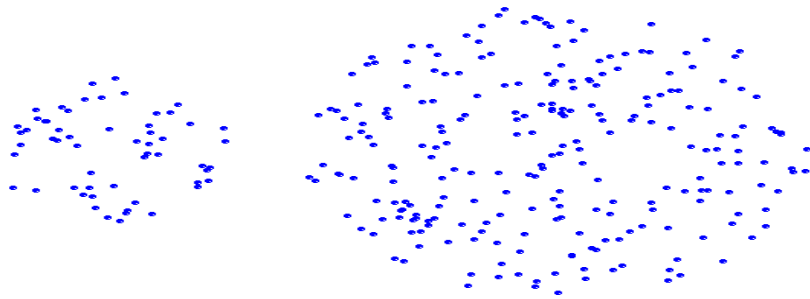
Nested Clusters

	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

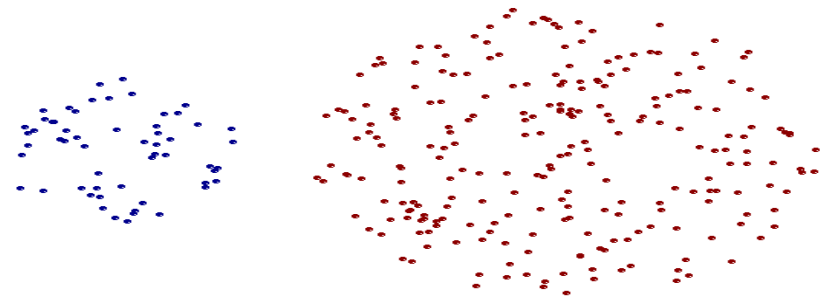
Dendrogram



Strength of MIN



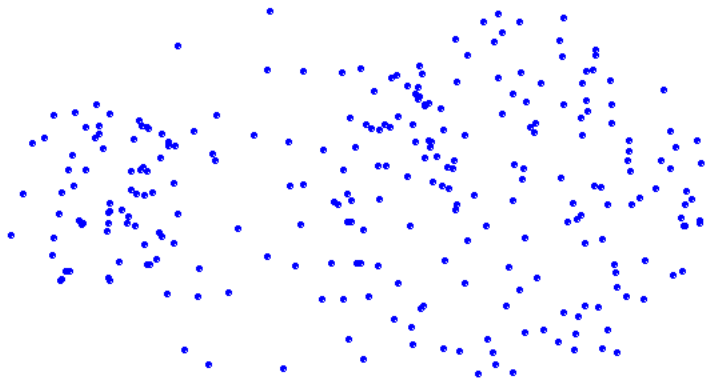
Original Points



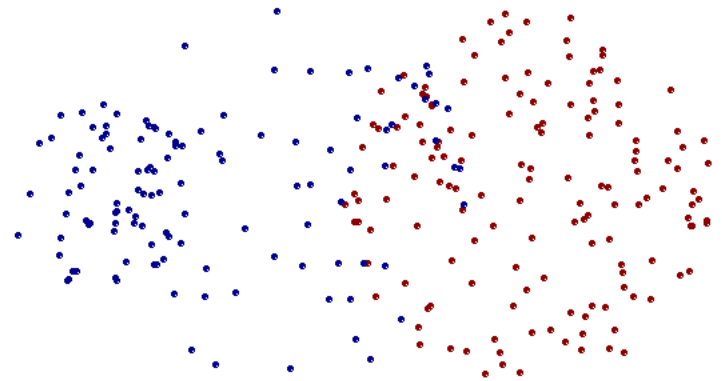
Two Clusters

- Can handle non-elliptical shapes

Limitations of MIN



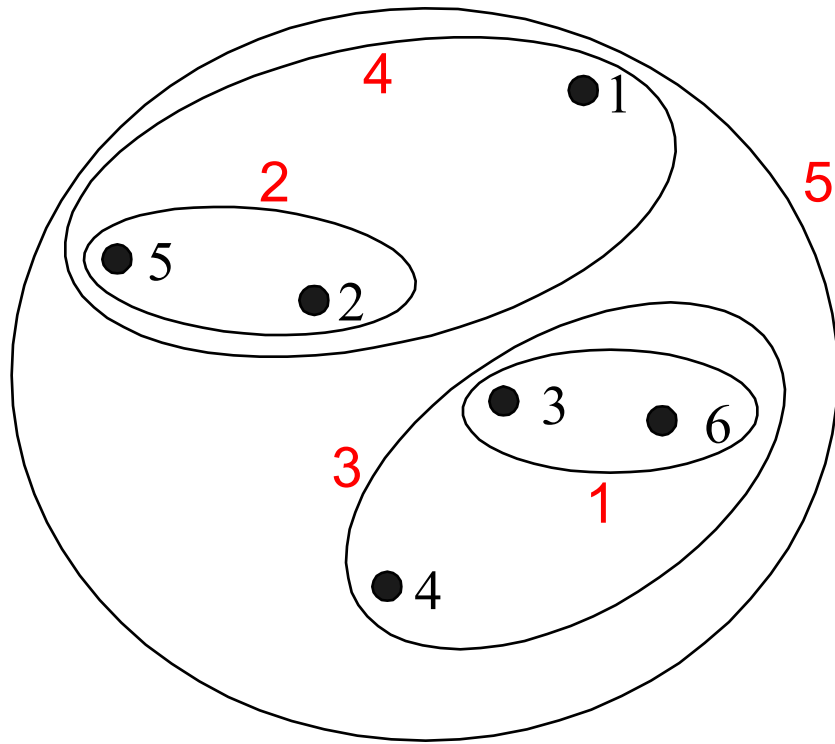
Original Points



Two Clusters

- Sensitive to noise and outliers

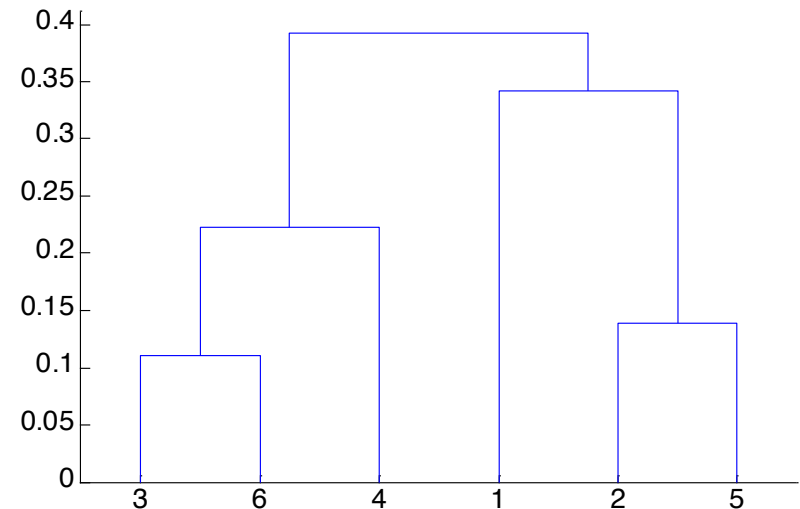
Hierarchical Clustering: MAX



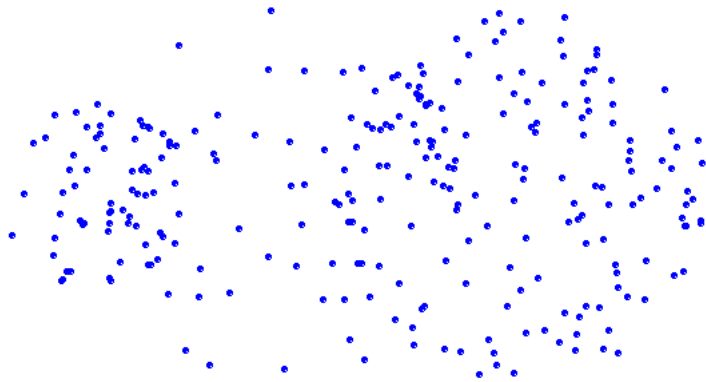
Nested Clusters

	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

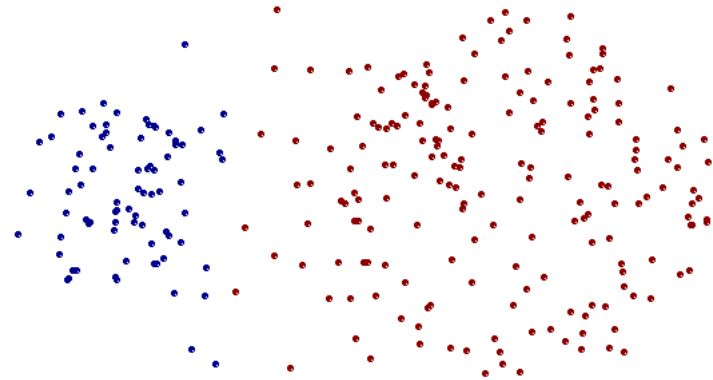
Dendrogram



Strength of MAX



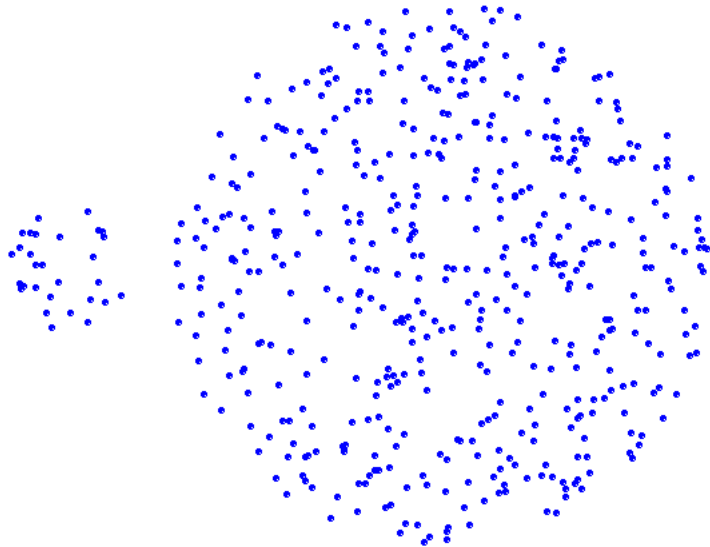
Original Points



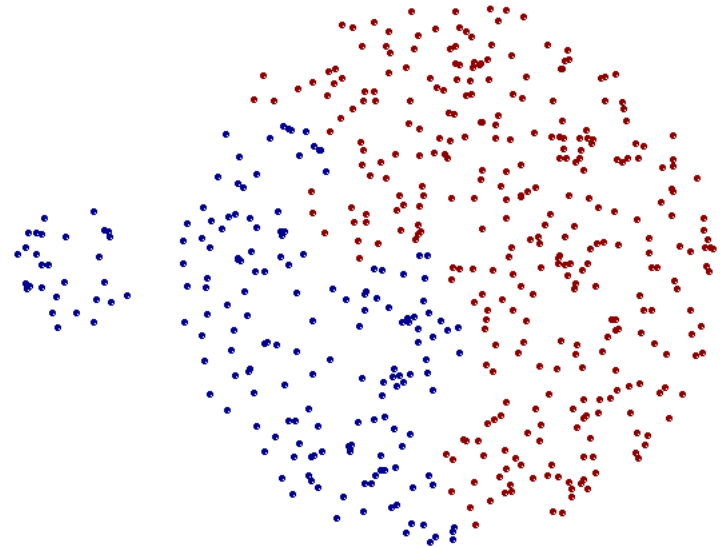
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

Cluster Similarity: Group Average

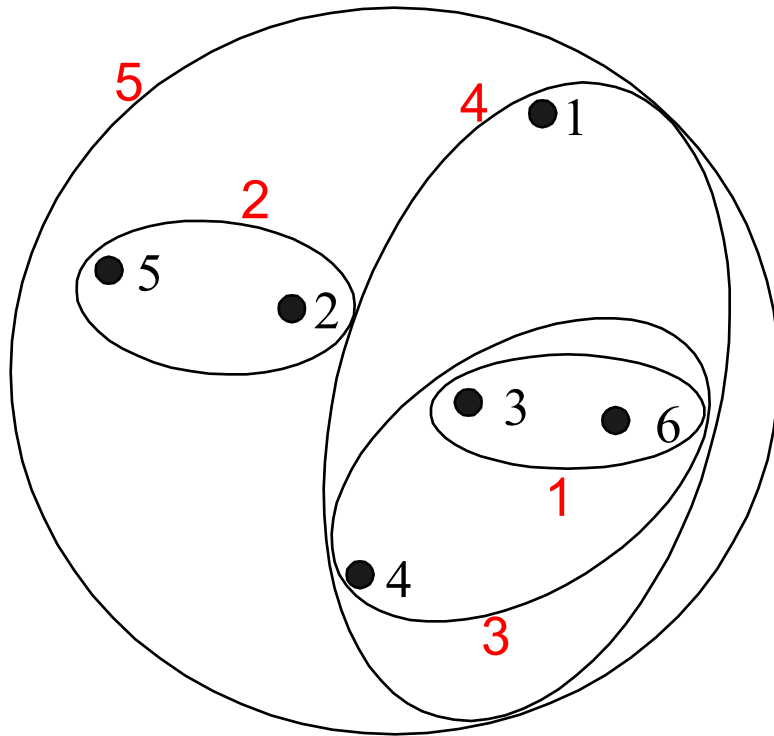
- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

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

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

	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

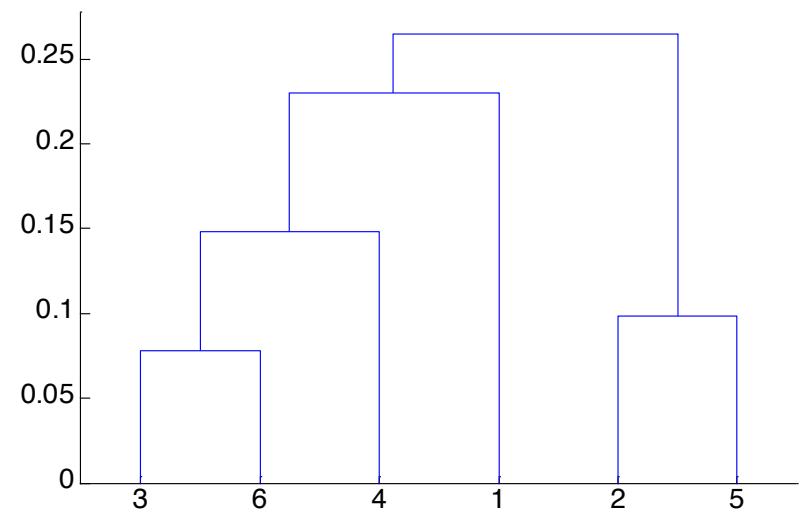
Hierarchical Clustering: Group Average



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



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
 - Breaking large clusters

DBSCAN

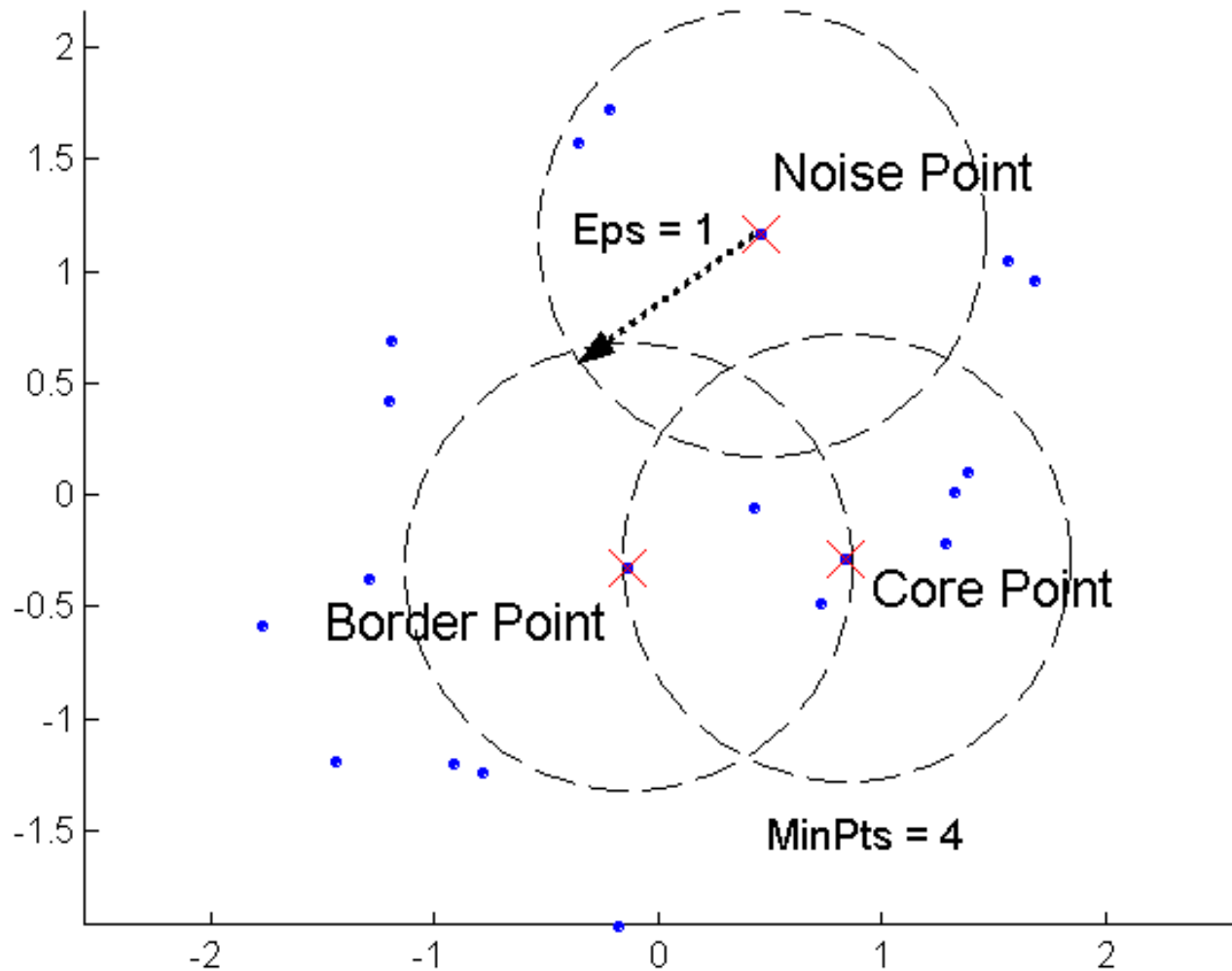
DBSCAN: Density-Based Clustering

- 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** 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.

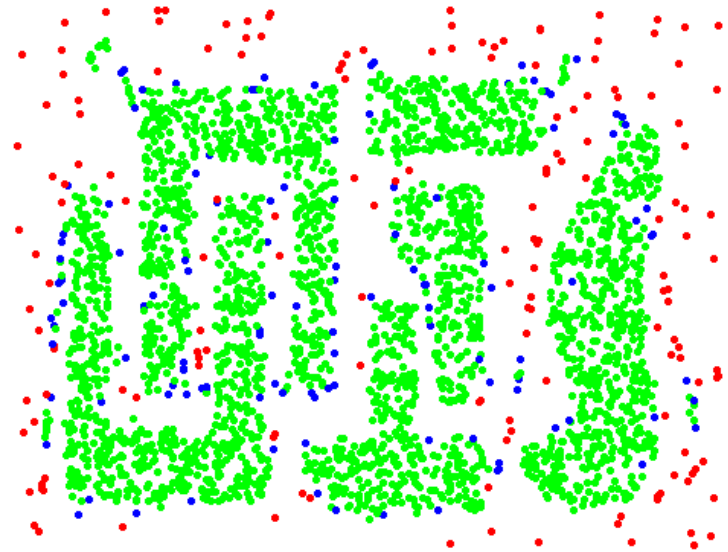
DBSCAN: Core, Border, and Noise Points



DBSCAN: Core, Border and Noise Points



Original Points

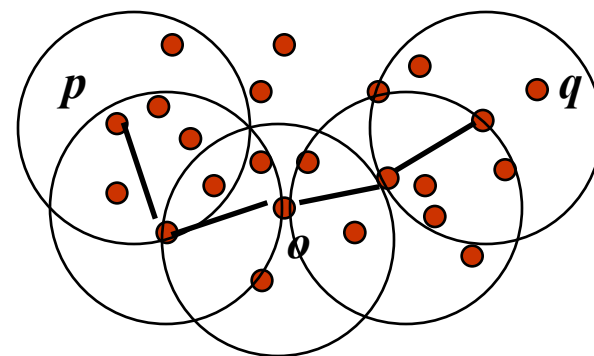
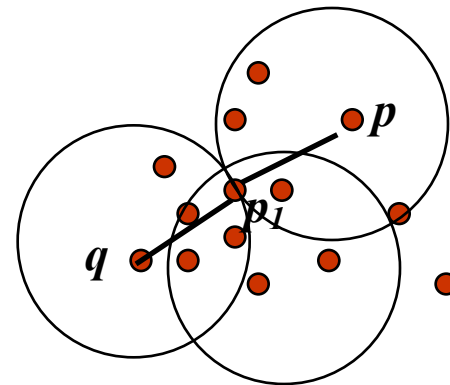


Point types: core,
border and noise

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**

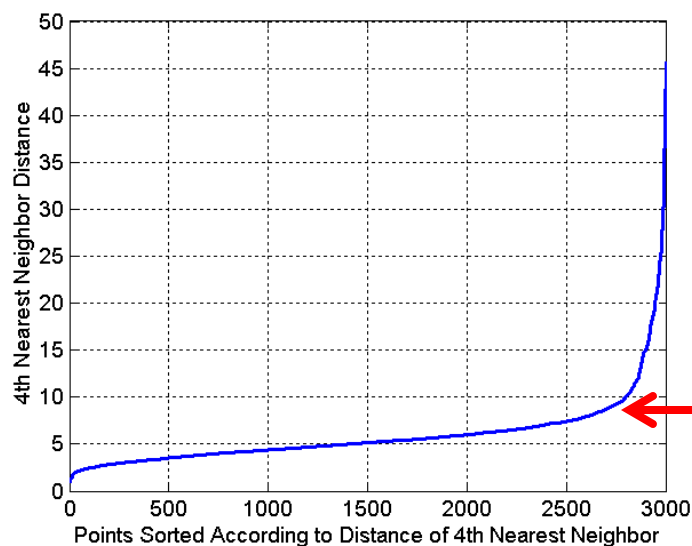


DBSCAN Algorithm

- 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 is that 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” in the curve
 - $\text{Eps} = d$, $\text{MinPts} = k$

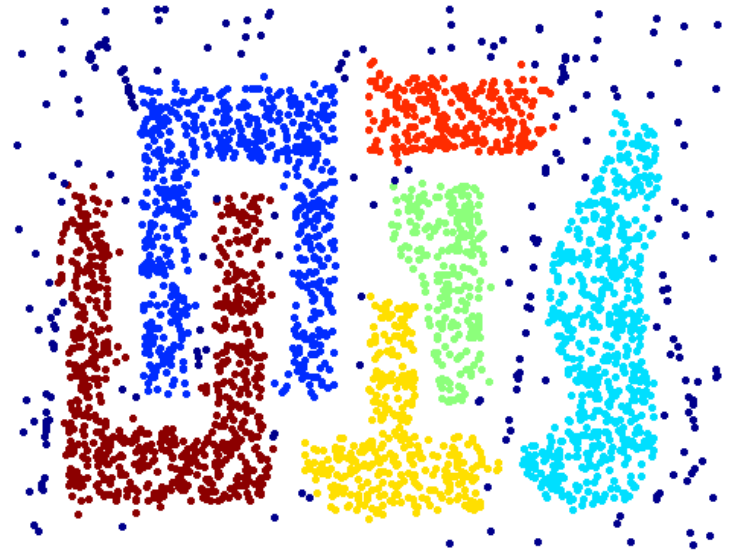


Eps ~ 7-10
MinPts = 4

When DBSCAN Works Well



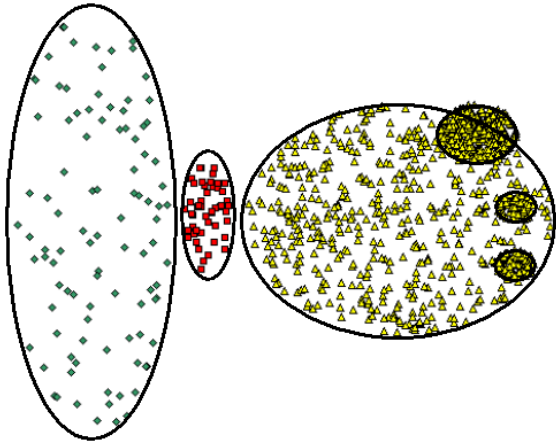
Original Points



Clusters

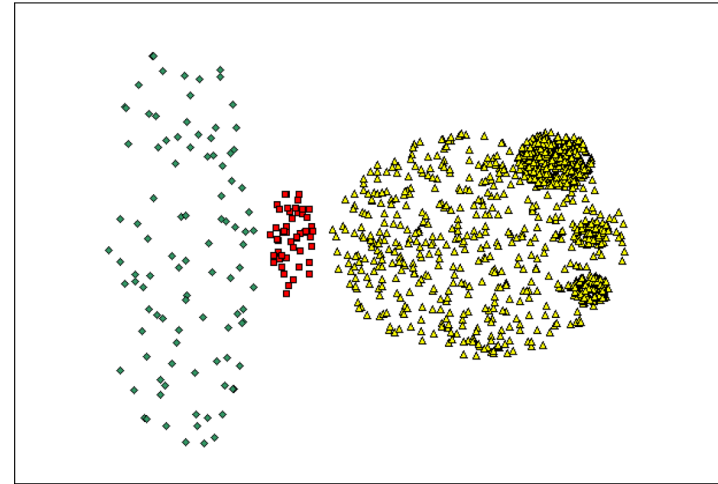
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN Does NOT Work Well

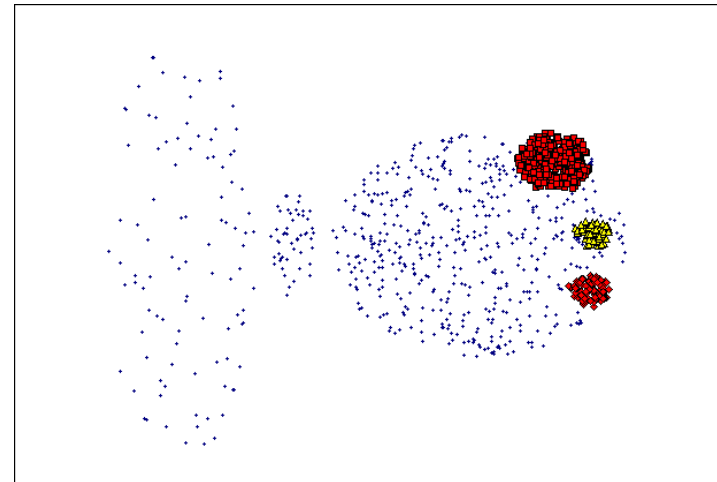


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

DBSCAN: Sensitive to Parameters

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

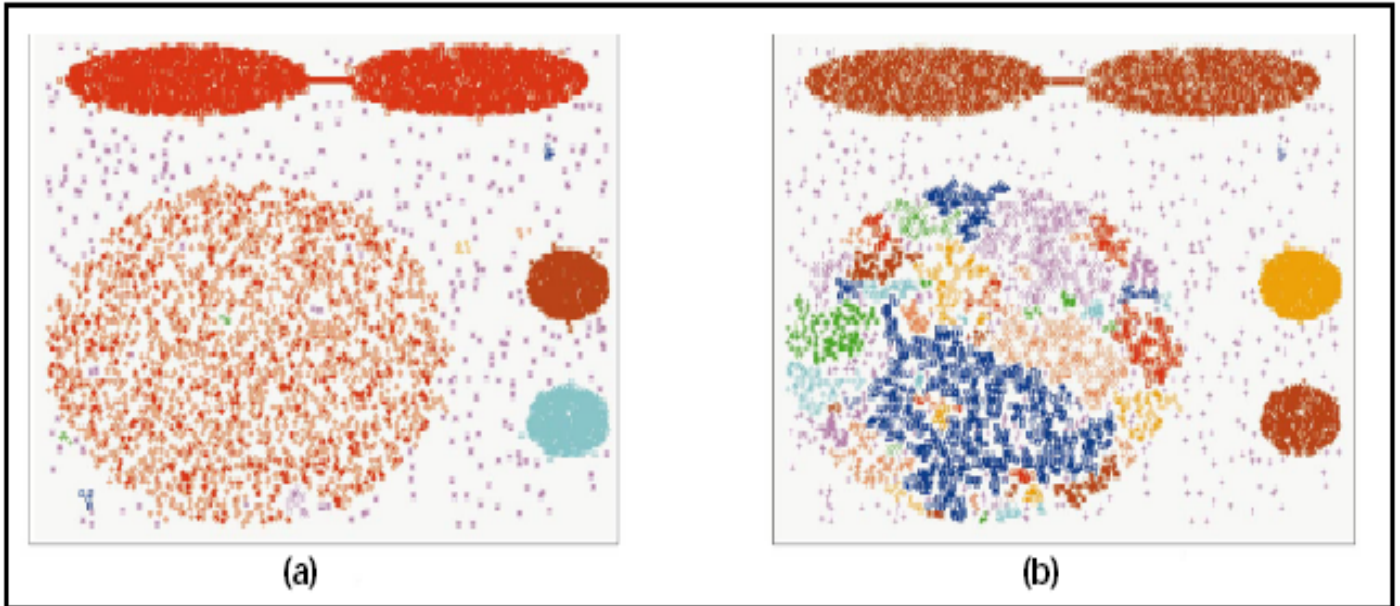
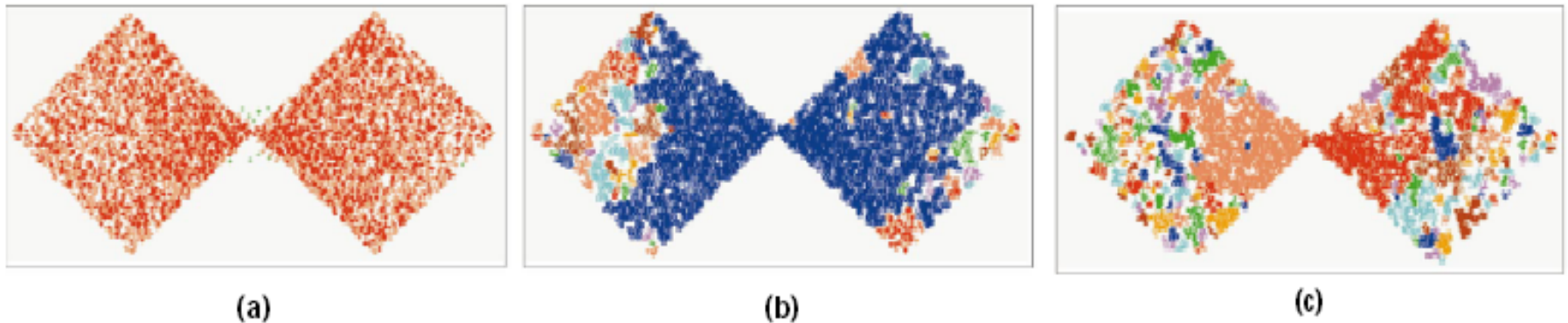


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



Slides source:

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