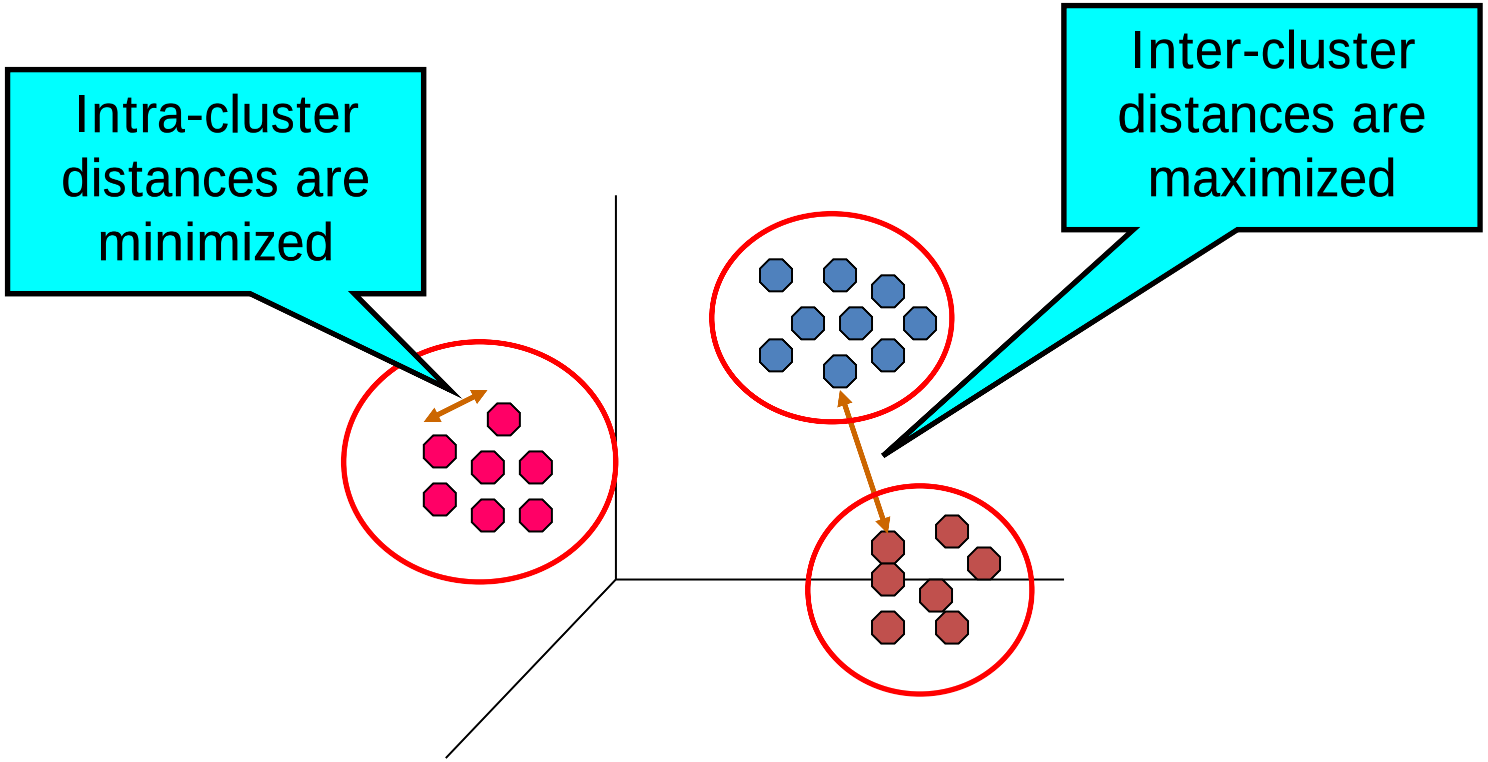
DATA MINING
CLUSTERING

The k-means algorithm

Hierarchical Clustering

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

Early applications of cluster analysis

- John Snow, London 1854

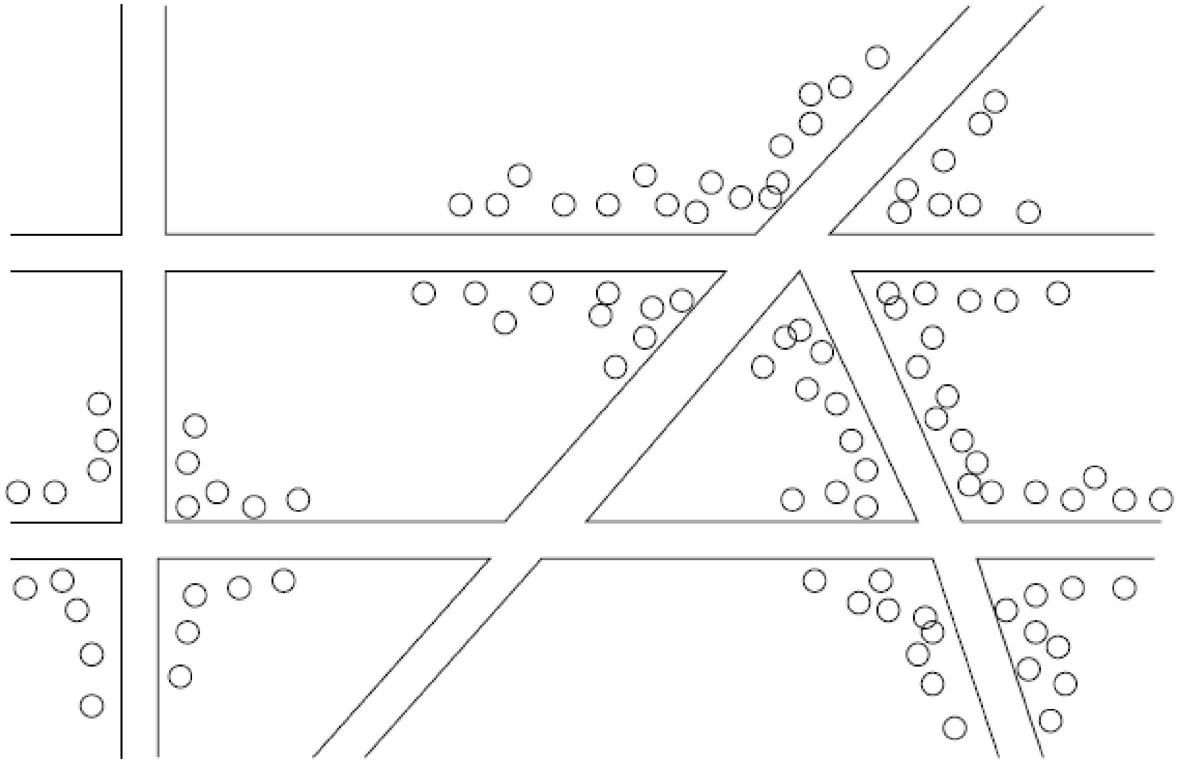


Figure 1.1: Plotting cholera cases on a map of London

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

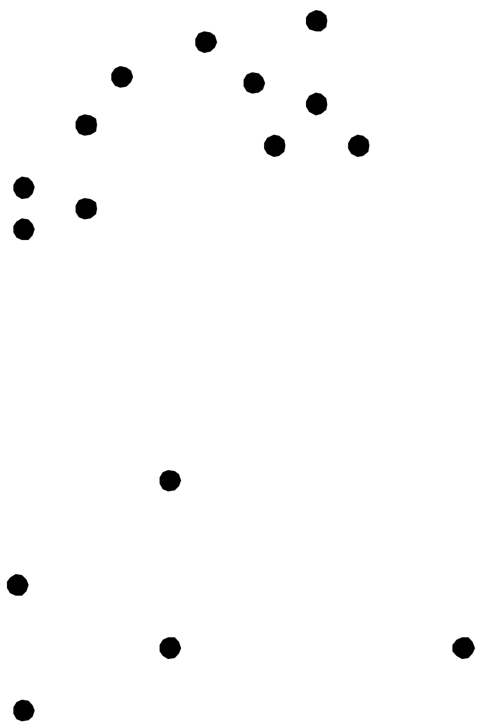
Two Clusters

Four Clusters

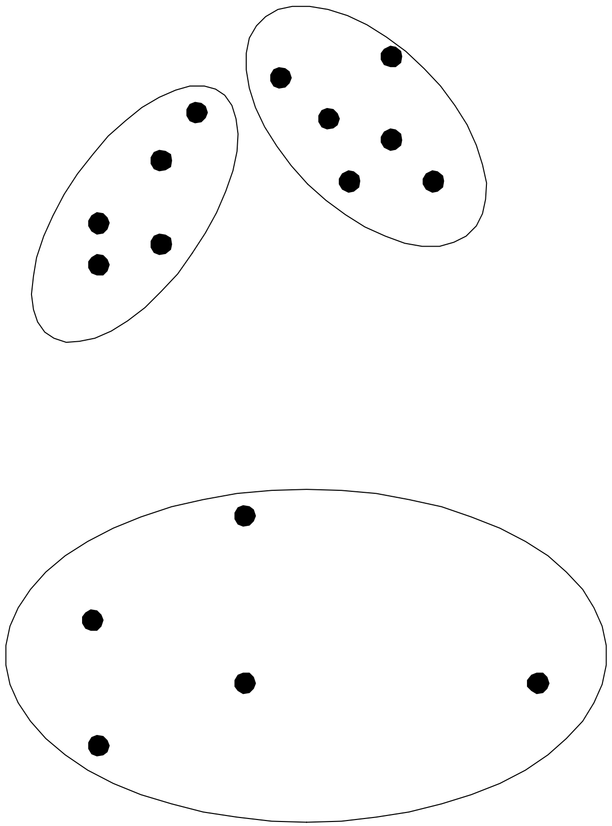
Types of Clusterings

- 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

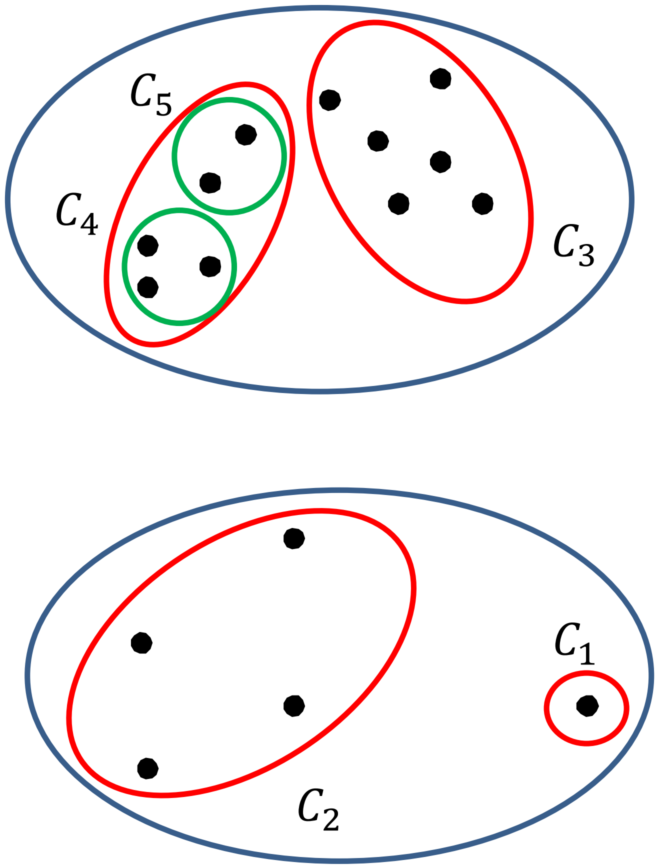


Original Points

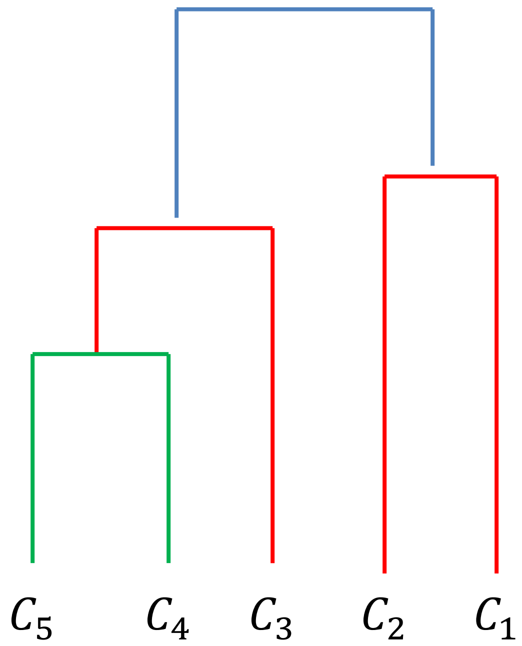


A Partitional Clustering

Hierarchical Clustering



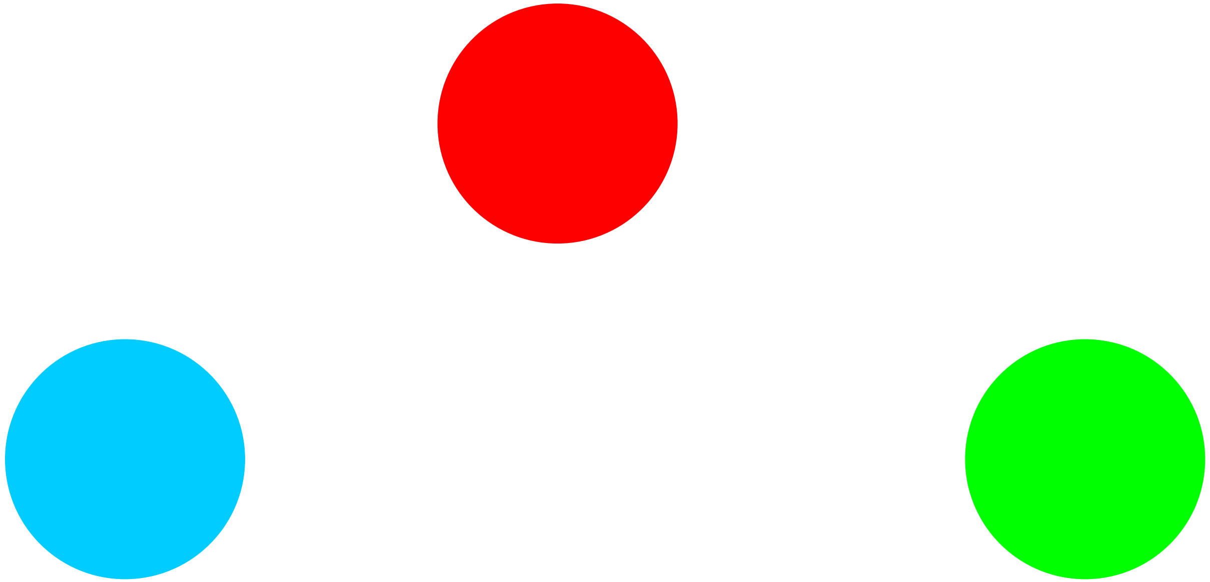
Hierarchical Clustering



Hierarchical Clustering dendrogram

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.



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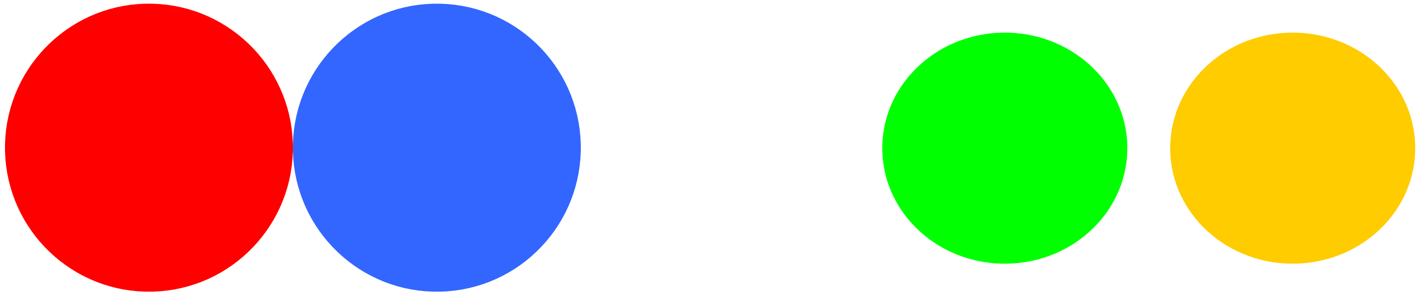
3 well-separated clusters

Clustering objectives

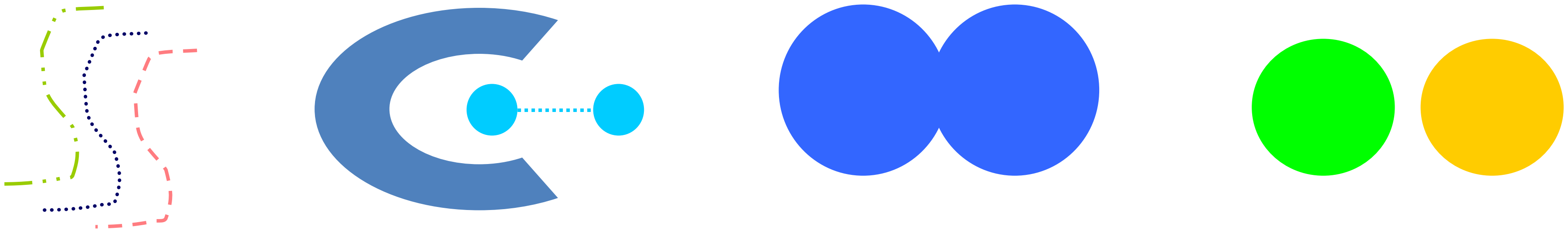
- Center-based Clusters:
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the minimizer of distances from all the points in the cluster



4 center-based clusters

Clustering objectives

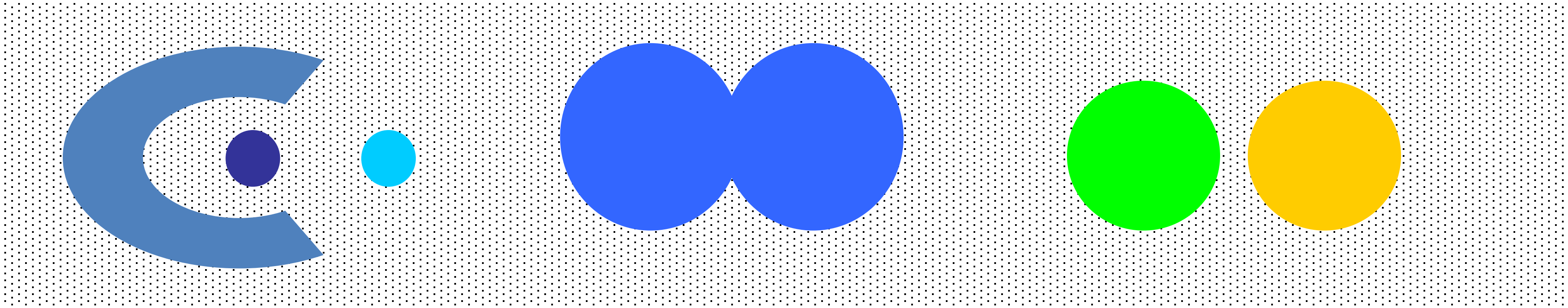
- Contiguous Clusters (Nearest neighbor or Transitive)
  - A cluster is a set of points such that for any point in the cluster, its nearest neighbor is in the same cluster.



8 contiguous clusters

Clustering Objectives

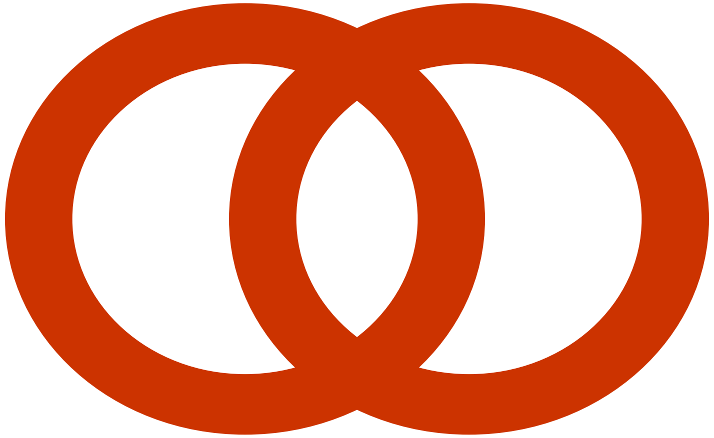
- Density-based clusters
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



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 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

- Most common definition is with Euclidean distance, minimizing the Sum of Squared Error (SSE) – distance 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 $C = \{C_1, C_2, \ldots, Ck\}$ such that

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

Sum of Squared Error (SSE)

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

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

K-means Algorithm

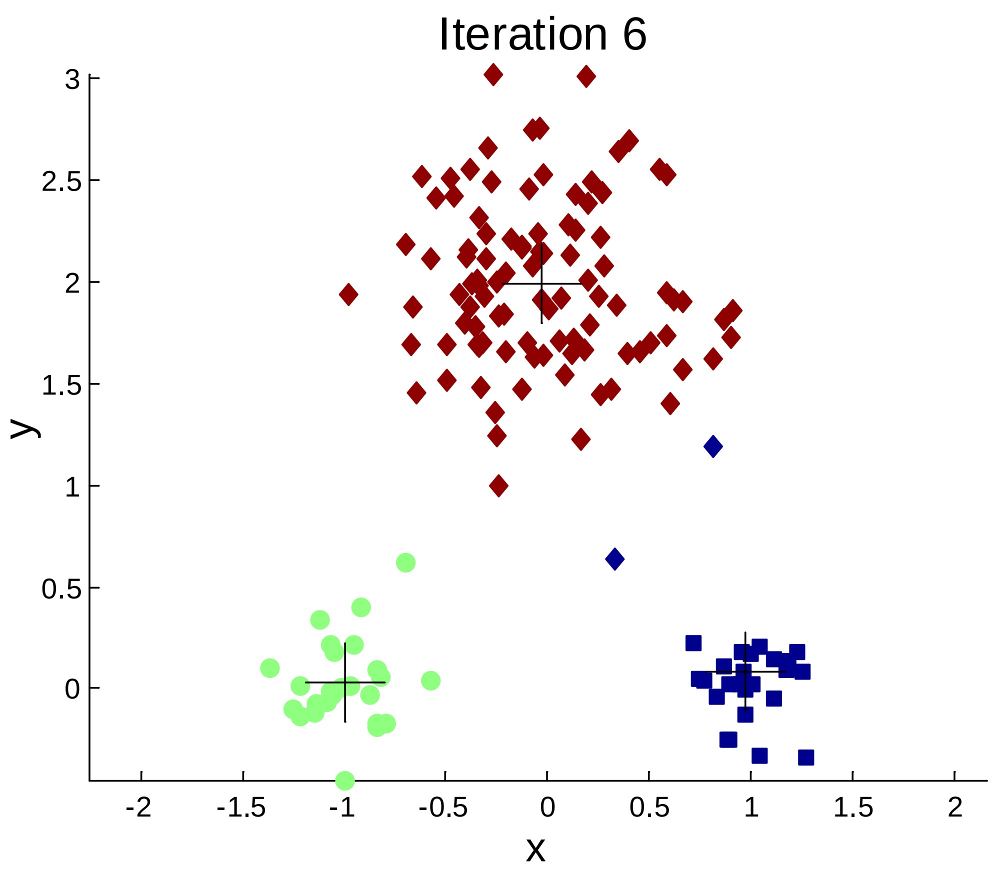
- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

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

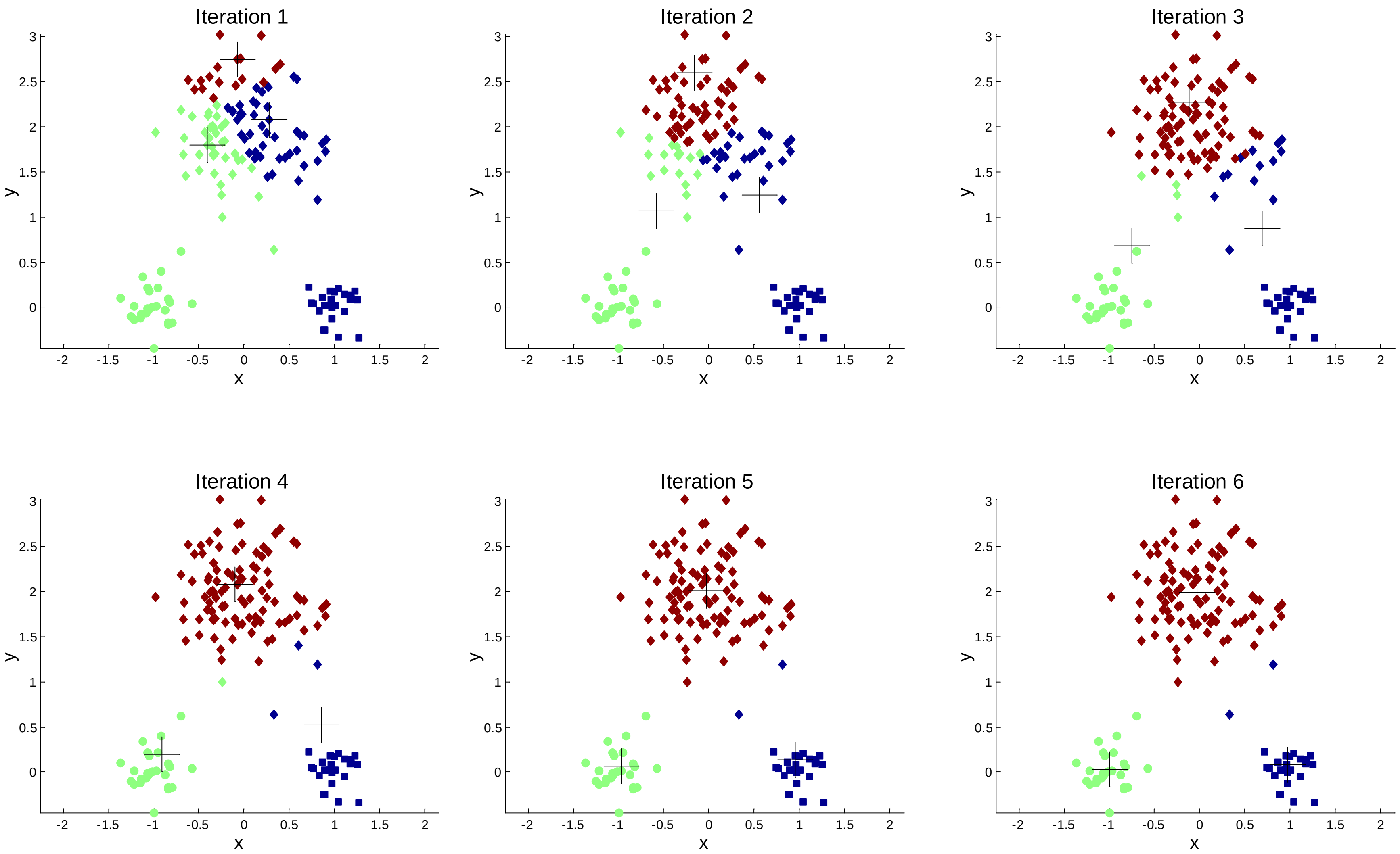
e.g. take mean of all points in a cluster to compute its centroid

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

Example



Example

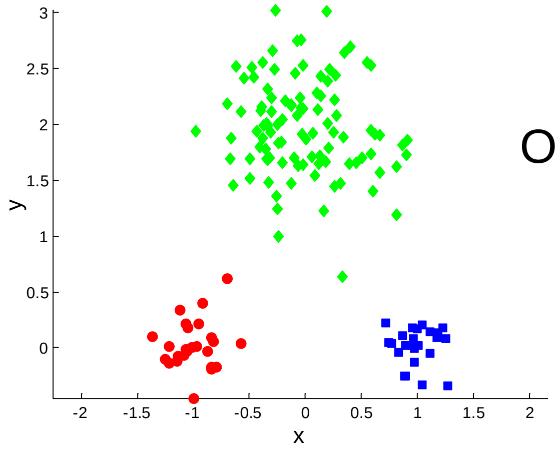


Iteration 1
Iteration 2
Iteration 3
Iteration 4
Iteration 5
Iteration 6
x
y

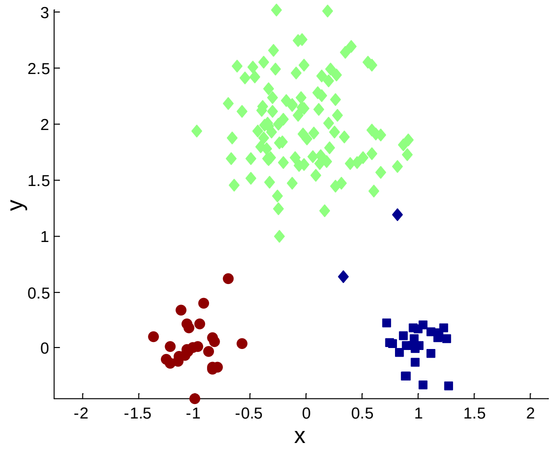
K-means Algorithm – Initialization

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

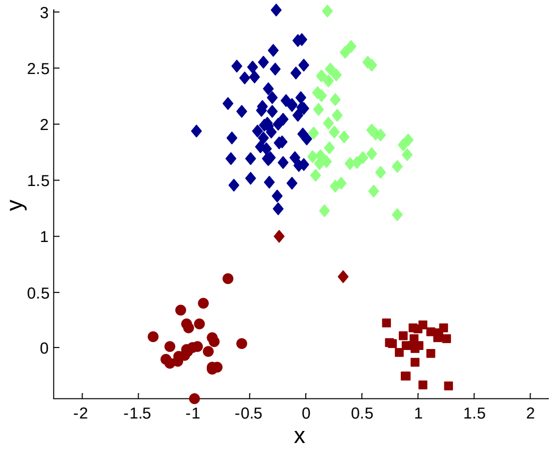
Two different K-means Clusterings



Original Points

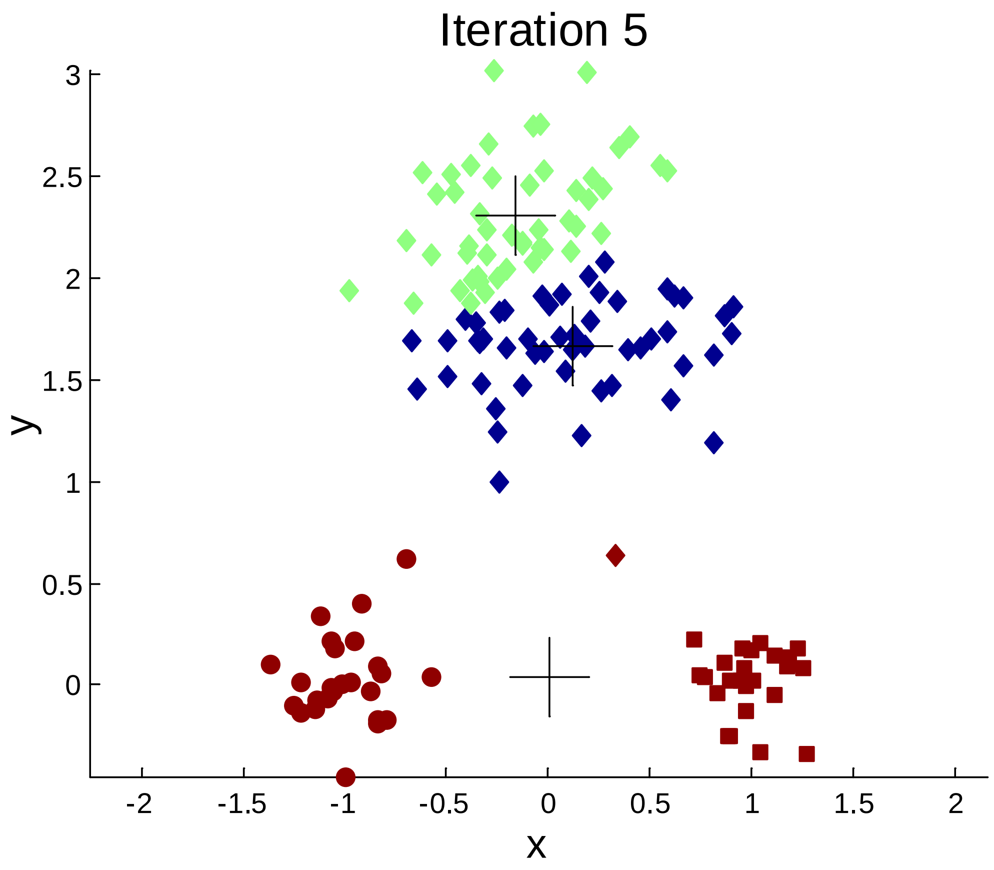


Optimal Clustering

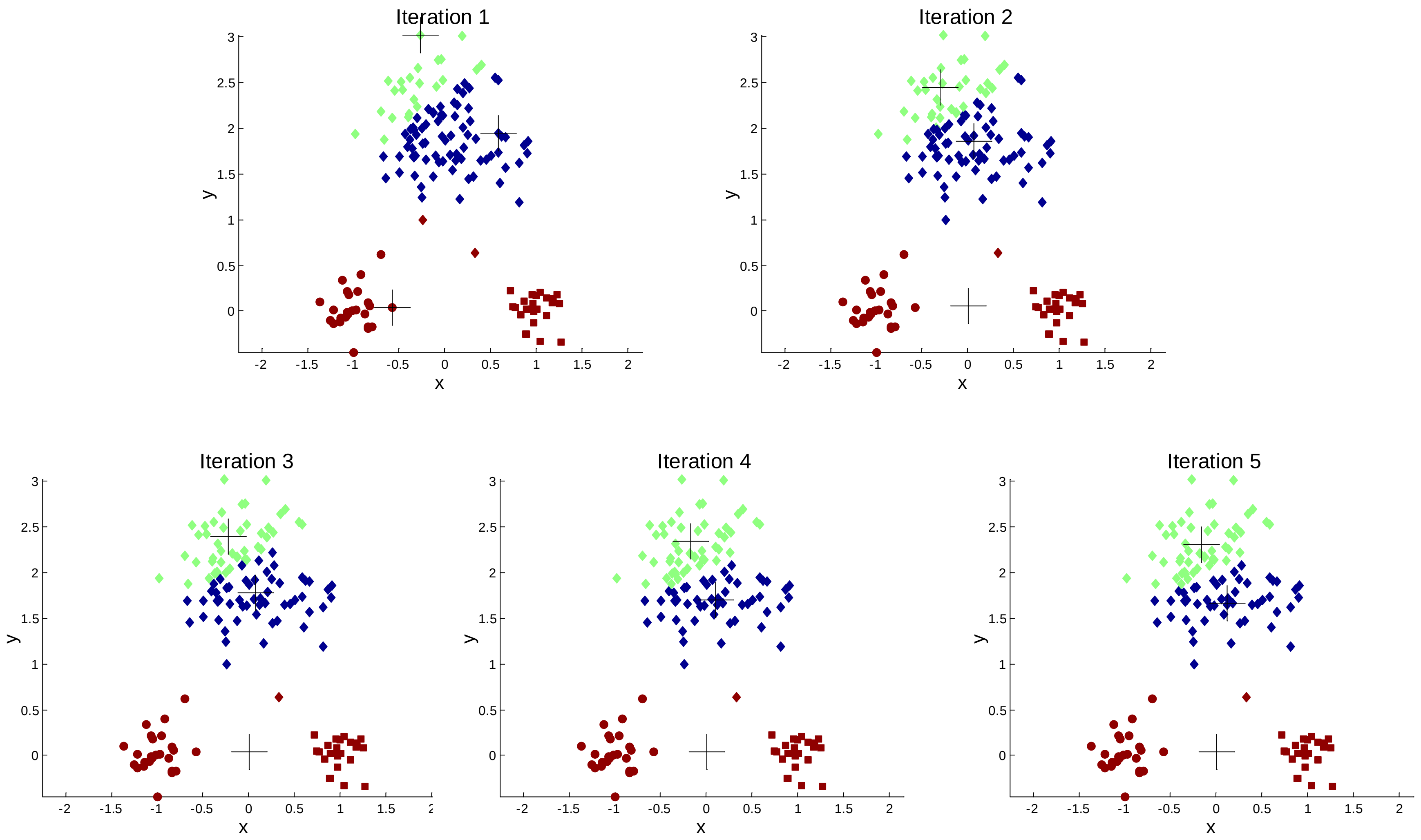


Sub-optimal Clustering

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., 1. pick one center; 2. when picking the next center, pick the most distant (from previously picked centers) point as cluster center (K-means++ algorithm); 3. repeat 2.

K-means Algorithm – Convergence

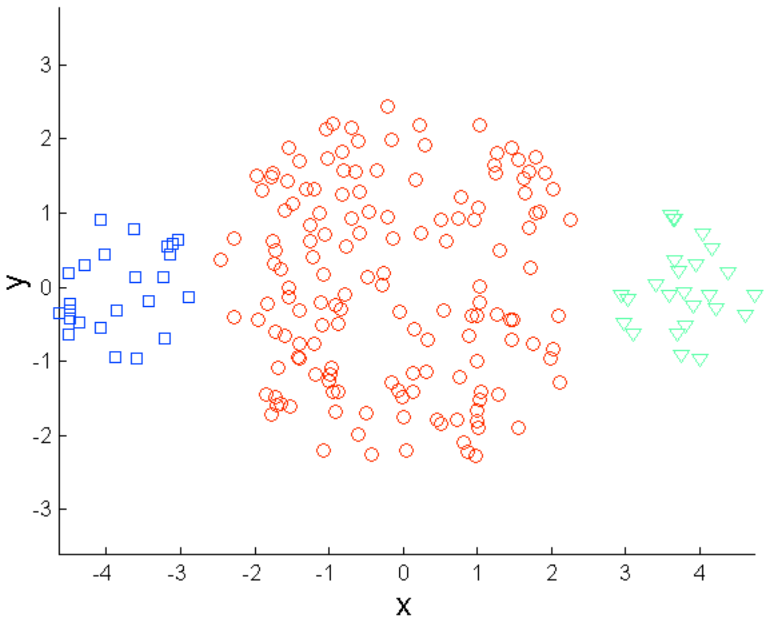
- K-means will converge for common similarity measures mentioned above.
  - Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'
- Complexity is $O(n * K * I * d)$
  - n = number of points,
  - K = number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

Limitations of K-means

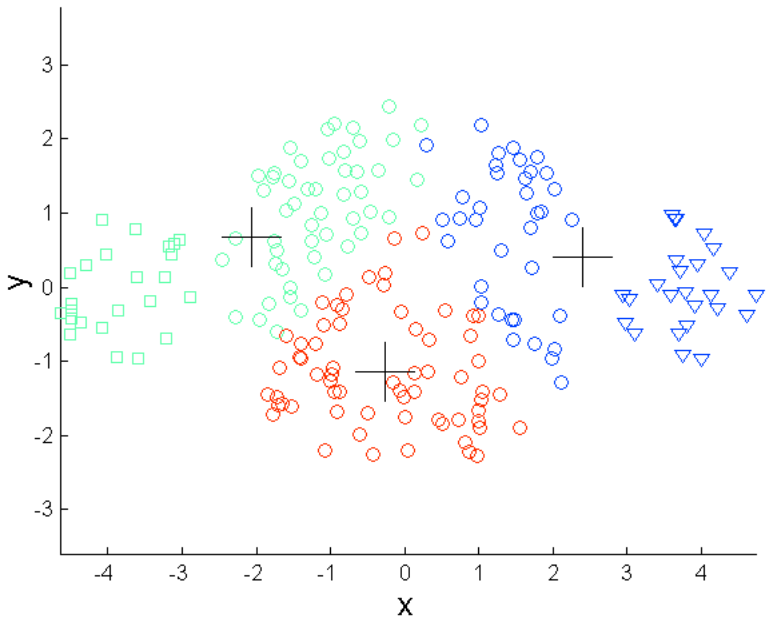
- K-means has problems when clusters are of different:
  - sizes
  - densities
  - non-globular shapes

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

Limitations of K-means: Differing Sizes

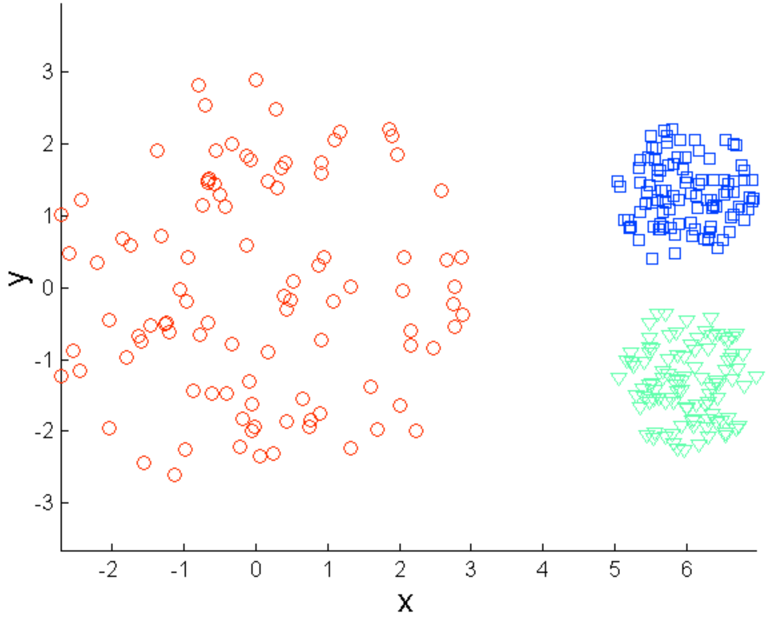


Original Points

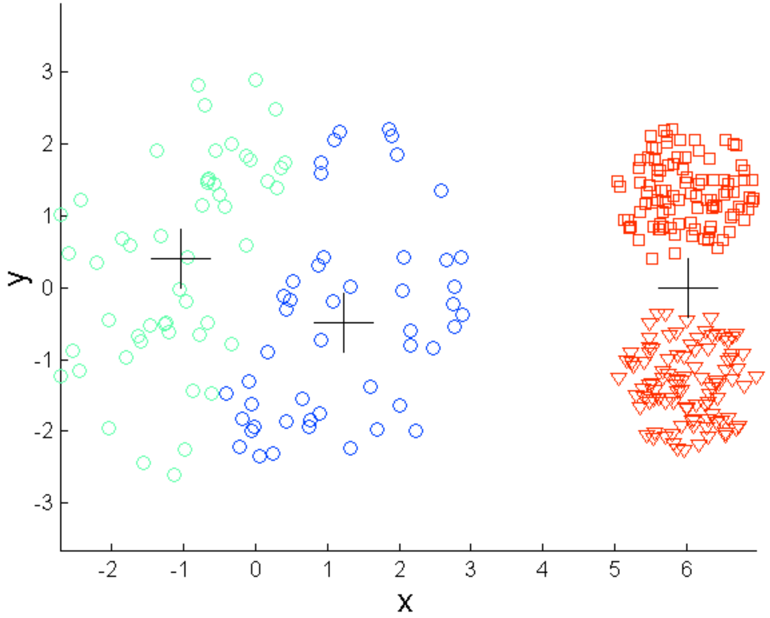


K-means (3 Clusters)

Limitations of K-means: Differing Density

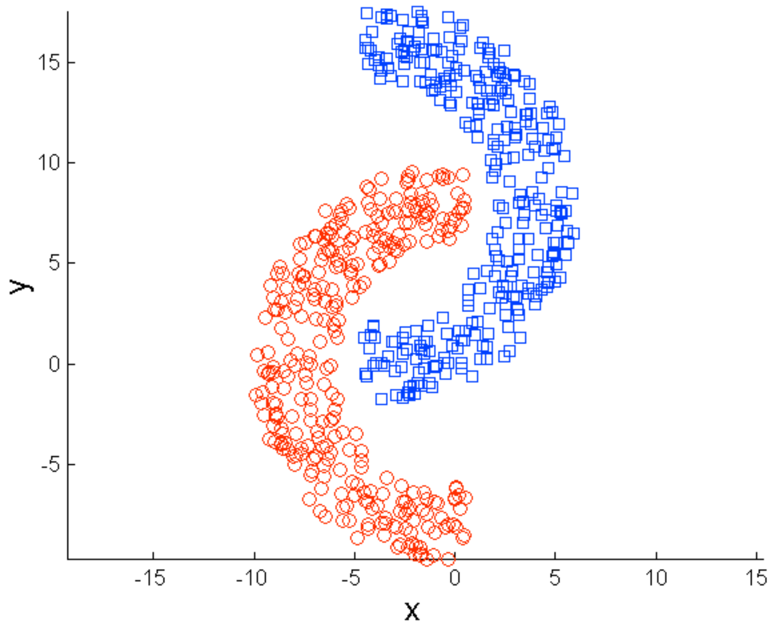


Original Points

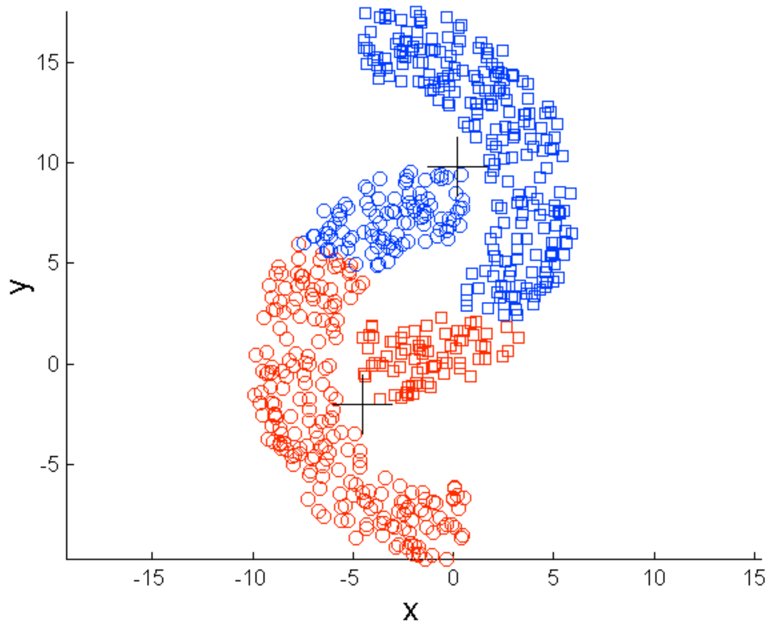


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

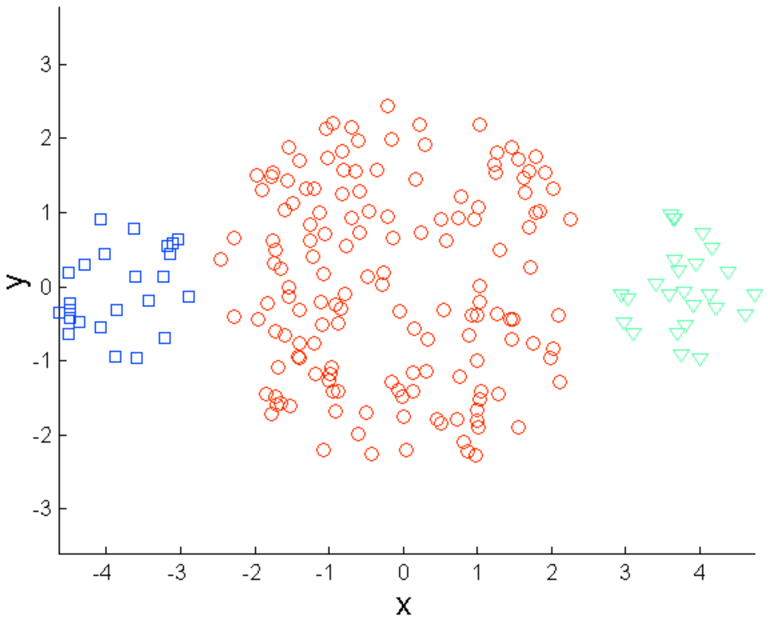


Original Points

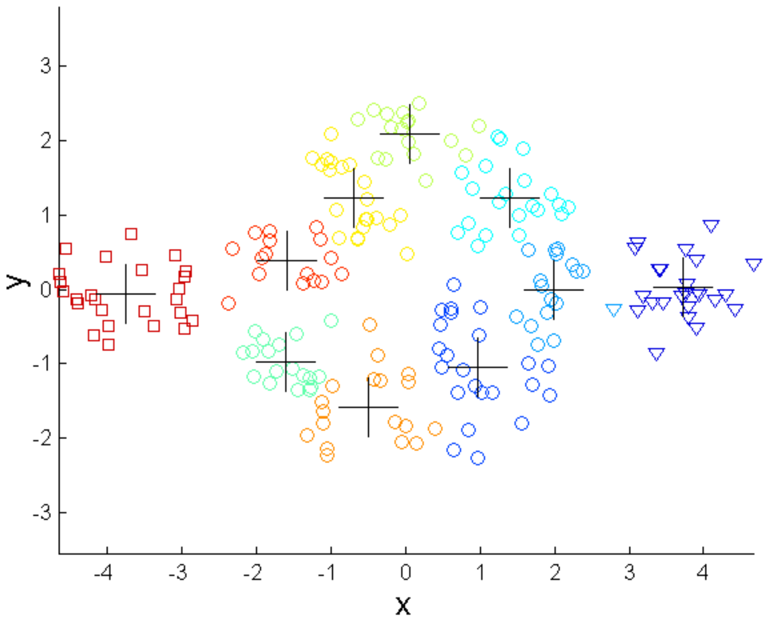


K-means (2 Clusters)

Overcoming K-means Limitations



Original Points

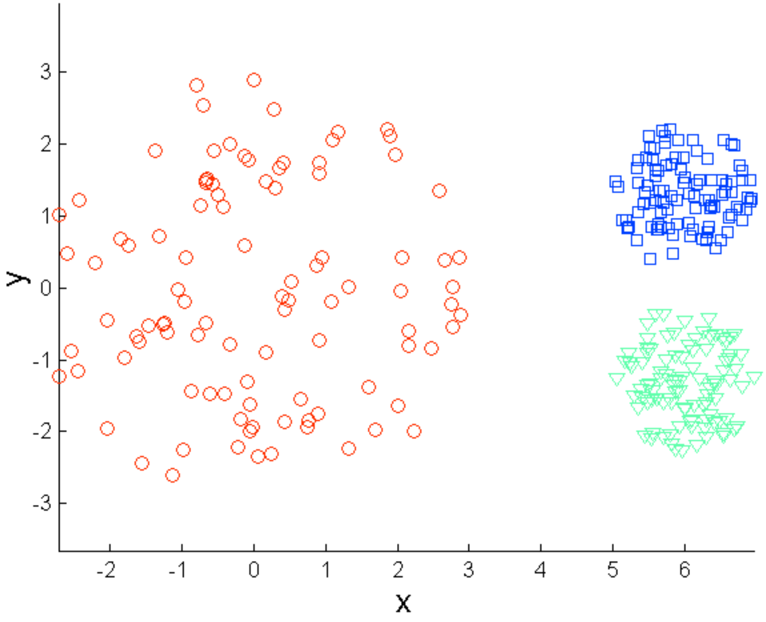


K-means Clusters

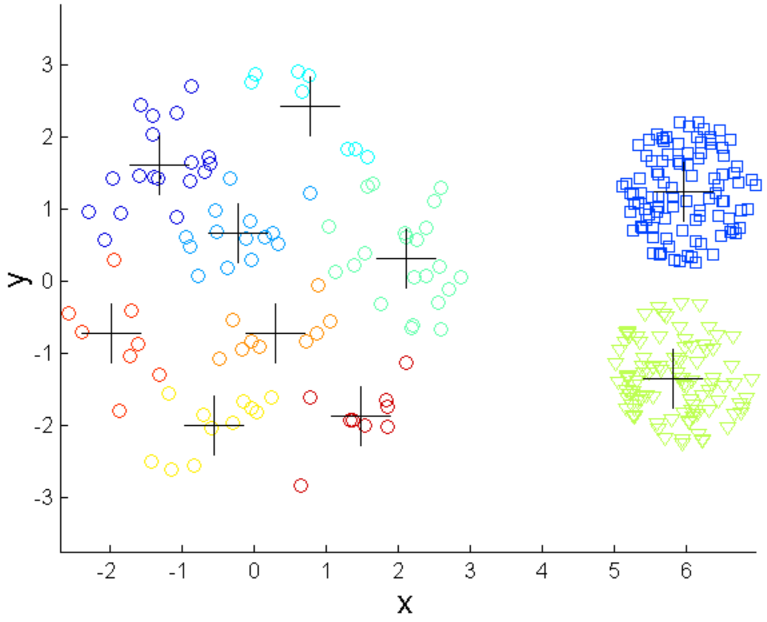
One solution is to use many clusters.

Find parts of clusters, but need to put together.

Overcoming K-means Limitations

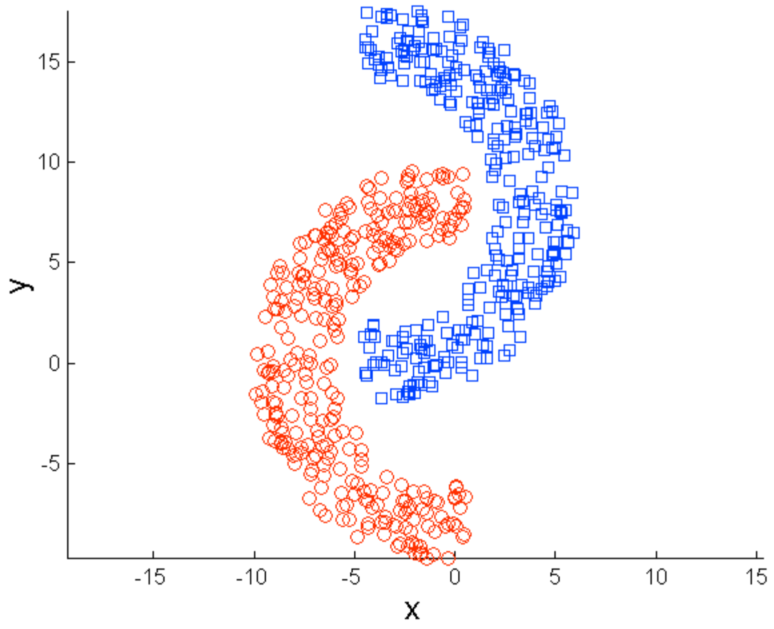


Original Points

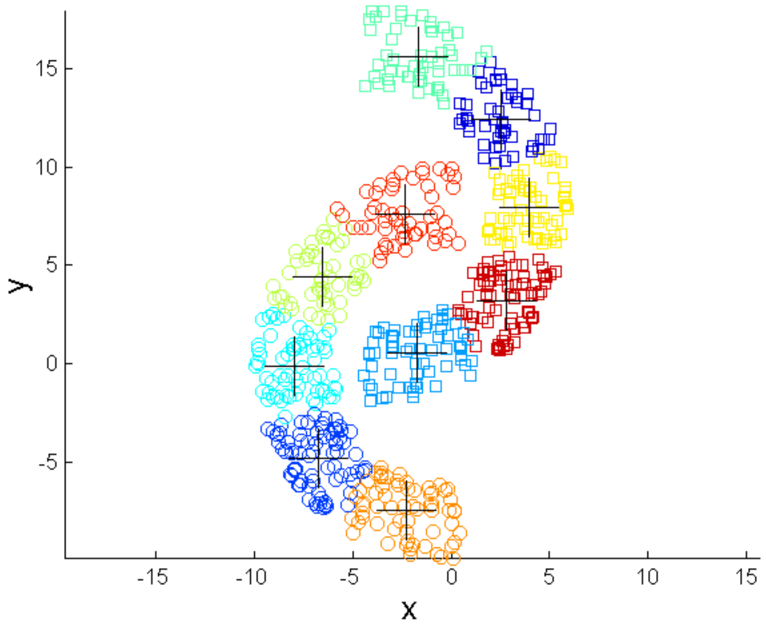


K-means Clusters

Overcoming K-means Limitations



Original Points



K-means Clusters

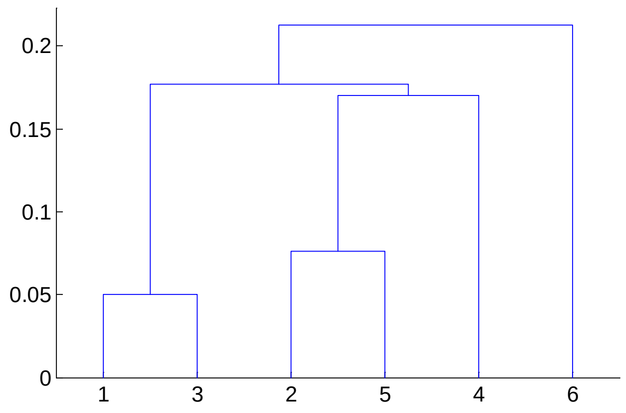
HIERARCHICAL CLUSTERING

Hierarchical Clustering

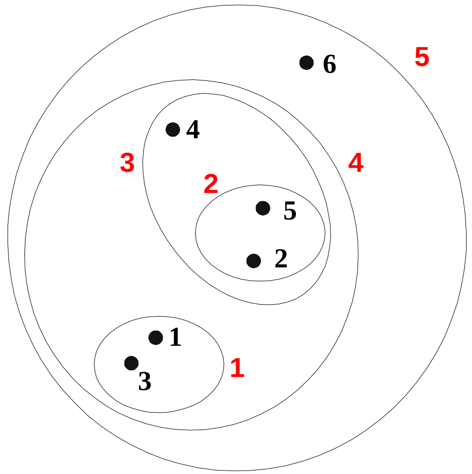
- Two main types of hierarchical clustering
  - Agglomerative（凝聚式）:
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive（分裂式）:
    - Start with one, all-inclusive cluster
    - At each step, 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）or nested cluster diagram（嵌套簇图）
  - A tree like diagram that records the sequences of merges or splits



dendrogram



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

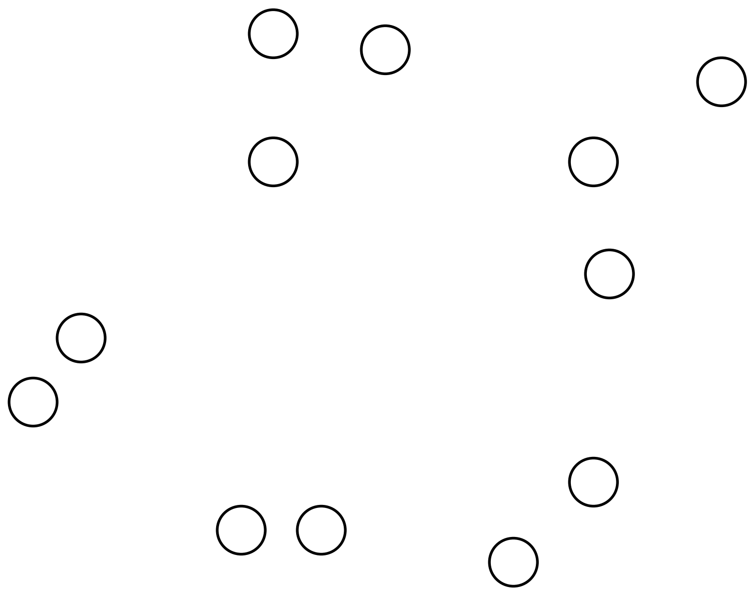
- Dendrograms may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom …)

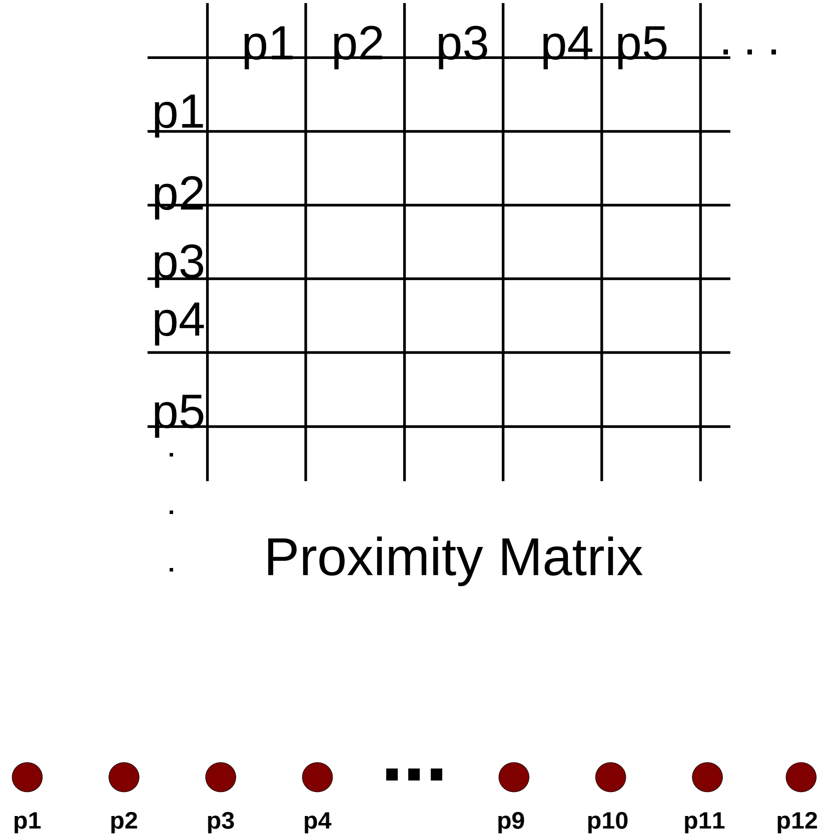
Agglomerative Clustering Algorithm

- Most popular hierarchical clustering technique
- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. **Repeat**
  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

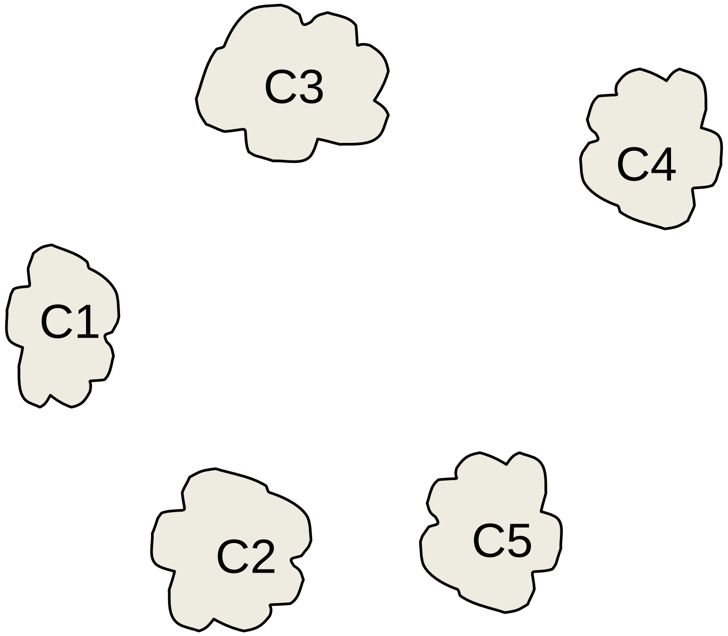
- Start with single-point clusters and a proximity matrix between points





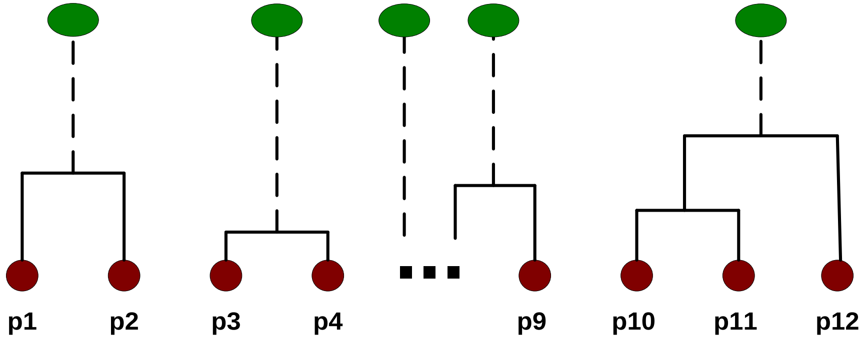
Intermediate Situation

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



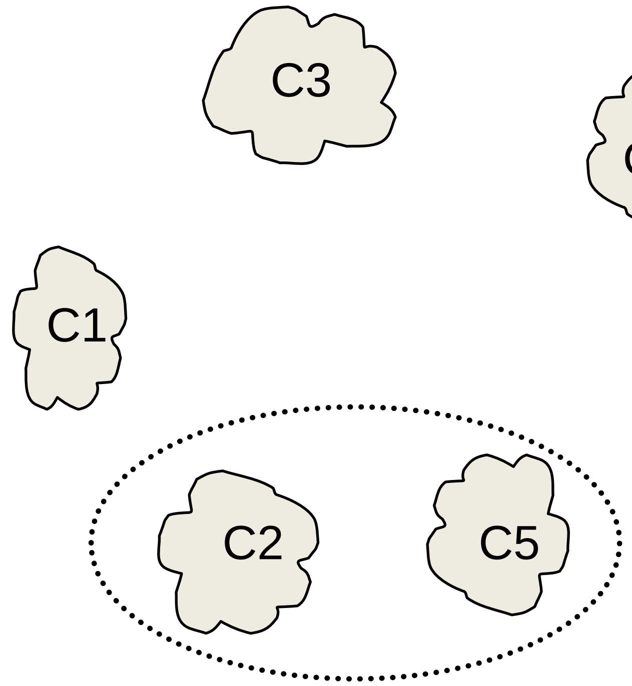
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

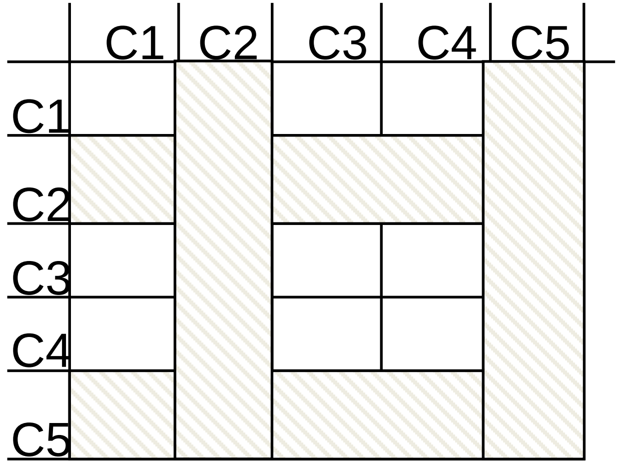
Proximity Matrix



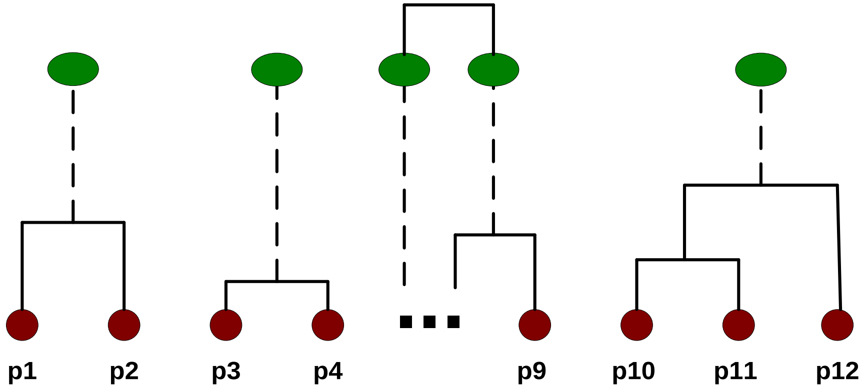
Intermediate Situation

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



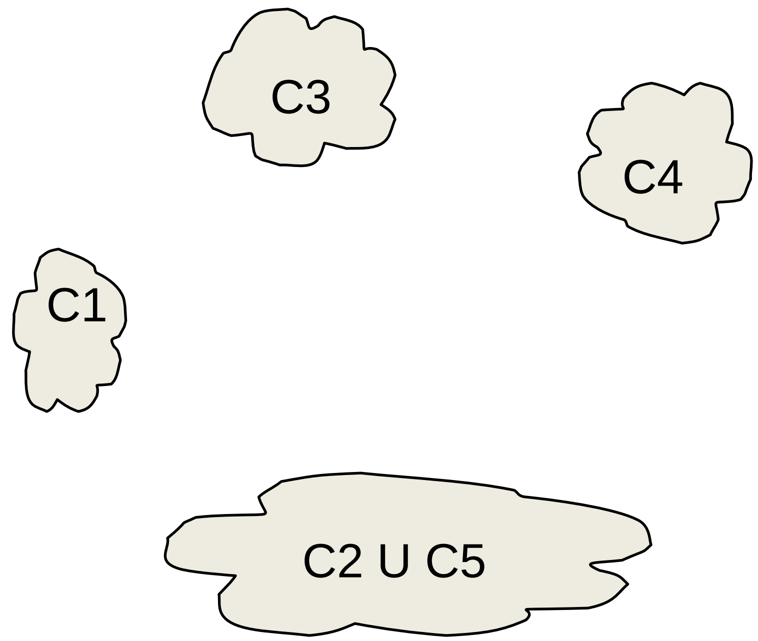


Proximity Matrix



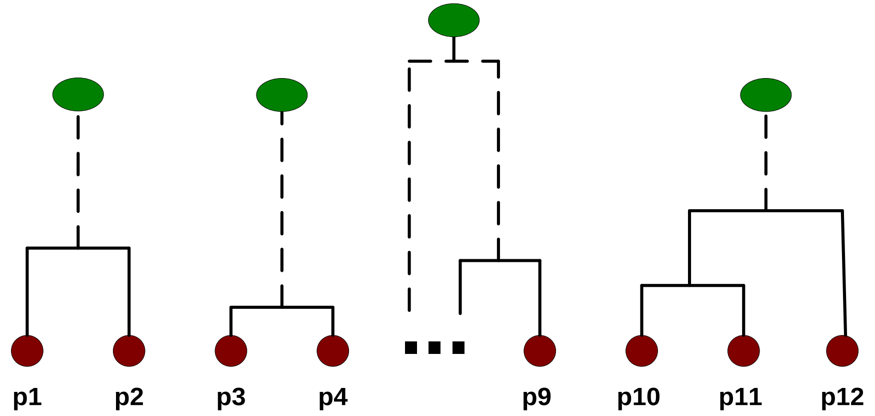
After Merging

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

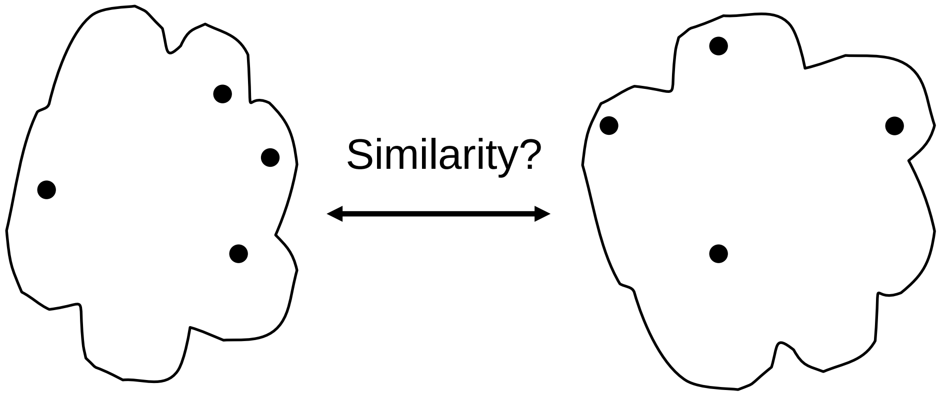


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Similarity

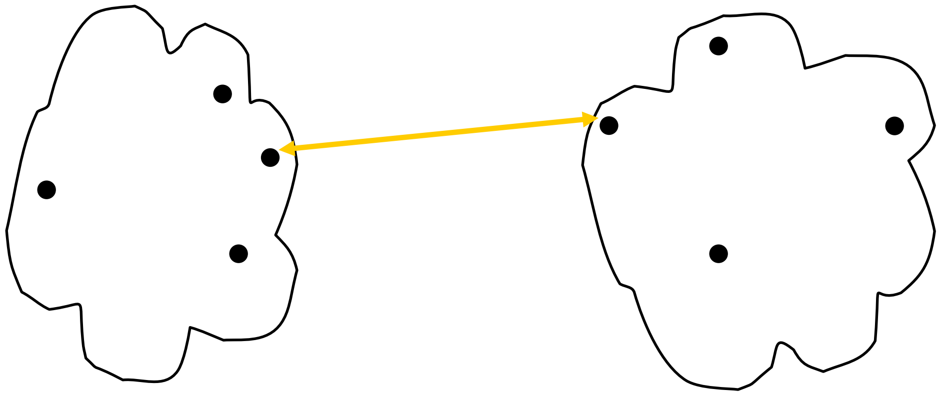


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

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						
.						
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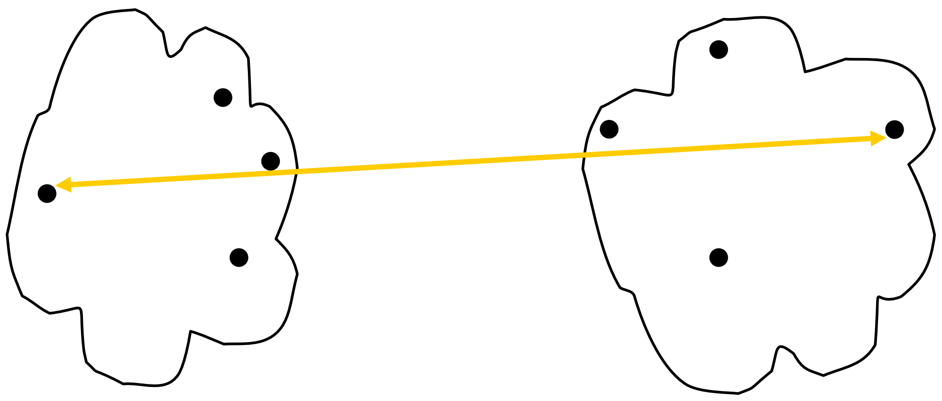

	p1	p2	p3	p4	p5	. . .
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p2						
p3						
p4						
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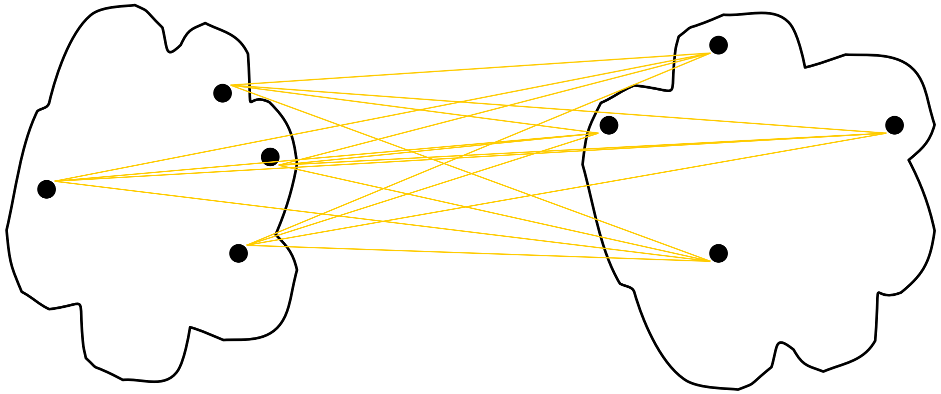

	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
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Proximity Matrix

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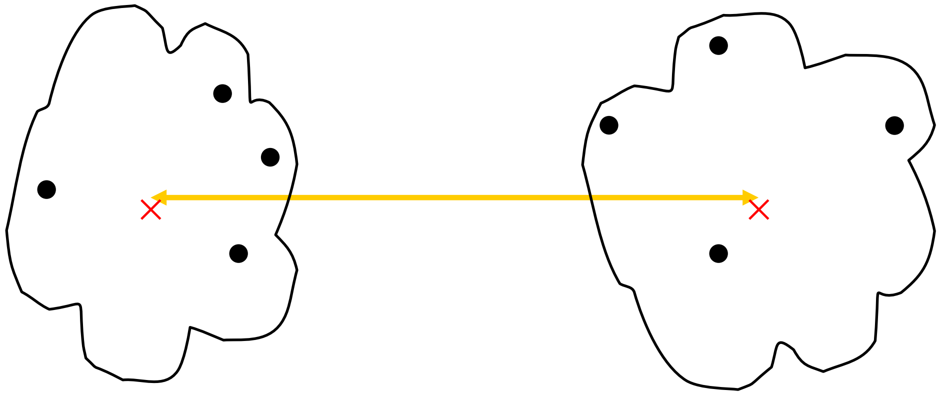
$$\text{proximity}(\text{Cluster}_i,\text{Cluster}_j) = \frac{\sum\limits_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i,p_j)}{|\text{Cluster}_i| * |\text{Cluster}_j|}$$

How to Define Inter-Cluster Similarity



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

Proximity Matrix

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- MAX
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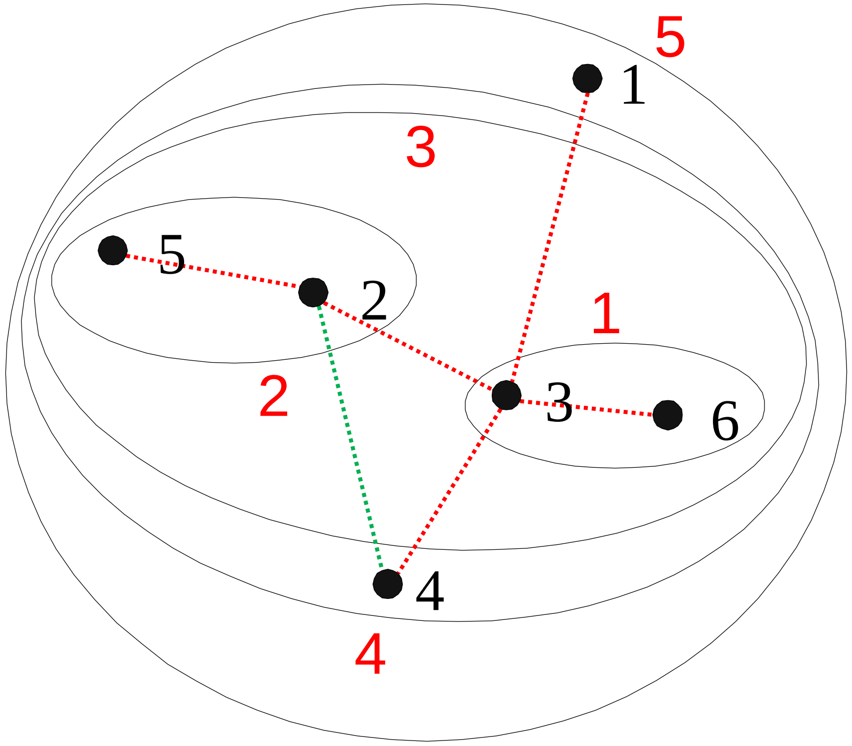
Single Link – Complete Link

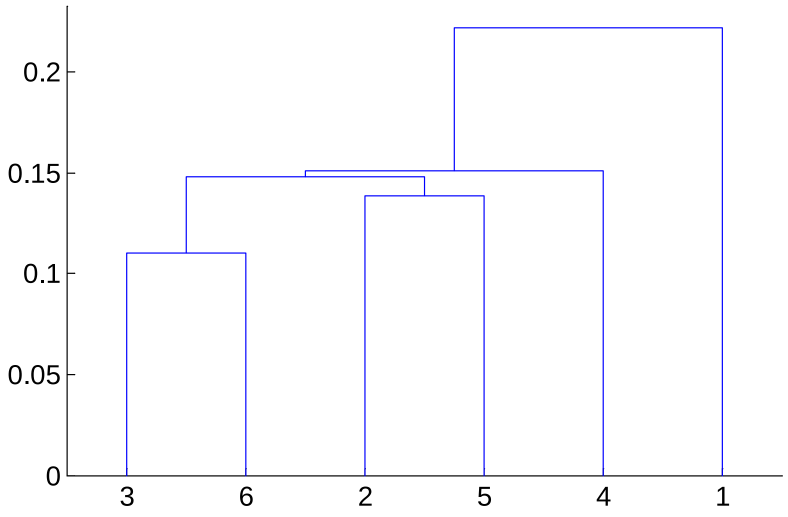
- Another way to view the processing of the hierarchical algorithm is that we create links between the elements in order of increasing distance
  - The MIN – Single Link, will merge two clusters when a single pair of elements is linked
  - The MAX – Complete Linkage will merge two clusters when all pairs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

Hierarchical Clustering: MIN



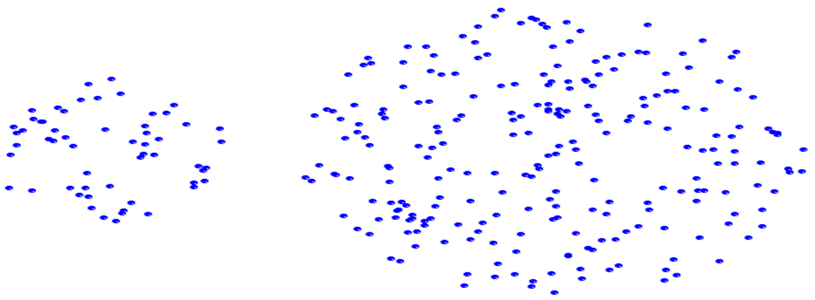
Nested Clusters

	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

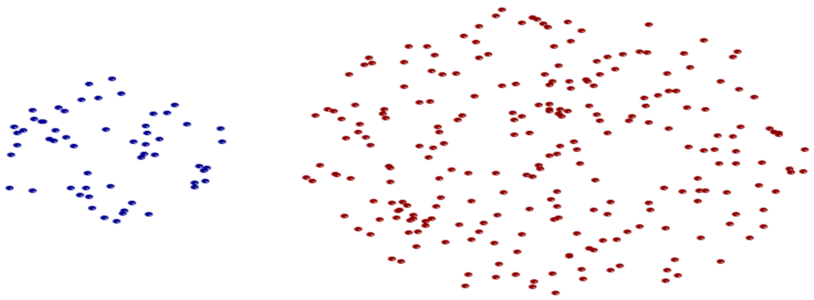


Dendrogram

Strength of MIN



Original Points

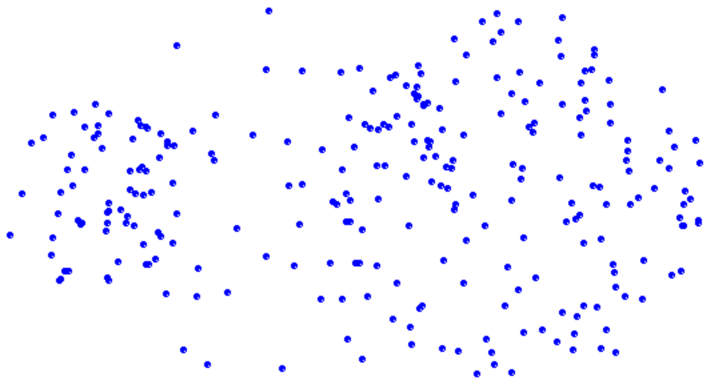


Two Clusters

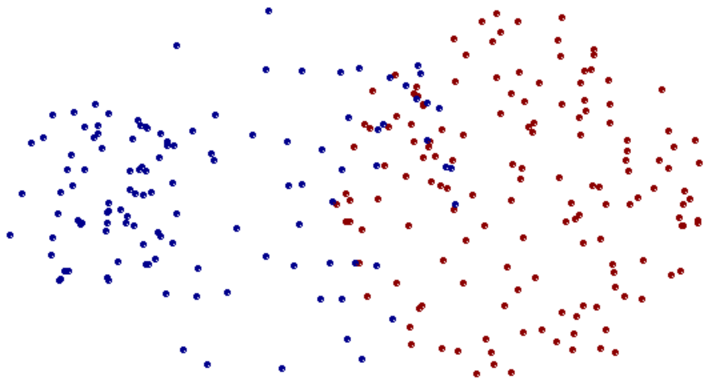
• Can handle non-elliptical shapes

single link method is also called *nearest neighbor* method.

Limitations of MIN



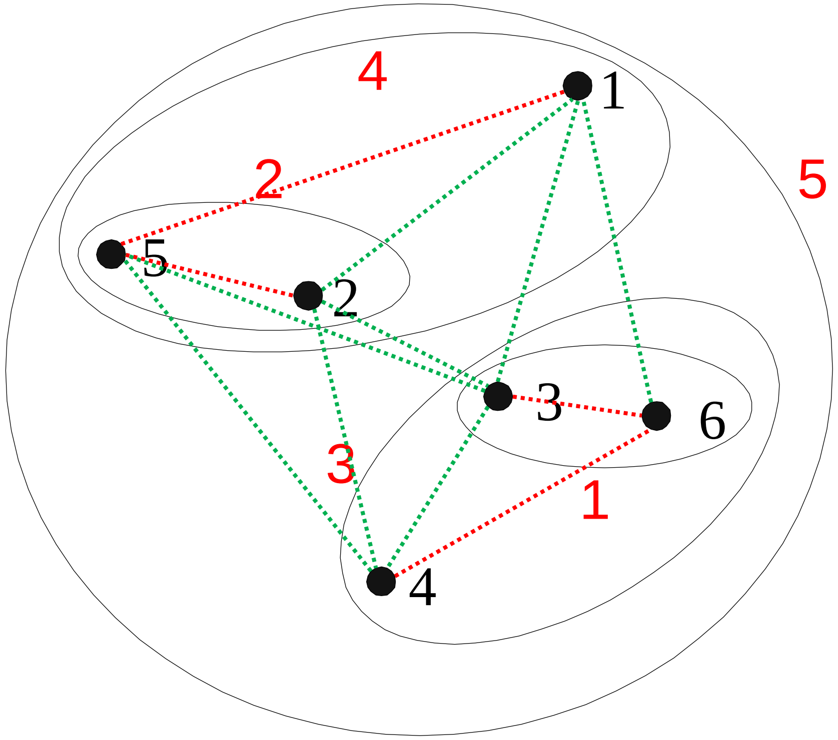
Original Points



Two Clusters

- Sensitive to noise and outliers

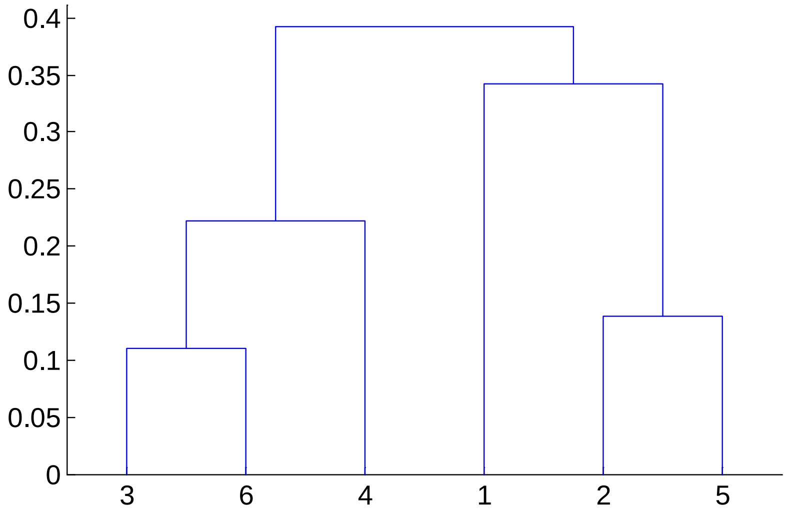
Hierarchical Clustering: MAX



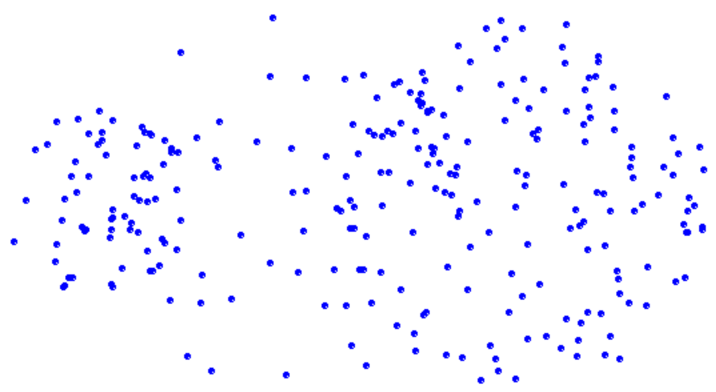
Nested Clusters

Dendrogram

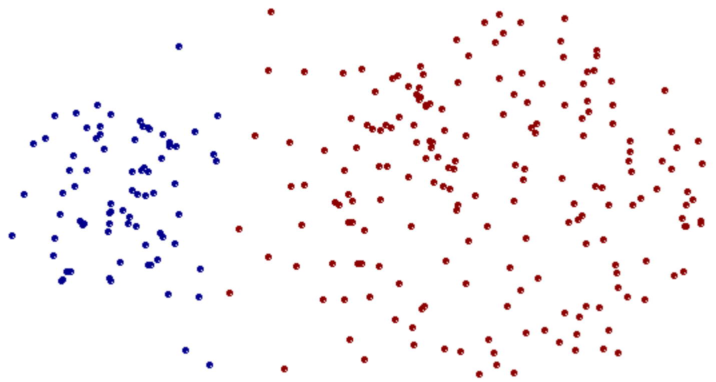
	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Strength of MAX



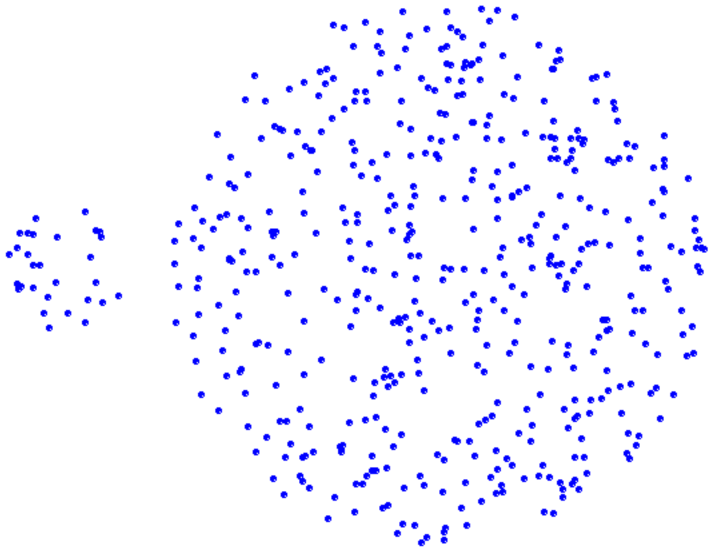
Original Points



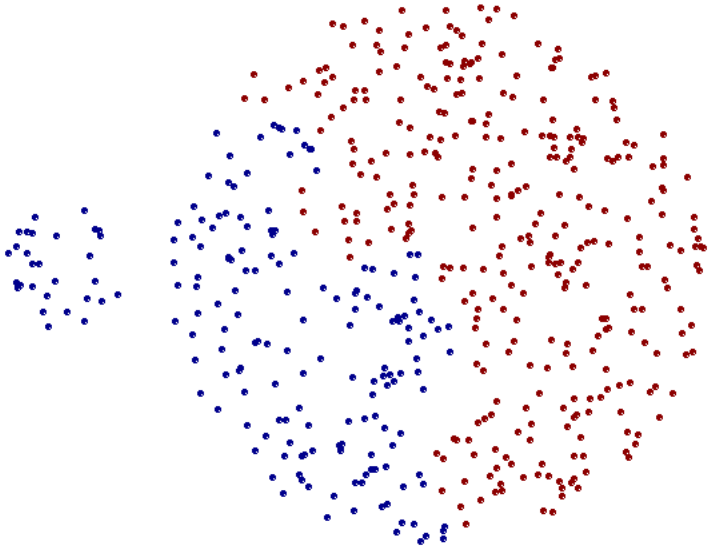
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points

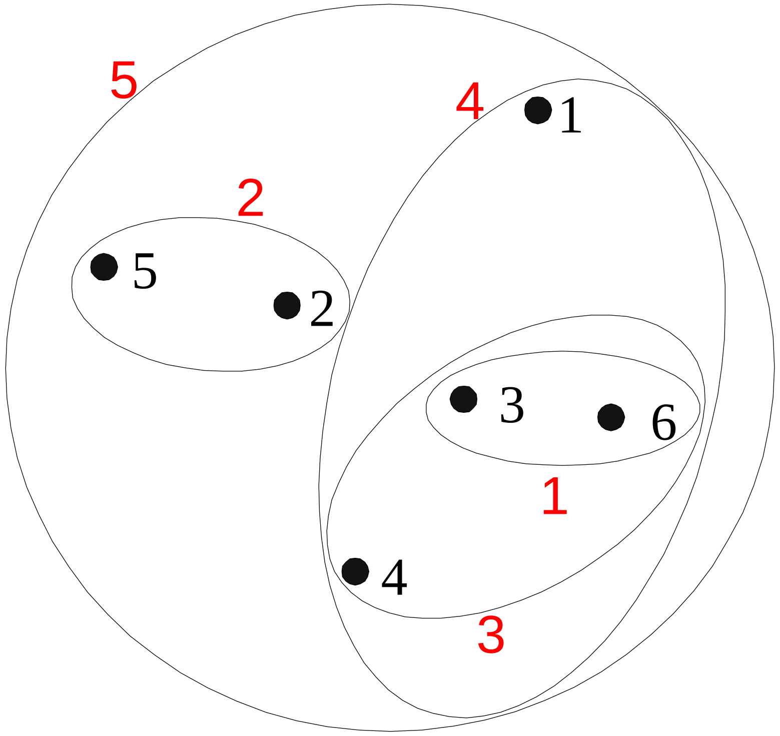


Two Clusters

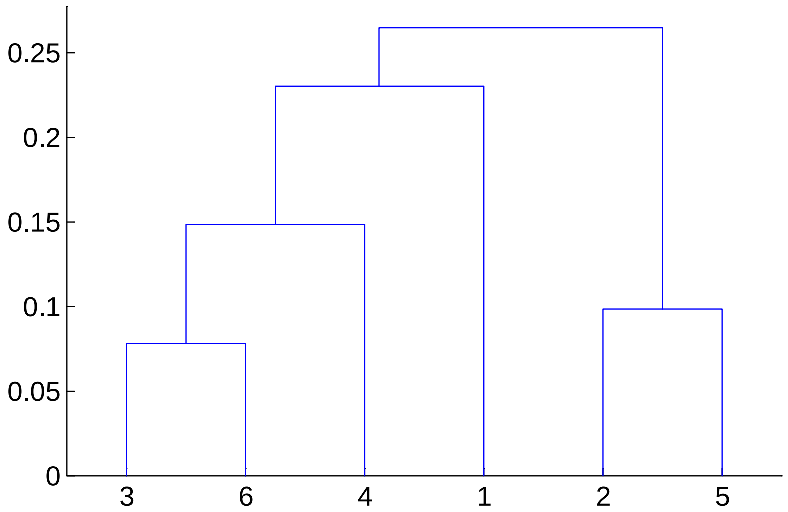
- Tends to break large clusters
- Biased towards globular clusters

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 to noise and outliers

- Limitations
  - Biased towards globular clusters

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

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

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