Ontario Tech Science

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Clustering: Advanced Concepts and Algorithms

CSCI 4150U: Data Mining

Outline

- Soft Clustering
  - Fuzzy c-means
- CURE
- Graph-based Clustering
  - Chameleon
  - Jarvis-Patrick
  - SNN (Density) Clustering
- Characteristics of Clustering Algorithms

Hard (Crisp) vs Soft (Fuzzy) Clustering

- Hard (Crisp) vs. Soft (Fuzzy) clustering
  - For soft clustering allow point to belong to more than one cluster
  - For K-means, generalize objective function

Hard clustering: $w_{ij} \in \{0,1\}$

$$SSE = \sum_{j=1}^{k} \sum_{i=1}^{m} w_{ij}\, dist(\boldsymbol{x}_i, \boldsymbol{c}_j)^2 \qquad \sum_{j=1}^{k} w_{ij} = 1$$

  - w_{ij}: weight with which object x_i belongs to cluster $\boldsymbol{c}_j$

K-means Algorithm

  - To minimize SSE, repeat the following steps:
    - Fix $\boldsymbol{c}_j$ and determine w_{ij} (cluster assignment)
    - Fix w_{ij} and re-compute $\boldsymbol{c}_j$

Fuzzy C-means

p: fuzzifier (p > 1)

- Objective function

Fuzzy C-means: $w_{ij} \in [0,1]$

$$SSE = \sum_{j=1}^{k} \sum_{i=1}^{m} w_{ij}^{p}\, dist(\boldsymbol{x}_i, \boldsymbol{c}_j)^2 \qquad \sum_{j=1}^{k} w_{ij} = 1$$

- w_{ij}: weight with which object $\boldsymbol{x}_i$ belongs to cluster $\boldsymbol{c}_j$
- p: a power for the weight not a superscript and controls how “fuzzy” the clustering is

- To minimize objective function, repeat the following:
  - Fix $\boldsymbol{c}_j$ and determine w_{ij}
  - Fix w_{ij} and re-compute $\boldsymbol{c}$

(Bezdek, James C. Pattern recognition with fuzzy objective function algorithms. Kluwer Academic Publishers, 1981)

Fuzzy C-means

- Objective function:

p: fuzzifier (p > 1)

$$SSE = \sum_{j=1}^{k}\sum_{i=1}^{m} w_{ij}^{p}\, dist(\boldsymbol{x}_i, \boldsymbol{c}_j)^2 \qquad \sum_{j=1}^{k} w_{ij} = 1$$

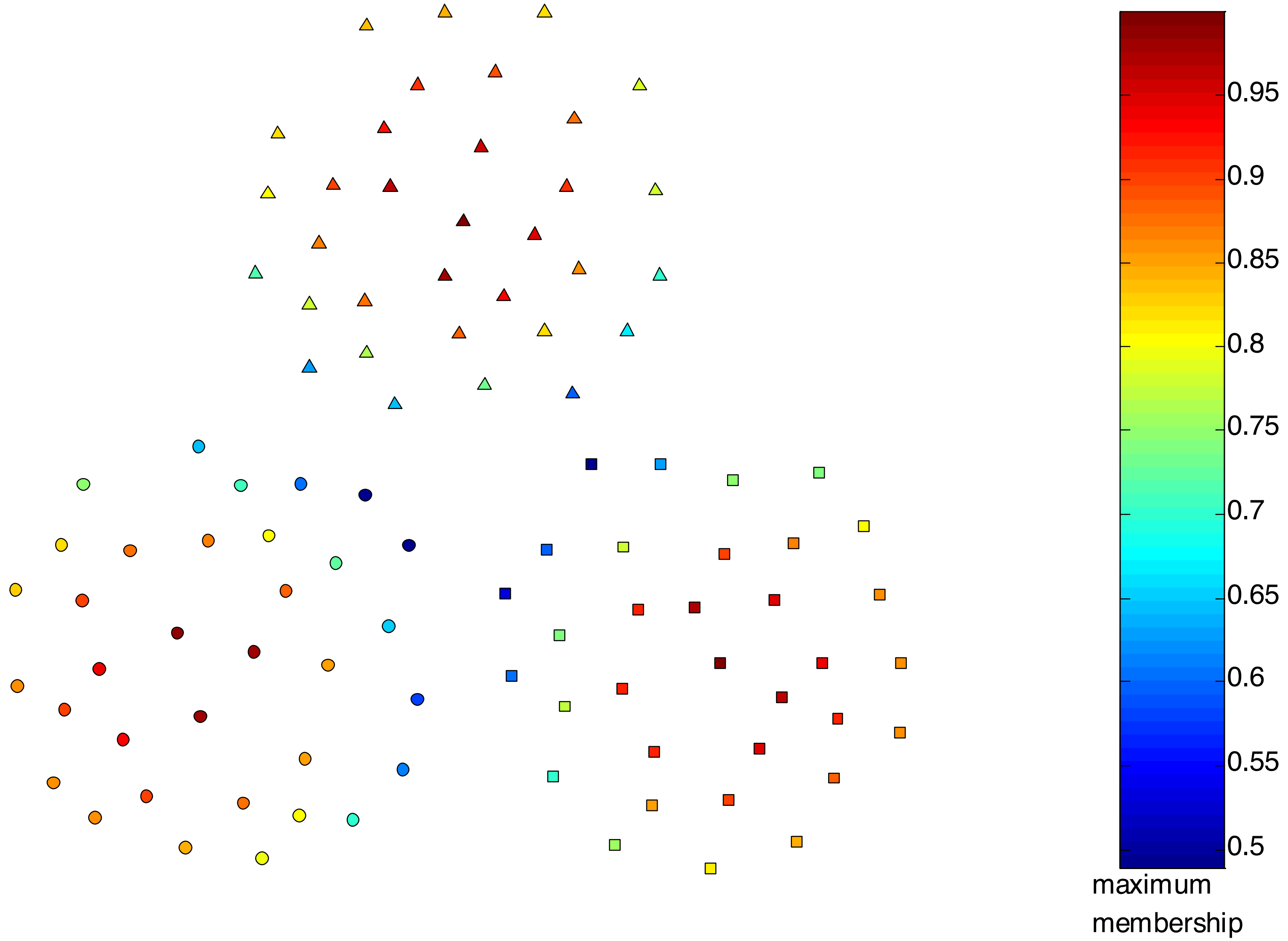
- Initialization: choose the weights w_{ij} randomly
- Repeat:
  - Update centroids: $\boldsymbol{c}_j = \sum_{i=1}^{m} w_{ij}\boldsymbol{x}_i \,/\, \sum_{i=1}^{m} w_{ij}$

C-Means Algorithm

  - Update weights:

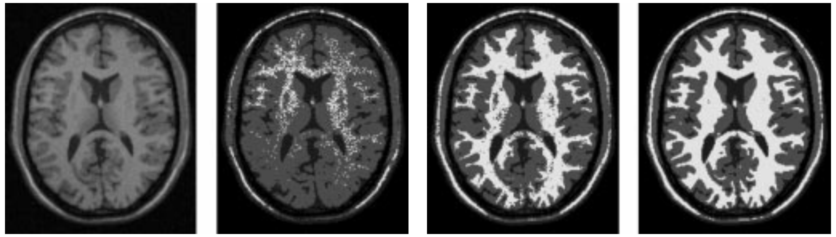
$$w_{ij} = (1/dist(\boldsymbol{x}_i, \boldsymbol{c}_j)^2)^{\frac{1}{p-1}} / \sum_{j=1}^{k} (1/dist(\boldsymbol{x}_i, \boldsymbol{c}_j)^2)^{\frac{1}{p-1}}$$

Fuzzy K-means Applied to Sample Data



An Example Application: Image Segmentation

- Modified versions of fuzzy c-means have been used for image segmentation
  - Especially fMRI images (functional magnetic resonance images)
- References
  - Gong, Maoguo, Yan Liang, Jiao Shi, Wenping Ma, and Jingjing Ma. "Fuzzy c-means clustering with local information and kernel metric for image segmentation." *Image Processing, IEEE Transactions on* 22, no. 2 (2013): 573-584.



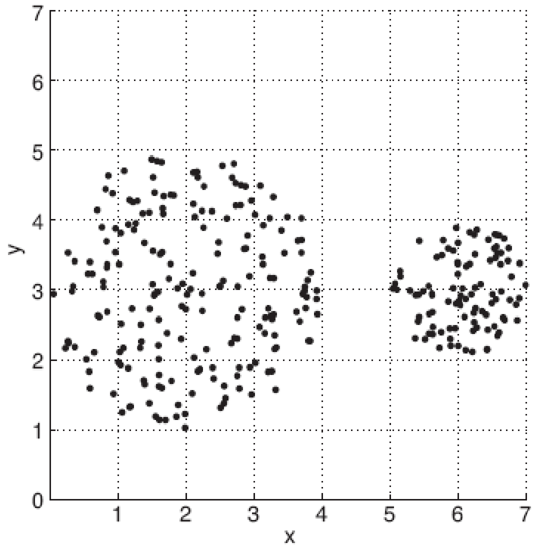
From left to right: original images, fuzzy c-means, EM, BCFCM

  - Ahmed, Mohamed N., Sameh M. Yamany, Nevin Mohamed, Aly A. Farag, and Thomas Moriarty. "A modified fuzzy c-means algorithm for bias field estimation and segmentation of MRI data." *Medical Imaging, IEEE Transactions on* 21, no. 3 (2002): 193-199.

Grid-based Clustering

Algorithm 9.4 Basic grid-based clustering algorithm.

1: Define a set of grid cells.
2: Assign objects to the appropriate cells and compute the density of each cell.
3: Eliminate cells having a density below a specified threshold, τ.
4: Form clusters from contiguous (adjacent) groups of dense cells.



0	0	0	0	0	0	0
0	0	0	0	0	0	0
4	**17**	**18**	**6**	0	0	0
14	**14**	**13**	**13**	0	**18**	**27**
11	**18**	**10**	**21**	0	**24**	**31**
3	**20**	**14**	**4**	0	0	0
0	0	0	0	0	0	0

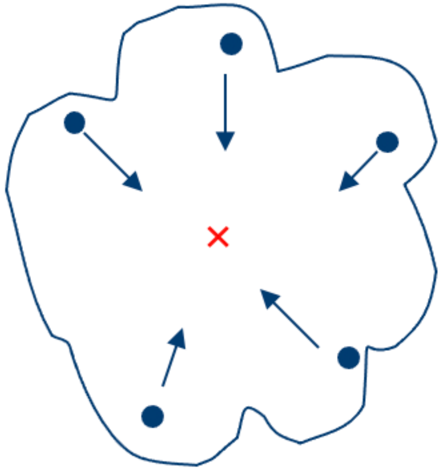
Hierarchical Clustering: Revisited

- Agglomerative hierarchical clustering algorithms vary in terms of how the proximity of two clusters are computed
  - MIN (single link)
    - susceptible to noise/outliers
  - MAX (complete link)/GROUP AVERAGE/Centroid:
    - may not work well with non-globular clusters

- CURE algorithm tries to handle both problems

CURE Algorithm

- Represents a cluster using **multiple representative** points



  - Representative points are found by selecting a constant number of points from a cluster
    - First representative point is chosen to be the point furthest from the center of the cluster
    - Remaining representative points are chosen so that they are farthest from all previously chosen points

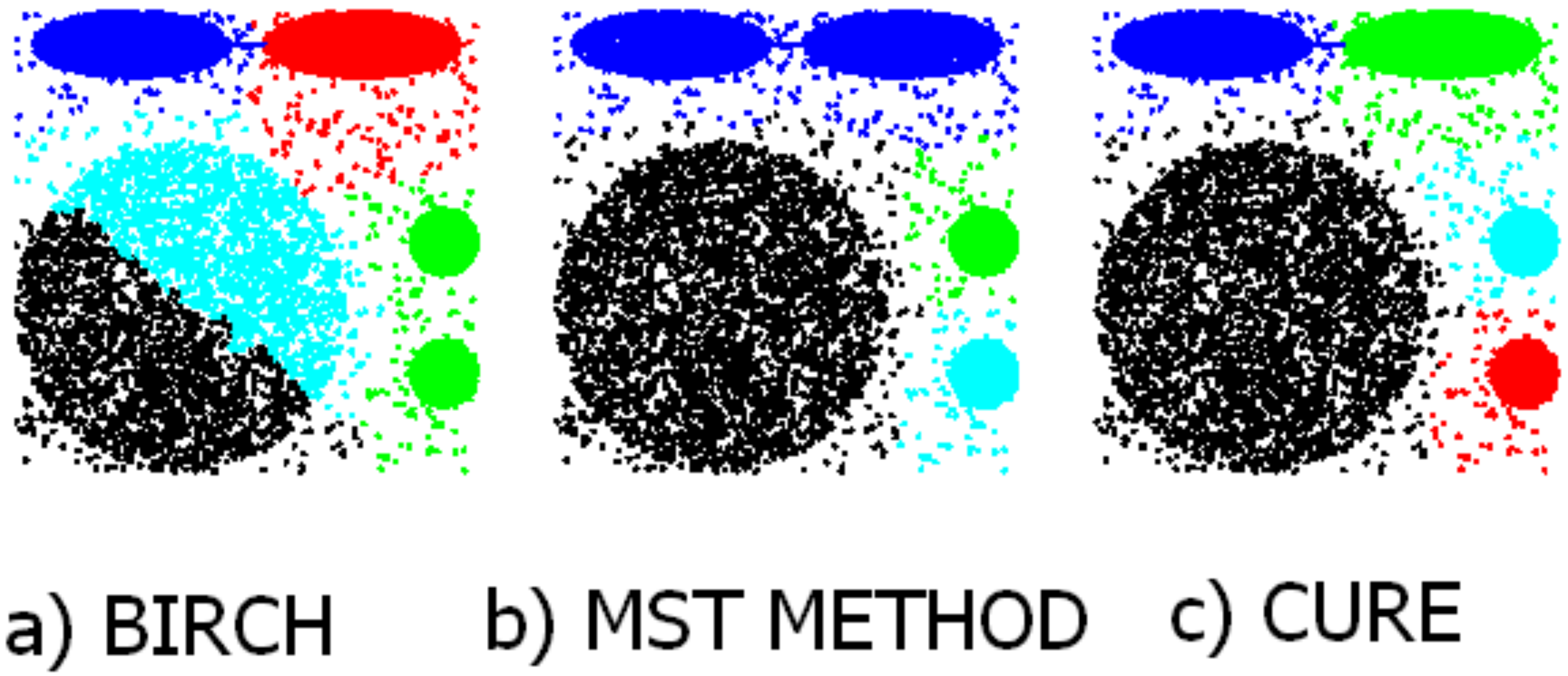
CURE Algorithm

- "Shrink" **representative points** toward the center of the cluster by a factor, α

- Cluster **similarity** is the similarity of the **closest pair** of representative points from different clusters

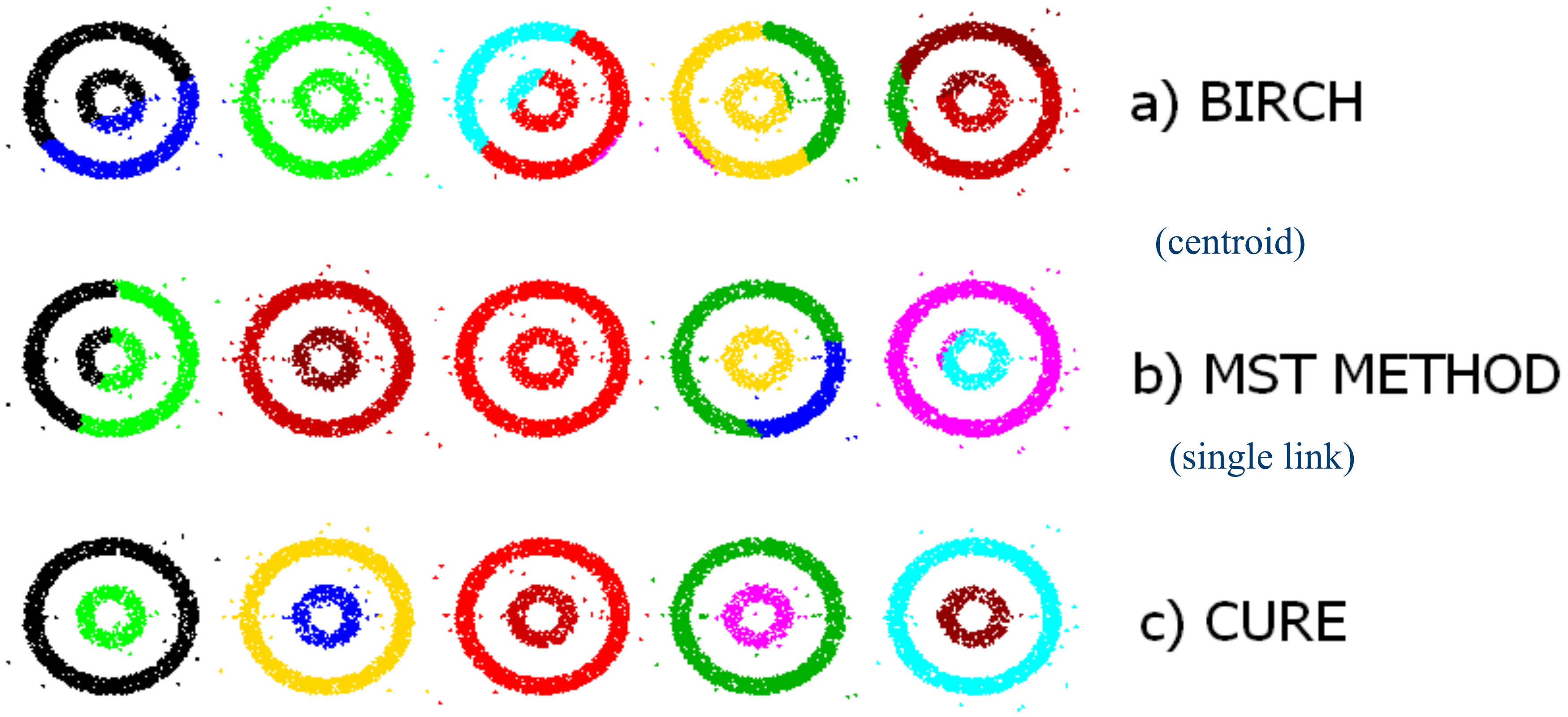
- CURE is better able to handle clusters of arbitrary shapes and sizes

Experimental Results: **CURE**



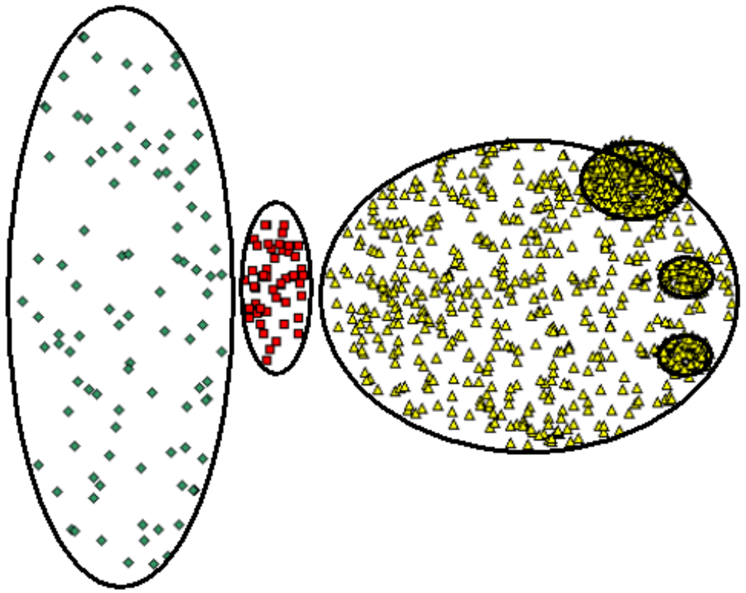
Picture from CURE, Guha, Rastogi, Shim.

Experimental Results: **CURE**

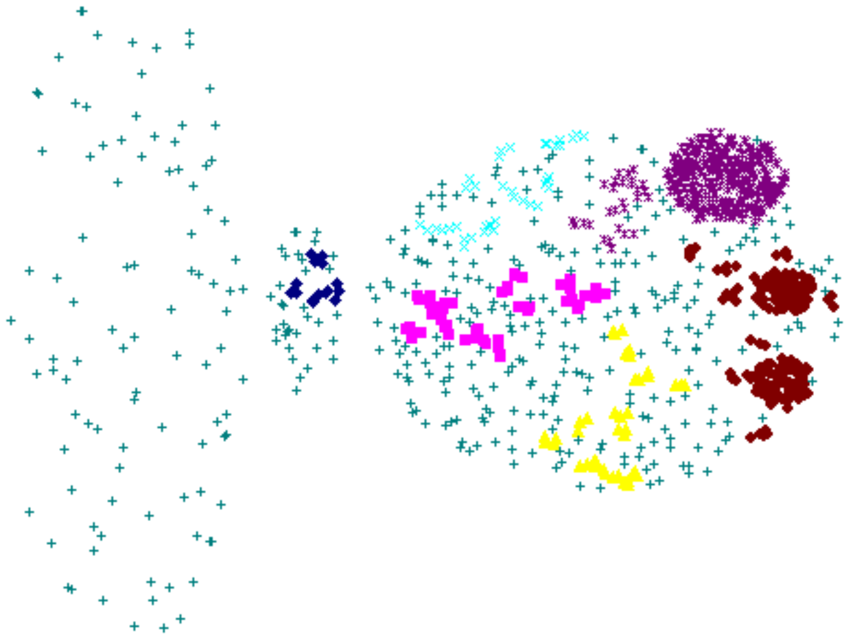


Picture from CURE, Guha, Rastogi, Shim.

CURE Cannot Handle Differing Densities



Original Points



CURE

Graph-Based Clustering: General Concepts

- 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 in graph terms

- In the simplest case, clusters are connected components in the graph.

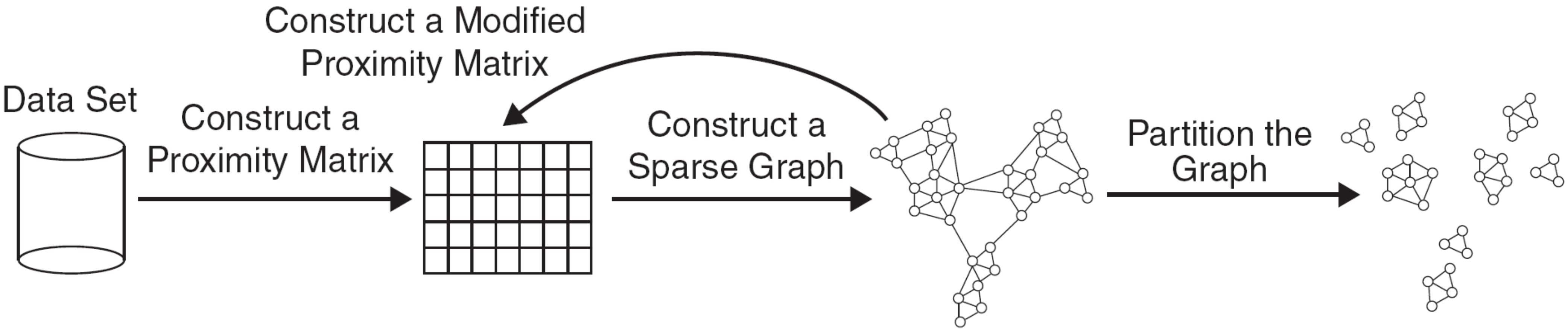
Graph-Based Clustering: Sparsification

- 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



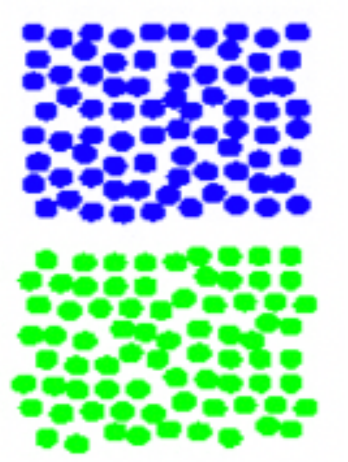
Limitations of Current Merging Schemes

- 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

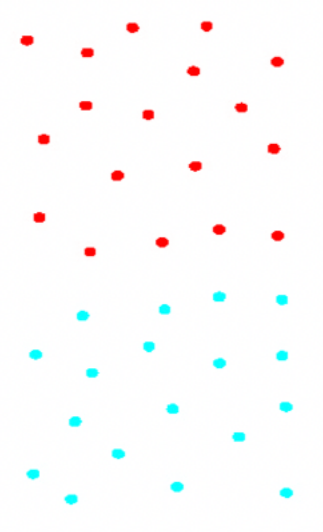
(a)

(b)



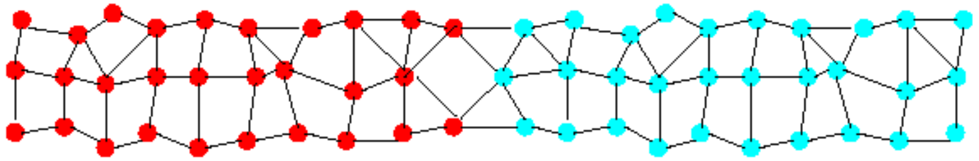
(a)

(b)

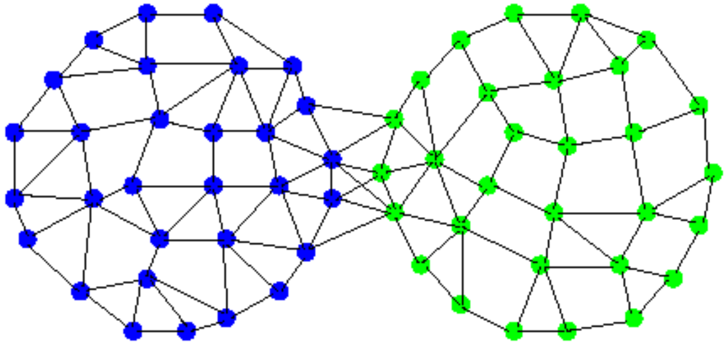


Closeness schemes will merge (a) and (b)

Limitations of Current Merging Schemes



(c) (d)



(c) (d)

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

Chameleon: Clustering Using Dynamic Modeling

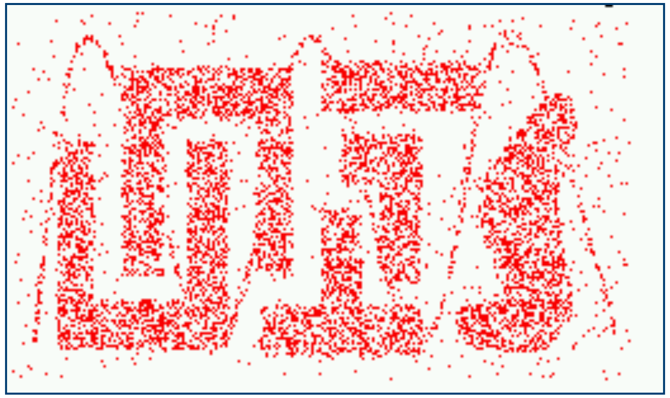
- Adapt to the characteristics of the data set to find the natural clusters
- Use a dynamic model to measure the similarity between clusters
  - Main property is the relative closeness and relative inter-connectivity of the cluster
  - Two clusters are combined if the resulting cluster shares certain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

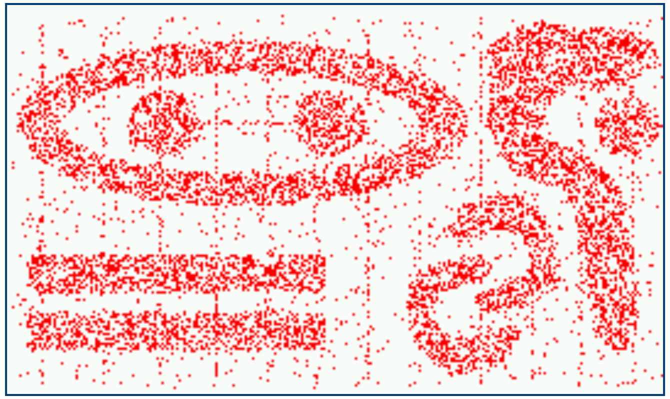
- One of the areas of application is spatial data

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

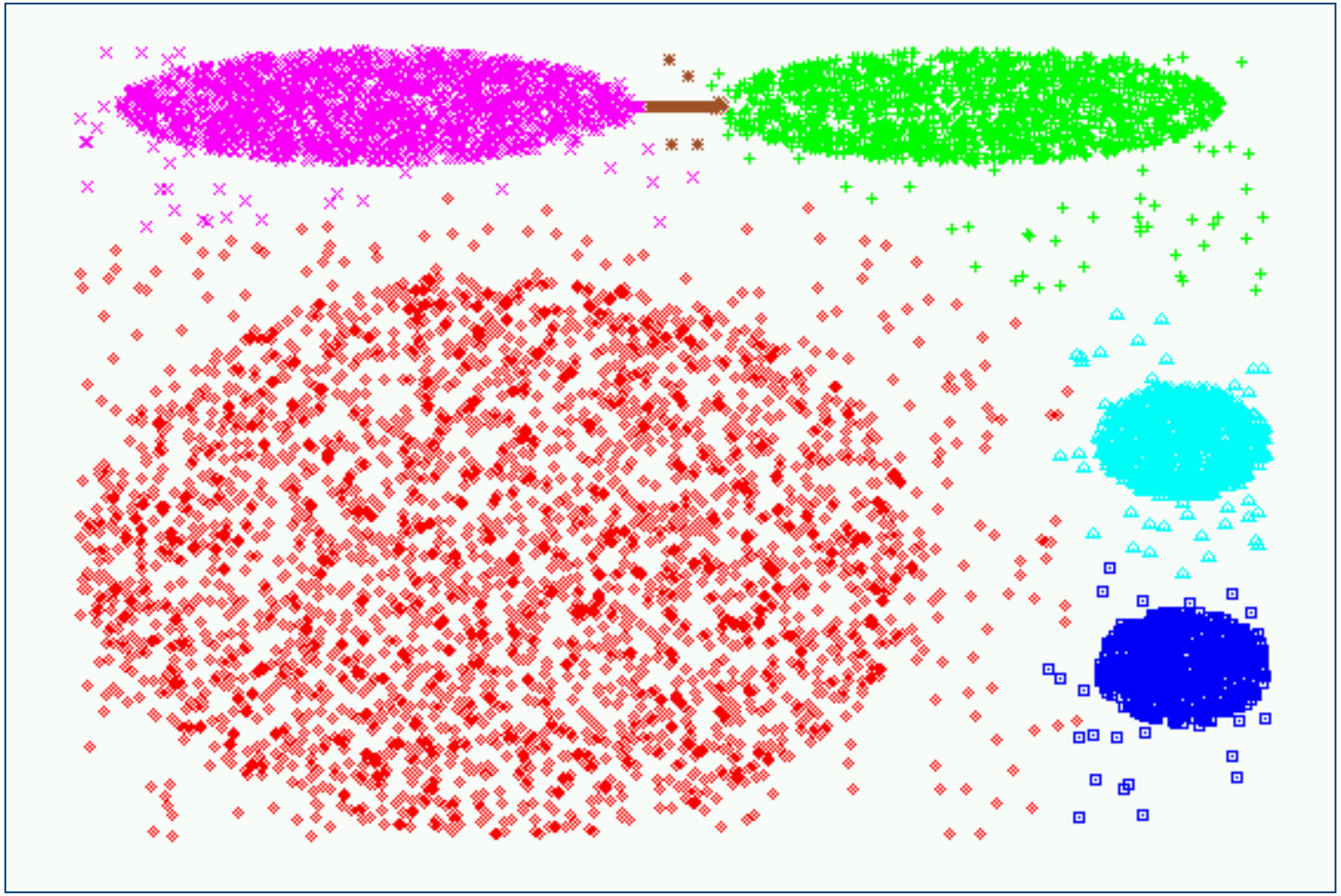
- Preprocessing Step: Represent the data by a Graph
  - Given a set of points, construct the k-nearest-neighbor (k-NN) graph to capture the relationship between a point and its k nearest neighbors
  - Concept of neighborhood is captured dynamically (even if region is sparse)

- 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., be a sub-cluster of a “real” cluster

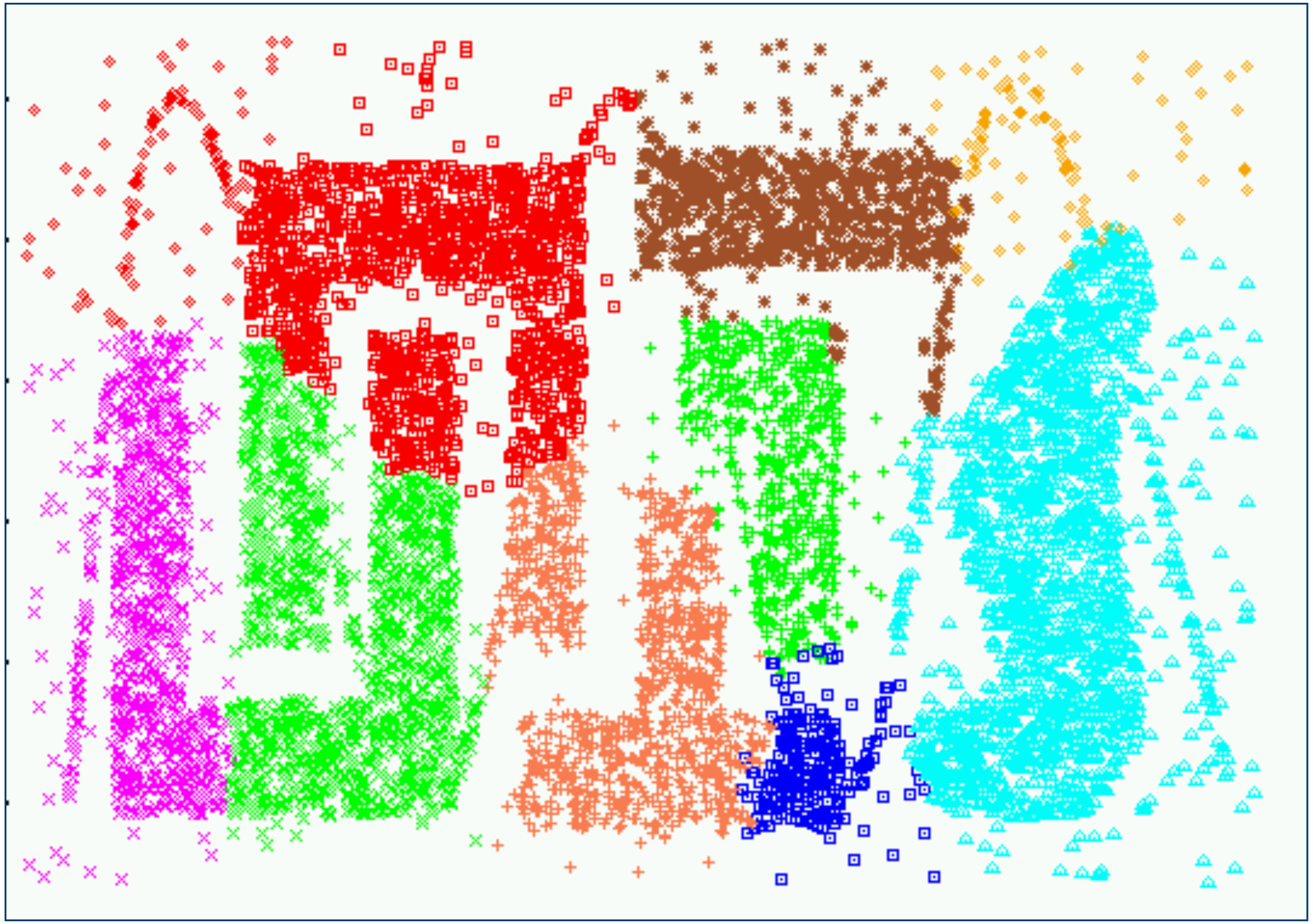
Chameleon: Steps …

- 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

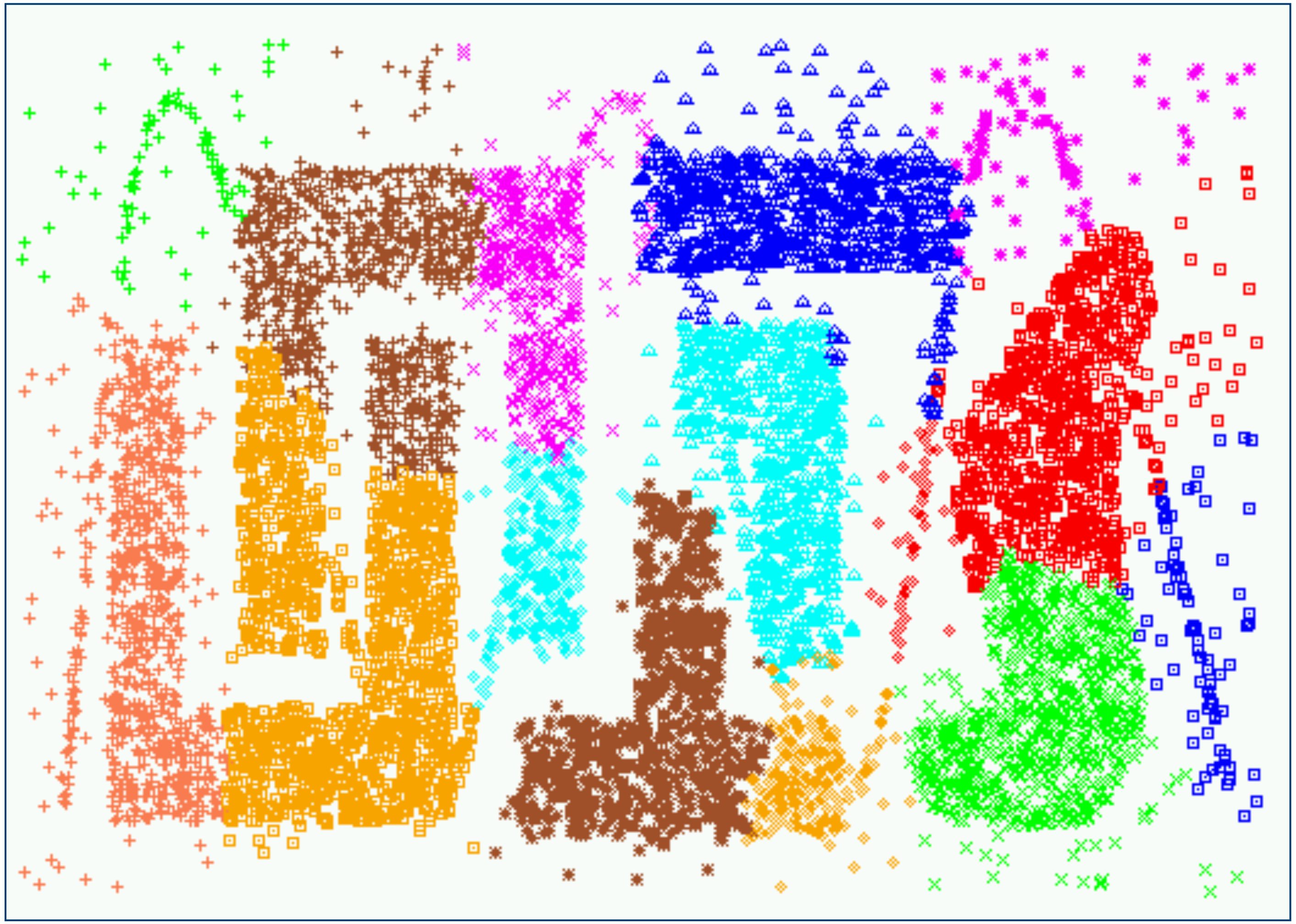
Experimental Results: CHAMELEON



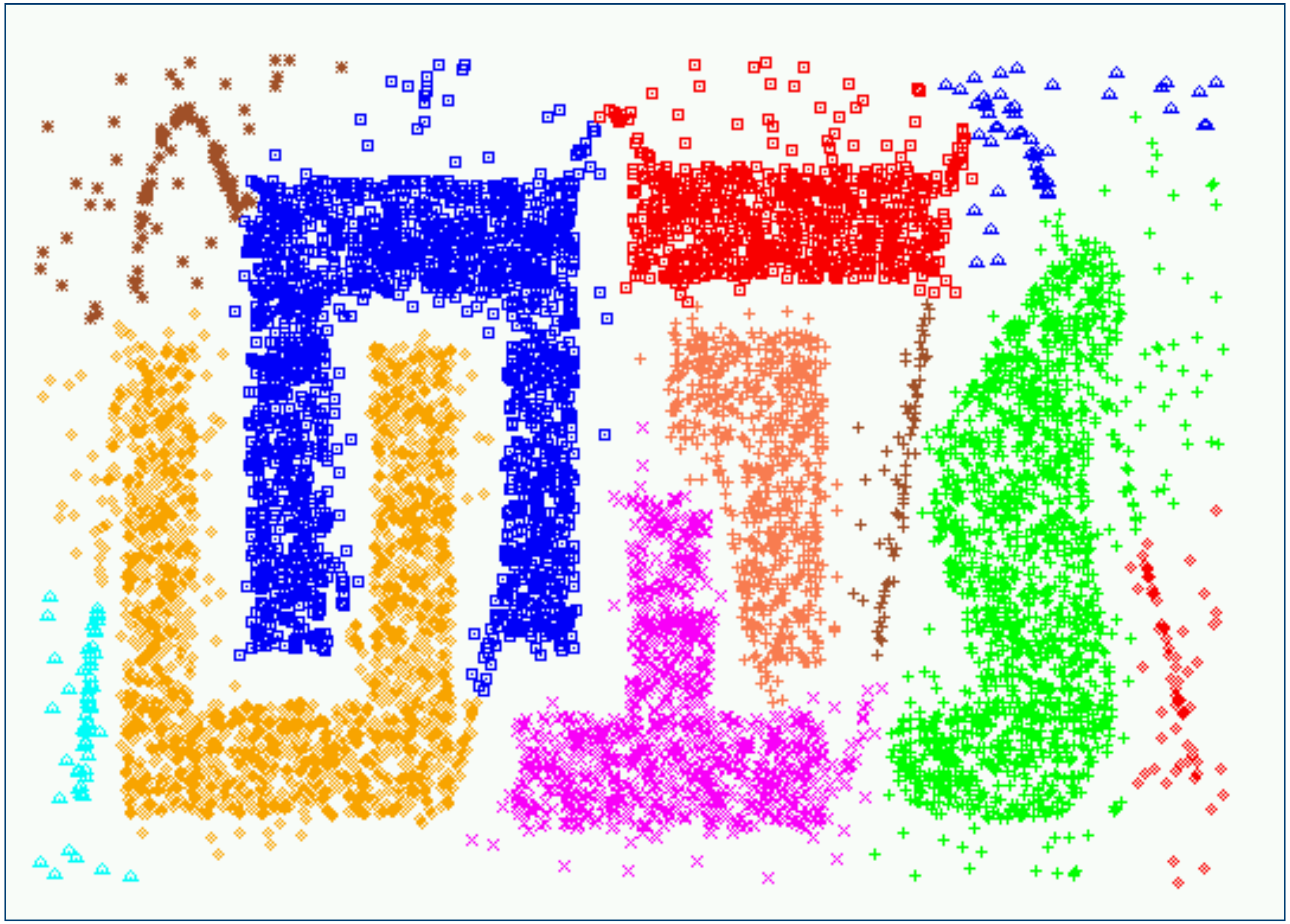
Experimental Results: CURE (10 clusters)



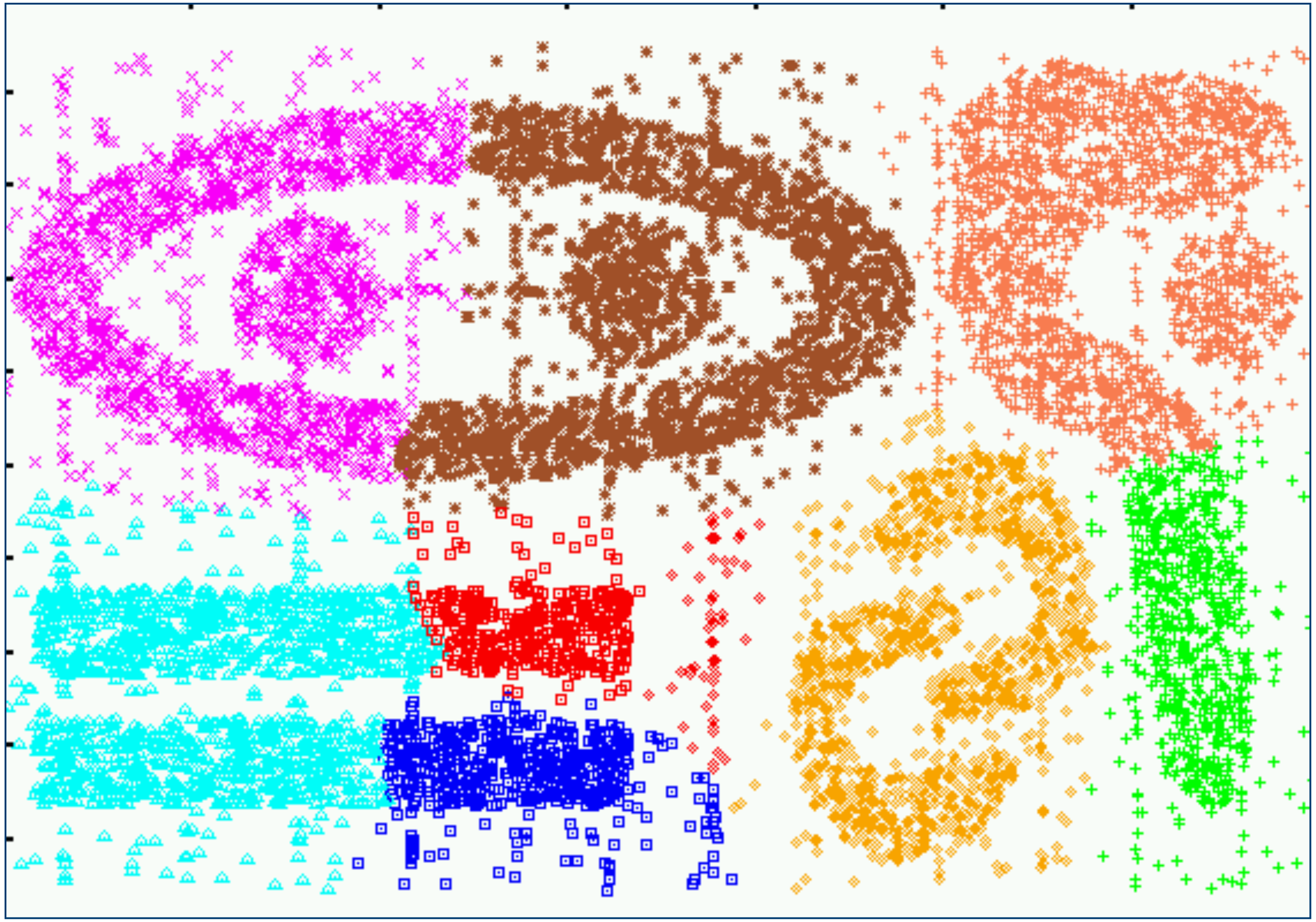
Experimental Results: CURE (15 clusters)



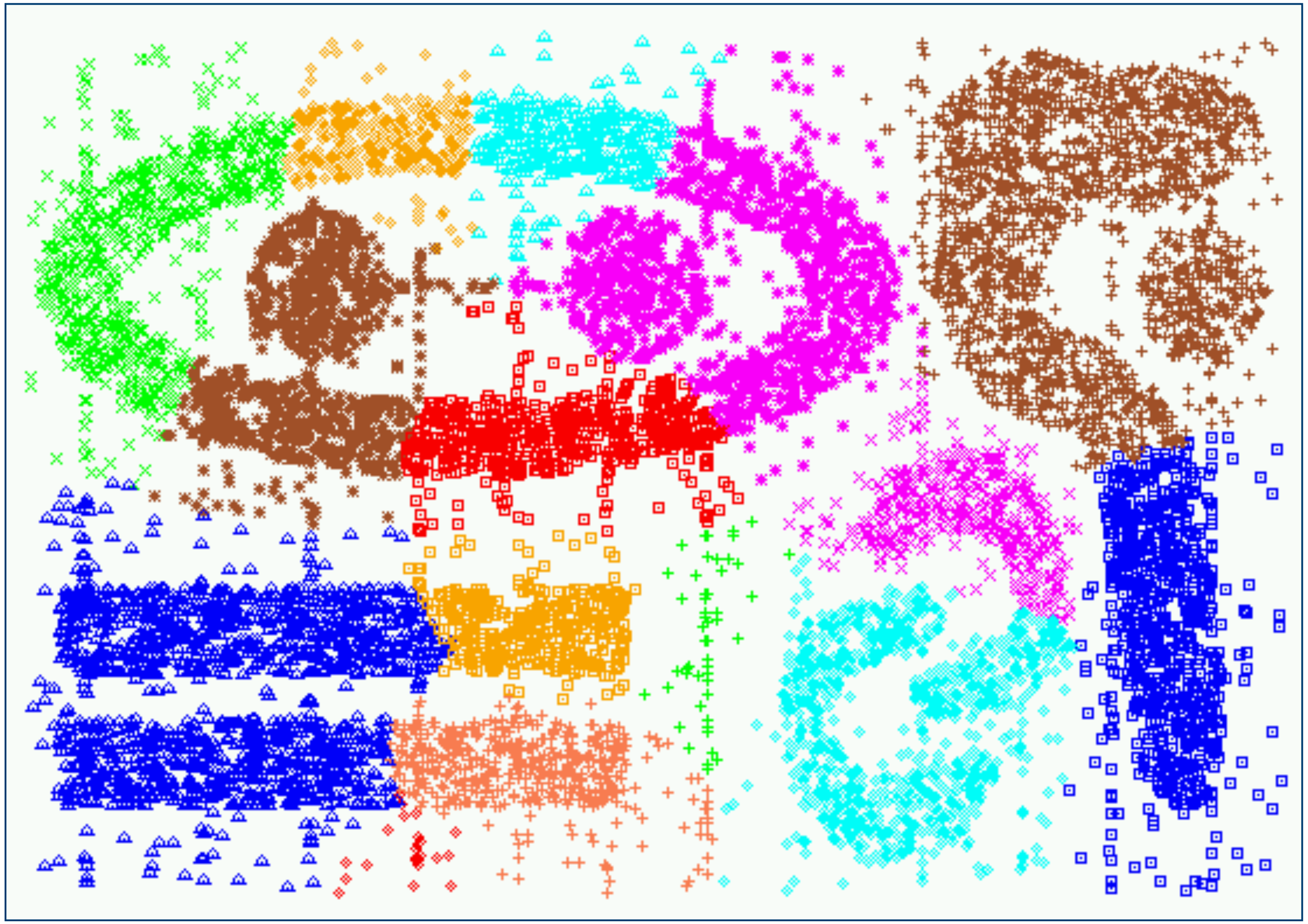
Experimental Results: CHAMELEON



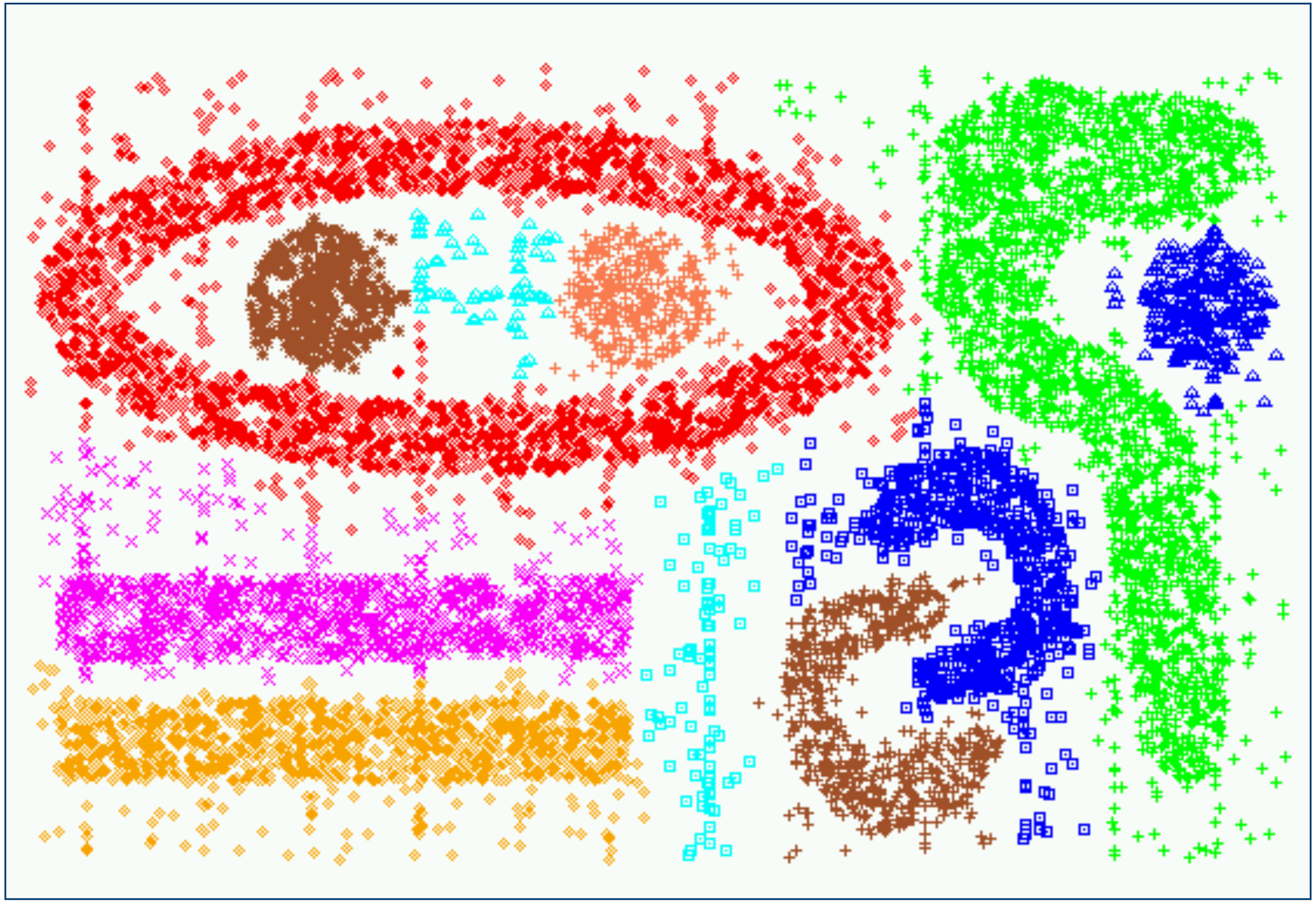
Experimental Results: CURE (9 clusters)



Experimental Results: CURE (15 clusters)

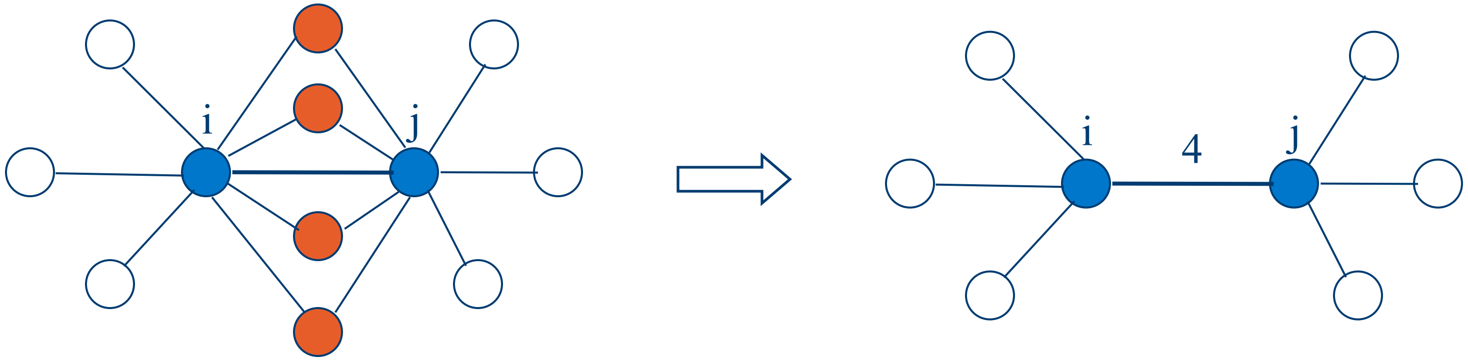


Experimental Results: CHAMELEON

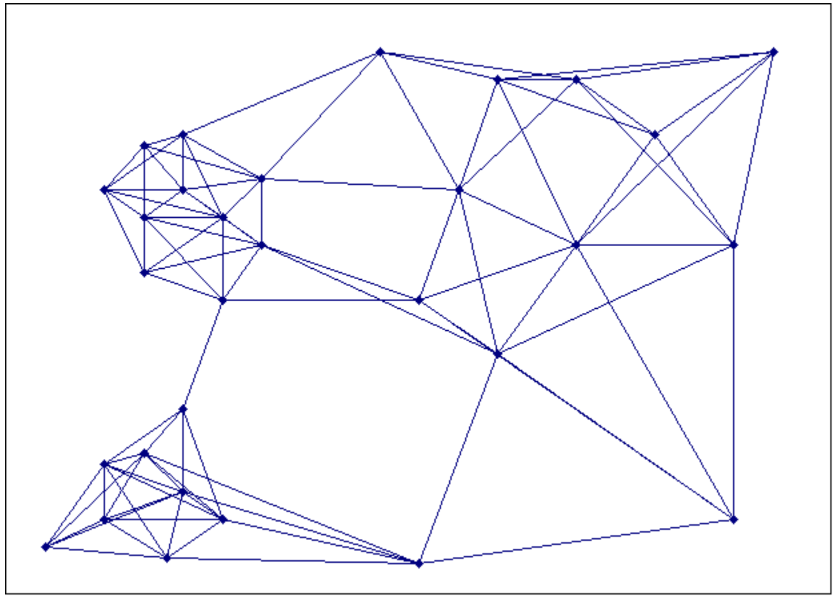


Graph-Based Clustering: SNN Approach

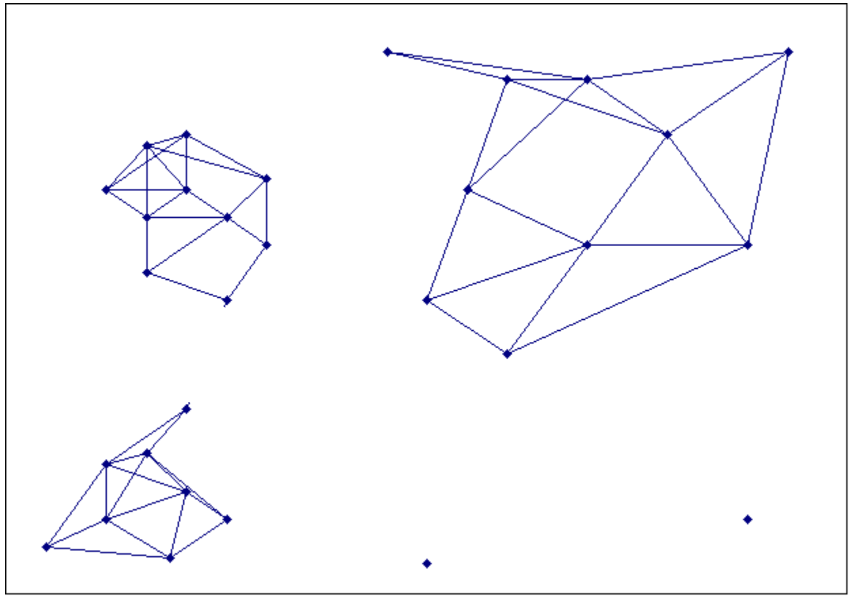
- Shared Nearest Neighbor (SNN) graph: the weight of an edge is the number of shared neighbors between vertices given that the vertices are connected



Creating the SNN Graph



Sparse Graph



Shared Near Neighbor Graph

Link weights are similarities between neighboring points

Link weights are **number of Shared Nearest** Neighbors

Example: SNN Similarity

- Given the following proximity matrix between 6 data points, calculate the Shared near neighbor similarity matrix with K=2 and K=3.

	A	B	C	D	E	F
A	1.000	**0.809**	**0.874**	**0.697**	**0.681**	**0.696**
B	**0.809**	1.000	0.746	**0.673**	0.590	0.594
C	**0.874**	**0.746**	1.000	0.603	**0.680**	**0.771**
D	0.697	0.673	0.603	1.000	0.514	0.543
E	0.681	0.590	0.680	0.514	1.000	0.622
F	0.696	0.594	**0.771**	0.543	0.622	1.000

K=2

	1st NN	2nd NN
A	C	B
B	A	C
C	A	F
D	A	B
E	A	C
F	C	A

	A	B	C	D	E	F
A	0	1	0	0	0	0
B		0	0	0	0	0
C			0	0	0	1
D				0	0	0
E					0	0
F						0

Example: SNN similarity (cont')

- K=3

	1st NN	2nd NN	3rd NN
A	C	B	D
B	A	C	D
C	A	F	B
D	A	B	C
E	A	C	F
F	C	A	E

	A	B	C	D	E	F
A	0	2	1	2	0	0
B		0	1	2	0	0
C			0	0	0	1
D				0	0	0
E					0	2
F						0

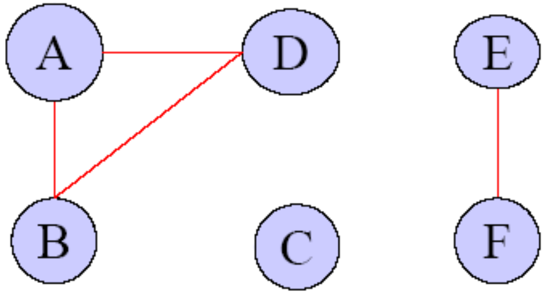
Jarvis-Patrick Clustering

- 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 k=20 and put points in the same cluster if they share more than T=10 near neighbors
- Jarvis-Patrick clustering is too brittle

Example: Jarvis-Patrick Clustering

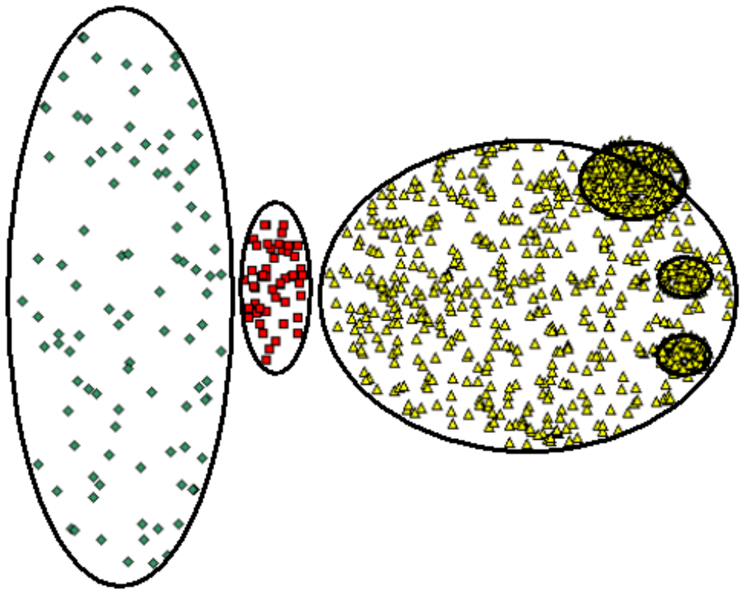
- Jarvis-Patrick Clustering for K=3 and T=2

	A	B	C	D	E	F
A	0	2	1	2	0	0
B		0	1	2	0	0
C			0	0	0	1
D				0	0	0
E					0	2
F						0

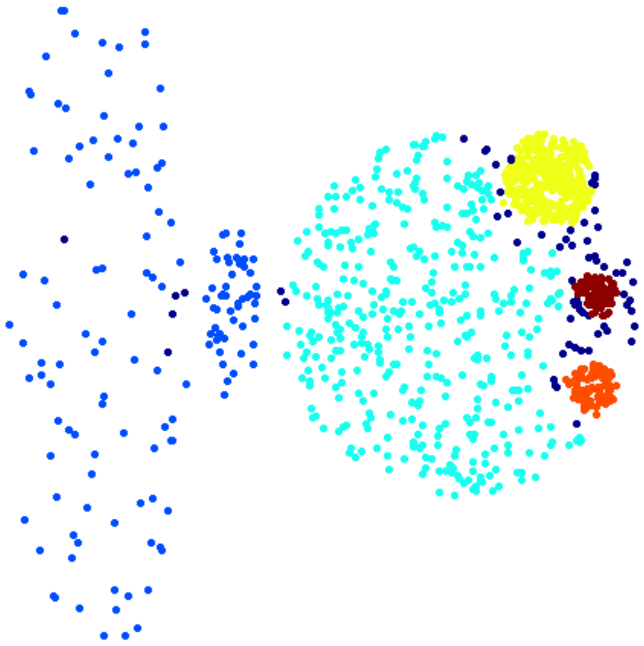


- Thus, three clusters are obtained: {A, B, D}, {C}, {E, F}

When Jarvis-Patrick Works Reasonably Well



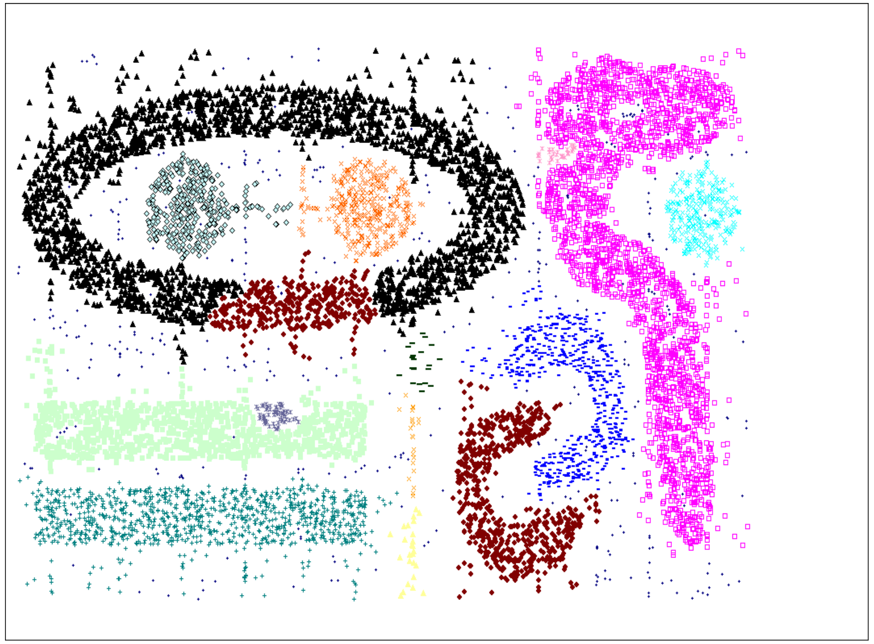
Original Points



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 Density-Based Clustering

- Combines:
  - Graph based clustering (similarity definition based on number of shared nearest neighbors)
  - Density based clustering (DBSCAN-like approach)

- SNN density measures whether a point is surrounded by similar points (with respect to its nearest neighbors)

SNN Density-Based Clustering

1. 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

2. 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

3. 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)

4. 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 Density-Based Clustering…

5. **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*

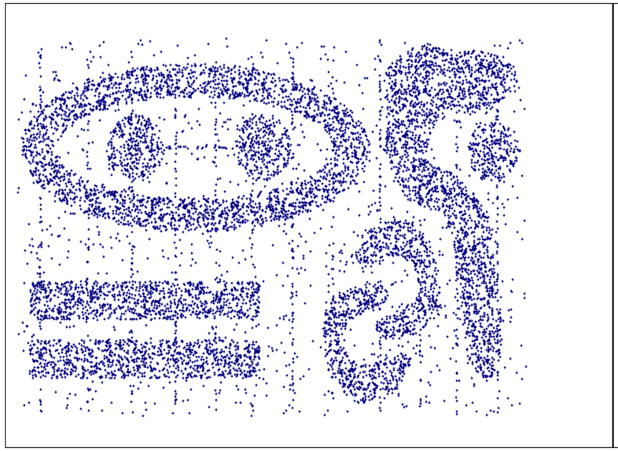
6. **Form clusters from the core points**
   If two core points are within a "radius", *Eps*, of each other they are placed in the same cluster

7. **Discard all noise points**
   All non-core points that are not within a "radius" of *Eps* of a core point are discarded

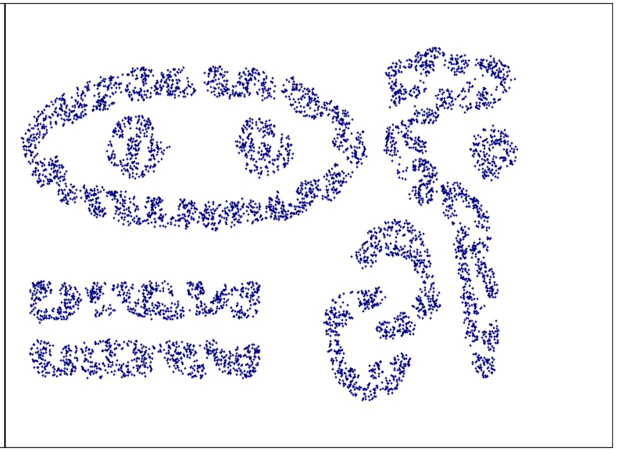
8. **Assign all non-noise, non-core points to clusters**
   This can be done by assigning such points to the nearest core point

(Note that steps 4-8 are DBSCAN)

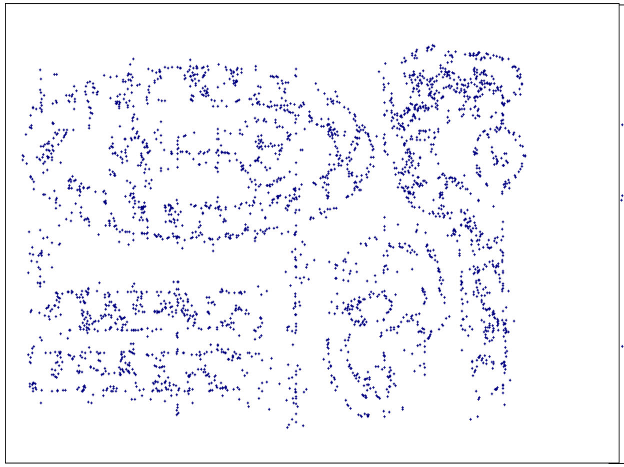
SNN Density



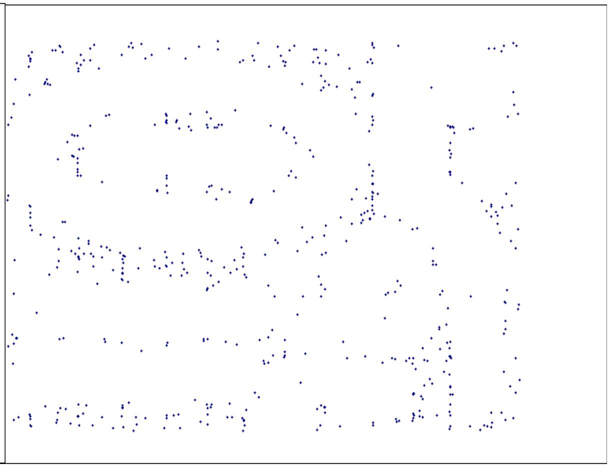
a) All Points



b) High SNN Density

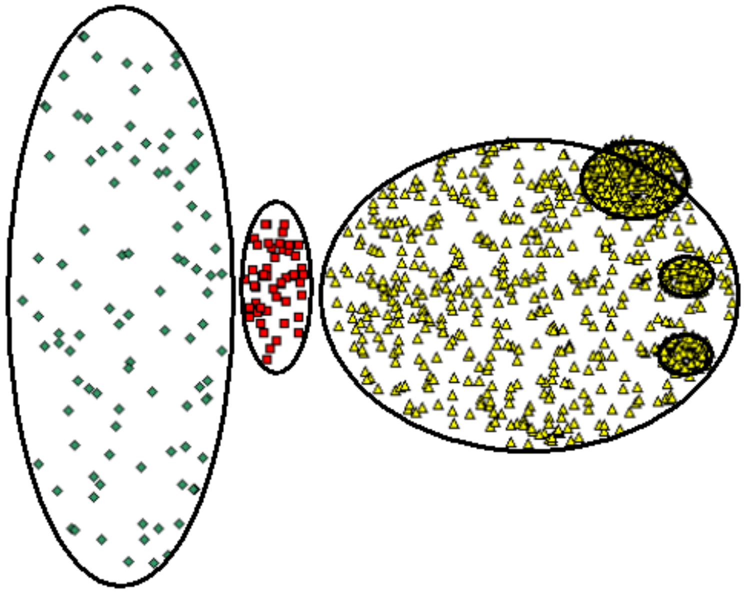


c) Medium SNN Density

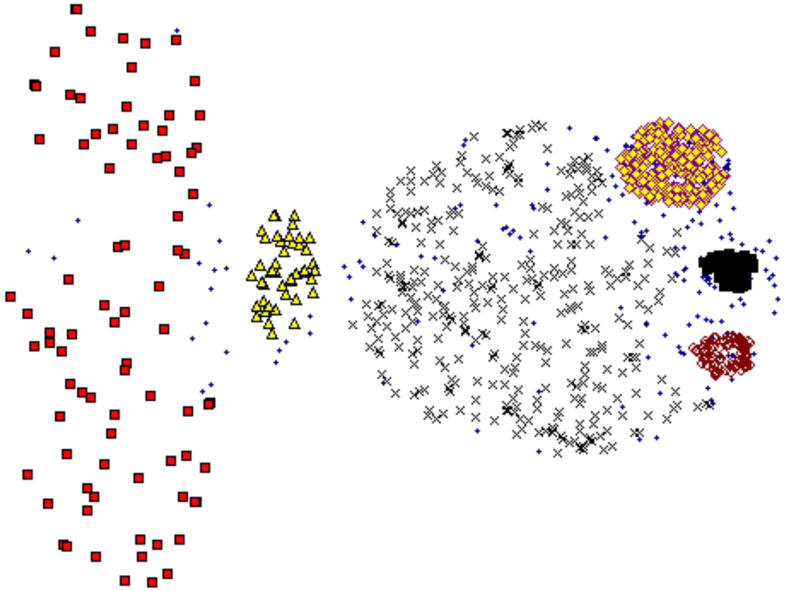


d) Low SNN Density

SNN Clustering Can Handle Differing Densities

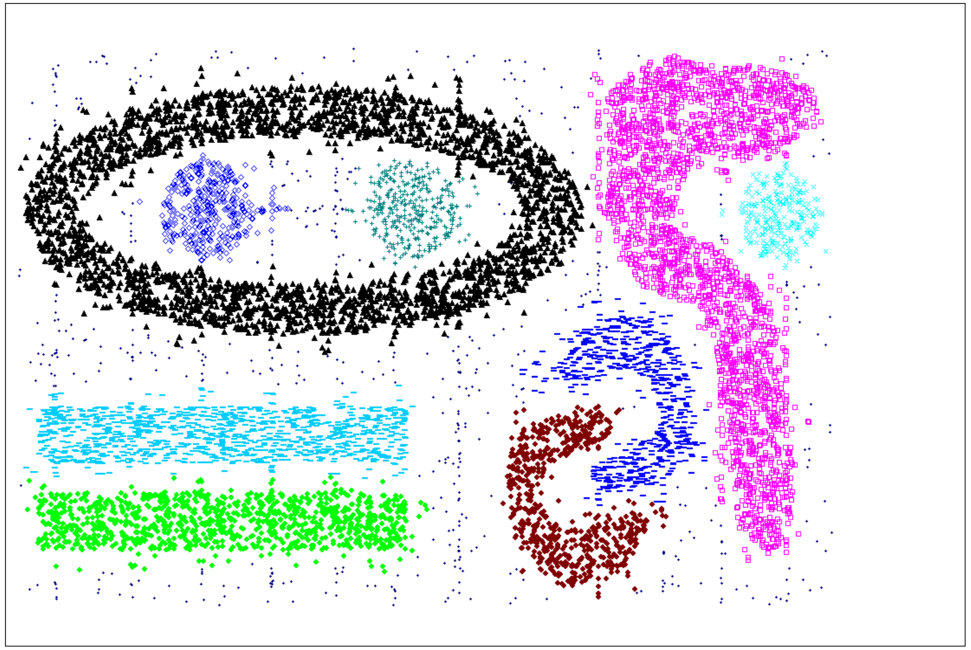


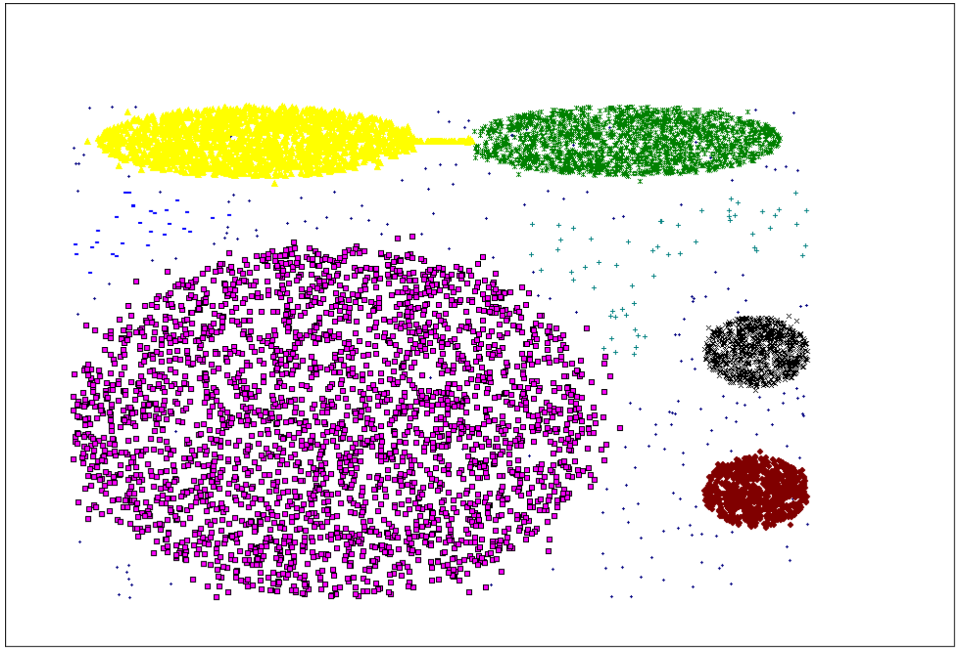
Original Points



SNN Clustering

SNN Clustering Can Handle Other Difficult Situations





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 $O(n^2)$
  - For lower dimensions, there are more efficient ways to find the nearest neighbors
    - R* Tree
    - k-d Trees

- Parameterization is not easy

Characteristics of Data, Clusters, and Clustering Algorithms

- A cluster analysis is affected by characteristics of
  - Data
  - Clusters
  - Clustering algorithms

- Looking at these characteristics gives us a number of dimensions that you can use to describe clustering algorithms and the results that they produce