CLUSTERING

Sanjay Ranka
Distinguished Professor
Department of Computer and Information Science and Engineering
www.sanjayranka.com
sanjayranka@gmail.com
352 514 4213

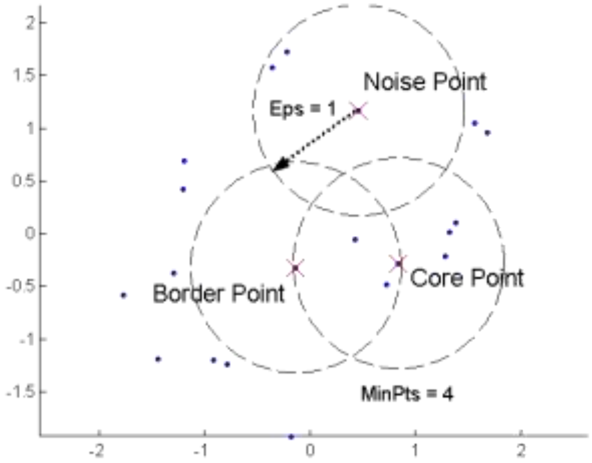
1

DBSCAN

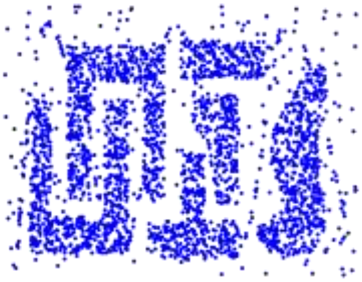
- DBSCAN is a density based clustering algorithm
- Density = number of points within a specified radius (*Eps*)
- A point is a *core point* if it has more than specified number of points (*MinPts*) within *Eps*
  - Core point is in the interior of a cluster
- A *border point* has fewer than *MinPts* within *Eps* but is in neighborhood of a core point
- A *noise point* is any point that is neither a core point nor a border point

2

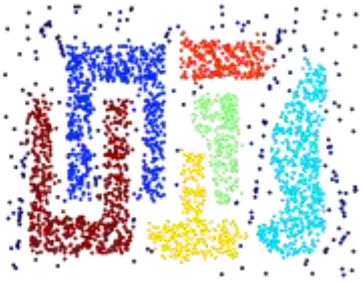
DBSCAN: Core, Border and Noise points



When DBSCAN works well

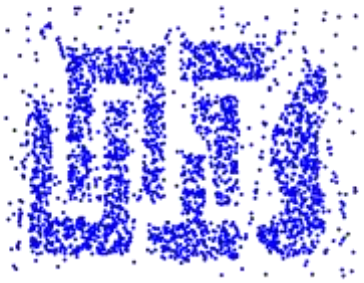


Original Dataset

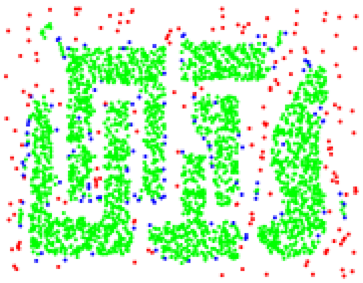


Clusters found by DBSCAN

DBSCAN: Core, Border and Noise points



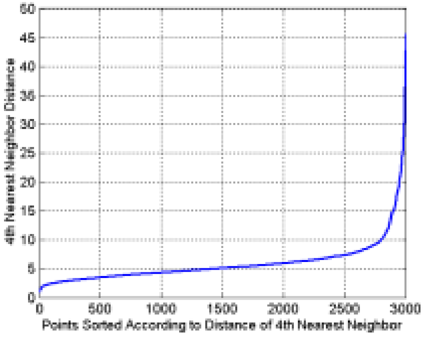
Original Points



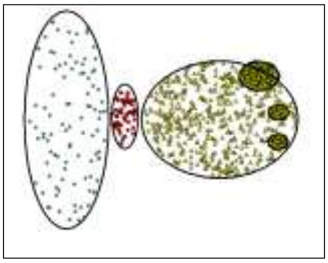
Eps = 10, Minpts = 4
Point types:
Core
Border
Noise

DBSCAN: Determining Eps and MinPts

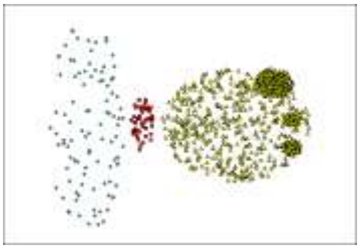
- Idea is that for points in a cluster, there k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor. (k=4 used for 2D points)



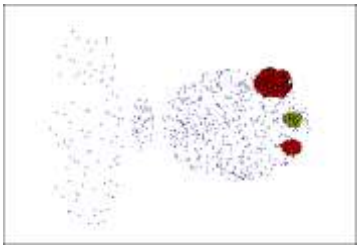
Where DBSCAN doesn’t work well



Original Points



Minpts = 4, Eps = 9.75

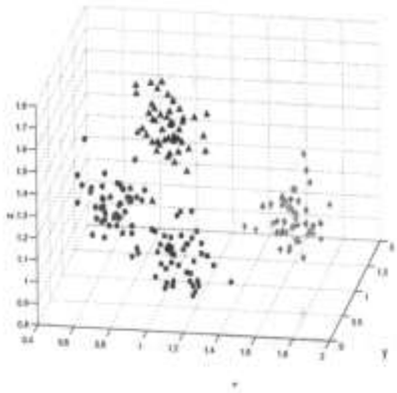


MinPts = 4, Eps = 9.92

Subspace clustering

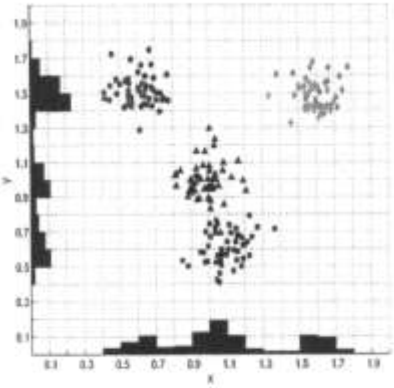
- Instead of using all the attributes (features) of a dataset, if we consider only subset of the features (subspace of the data), then the clusters that we find can be quite different from one subspace to another
- The clusters we find depend on the subset of the attributes that we consider

Subspace clustering



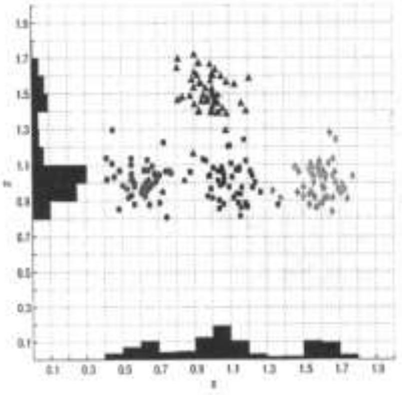
(a) Four clusters in three dimensions.

Subspace clustering



(b) View in the XY plane.

Subspace Clustering

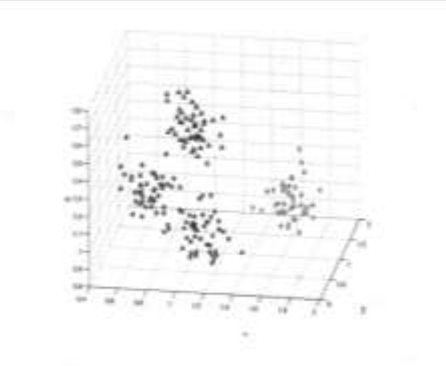


(c) View in the XZ plane.

CLIQUE

- CLIQUE is a grid based clustering algorithm
- CLIQUE splits each dimension (attribute) in to a fixed number (ξ) of equal length intervals. This partitions the data space in to rectangular *units* of equal volume
- We can measure the density of each unit by the fraction of points it contains
- A unit is considered dense if its density > user specified threshold τ
- A cluster is a group of contiguous (touching) dense units

CLIQUE: Example



(a) Four clusters in three dimensions.

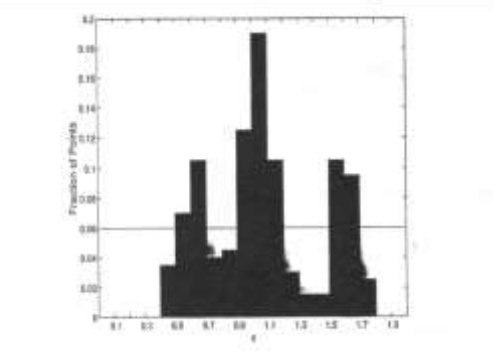


Figure 5.36. Histogram showing distribution of points for the X attribute.

CLIQUE

- CLIQUE starts by finding all the dense areas in the one dimensional spaces associated with each attribute
- Then it generates the set of two dimensional cells that might possibly be dense by looking at pairs of dense one dimensional cells
- In general, CLIQUE generates the possible set of k-dimensional cells that might possibly be dense by looking at dense (k-1)-dimensional cells. This is similar to APRIORI algorithm for finding frequent item sets
- It then finds clusters finds clusters by taking union of all adjacent high density cells

MAFIA

- Merging of Adaptive Finite Intervals (MAFIA) is a modification of CLIQUE that runs faster and finds better quality clusters.
- The main modification over CLIQUE is the use of an adaptive grid
- Initially each dimension is partitioned into a large number of intervals. A histogram is generated that shows the number of data points in each interval
- Groups of adjacent intervals are grouped in to windows, and the maximum number of points in the window's intervals becomes the value associated with the window

MAFIA

- Adjacent windows are grouped together if the values of the two windows are close
- As a special case, if all windows are combined into one window, the dimensions is partitioned in to a fixed number of cells and the threshold for being considered a dense unit is increased for that dimension

Limitations of CLIQUE and MAFIA

- Time complexity is exponential in the number of dimensions
- Will have difficulty if “too many” dense units are generated at lower stages
- May fail if clusters are of widely differing densities, since the threshold is fixed
- Determining the appropriate τ and ξ for a variety of data sets can be challenging
- It is not typically possible to find all clusters using the same threshold

Clustering Scalability for Large Datasets

- One very common solution is sampling, but the sampling could miss small clusters.
    - Data is sometimes not organized to make valid sampling easy or efficient.
- Another approach is to compress the data or portions of the data.
    - Any such approach must ensure that not too much information is lost. (*Scaling Clustering Algorithms to Large Databases*, Bradley, Fayyad and Reina.)

Scalable Clustering: BIRCH

- BIRCH (Balanced and Iterative Reducing and Clustering using Hierarchies)
  - BIRCH can efficiently cluster data with a single pass and can improve that clustering in additional passes.
  - Can work with a number of different distance metrics.
  - BIRCH can also deal effectively with outliers.

Scaleable Clustering: BIRCH

- BIRCH is based on the notion of a clustering feature (CF) and a CF tree.
- A cluster of data points (vectors) can be represented by a triplet of numbers
  - (N, LS, SS)
  - N is the number of points in the cluster
  - LS is the linear sum of the points
  - SS is the sum of squares of the points.
- Points are processed incrementally.
  - Each point is placed in the leaf node corresponding to the “closest” cluster (CF).
  - Clusters (CFs) are updated.

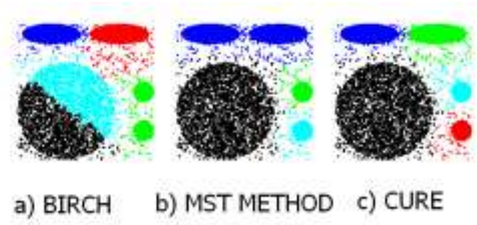
Scalable Clustering: BIRCH

- Basic steps of BIRCH
  - Load the data into memory by creating a CF tree that “summarizes” the data.
  - Perform global clustering.
    - Produces a better clustering than the initial step.
    - An agglomerative, hierarchical technique was selected.
  - Redistribute the data points using the centroids of clusters discovered in the global clustering phase, and thus, discover a new (and hopefully better) set of clusters.

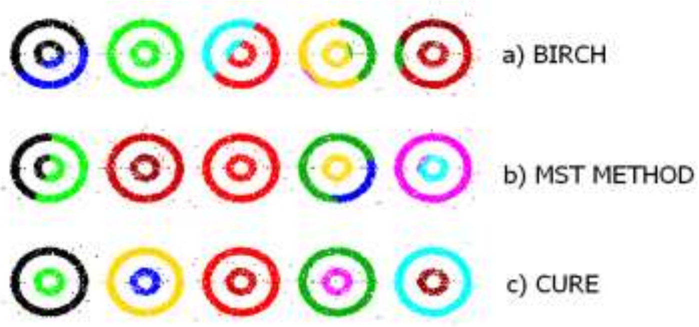
Scalable Clustering: CURE

- Clustering Using Representatives
- Uses a number of points to represent a cluster
- Representative points are found by selecting a constant number of points from a cluster and then “shrinking” them toward the center of the cluster
- Cluster similarity is the similarity of the closest pair of representative points from different clusters
- Shrinking representative points toward the center helps avoid problems with noise and outliers
- CURE is better able to handle clusters of arbitrary shapes and sizes

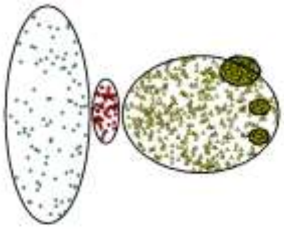
Experimental results: CURE



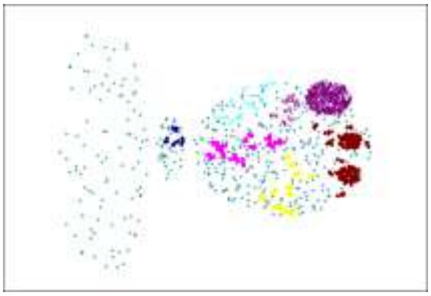
Experimental Results: CURE



CURE can not handle differing densities



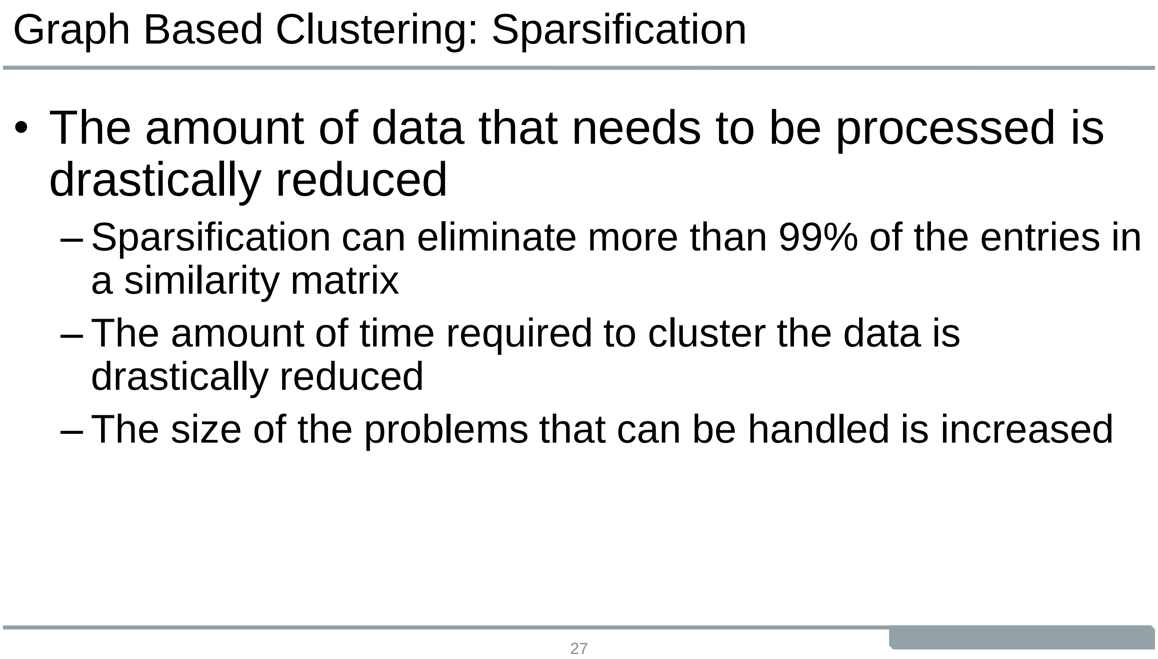
Original Points



CURE

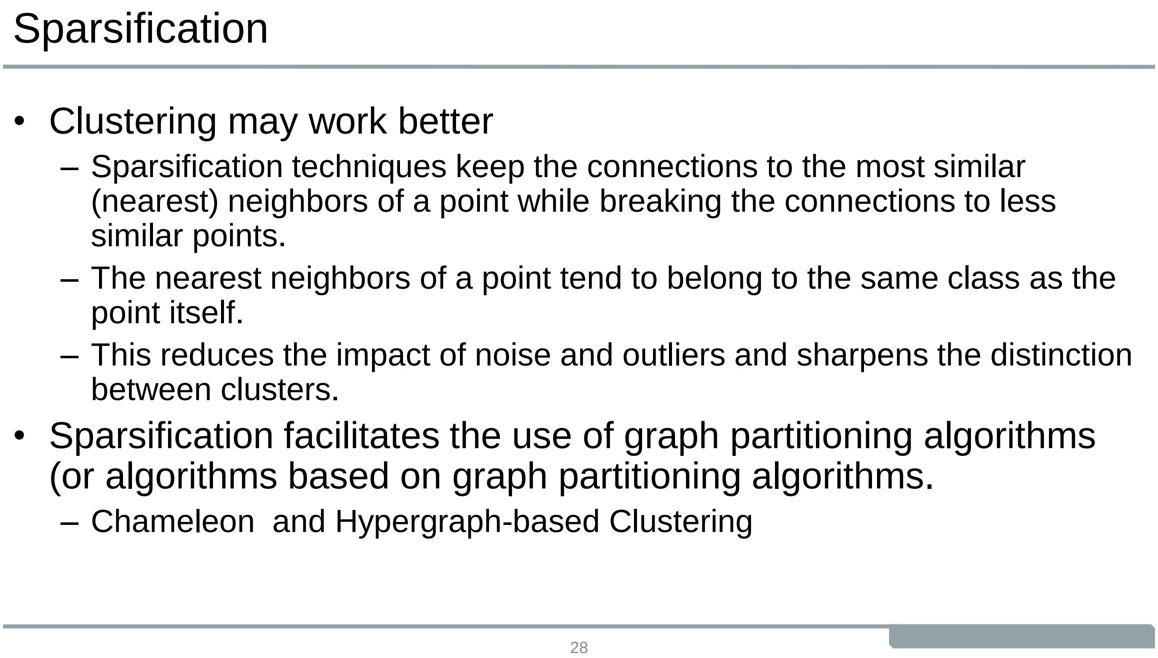
Graph Based Clustering

- Graph-Based clustering uses the proximity graph
  - Start with the proximity matrix
  - Consider each point as a node in a graph
  - Each edge between two nodes has a weight which is the proximity between the two points
  - Initially the proximity graph is fully connected
  - MIN (single-link) and MAX (complete-link) can be viewed as starting with this graph
- In the most simple case, clusters are connected components in the graph



Graph Based Clustering: Sparsification

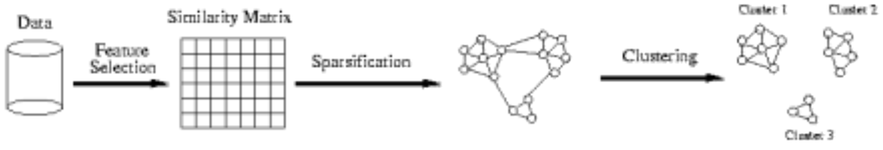
- The amount of data that needs to be processed is drastically reduced
  - Sparsification can eliminate more than 99% of the entries in a similarity matrix
  - The amount of time required to cluster the data is drastically reduced
  - The size of the problems that can be handled is increased



Sparsification

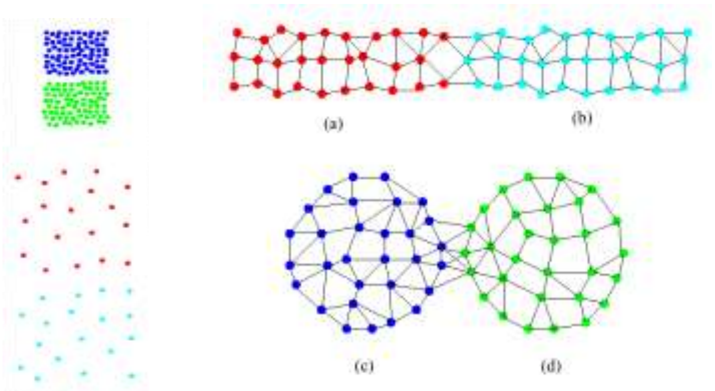
- Clustering may work better
  - Sparsification techniques keep the connections to the most similar (nearest) neighbors of a point while breaking the connections to less similar points.
  - The nearest neighbors of a point tend to belong to the same class as the point itself.
  - This reduces the impact of noise and outliers and sharpens the distinction between clusters.
- Sparsification facilitates the use of graph partitioning algorithms (or algorithms based on graph partitioning algorithms.
  - Chameleon and Hypergraph-based Clustering

Sparsification



Limitations of Current Merging Schemes

- Existing merging schemes are static in nature

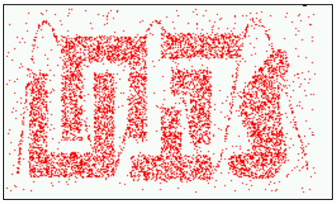


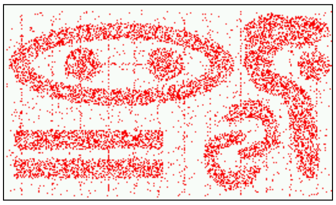
Chameleon: Clustering Using Dynamic Modeling

- Adapt to the characteristics of the data set to find the natural clusters.
- Use a dynamic model to measure the similarity between clusters.
  - Main property is the relative closeness and relative inter-connectivity of the cluster.
  - Two clusters are combined if the resulting cluster shares certain *properties* with the constituent clusters.
  - The merging scheme preserves *self-similarity*.
- One of the areas o a.

Characteristics of Spatial Datasets

- Clusters are defined as densely populated regions of the space
- Clusters have arbitrary shapes, orientation, and non-uniform sizes
- Difference in densities across clusters and variation in density within clusters
- Existence of special artifacts (*streaks*) and noise
- The clustering algorithm must address the above characteristics and also require minimal supervision





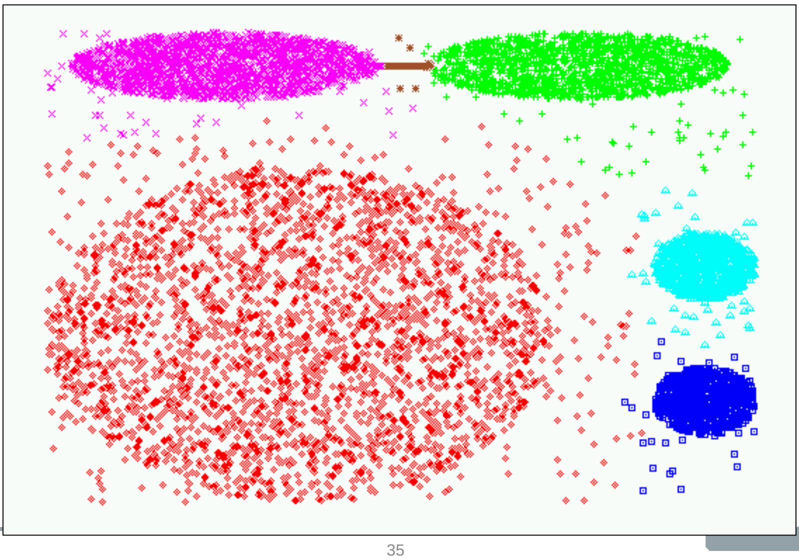
Chameleon

- Preprocessing Step: Represent the Data by a Graph
  - Given a set of points, we construct the *k-nearest-neighbor* (*k-NN*) graph to capture the relationship between a point and its *k* nearest neighbors.
- Phase 1: Use a multilevel graph partitioning algorithm on the graph to find a large number of clusters of well-connected vertices.
  - Each cluster should contain mostly points from one “true” cluster, i.e., is a sub-cluster of a “real” cluster.
  - Graph algorithms take into account global structure.

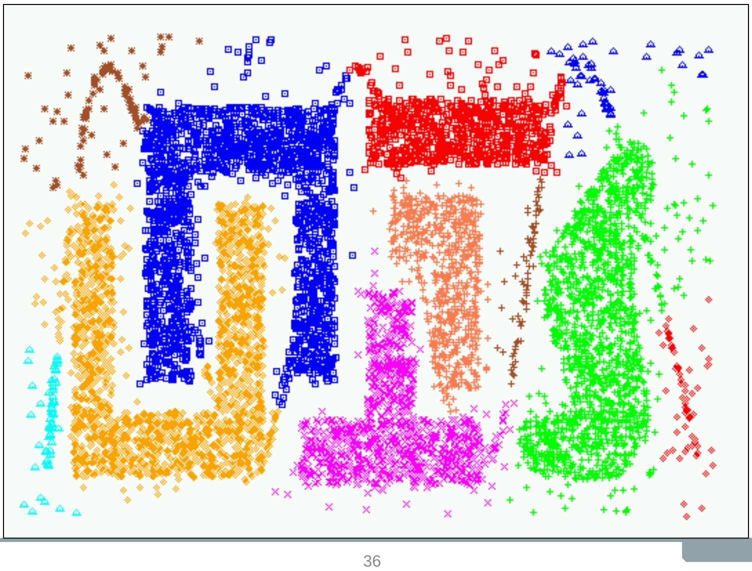
Chameleon

- Phase 2: Use Hierarchical Agglomerative Clustering to merge sub-clusters.
  - Two clusters are combined if the resulting cluster shares certain *properties* with the constituent clusters.
  - Two key properties are used to model cluster similarity:
    - Relative Interconnectivity: Absolute interconnectivity of two clusters normalized by the internal connectivity of the clusters.
    - Relative Closeness: Absolute closeness of two clusters normalized by the internal closeness of the clusters.

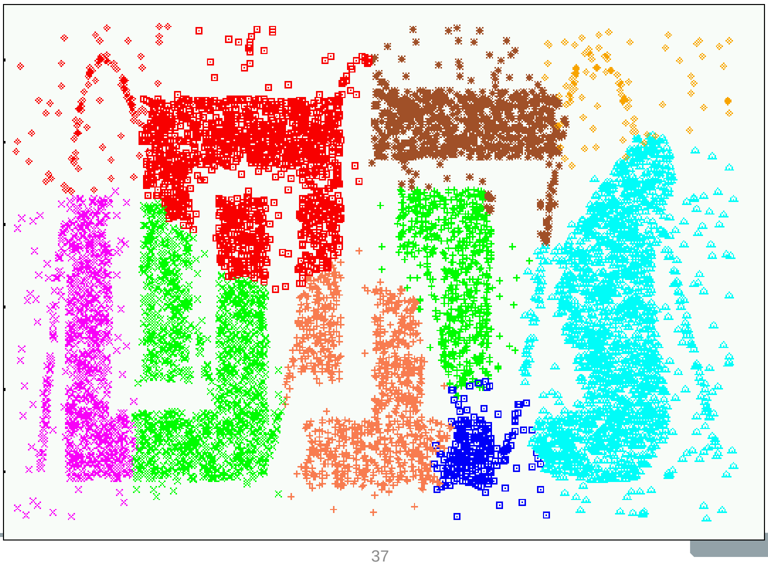
Experimental Results: Chameleon



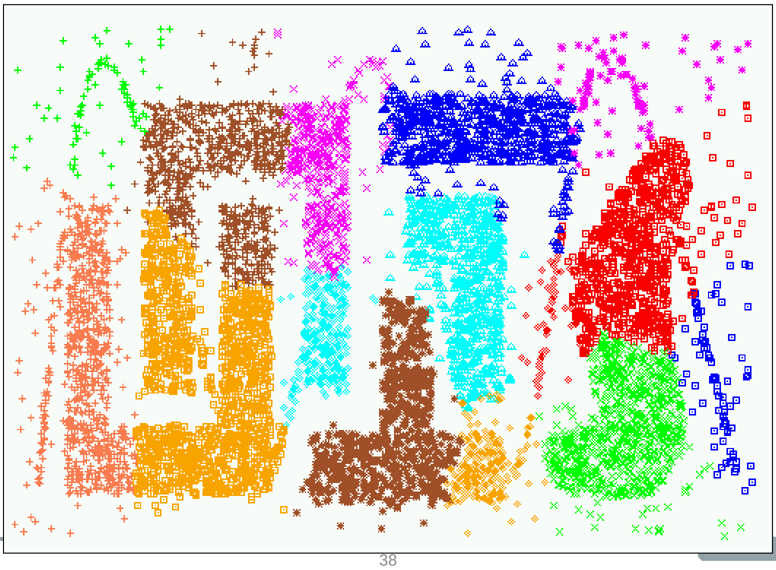
Experimental Results: Chameleon



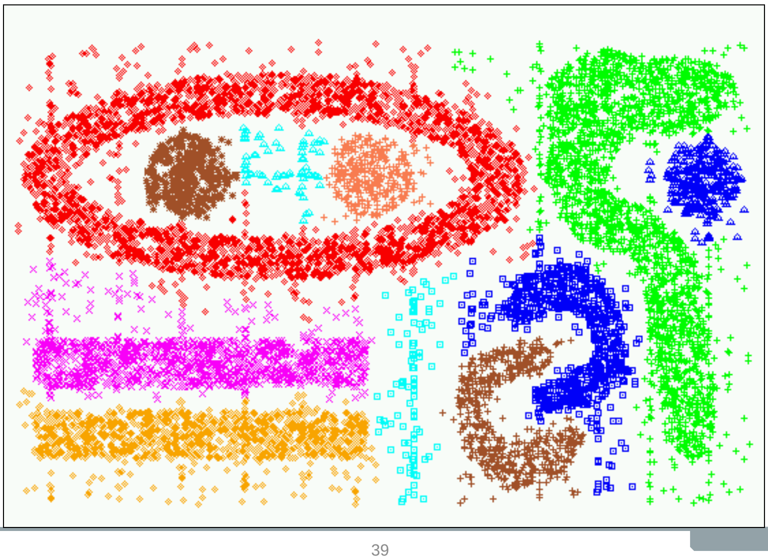
Experimental Results: CURE (10 clusters)



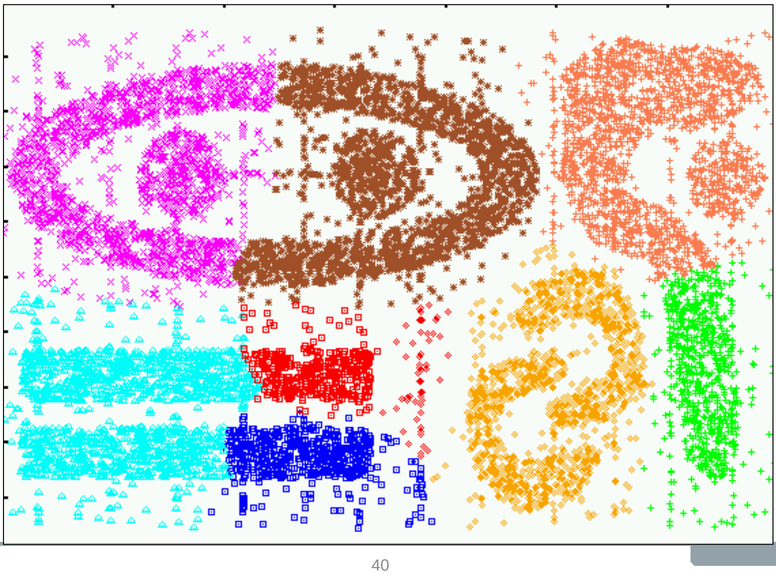
Experimental Results: CURE (15 clusters)



Experimental Results: Chameleon



Experimental Results: CURE (9 clusters)



Experimental Results: CURE (15 clusters)