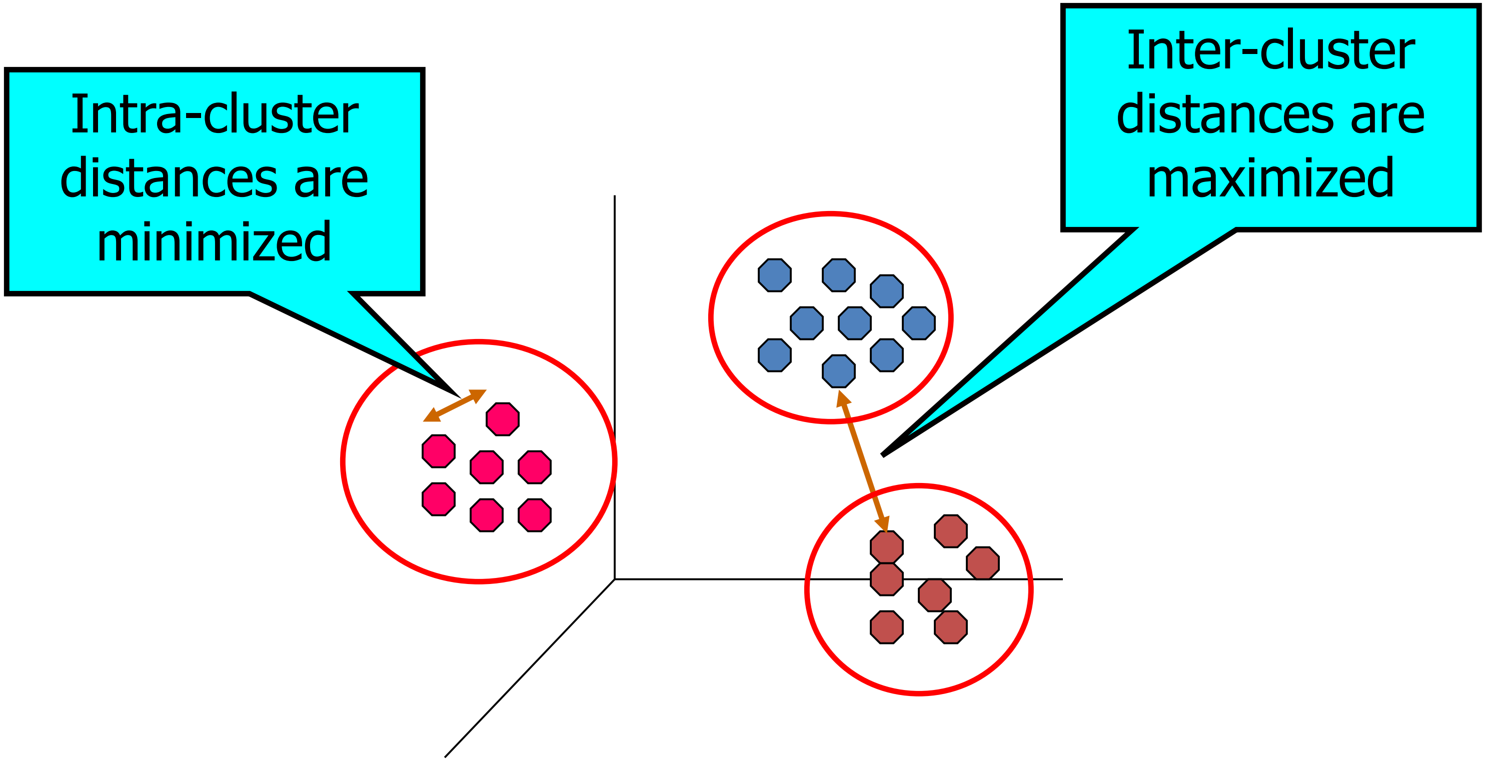
# DATA MINING
# LECTURE 7

Clustering

# 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

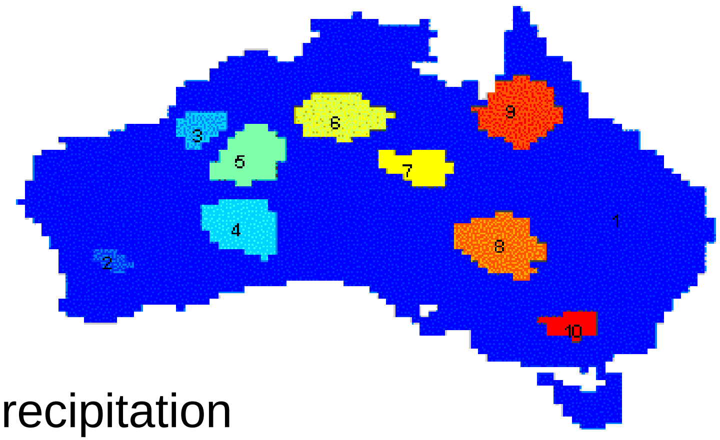


# Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

| | *Discovered Clusters* | *Industry Group* |
|---|---|---|
| **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 |

- **Summarization**
  - Reduce the size of large data sets




Clustering precipitation in Australia

# Early applications of cluster analysis

- John Snow, London 1854

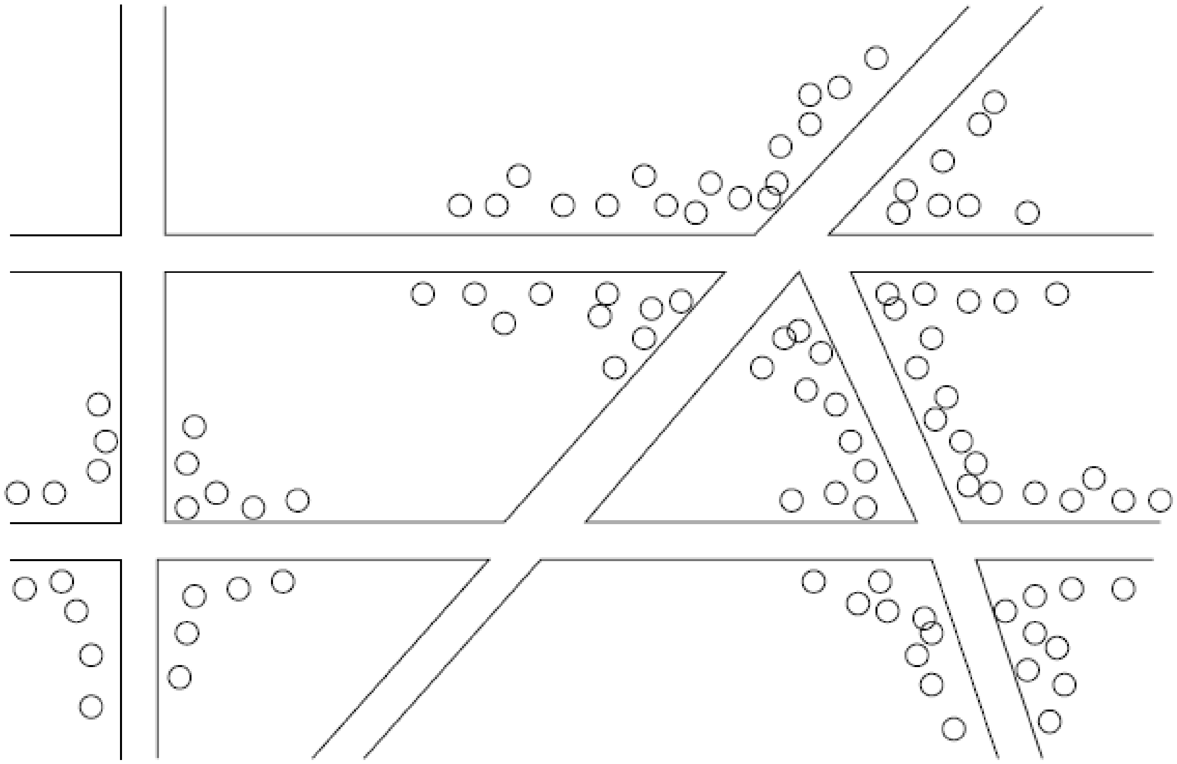


Figure 1.1: Plotting cholera cases on a map of London

# Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

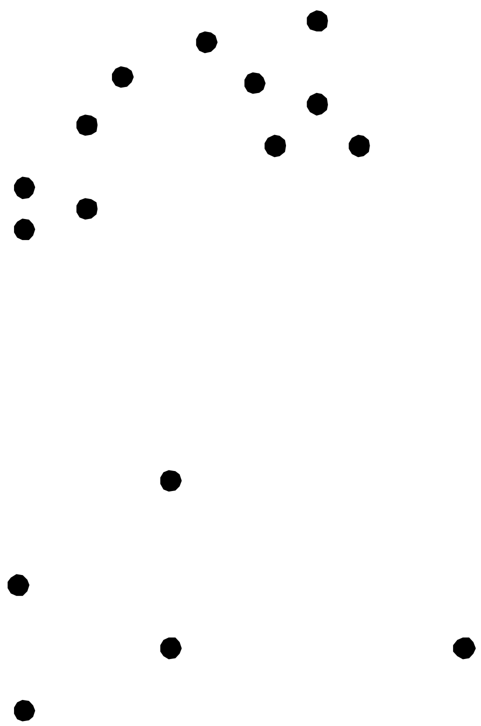
Two Clusters

Four Clusters

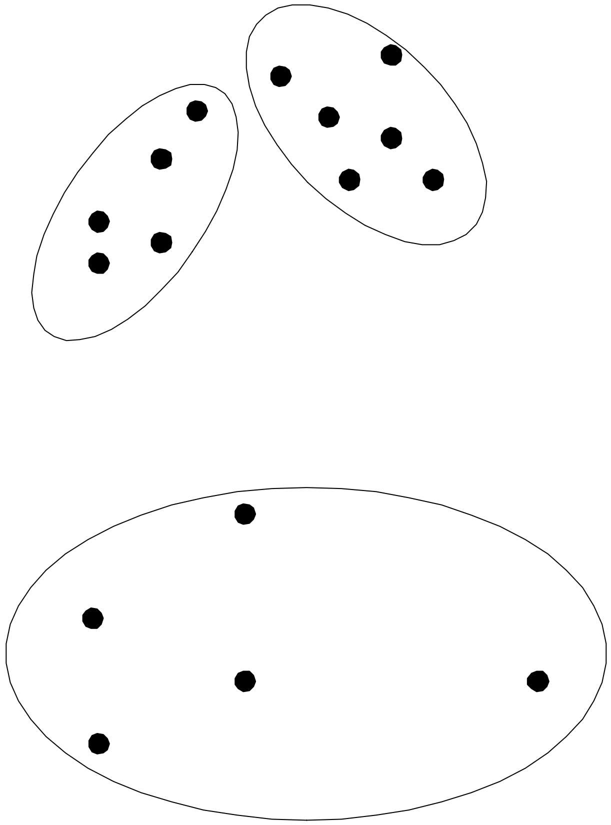
# Types of Clusterings

- 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

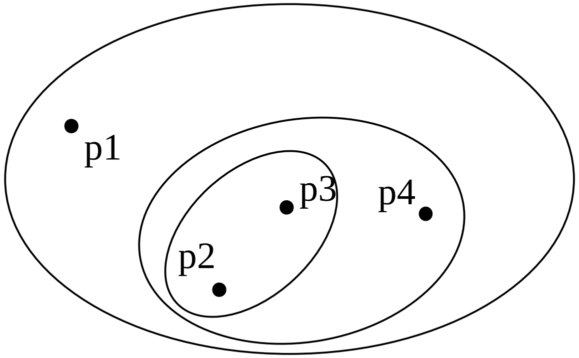


Original Points

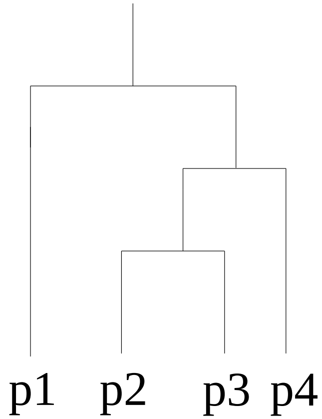


A Partitional  Clustering

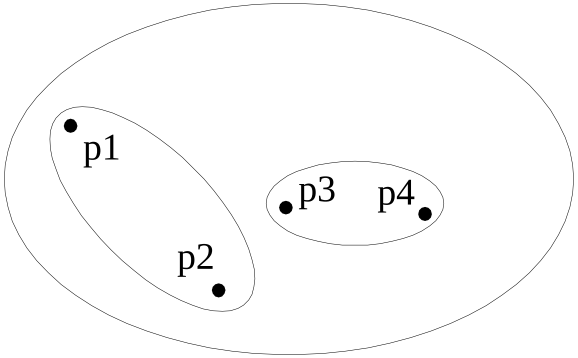
# Hierarchical Clustering



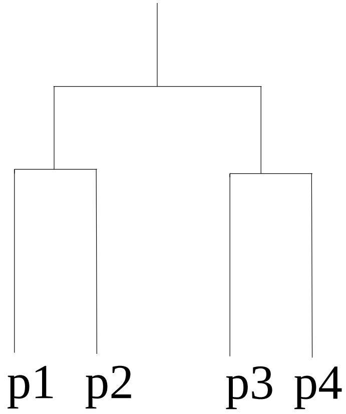

Traditional Hierarchical Clustering




Traditional Dendrogram




Non-traditional Hierarchical Clustering



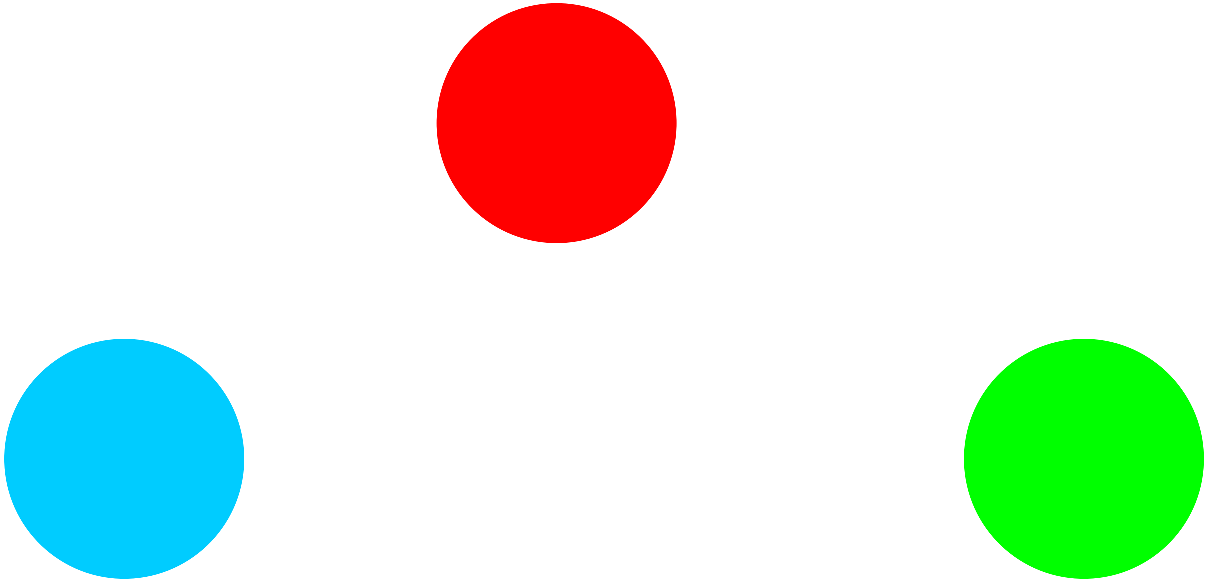

Non-traditional Dendrogram

# 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: Well-Separated

- 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

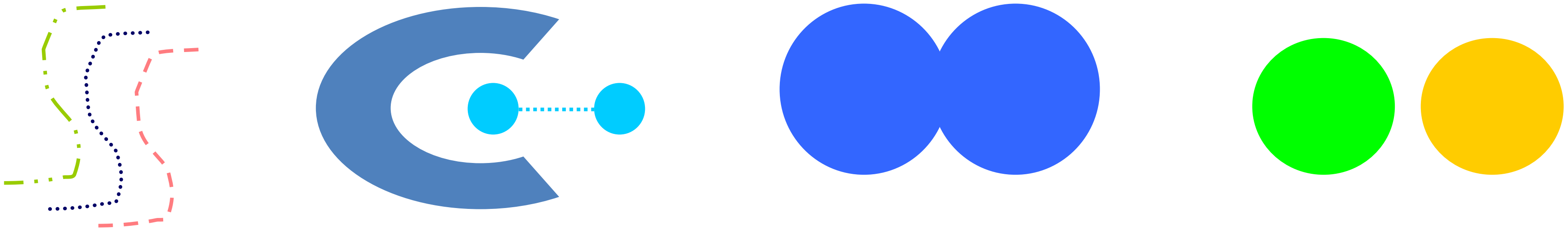
# Types of Clusters: Center-Based

- Center-based
  - 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

4 center-based clusters

# Types of Clusters: Contiguity-Based

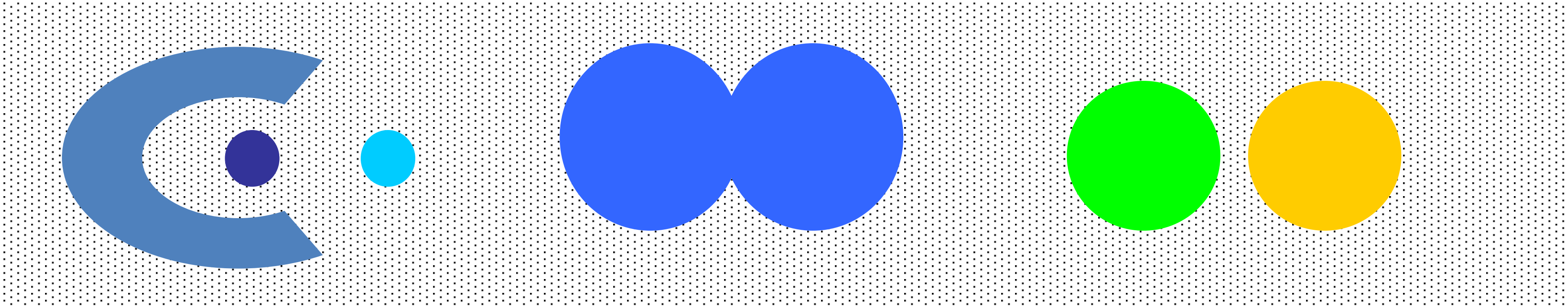
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

# Types of Clusters: Density-Based

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



6 density-based clusters

# Types of Clusters: Conceptual Clusters

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

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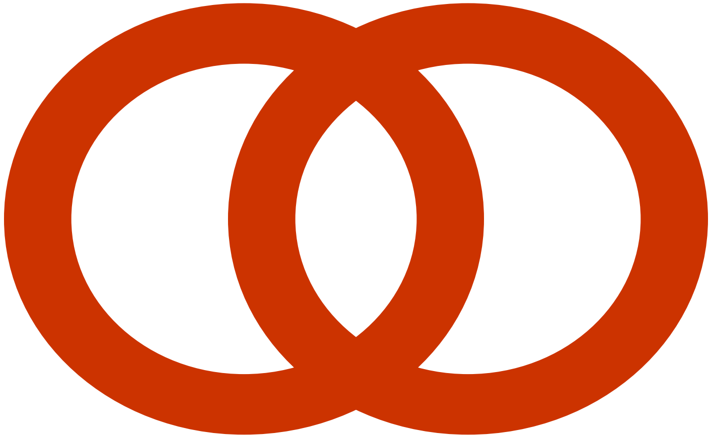


2 Overlapping Circles

# 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 $C = \{C_1, C_2, \ldots, C_k\}$ such that

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

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 $C = \{C_1, C_2, \ldots, C_k\}$ 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>=2**)
  - Finding the best solution in polynomial time is infeasible

- For **d=1** the problem is solvable in polynomial time (how?)

- A simple iterative algorithm works quite well in practice

# K-means Algorithm

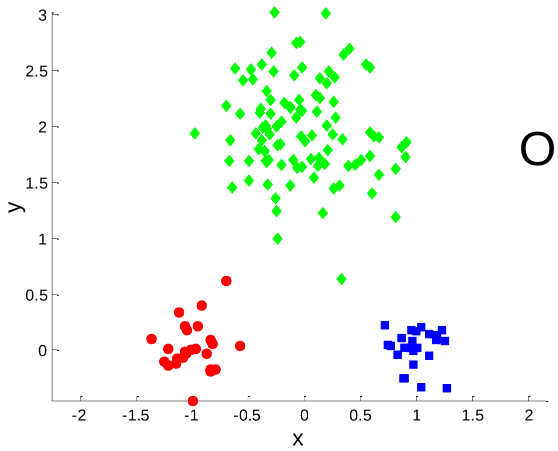
- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

```
Select K points as the initial centroids.
repeat
    Form K clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
until The centroids don't change
```

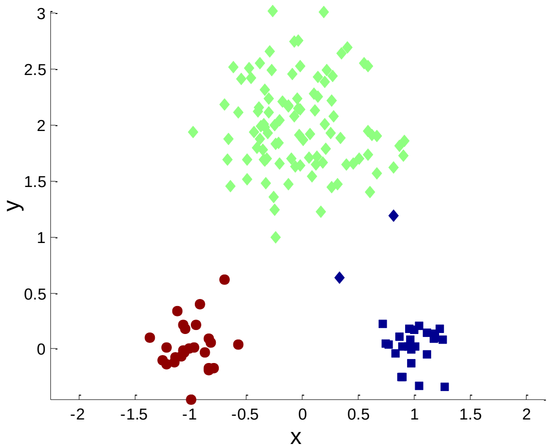
# K-means Algorithm – Initialization

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

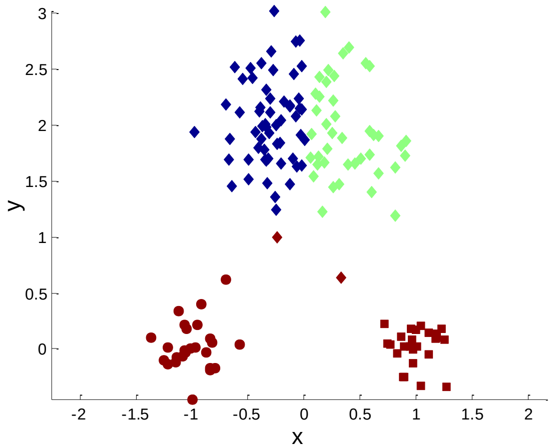
# Two different K-means Clusterings




Original Points

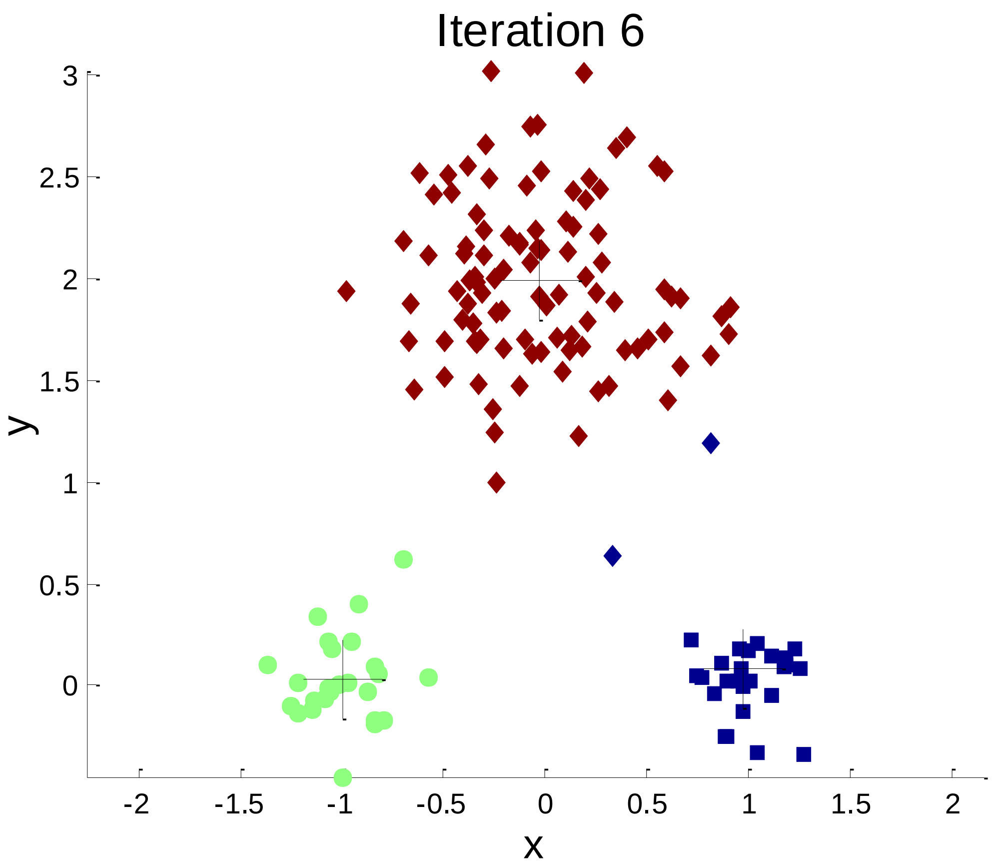



Optimal Clustering

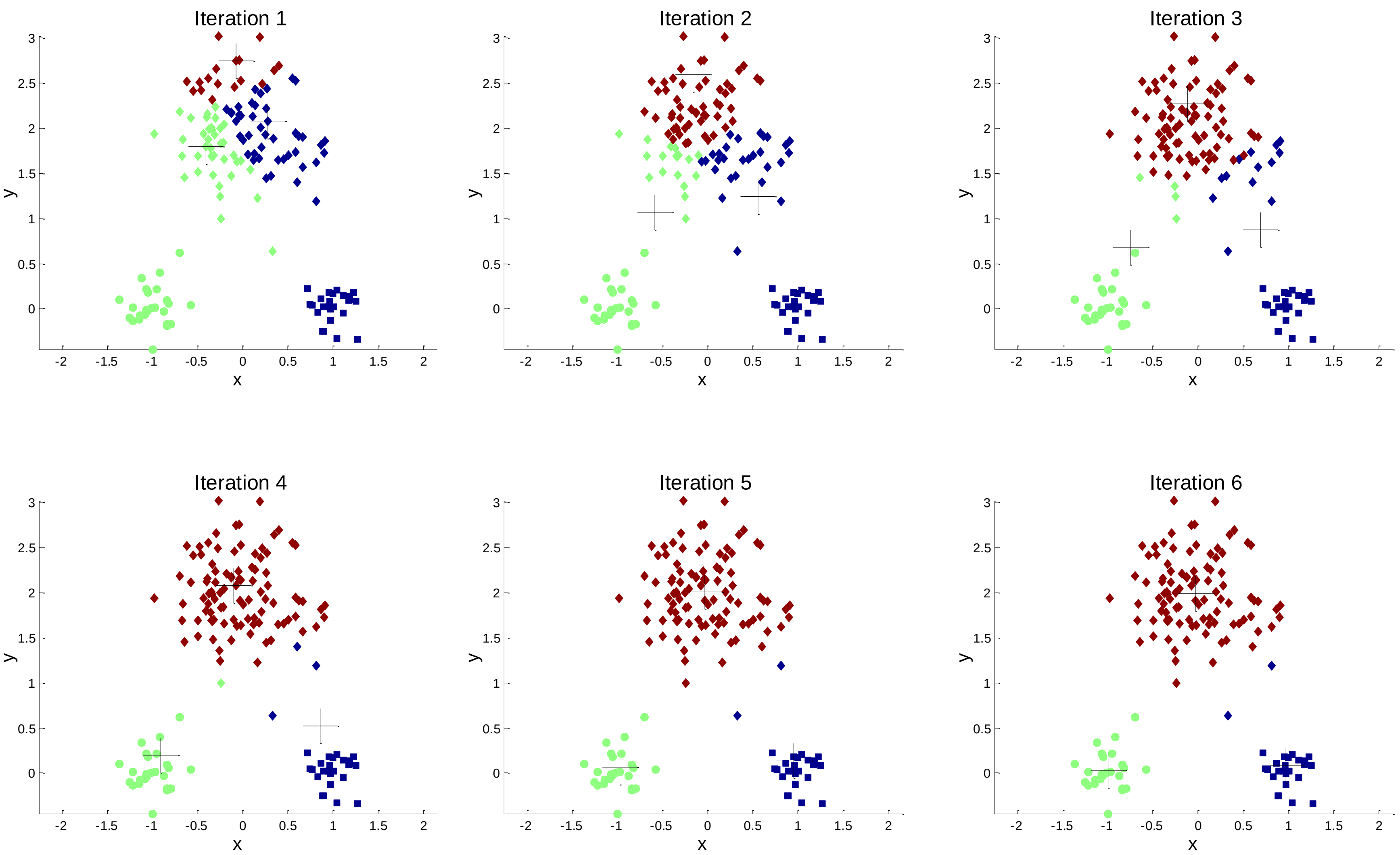



Sub-optimal Clustering

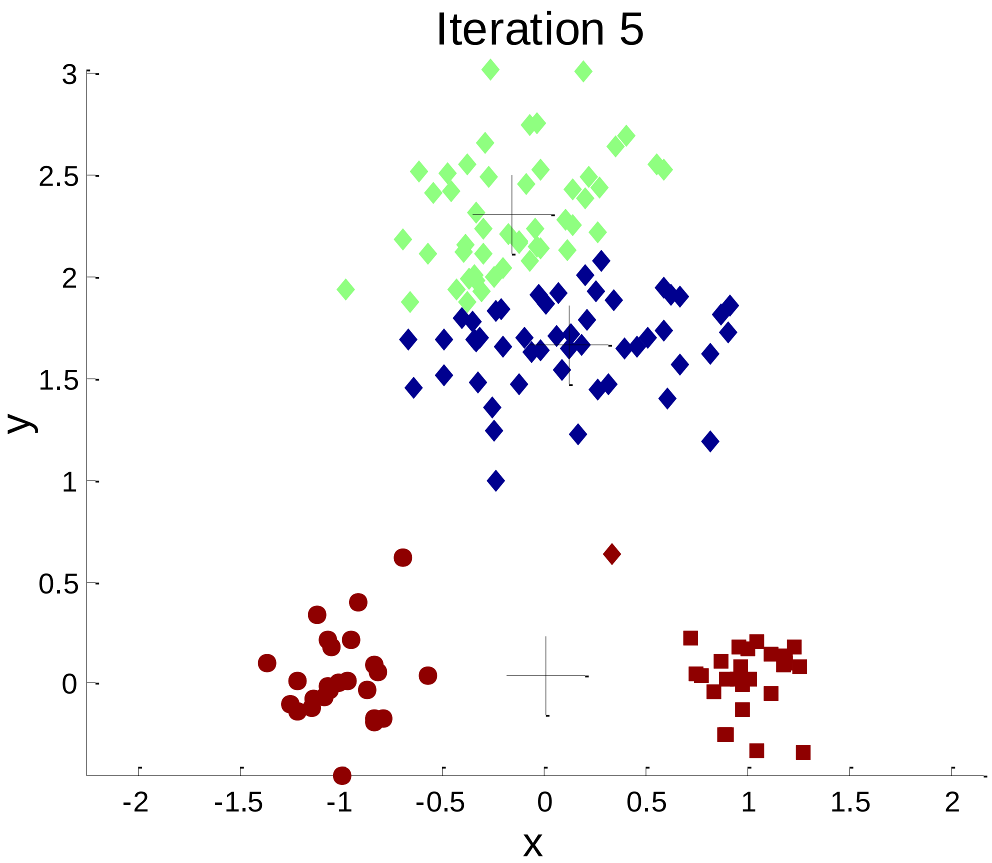
# Importance of Choosing Initial Centroids



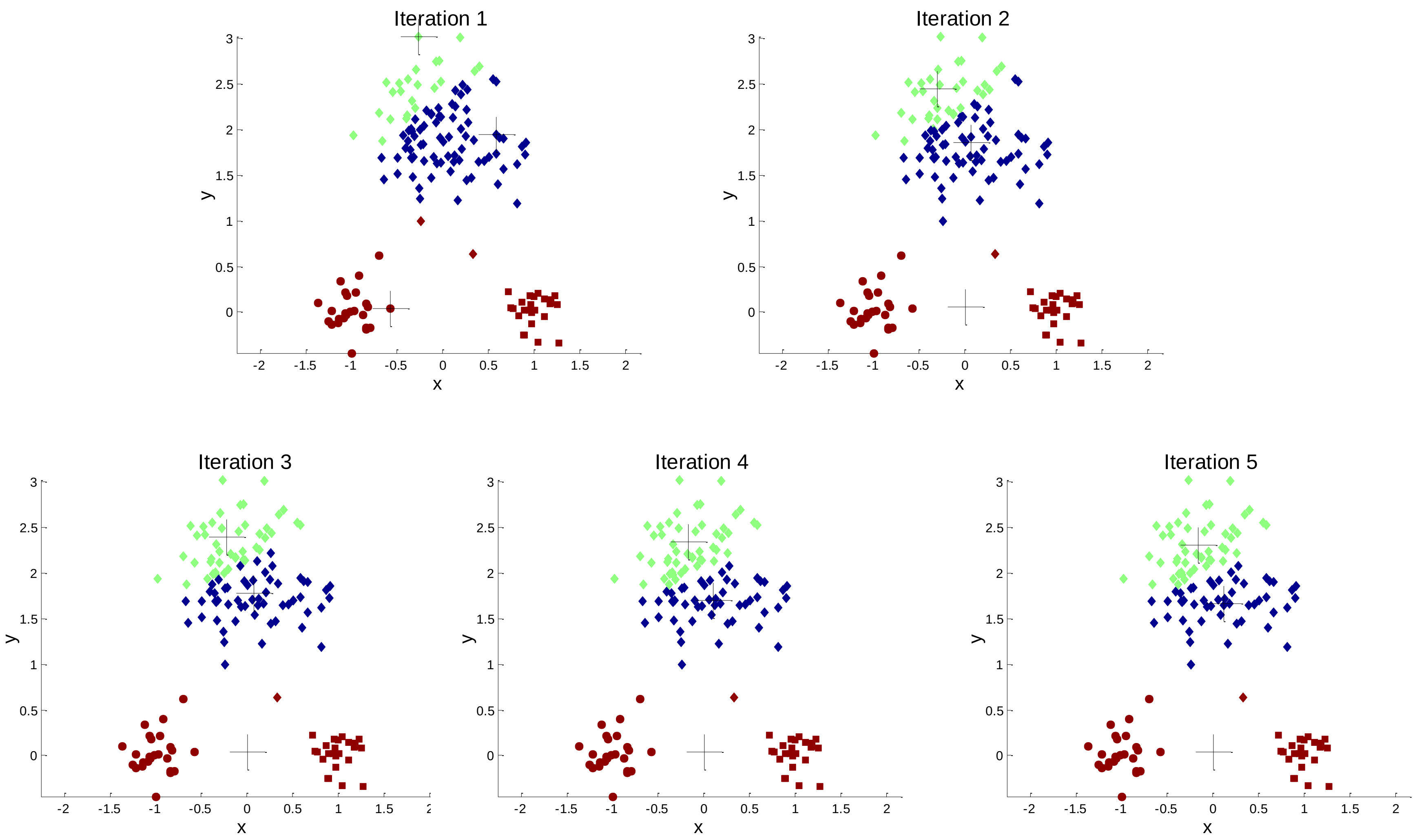
# Importance of Choosing Initial Centroids



# 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

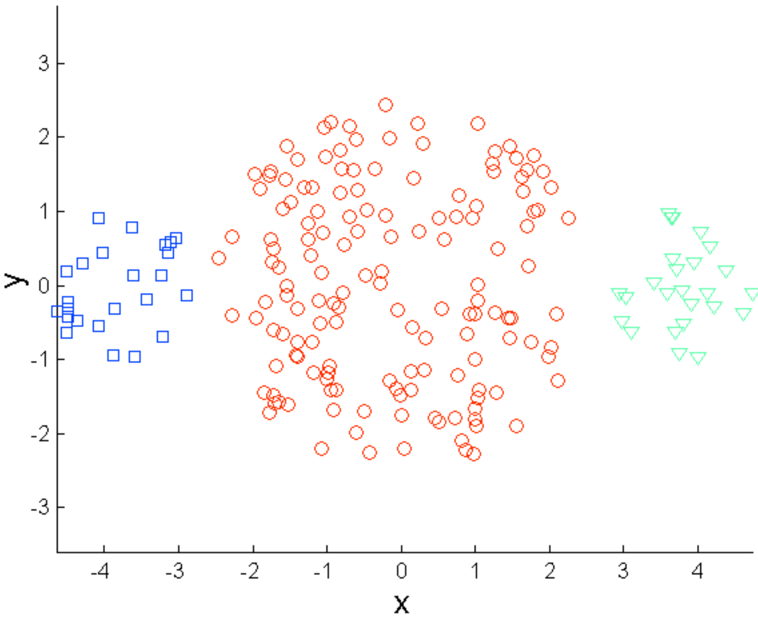
- K-means will converge for common similarity measures mentioned above.
  - Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is O( n * K * I * d )
  - n = number of points, K = number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

# Limitations of K-means

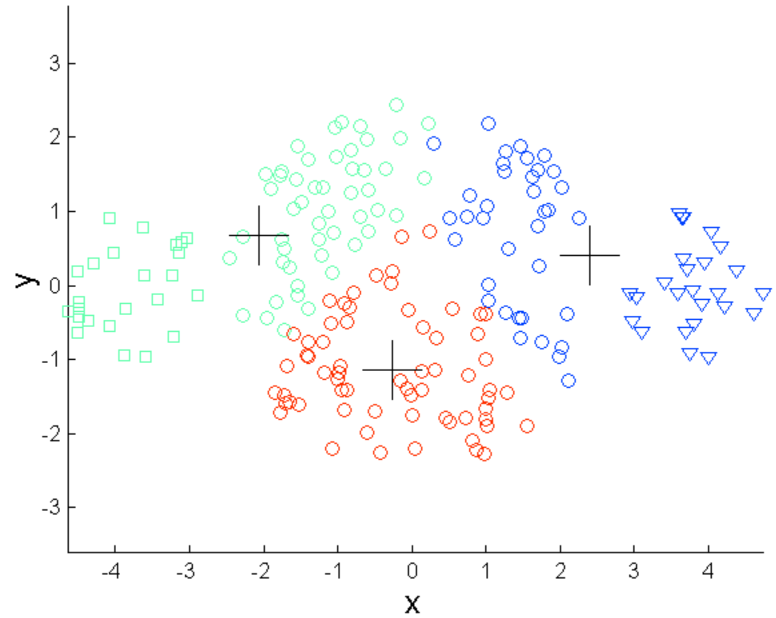
- K-means has problems when clusters are of different
  - Sizes
  - Densities
  - Non-globular shapes

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

# Limitations of K-means: Differing Sizes

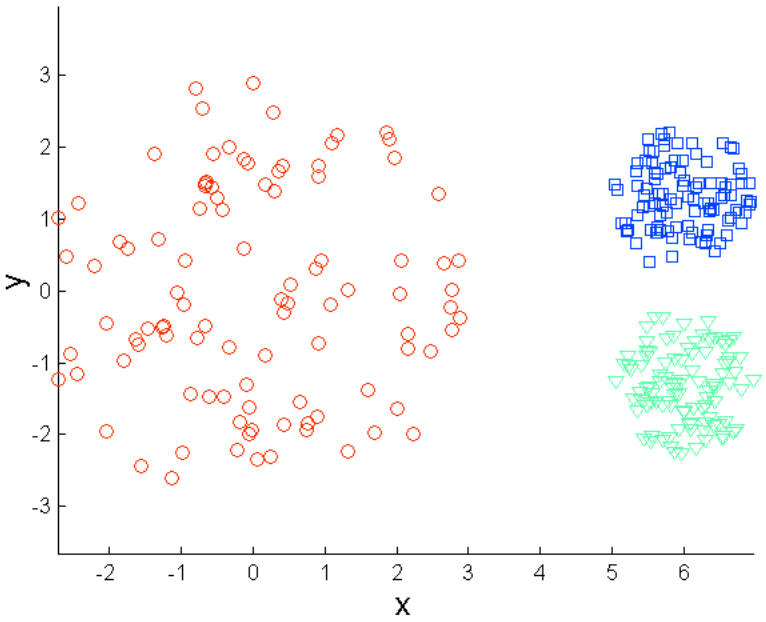



Original Points

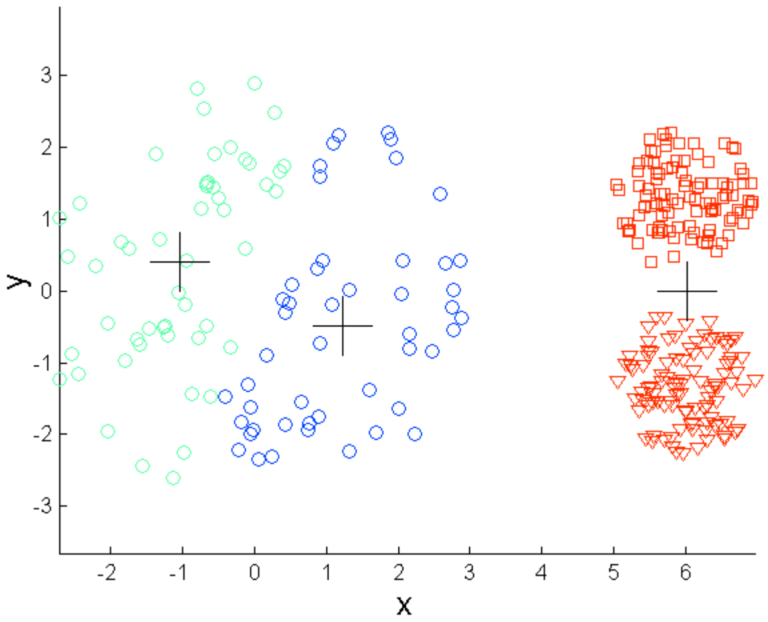



K-means (3 Clusters)

# Limitations of K-means: Differing Density

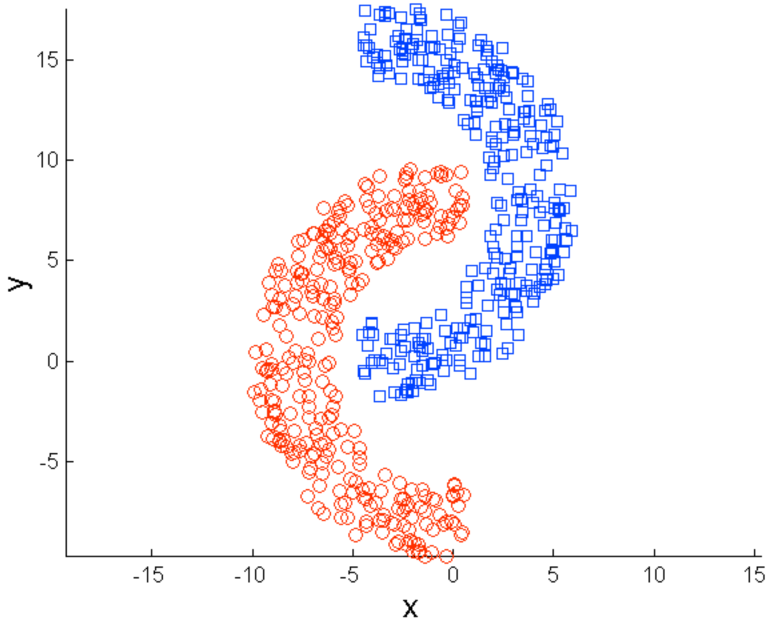



Original Points

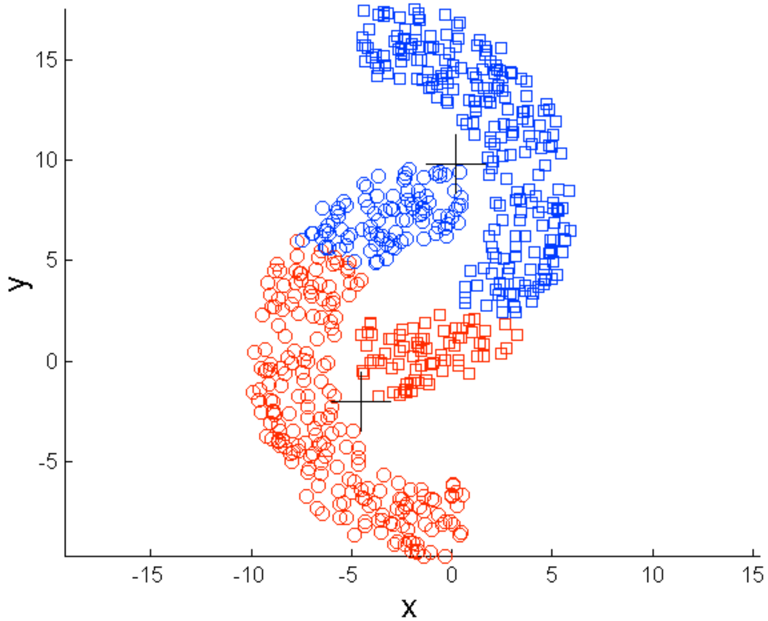



K-means (3 Clusters)

# Limitations of K-means: Non-globular Shapes

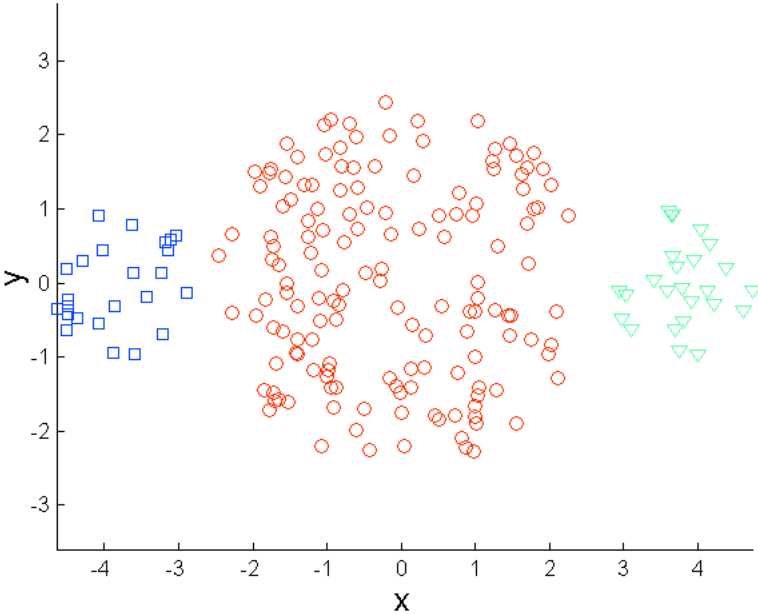



Original Points

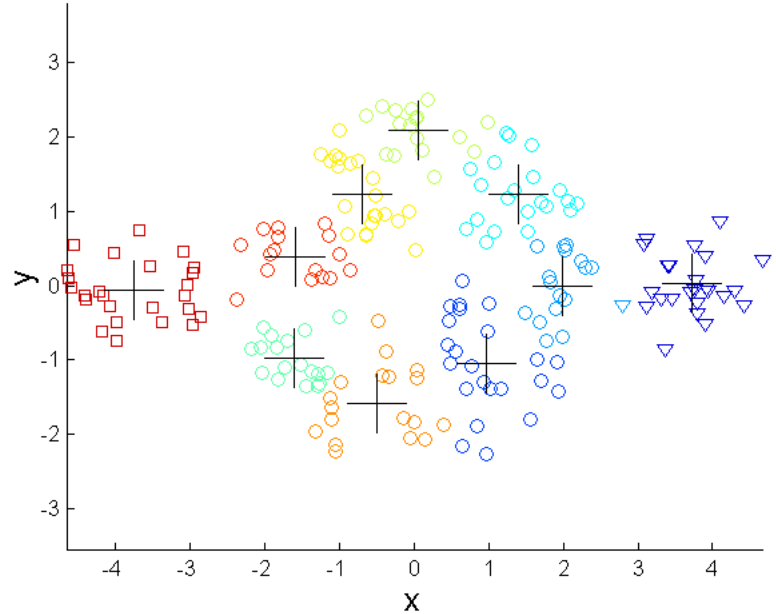



K-means (2 Clusters)

# Overcoming K-means Limitations




Original Points

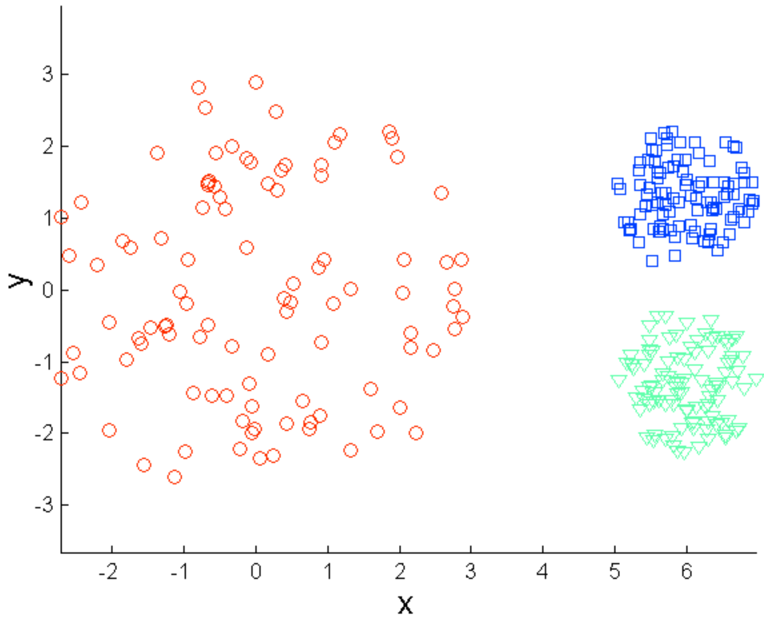



K-means Clusters

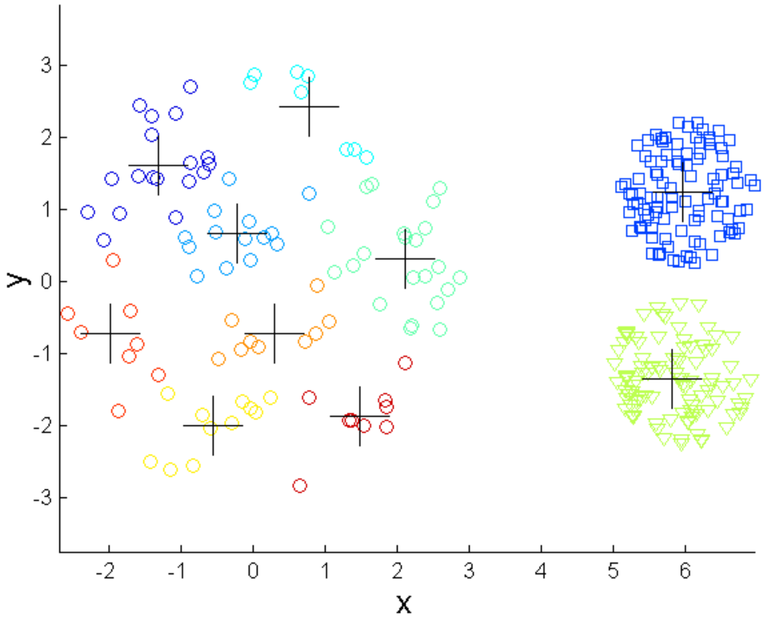
One solution is to use many clusters.

Find parts of clusters, but need to put together.

# Overcoming K-means Limitations

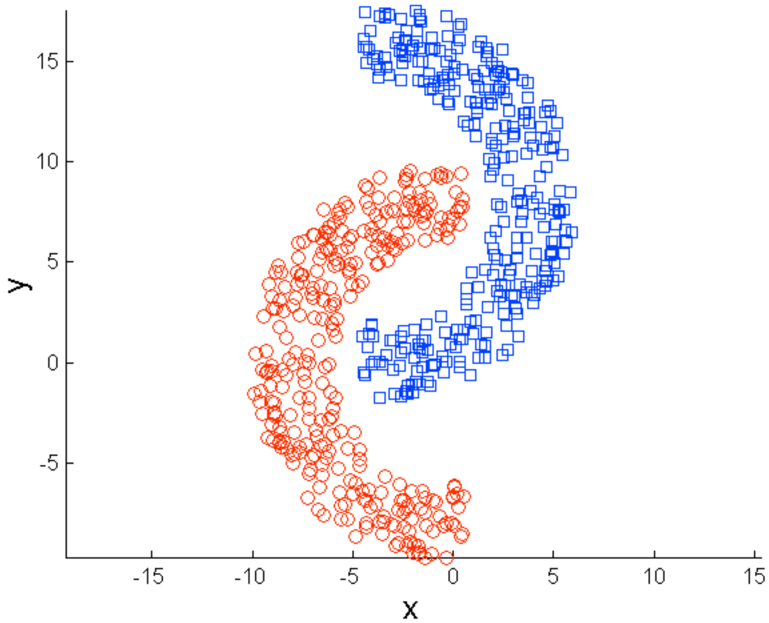


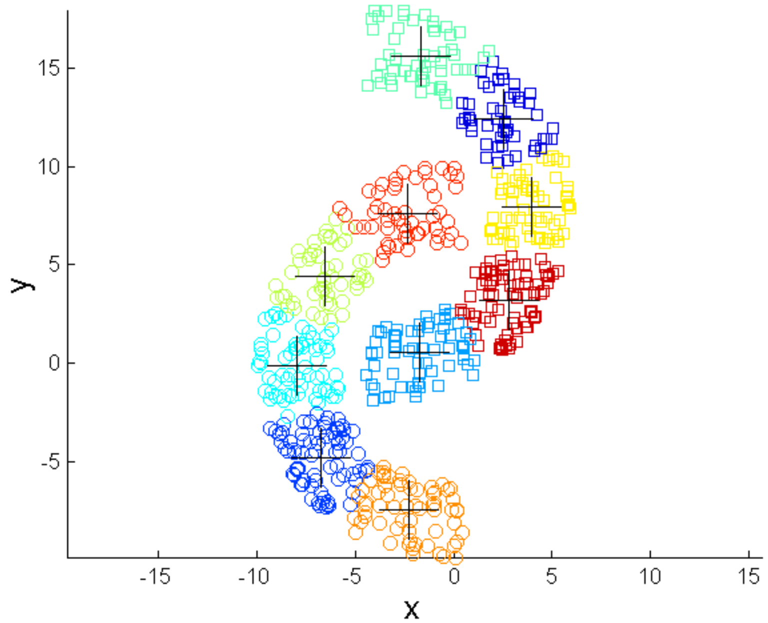

Original Points




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).

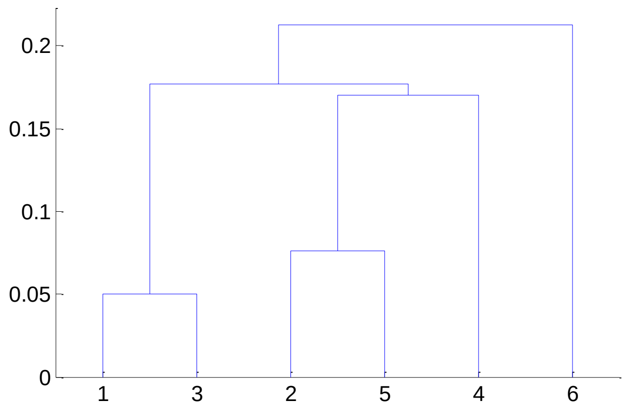
# HIERARCHICAL CLUSTERING

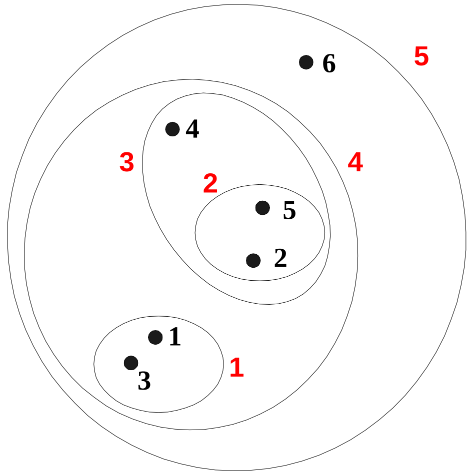
# Hierarchical Clustering

- 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 dendogram at the proper level

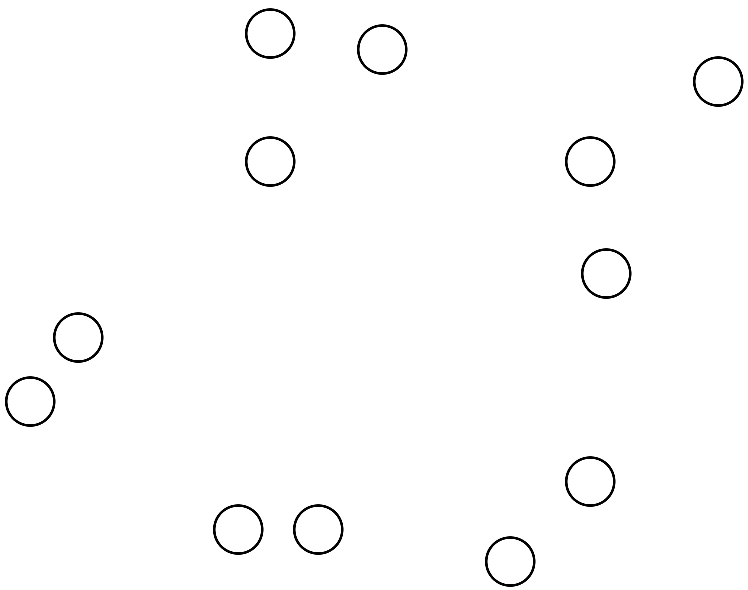
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

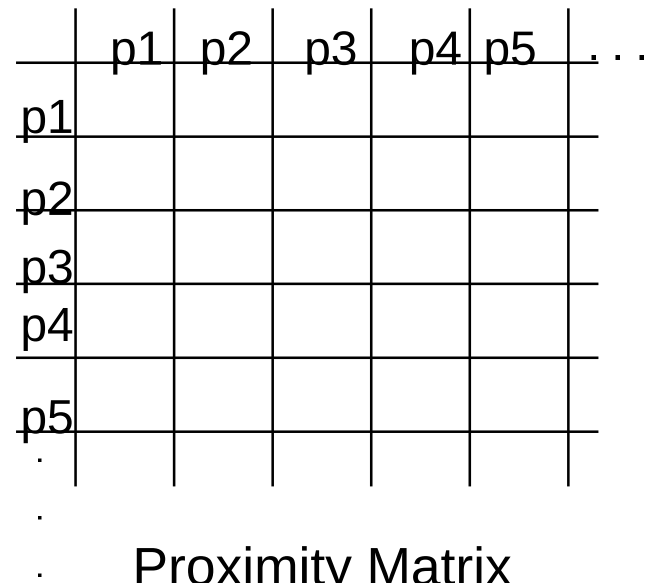
# Agglomerative Clustering Algorithm

- 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

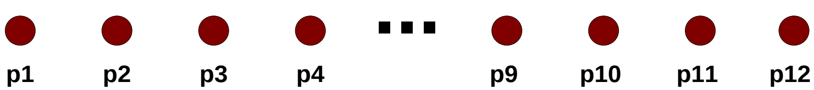
# Starting Situation

- Start with clusters of individual points and a proximity matrix



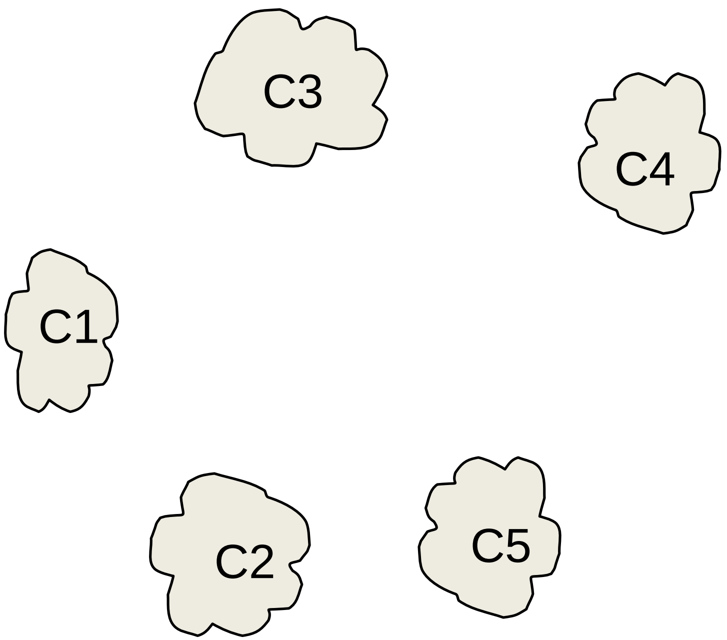



Proximity Matrix



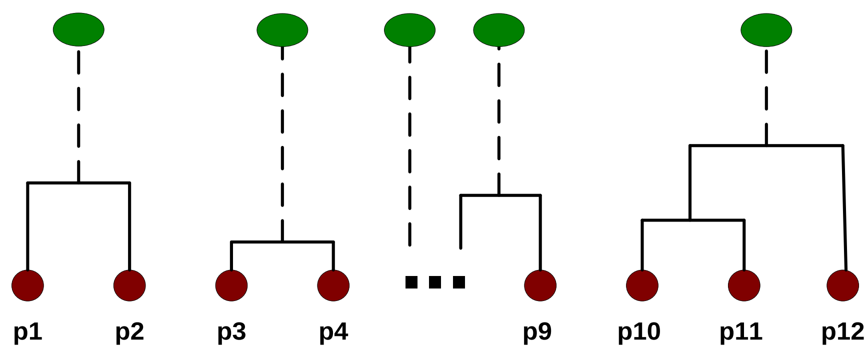
# Intermediate Situation

- After some merging steps, we have some clusters



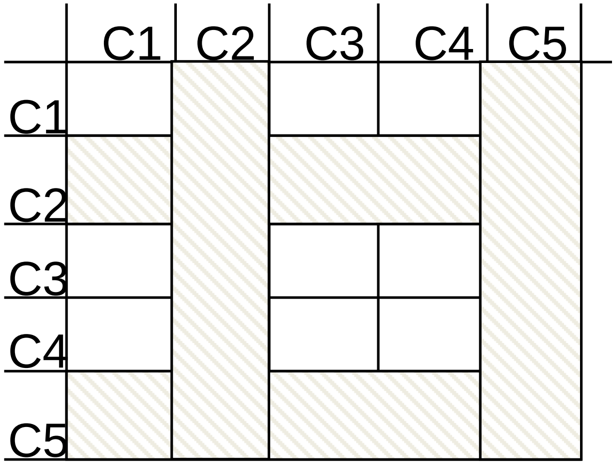

| | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| C1 | | | | | |
| C2 | | | | | |
| C3 | | | | | |
| C4 | | | | | |
| C5 | | | | | |

Proximity Matrix

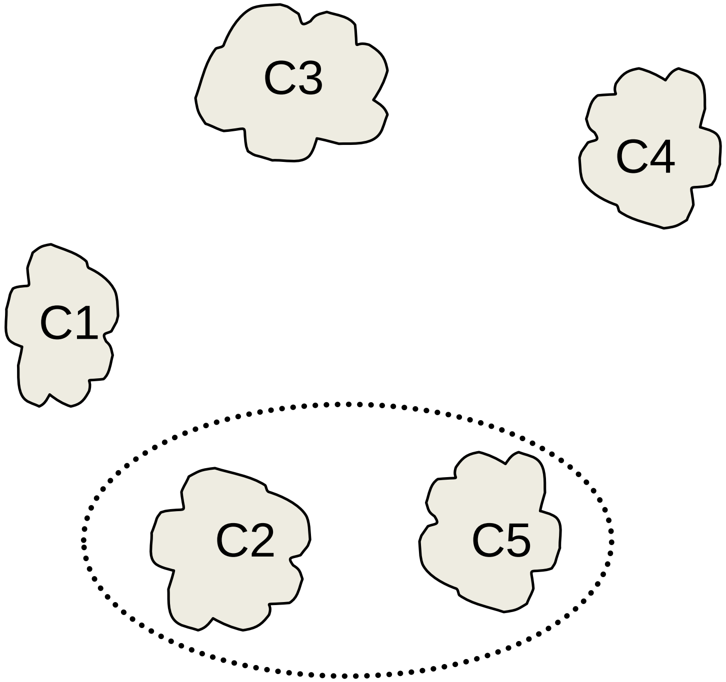


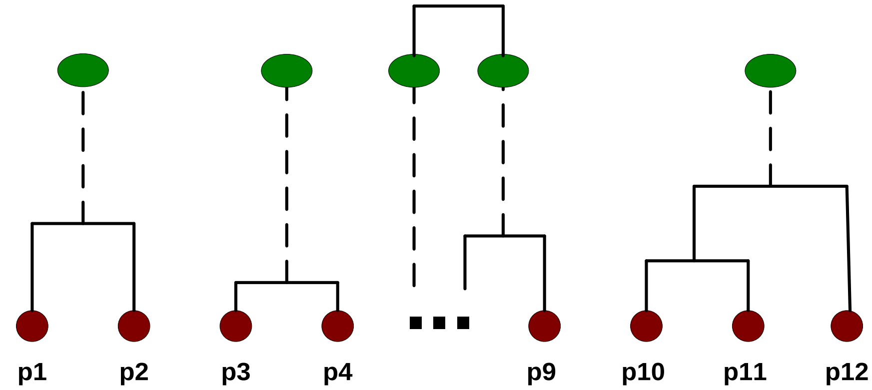
# Intermediate Situation

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




Proximity Matrix



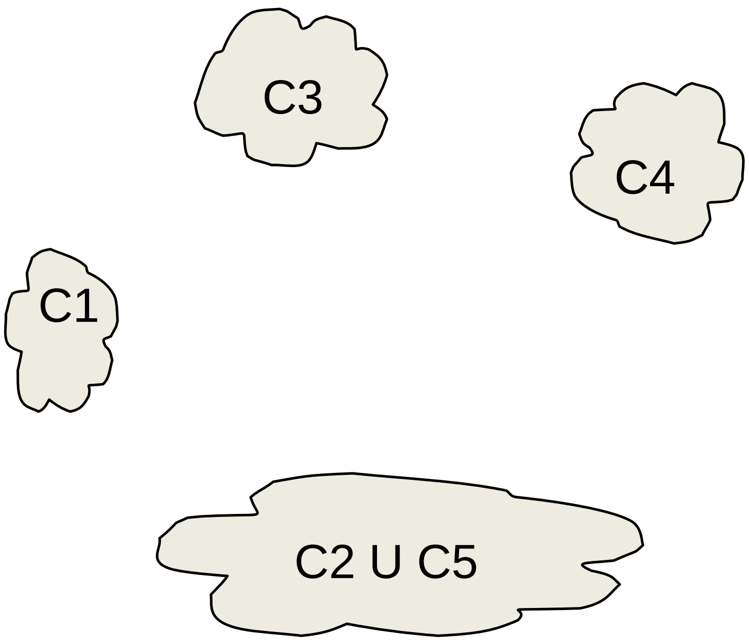



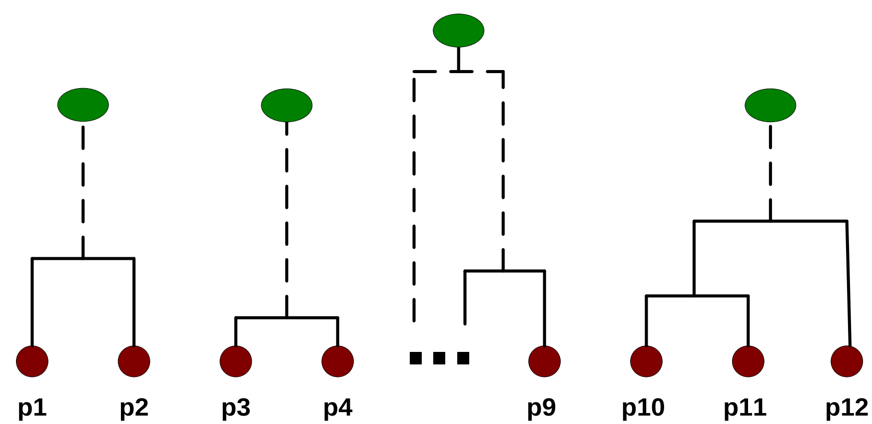
# After Merging

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

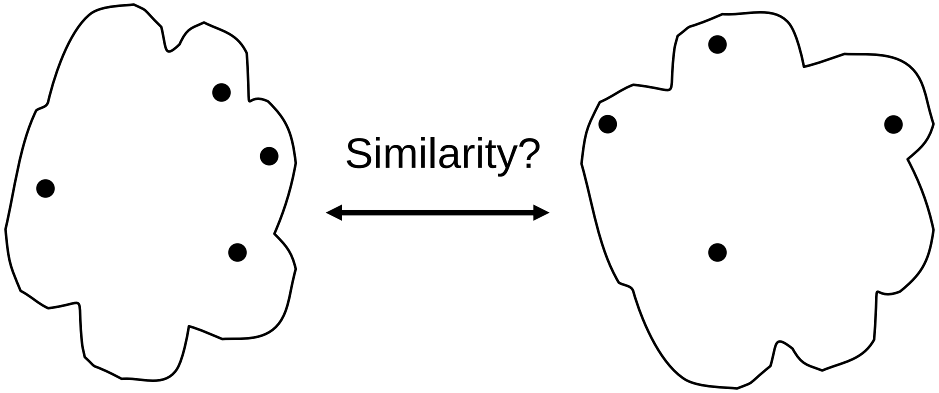
| | C1 | C2 U C5 | C3 | C4 |
|---|---|---|---|---|
| C1 | | ? | | |
| C2 U C5 | ? | ? | ? | ? |
| C3 | | ? | | |
| C4 | | ? | | |

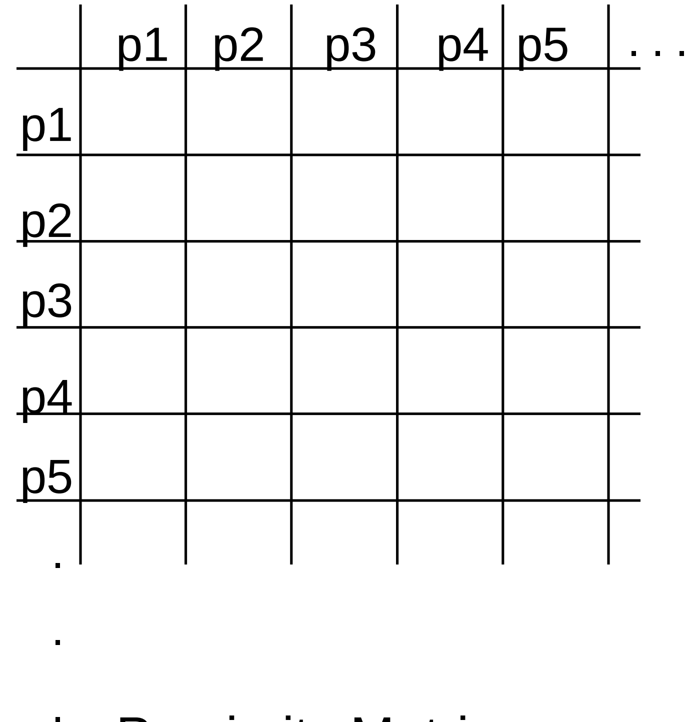
Proximity Matrix



# How to Define Inter-Cluster Similarity

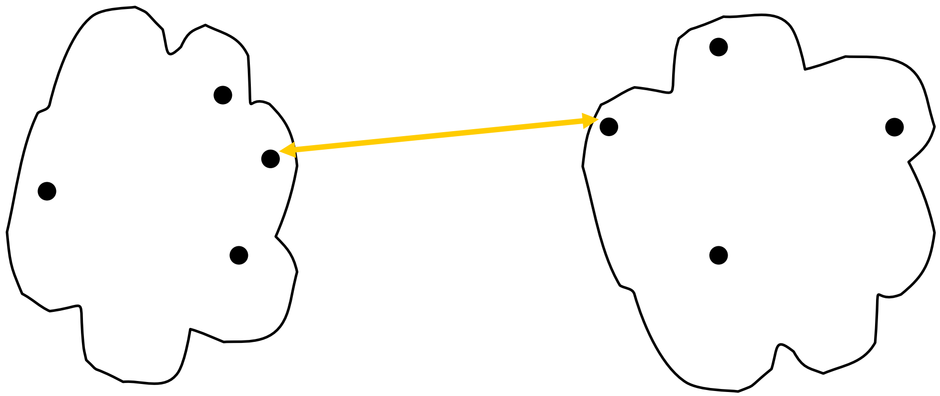



Proximity Matrix

- 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

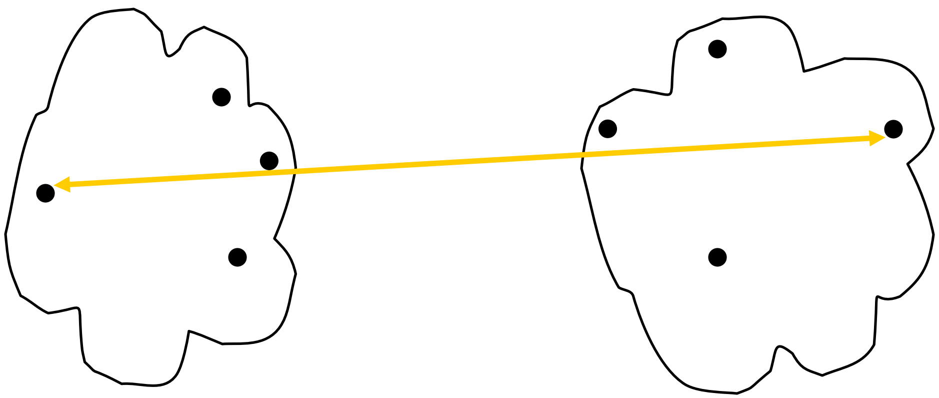


| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
| . | | | | | | |
| . | | | | | | |
| . | | | | | | |

Proximity Matrix

- MIN
- MAX
- 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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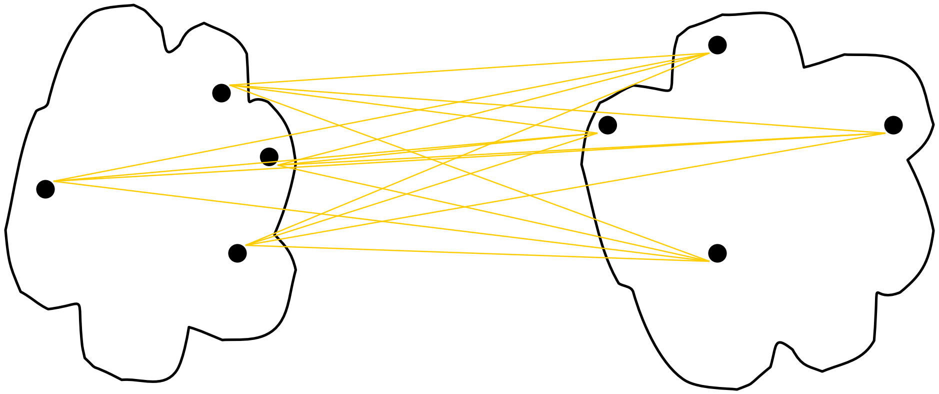

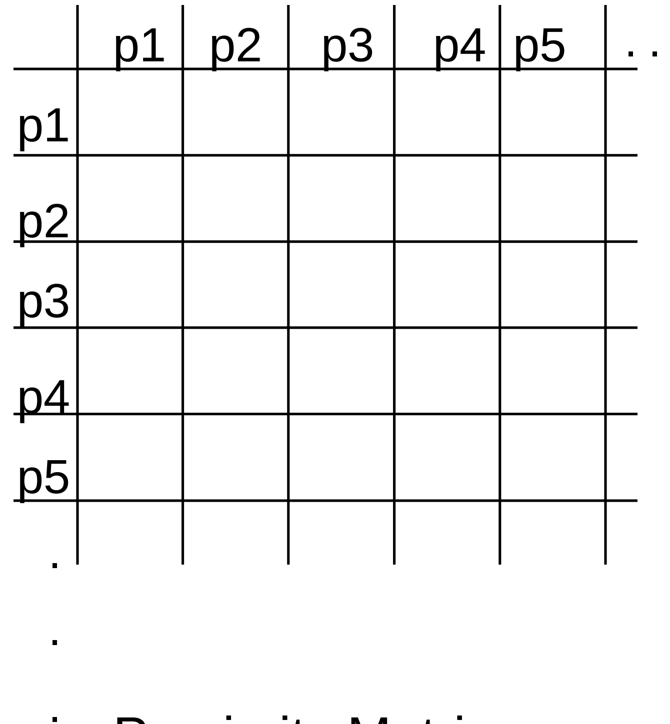


Proximity Matrix

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

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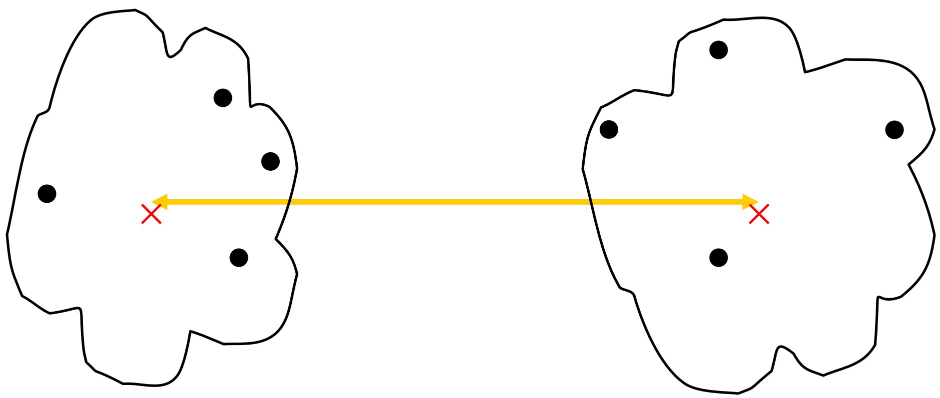


| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
| . | | | | | | |
| . | | | | | | |
| . | | | | | | |

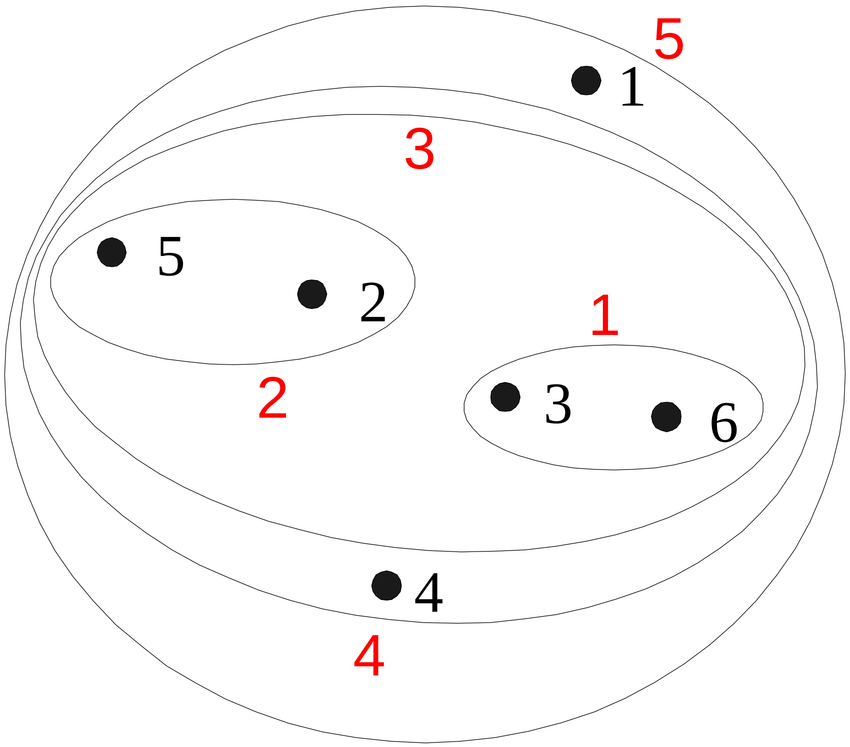
Proximity Matrix

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

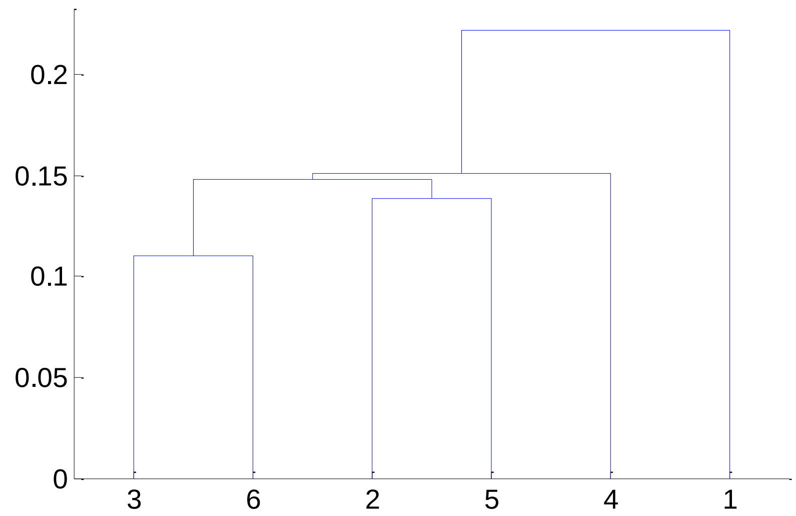
# Single Link – Complete Link

- Another way to view the processing of the hierarchical algorithm is that we create links between their 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



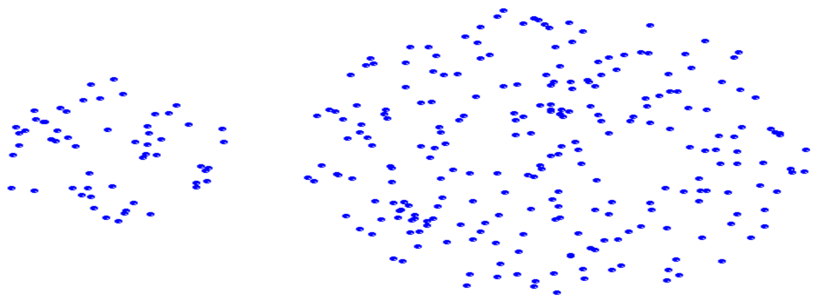

| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 0 | .24 | .22 | .37 | .34 | .23 |
| 2 | .24 | 0 | .15 | .20 | .14 | .25 |
| 3 | .22 | .15 | 0 | .15 | .28 | .11 |
| 4 | .37 | .20 | .15 | 0 | .29 | .22 |
| 5 | .34 | .14 | .28 | .29 | 0 | .39 |
| 6 | .23 | .25 | .11 | .22 | .39 | 0 |



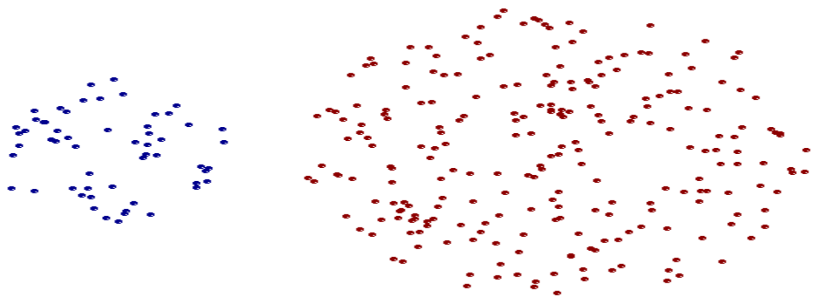

Nested Clusters

Dendrogram

# Strength of MIN



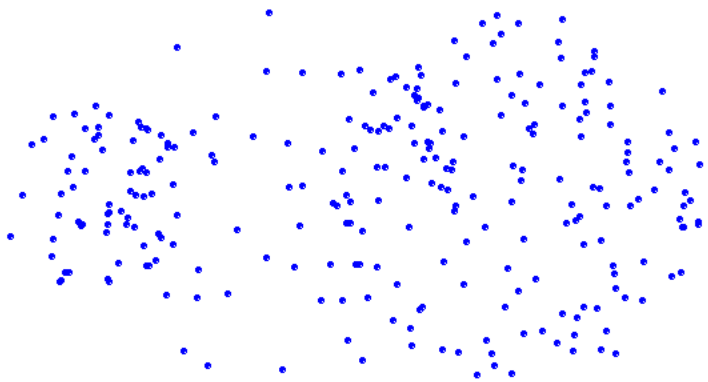
Original Points



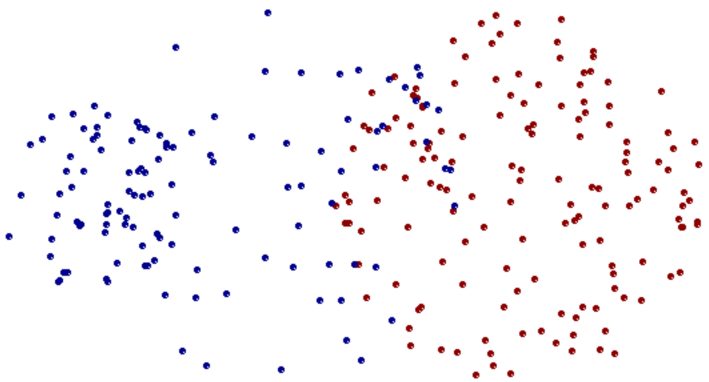
Two Clusters

- Can handle non-elliptical shapes

# Limitations of MIN



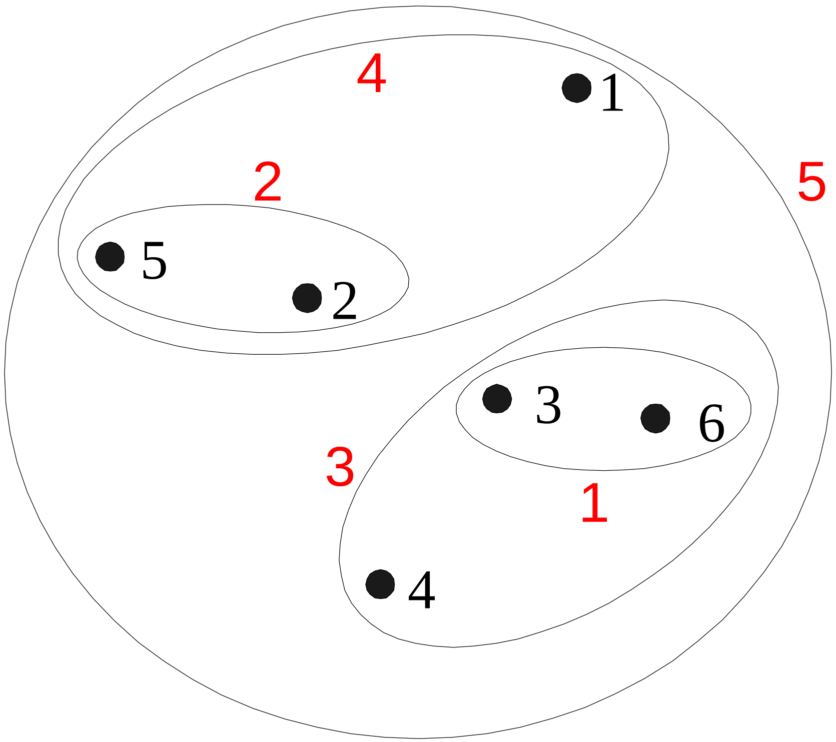
Original Points



Two Clusters

- Sensitive to noise and outliers

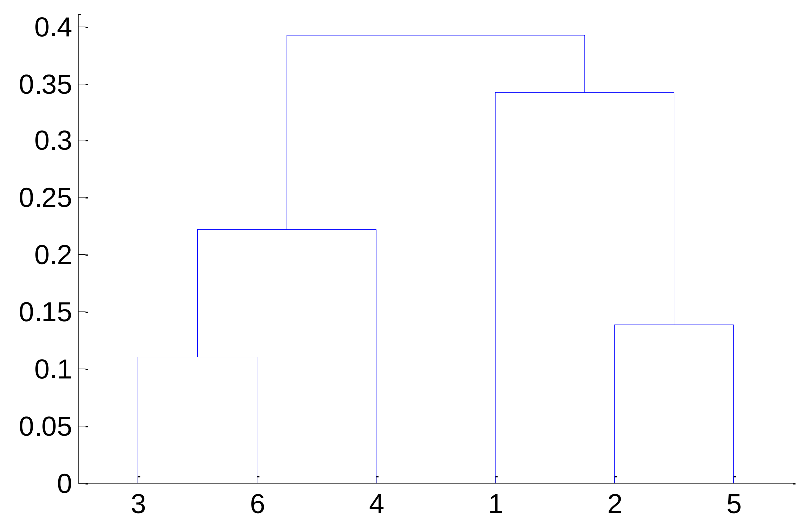
# Hierarchical Clustering: MAX



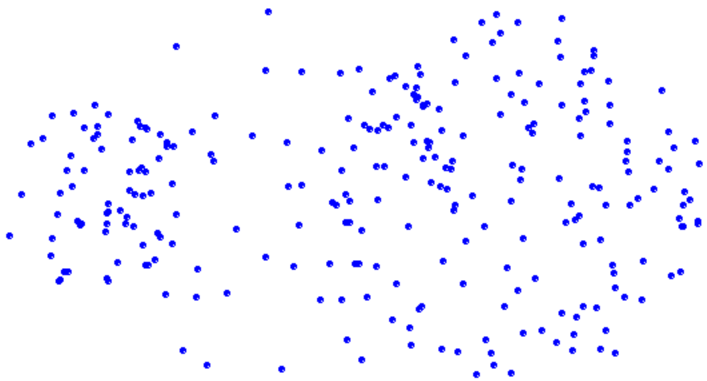

Nested Clusters

Dendrogram

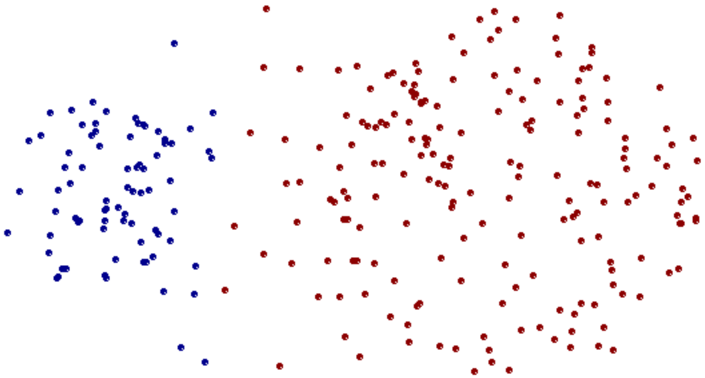
|   | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 0 | .24 | .22 | .37 | .34 | .23 |
| 2 | .24 | 0 | .15 | .20 | .14 | .25 |
| 3 | .22 | .15 | 0 | .15 | .28 | .11 |
| 4 | .37 | .20 | .15 | 0 | .29 | .22 |
| 5 | .34 | .14 | .28 | .29 | 0 | .39 |
| 6 | .23 | .25 | .11 | .22 | .39 | 0 |



# Strength of MAX



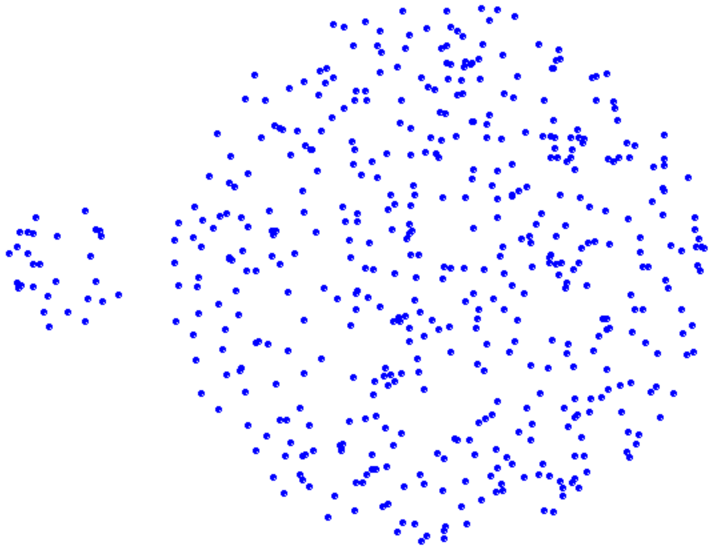
Original Points



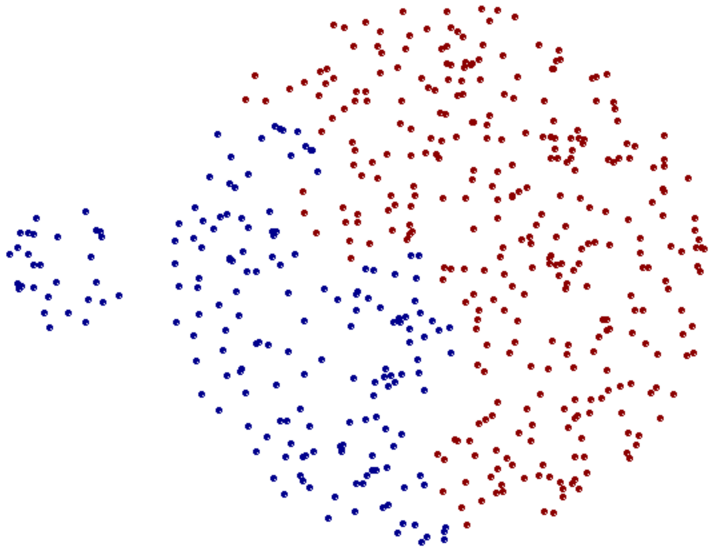
Two Clusters

- Less susceptible to noise and outliers

# Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

# Cluster Similarity: Group Average

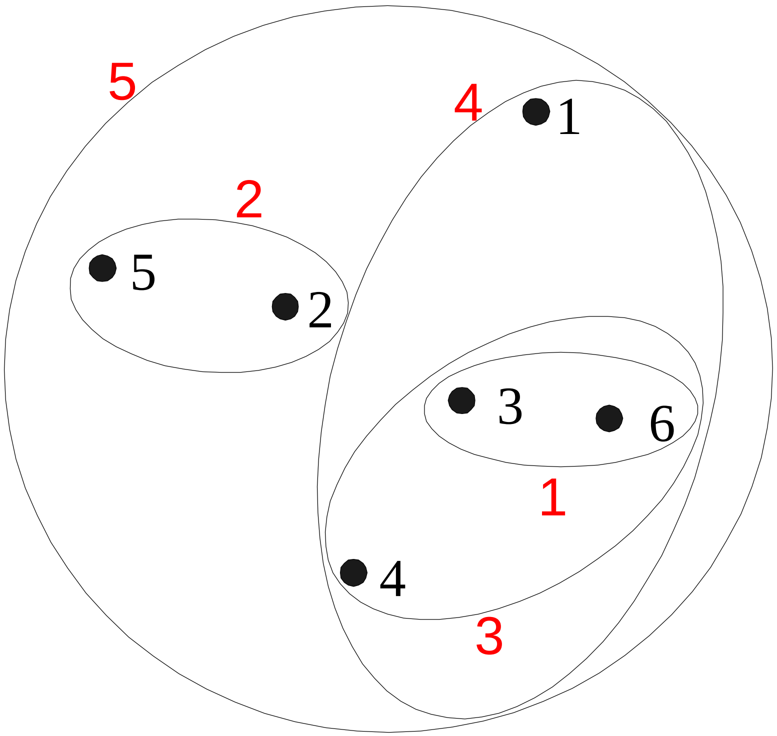
- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

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

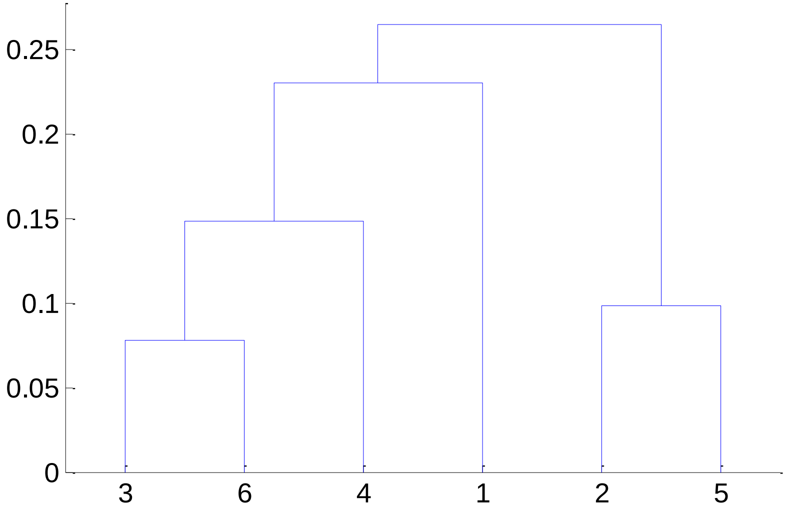
- Need to use average connectivity for scalability since total proximity favors large clusters

| | 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




| | 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

# Cluster Similarity: Ward's Method

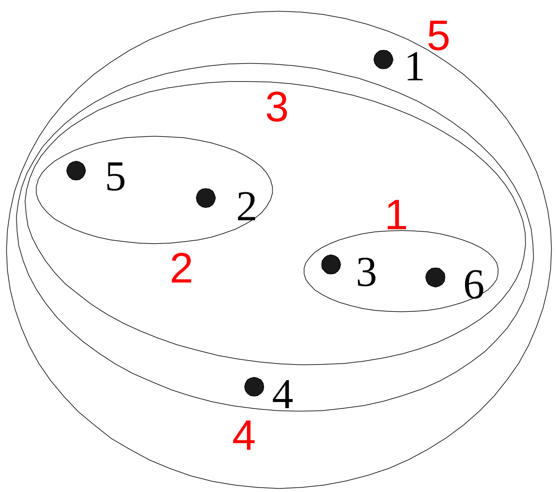
- Similarity of two clusters is based on the increase in squared error (SSE) when two clusters are merged
  - Similar to group average if distance between points is distance squared

- Less susceptible to noise and outliers

- Biased towards globular clusters

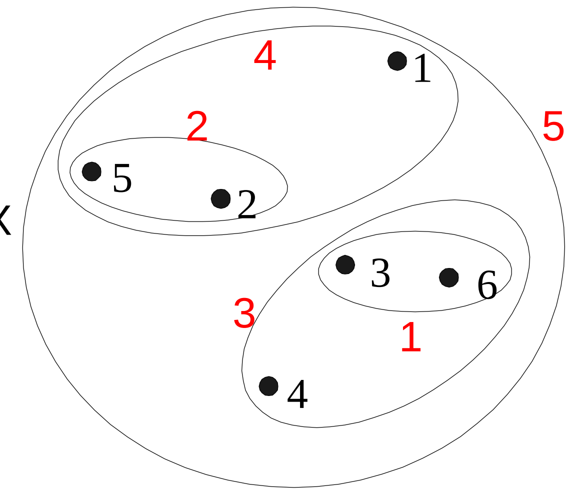
- Hierarchical analogue of K-means
  - Can be used to initialize K-means

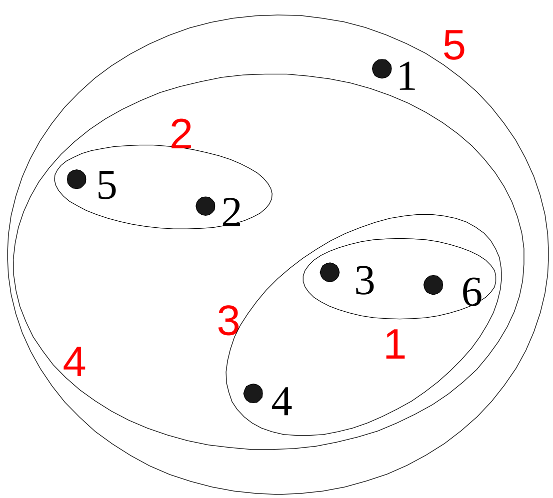
# Hierarchical Clustering: Comparison




MIN

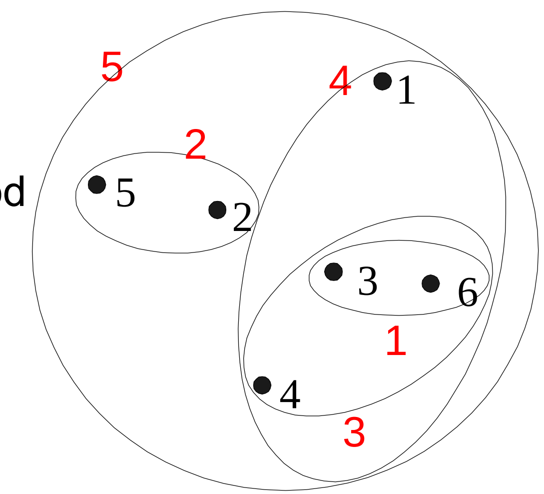
MAX




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
  - 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.

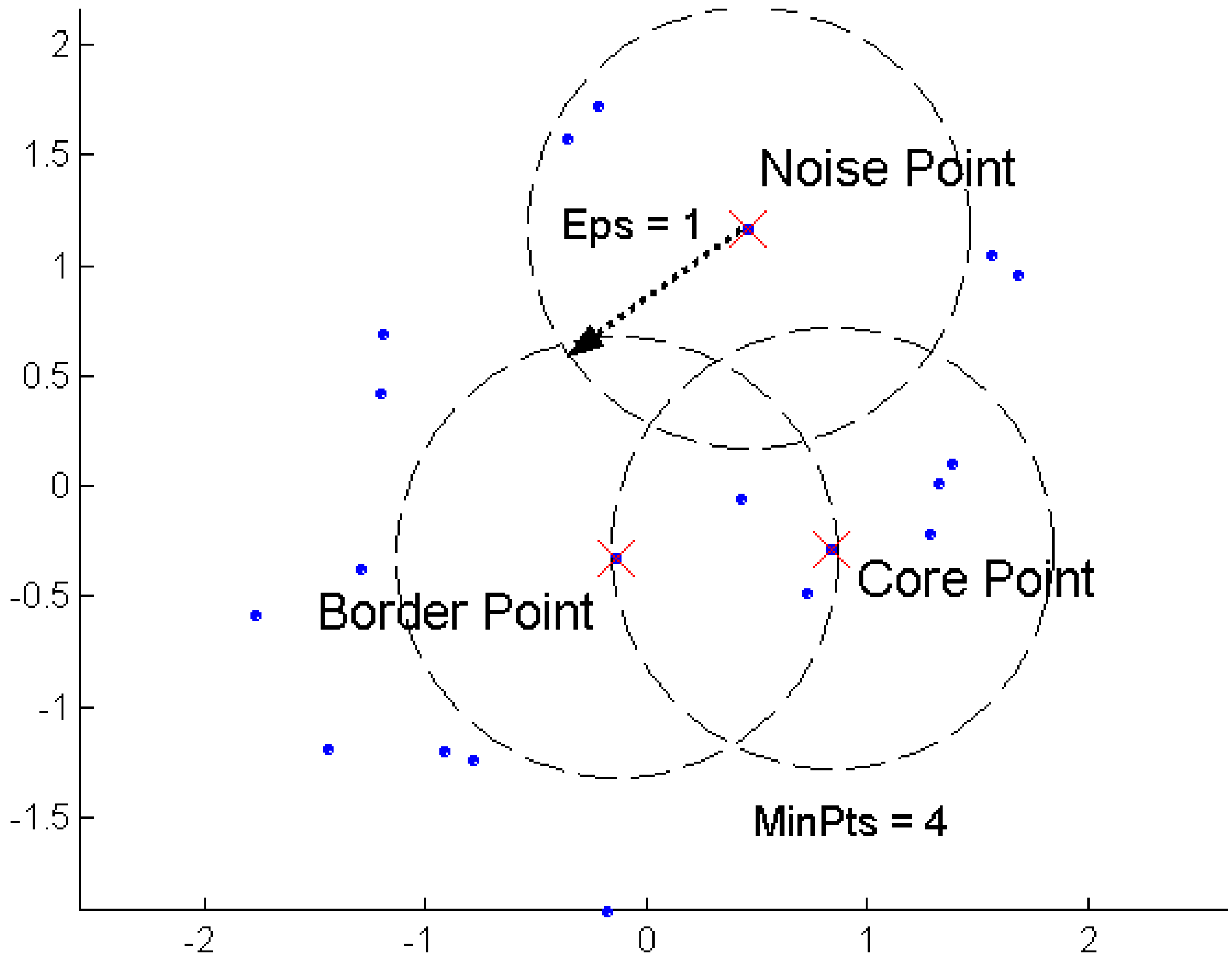
- Important Questions:
  - How do we measure density?
  - What is a dense region?

- 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

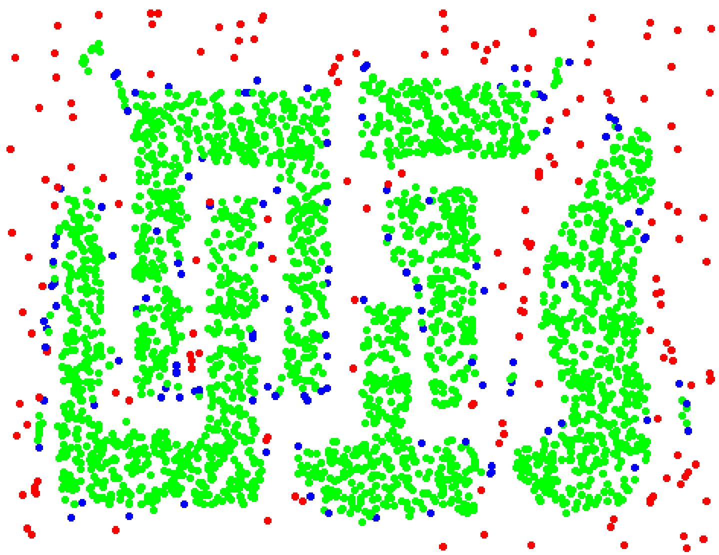
- Characterization of points
  - A point is a core point if it has more than a specified number of points (MinPts) within Eps
    - These points belong in a dense region and are at the interior of a cluster
  - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.
  - 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

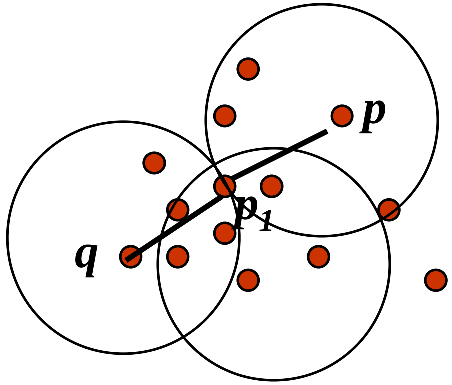


Point types: core, border and noise

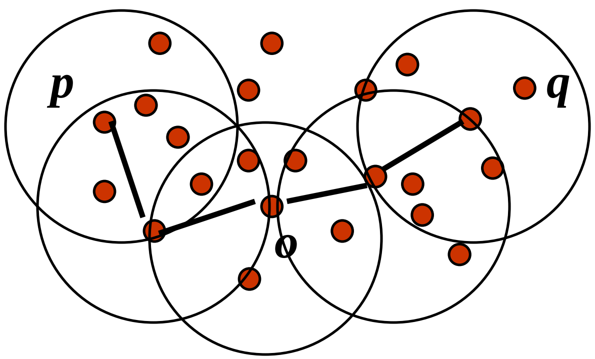
Eps = 10, MinPts = 4

# 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

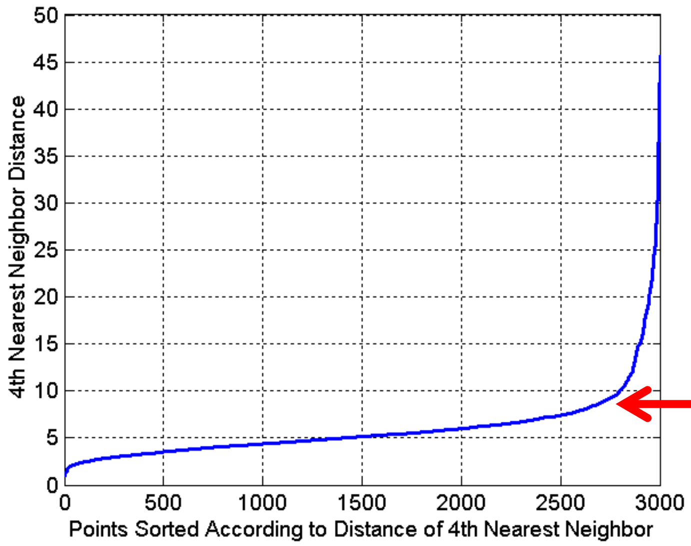


# DBSCAN Algorithm

- 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

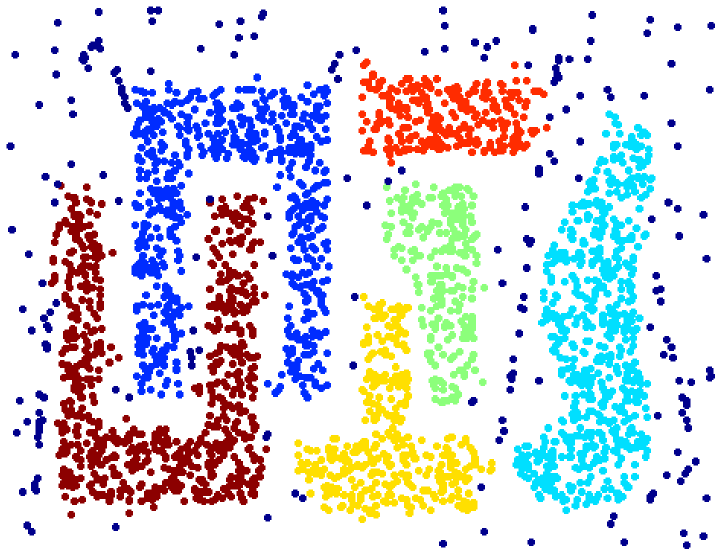
- Idea is that for points in a cluster, their $k^{th}$ nearest neighbors are at roughly the same distance
- Noise points have the $k^{th}$ nearest neighbor at farther distance
- So, plot sorted distance of every point to its $k^{th}$ nearest neighbor
- Find the distance d where there is a "knee" in the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




Eps ~ 7-10
MinPts = 4

# When DBSCAN Works Well

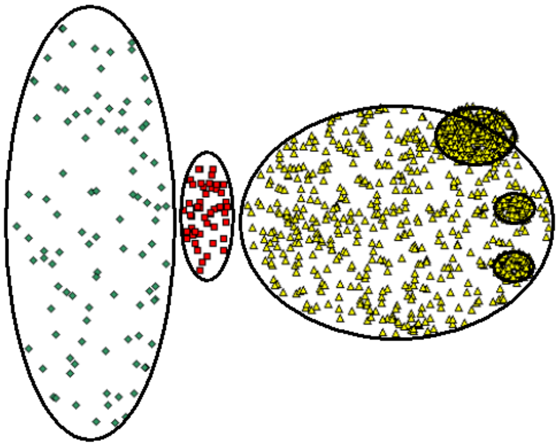
Original Points



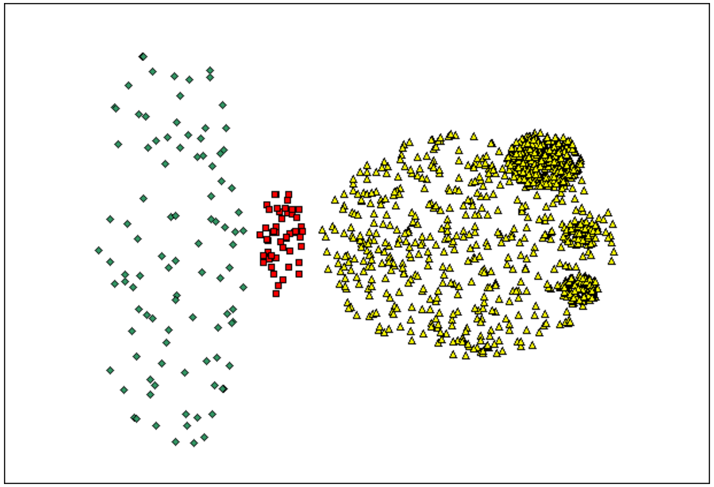
Clusters

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

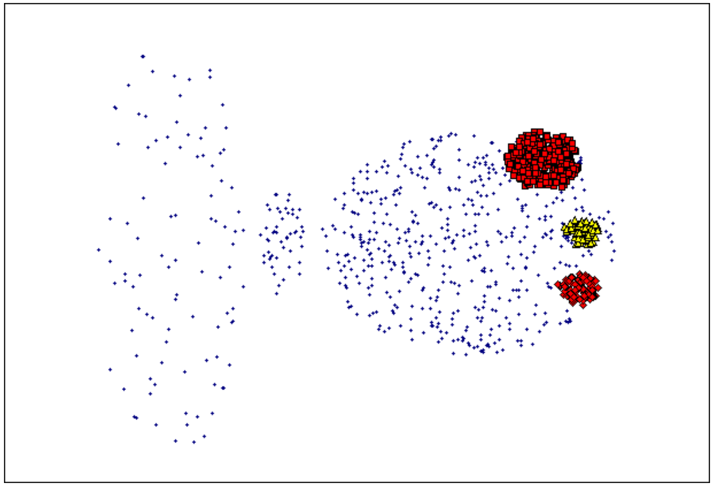
# When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

- Varying densities
- High-dimensional data

# DBSCAN: Sensitive to Parameters

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

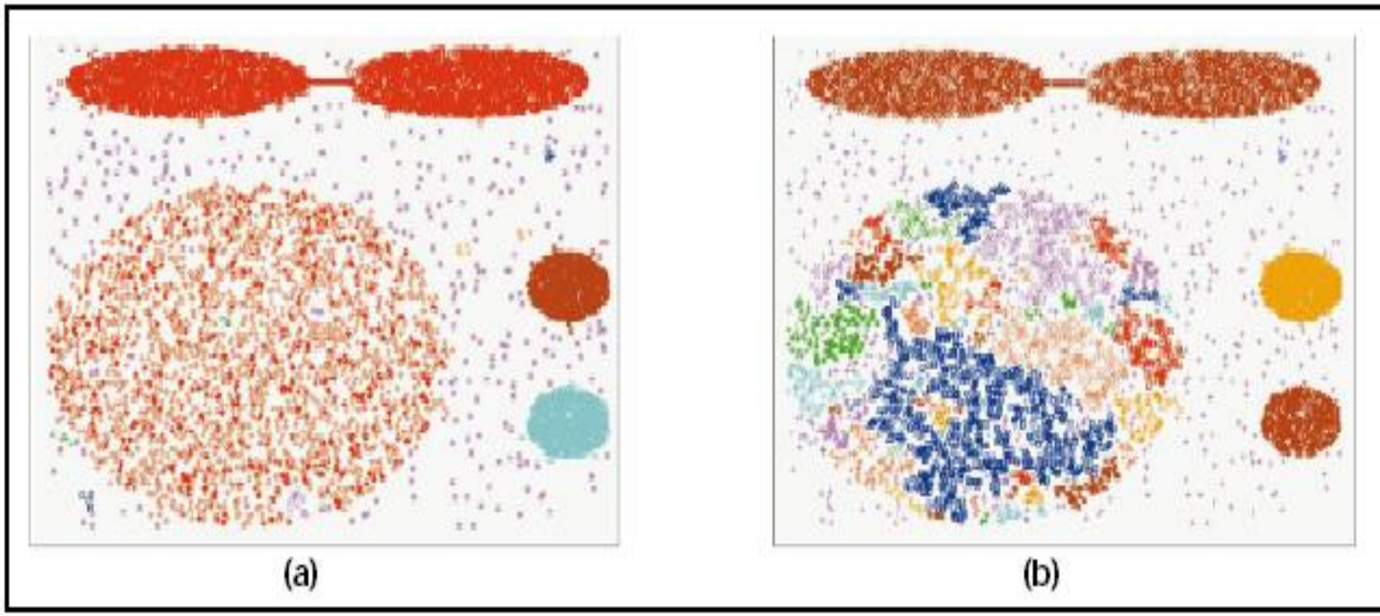
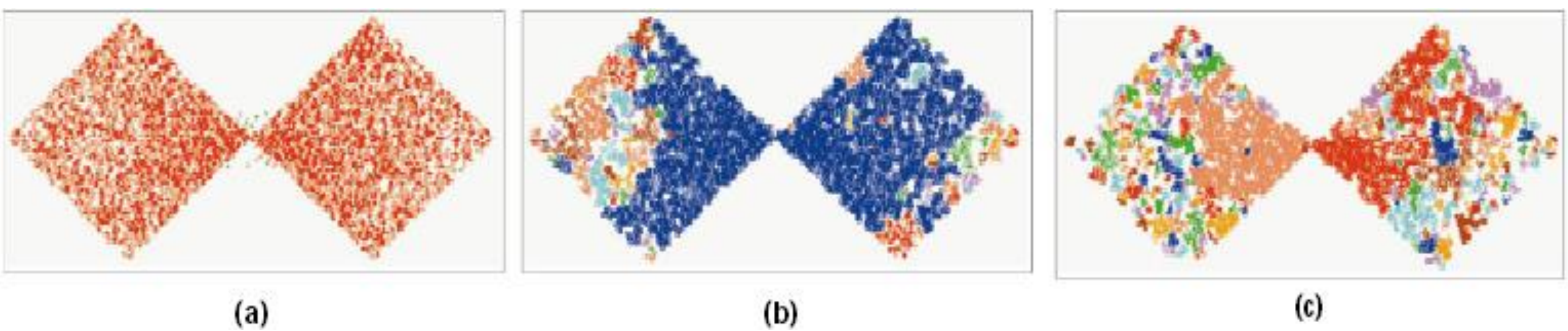



*Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.*



# 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