Data Mining 2025

Clustering Analysis and Unsupervised Learning III

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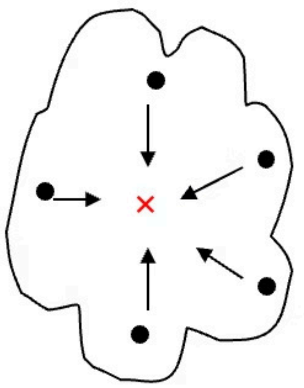
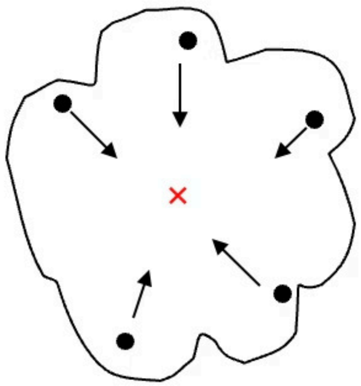
Hierarchical Clustering: Revisited

- Creates nested clusters
- Agglomerative clustering algorithms vary in terms of how the proximity of two clusters are computed
  - MIN (single link): susceptible to noise/outliers
  - MAX/GROUP AVERAGE: may not work well with non-globular clusters
- CURE algorithm tries to handle both problems
- Often starts with a proximity matrix
  - A type of graph-based algorithm

CURE: Another Hierarchical Approach

- 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

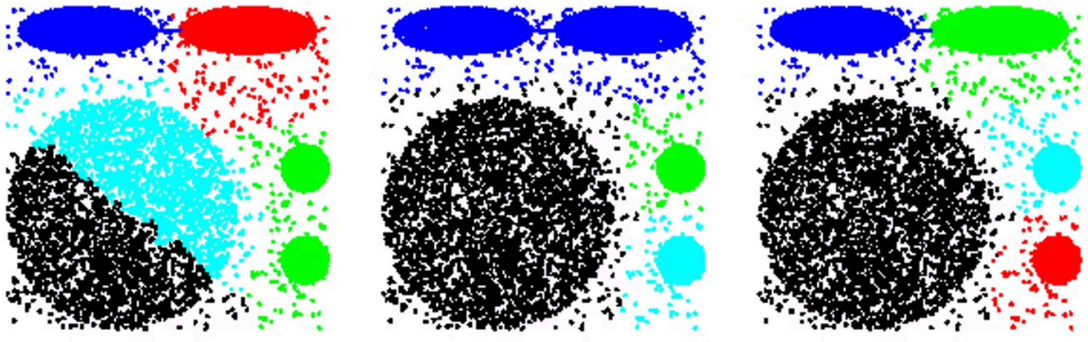




CURE

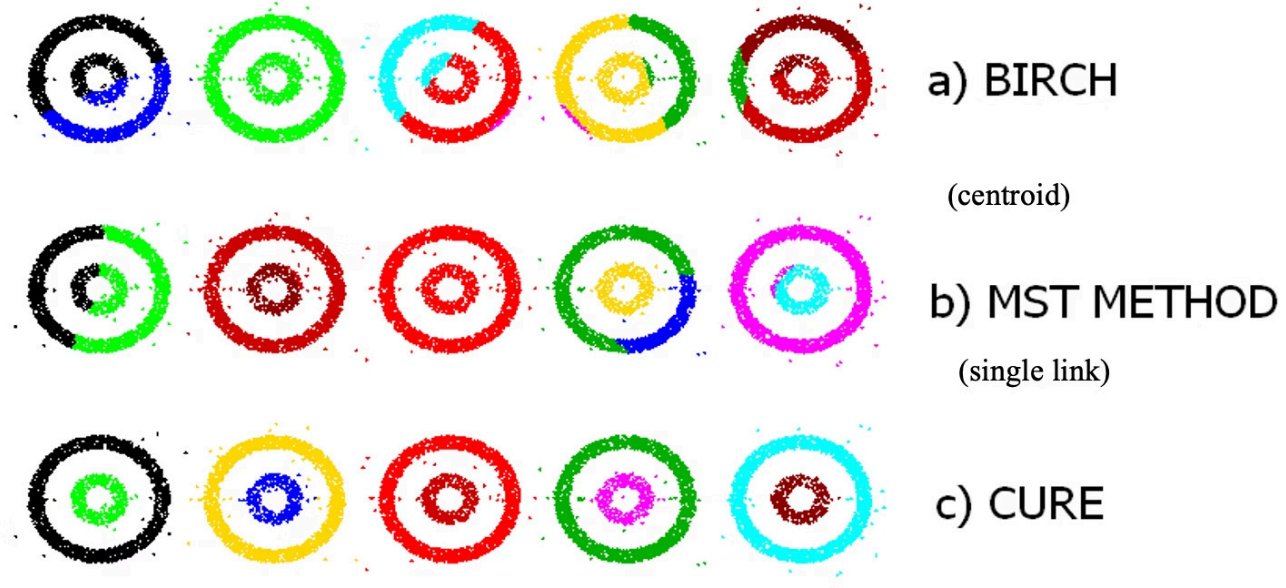
- Shrinking representative points toward the center helps avoid problems with noise and outliers
- CURE is better able to handle clusters of arbitrary shapes and sizes

Experimental Results: CURE

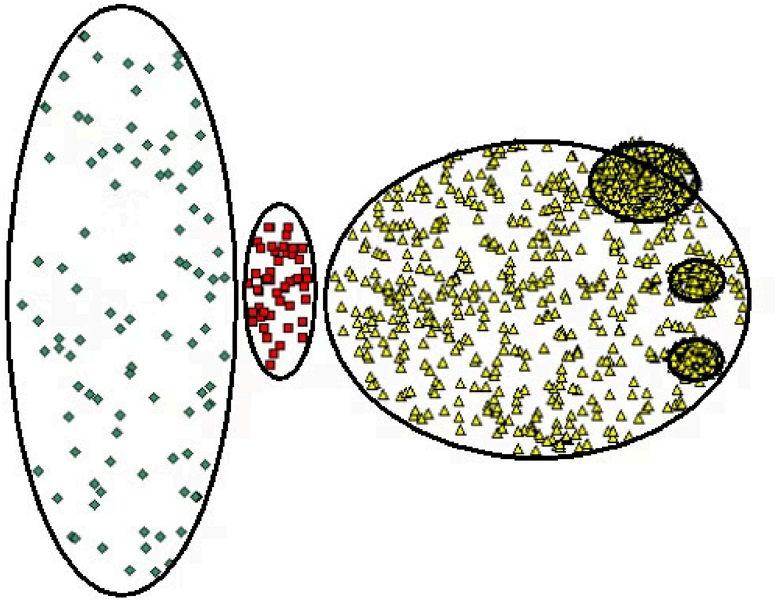


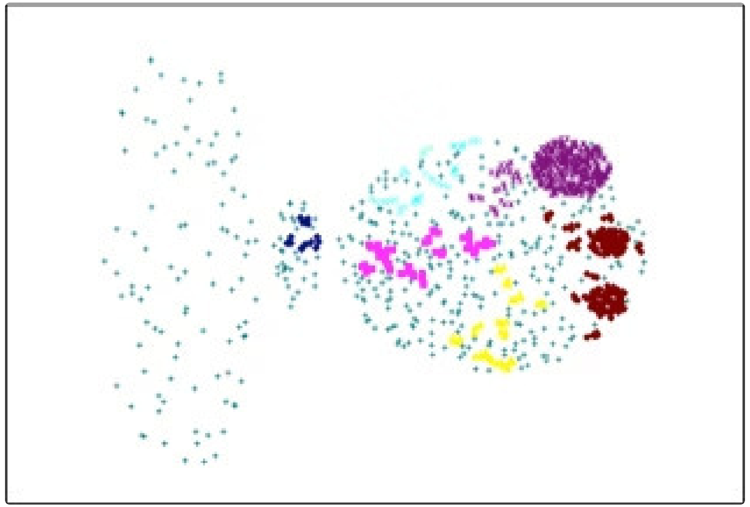
a) BIRCH b) MST METHOD c) CURE

Experimental Results: CURE



CURE Cannot Handle Differing Densities





CURE

Original Points

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 simplest 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 proximity matrix
  - The amount of time required to cluster the data is drastically reduced
  - The size of the problems that can be handled is increased

Graph-Based Clustering: Sparsification …

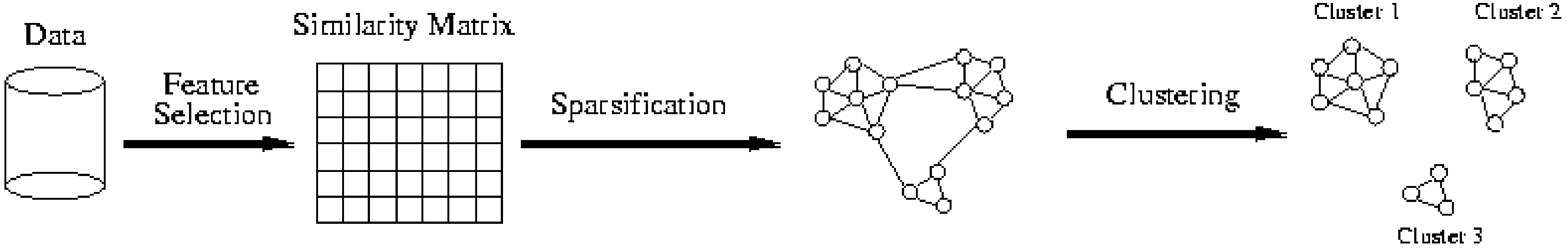
Clustering may work better

- 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

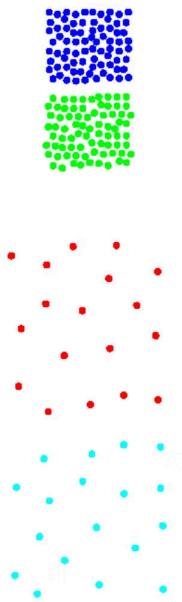
Sparsification in the Clustering Process

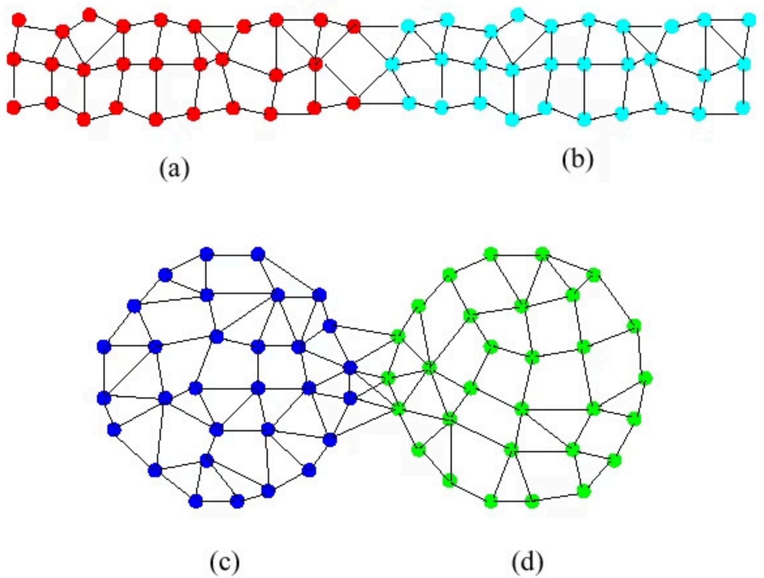


Limitations of Current Merging Schemes

- Existing merging schemes in hierarchical clustering algorithms are static in nature
  - MIN or CURE:
    - merge two clusters based on their *closeness* (or minimum distance)
  - GROUP-AVERAGE:
    - merge two clusters based on their average *connectivity*

Limitations of Current Merging Schemes



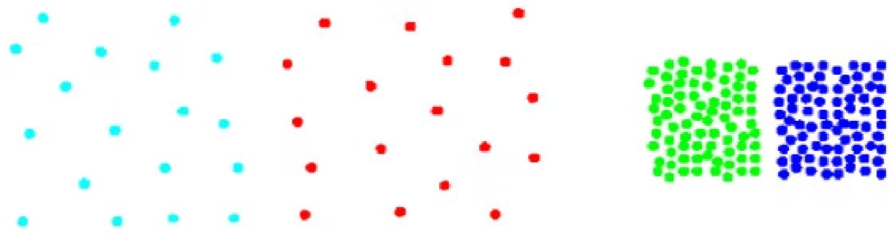


Closeness schemes will merge (a) and (b)

Average connectivity schemes will merge (c) and (d)

Chameleon: Clustering Using Dynamic Modeling

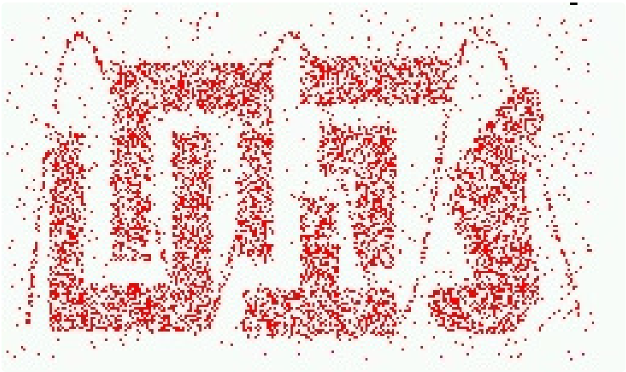
- Adapt to the characteristics of the data set to find the natural clusters
- Use a dynamic model to measure the similarity between clusters
  - Main property is the relative closeness and relative inter-connectivity of the cluster
  - Two clusters are combined if the resulting cluster shares certain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

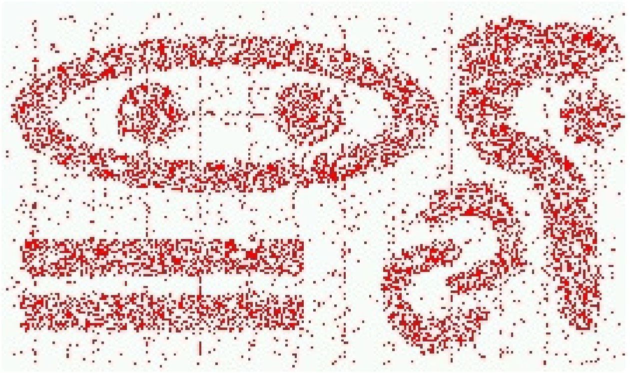


- One of the areas of application is **spatial data**

Characteristics of Spatial Data Sets

- 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: Steps

Preprocessing Step: Represent the Data by a Graph

- Given a set of points, construct the k-nearest-neighbor (k-NN) graph to capture the relationship between a point and its k nearest neighbors
- Concept of neighborhood is captured dynamically (even if region is sparse)

Phase 1: Use a multilevel graph partitioning algorithm on the graph to find a large number of clusters of well-connected vertices

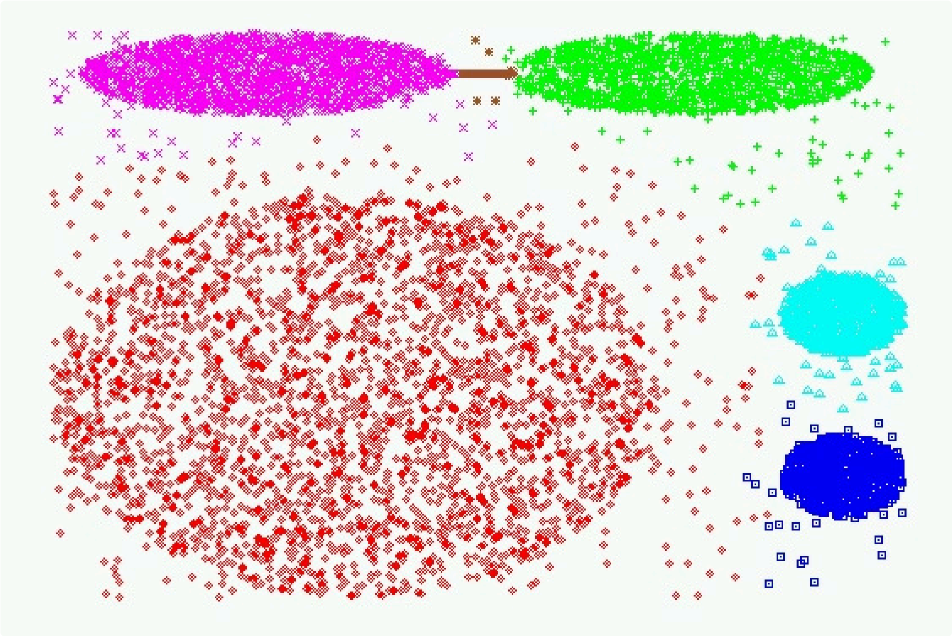
- Each cluster should contain mostly points from one "true" cluster, i.e., is a sub-cluster of a "real" cluster

Chameleon: Steps ...

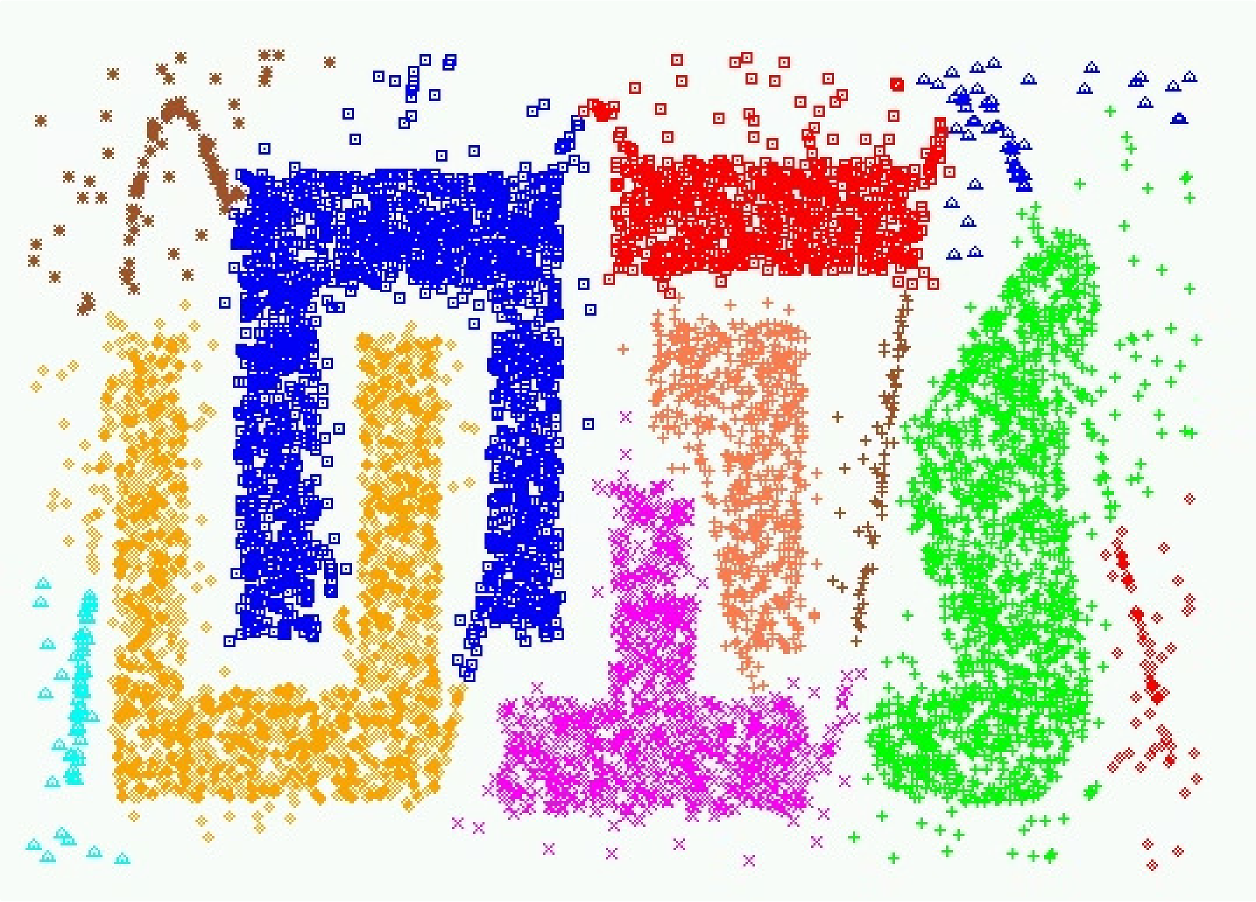
Phase 2: Use Hierarchical Agglomerative Clustering to merge sub-clusters

- Two clusters are combined if the *resulting cluster shares certain properties with the constituent clusters*
- Two key properties 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

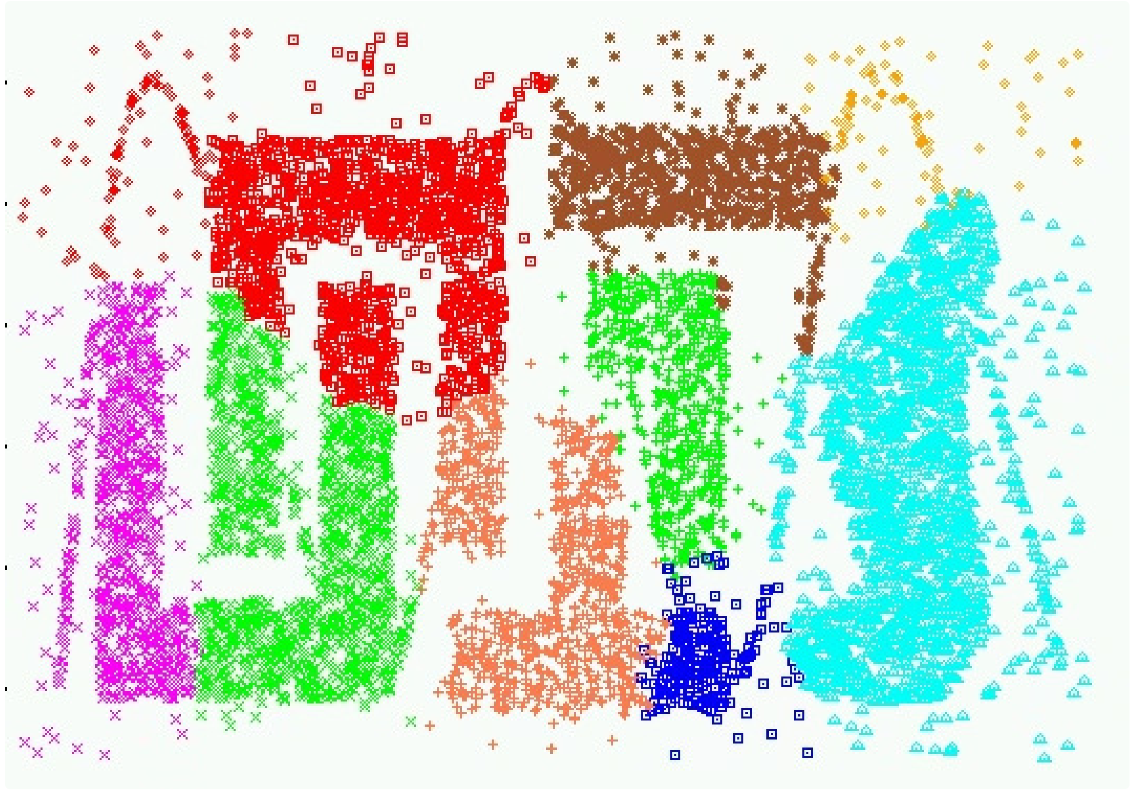
Experimental Results: CHAMELEON



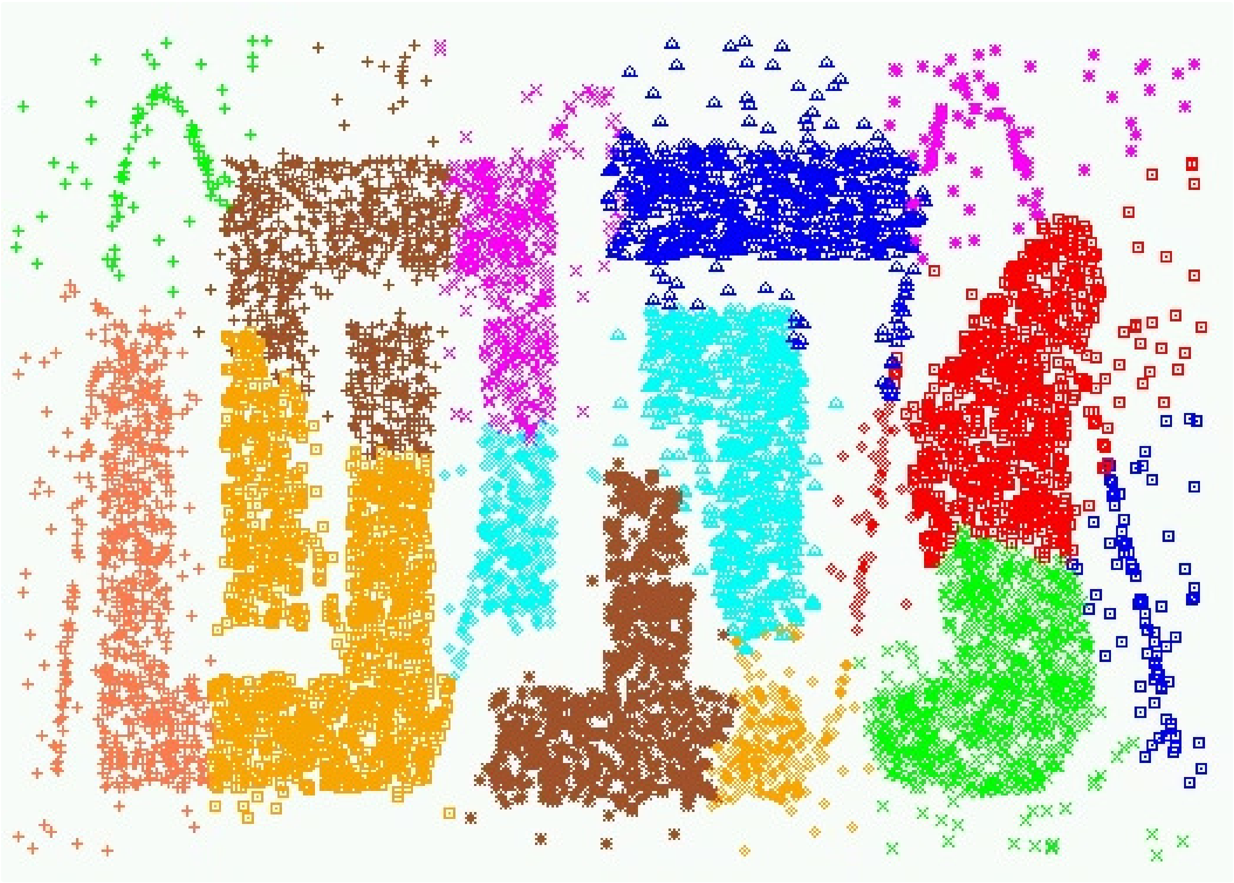
Experimental Results: CHAMELEON



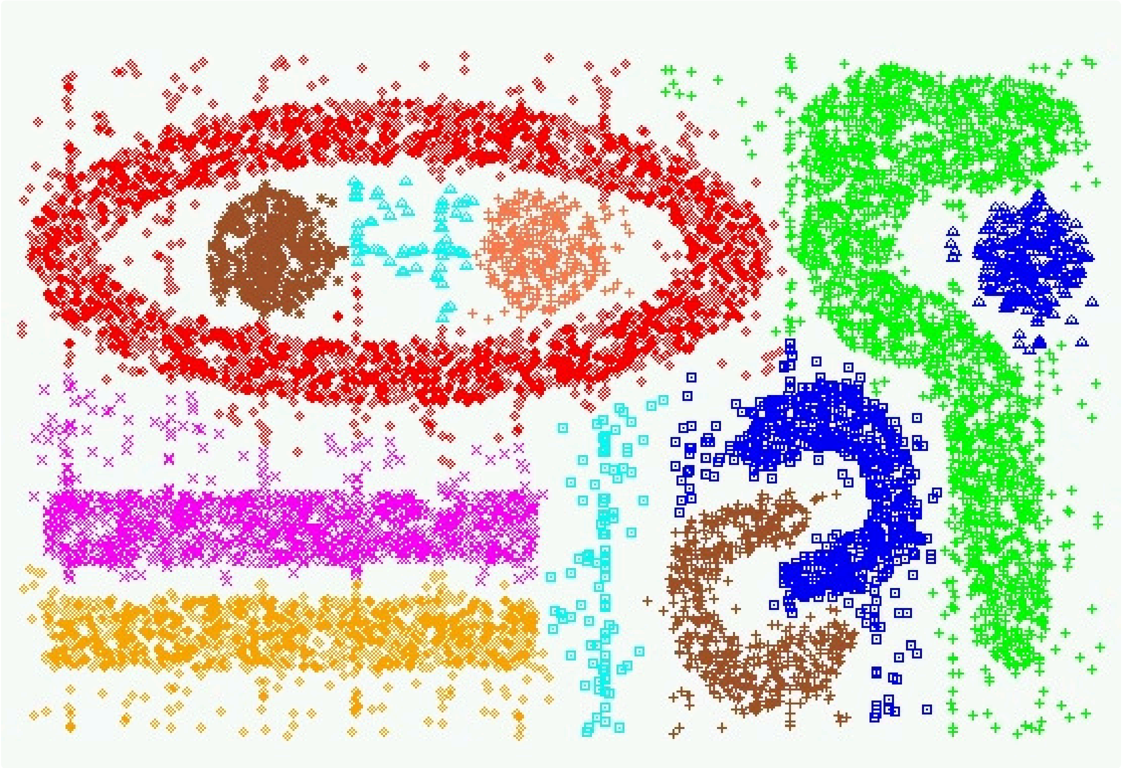
Experimental Results: CURE (*10 clusters*)



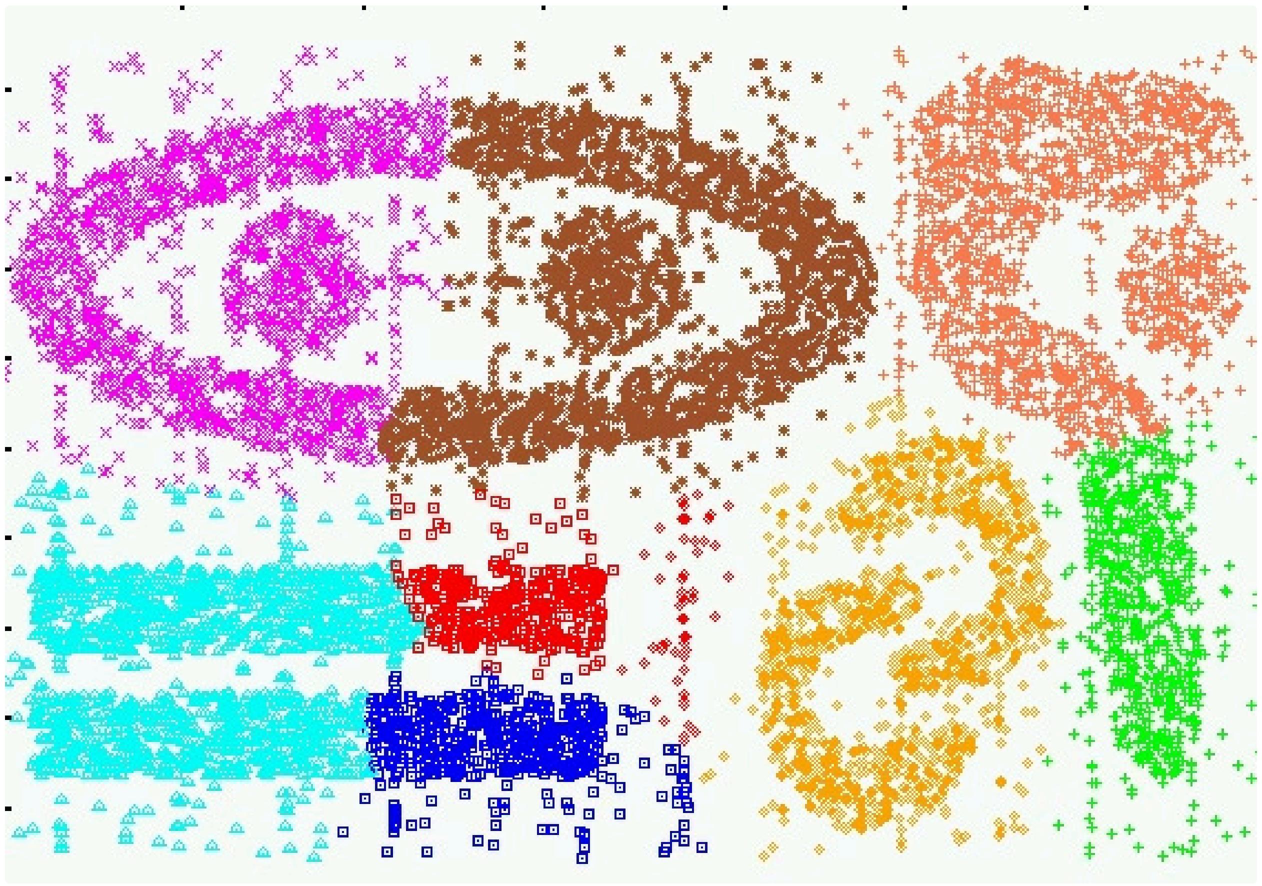
Experimental Results: CURE (*15 clusters*)



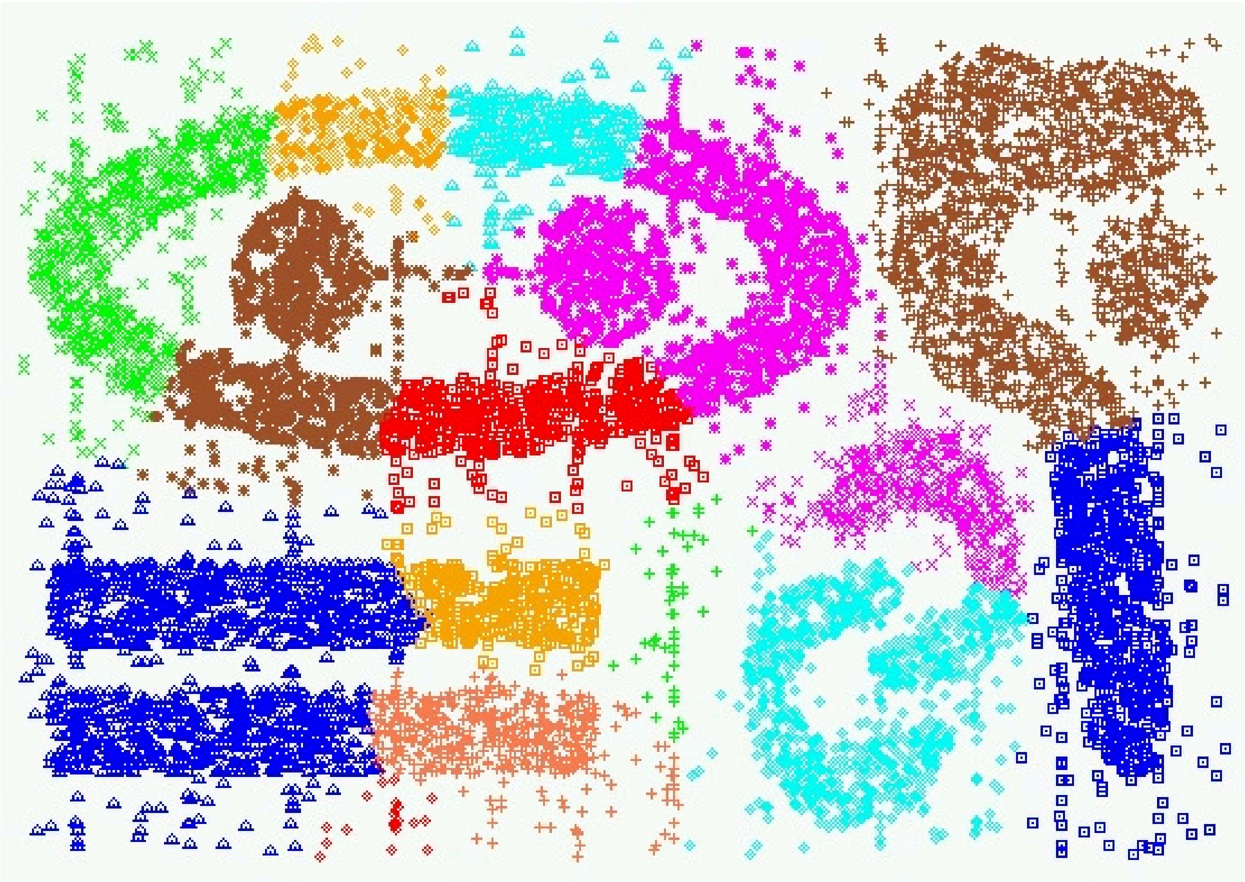
Experimental Results: CHAMELEON



Experimental Results: CURE (*9 clusters*)

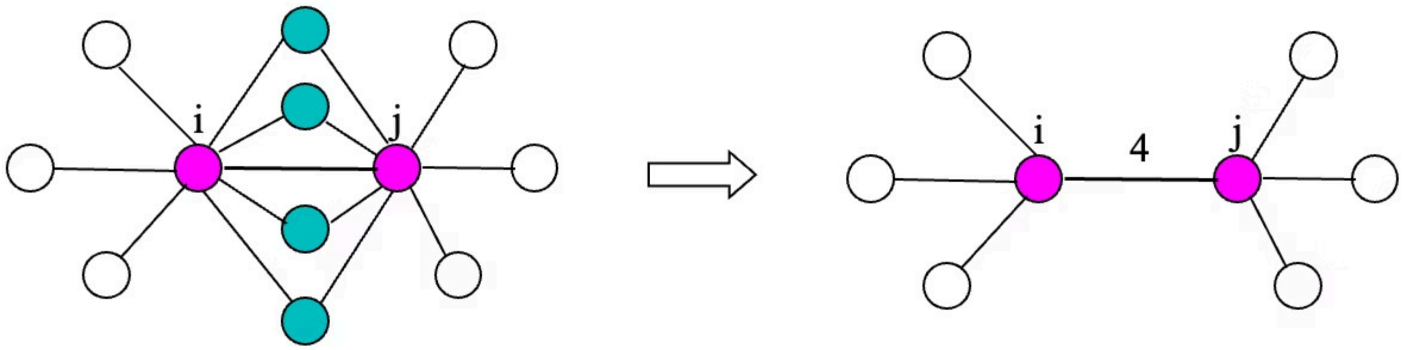


Experimental Results: CURE (*15 clusters*)

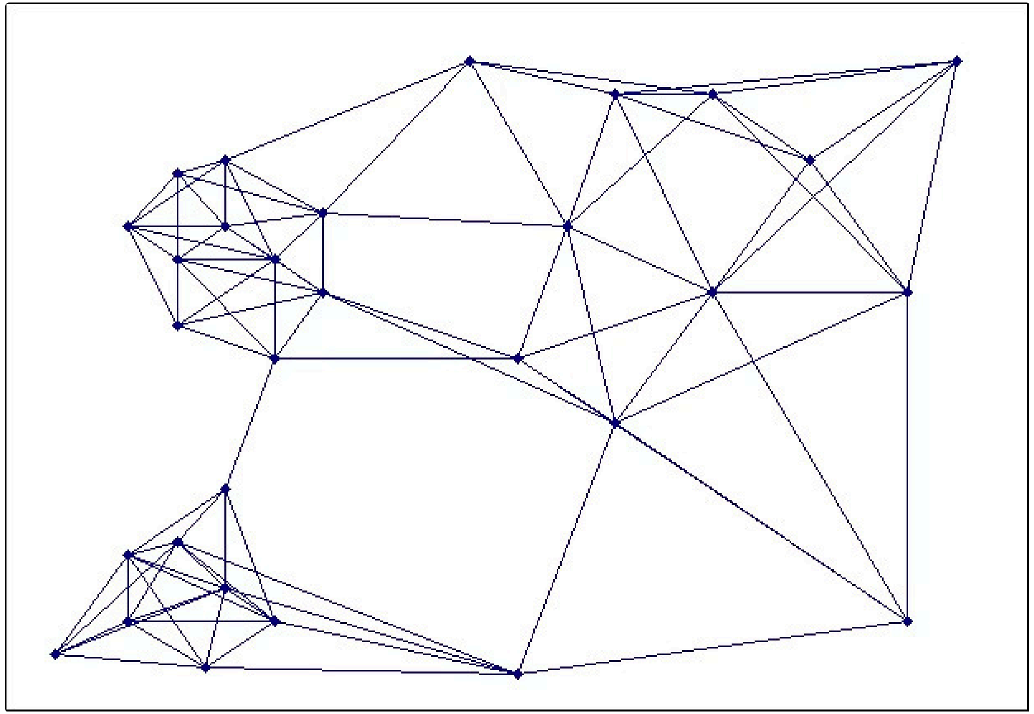


Shared Near Neighbor Approach

SNN graph: the weight of an edge is the number of shared neighbors between vertices given that the vertices are connected

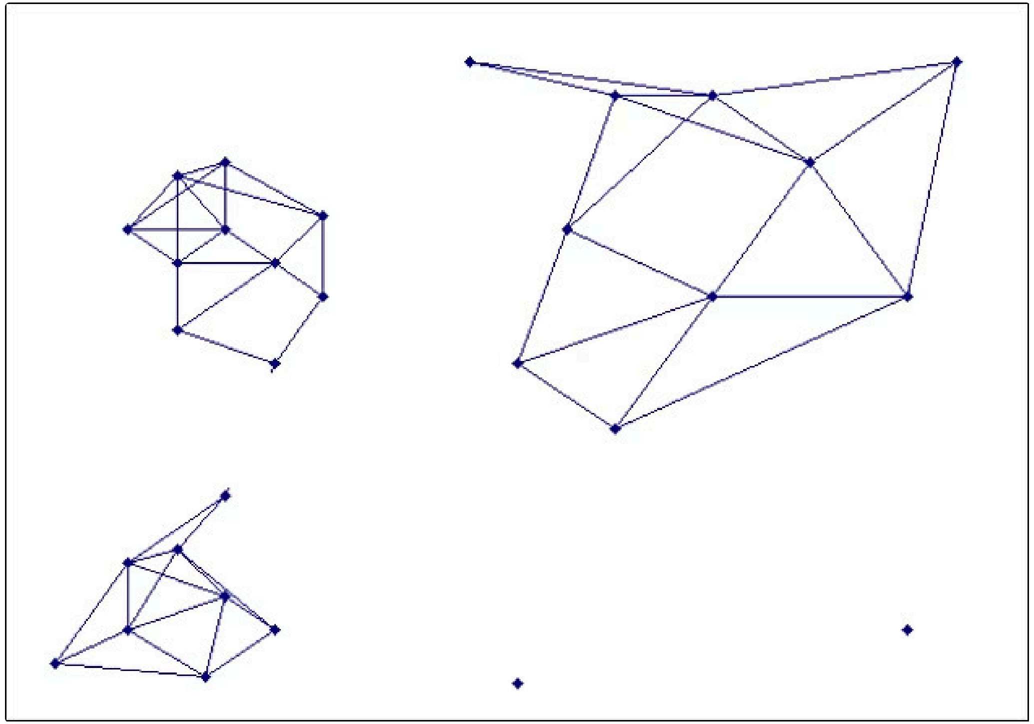


Creating the SNN Graph



Sparse Graph

Link weights are similarities between neighboring points



Shared Near Neighbor Graph

Link weights are number of Shared Nearest Neighbors

ROCK (RObust Clustering using linKs)

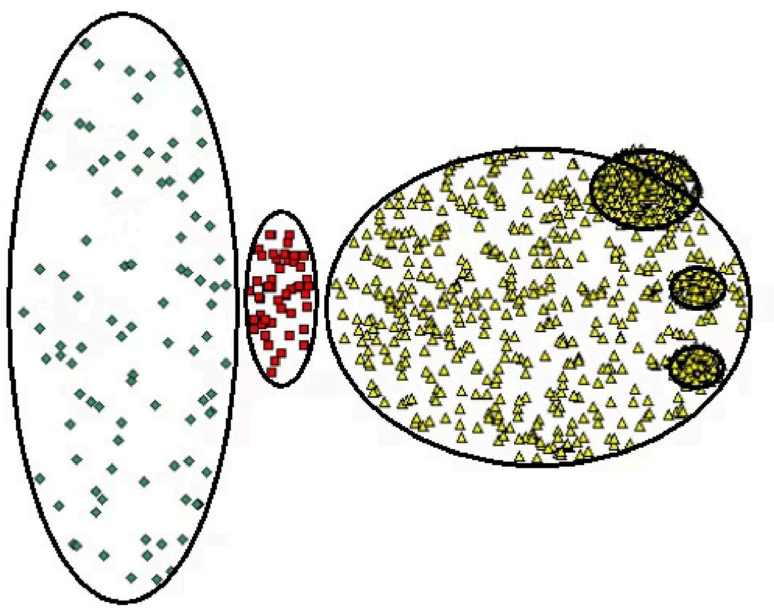
- Clustering algorithm for data with categorical and Boolean attributes
- A pair of points is defined to be neighbors if their similarity is greater than some threshold
- Use a hierarchical clustering scheme to cluster the data.

1. Obtain a sample of points from the data set
2. Compute the link value for each set of points, i.e., transform the original similarities (computed by Jaccard coefficient) into similarities that reflect the number of shared neighbors between points
3. Perform an agglomerative hierarchical clustering on the data using the "number of shared neighbors" as similarity measure and maximizing "the shared neighbors" objective function
4. Assign the remaining points to the clusters that have been found

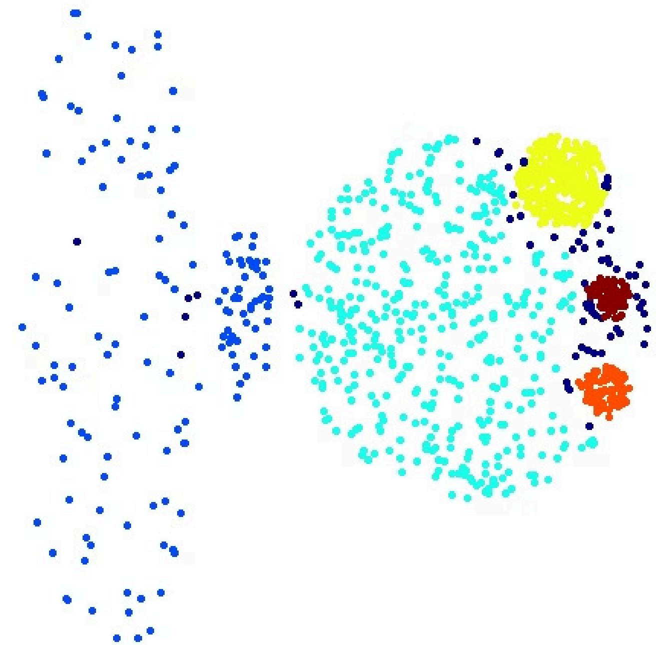
Jarvis-Patrick Clustering

- First, the k-nearest neighbors of all points are found
  - In graph terms this can be regarded as breaking all but the k strongest links from a point to other points in the proximity graph
- A pair of points is put in the same cluster if
  - any two points share more than T neighbors and
  - the two points are in each others k nearest neighbor list
- For instance, we might choose a nearest neighbor list of size 20 and put points in the same cluster if they share more than 10 near neighbors
- Jarvis-Patrick clustering is too brittle

When Jarvis-Patrick Works Reasonably Well



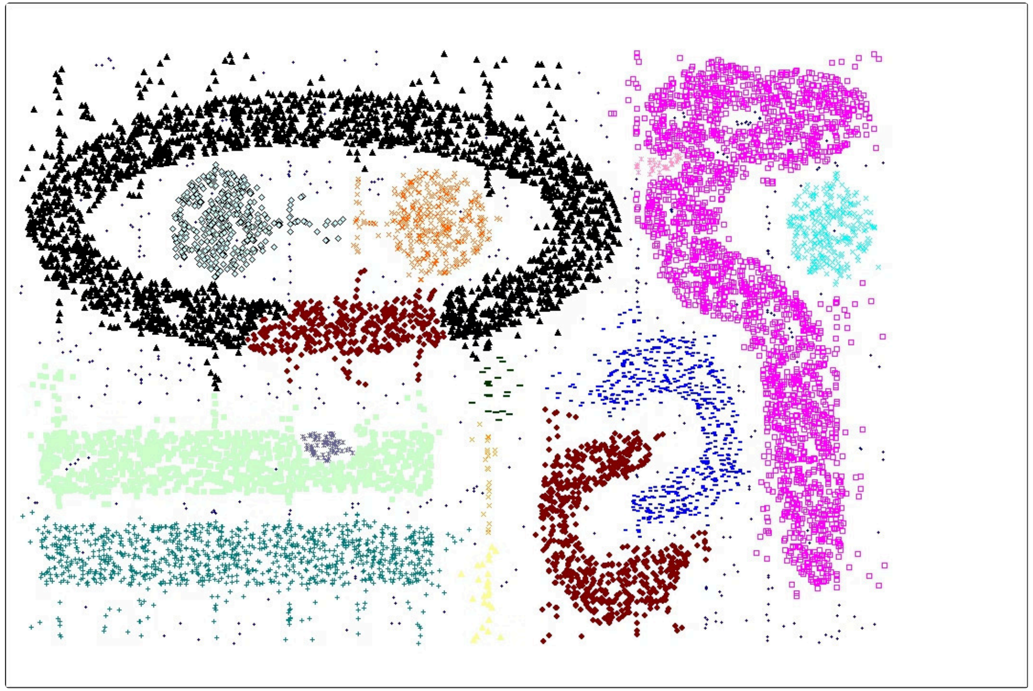
Original Points



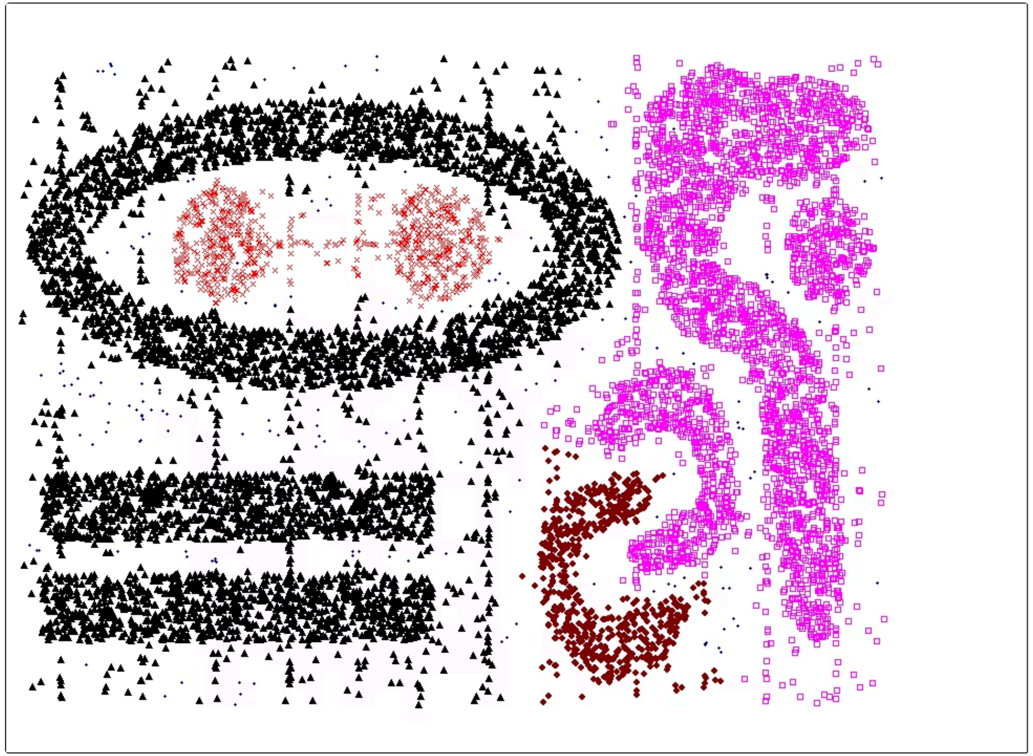
Jarvis Patrick Clustering

6 shared neighbors out of 20

When Jarvis-Patrick Does NOT Work Well



Smallest threshold, T, that does not merge clusters.



Threshold of T - 1

SNN Clustering Algorithm

Compute the similarity matrix

This corresponds to a similarity graph with data points for nodes and edges whose weights are the similarities between data points

Sparsify the similarity matrix by keeping only the *k* most similar neighbors

This corresponds to only keeping the *k* strongest links of the similarity graph

Construct the shared nearest neighbor graph from the sparsified similarity matrix

At this point, we could apply a similarity threshold and find the connected components to obtain the clusters (Jarvis-Patrick algorithm)

Find the SNN density of each Point

Using a user specified parameters, *Eps*, find the number points that have an SNN similarity of *Eps* or greater to each point. This is the SNN density of the point

SNN Clustering Algorithm …

Find the core points

Using a user specified parameter, *MinPts*, find the core points, i.e., all points that have an SNN density greater than *MinPts*

Form clusters from the core points

If two core points are within a radius, *Eps*, of each other they are place in the same cluster

Discard all noise points

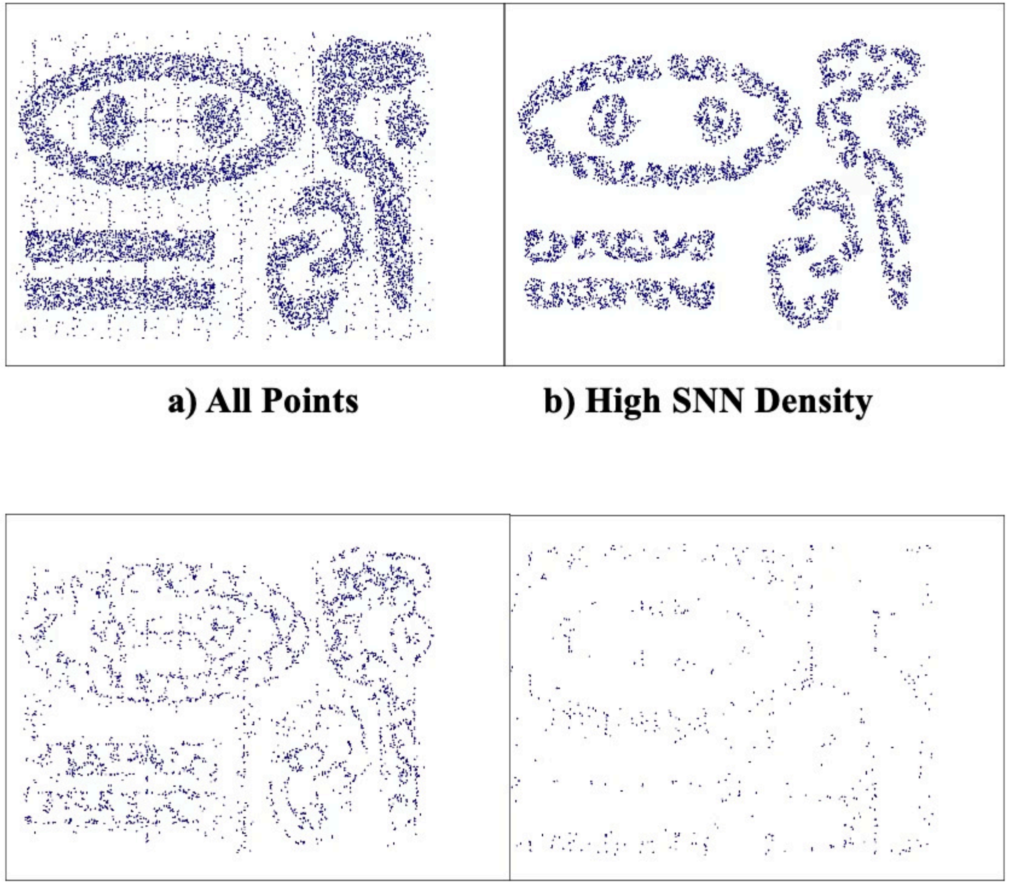
All non-core points that are not within a radius of *Eps* of a core point are discarded

Assign all non-noise, non-core points to clusters

This can be done by assigning such points to the nearest core point

(Note that steps 4-8 are DBSCAN)

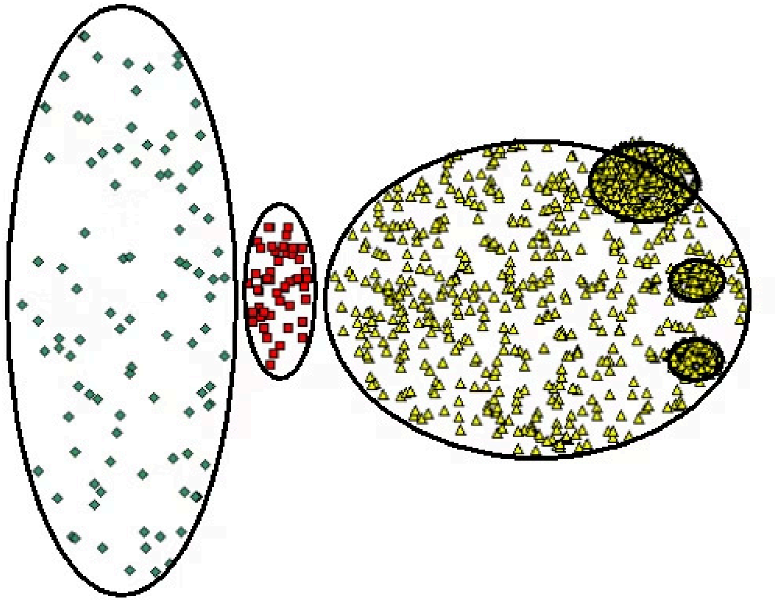
SNN Density



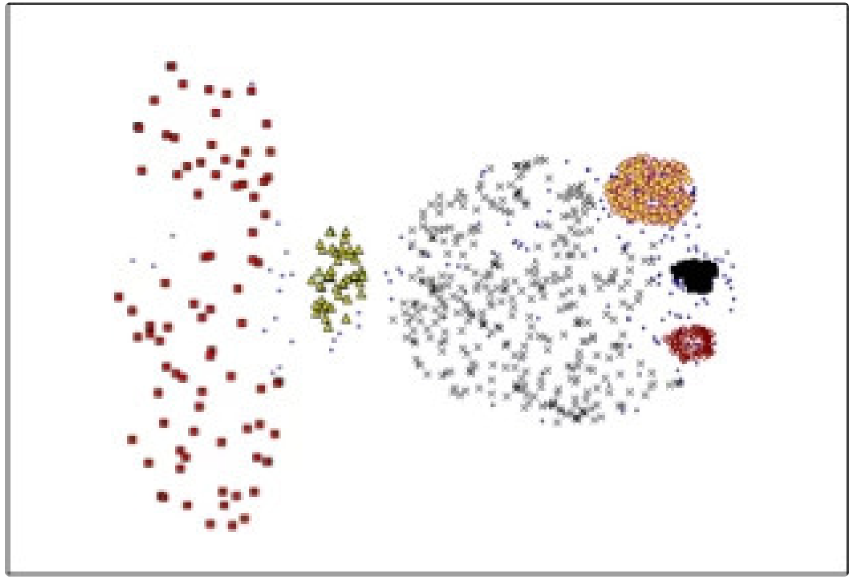
a) All Points　　b) High SNN Density

c) Medium SNN Density　　d) Low SNN Density

SNN Clustering Can Handle Differing Densities

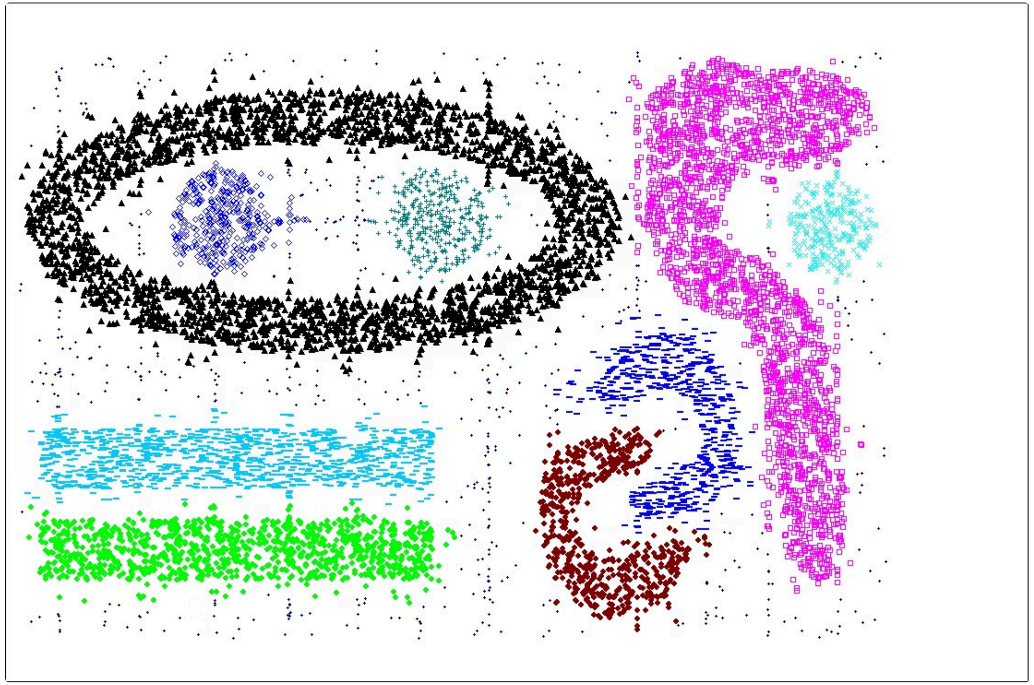


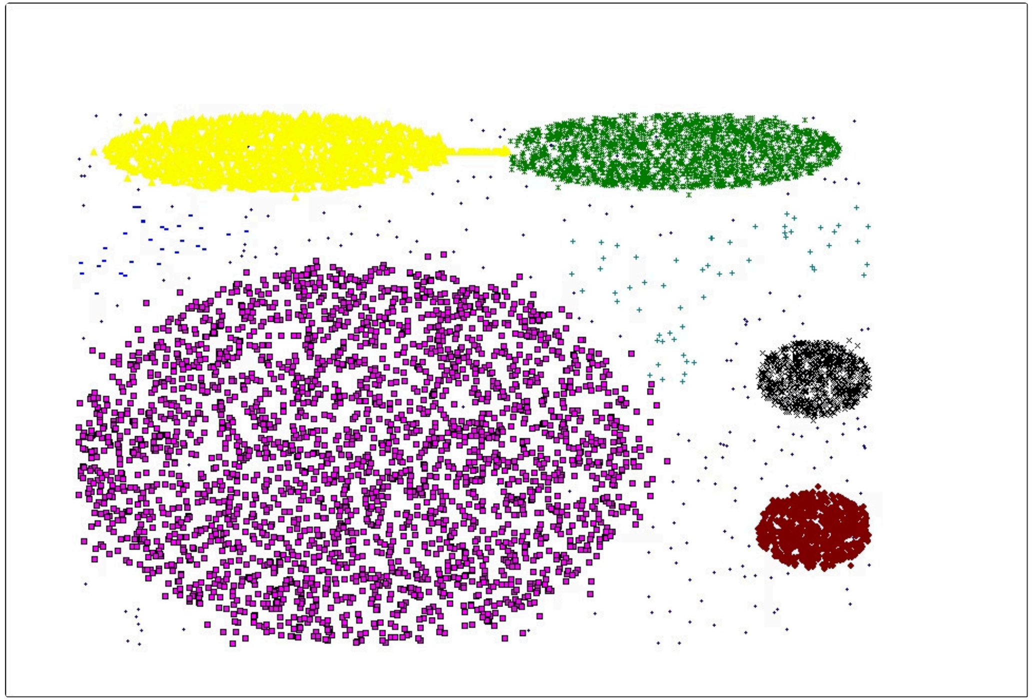
Original Points



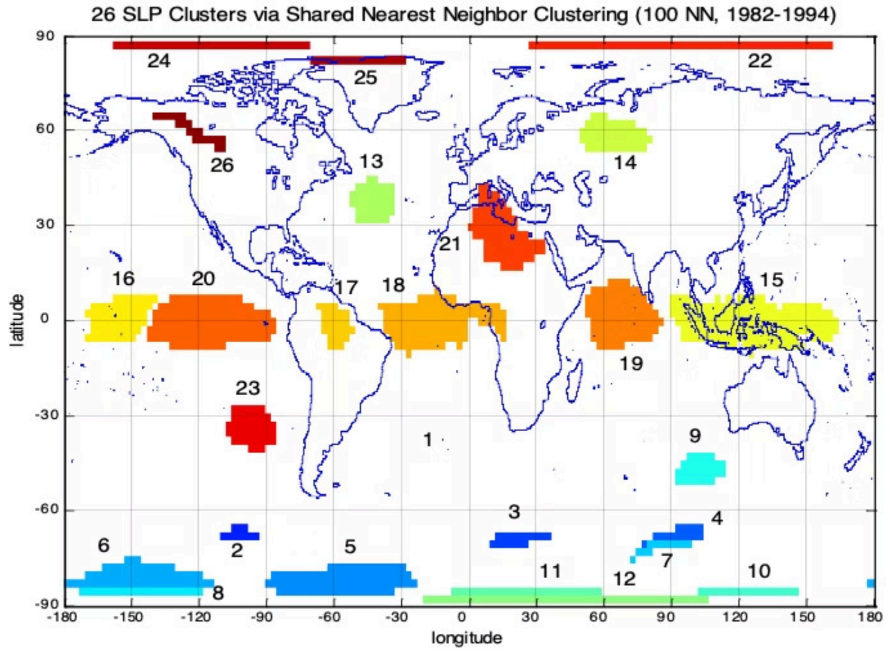
SNN Clustering

SNN Clustering Can Handle Other Difficult Situations

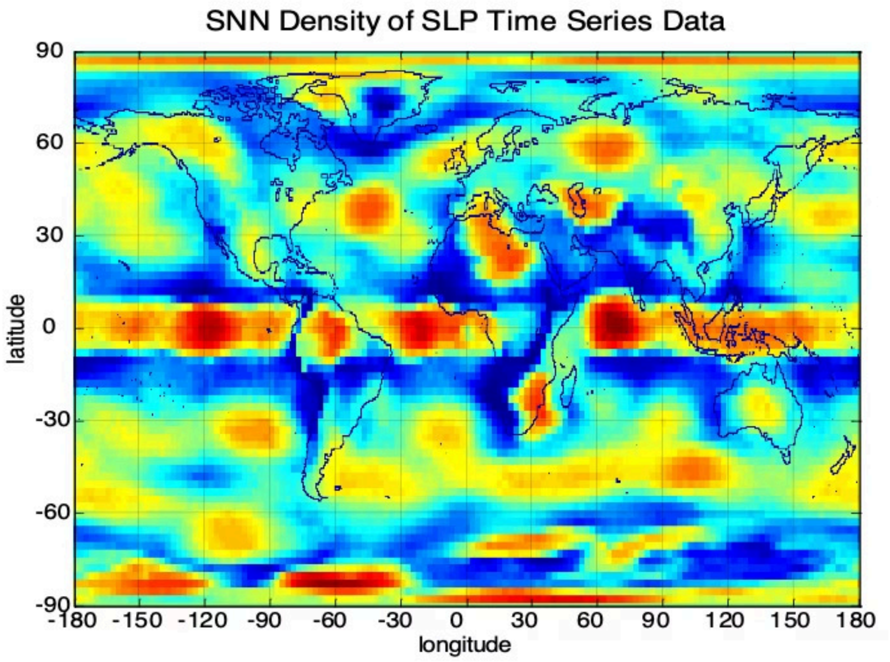




Finding Clusters of Time Series In Spatio-Temporal Data



SNN Clusters of SLP.



SNN Density of Points on the Globe.

Features and Limitations of SNN Clustering

- Does not cluster all the points
- Complexity of SNN Clustering is high
  - O(n * time to find numbers of neighbor within *Eps*)
  - In worst case, this is O(n2)
  - For lower dimensions, there are more efficient ways to find the nearest neighbors
    - R* Tree
    - k-d Trees