More Clustering Algorithms

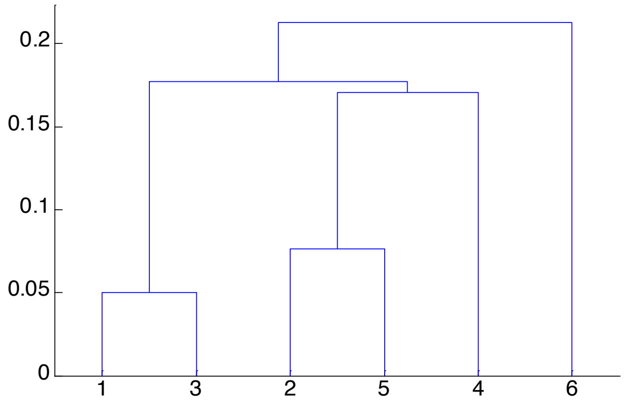
Blink Sakulkueakulsuk

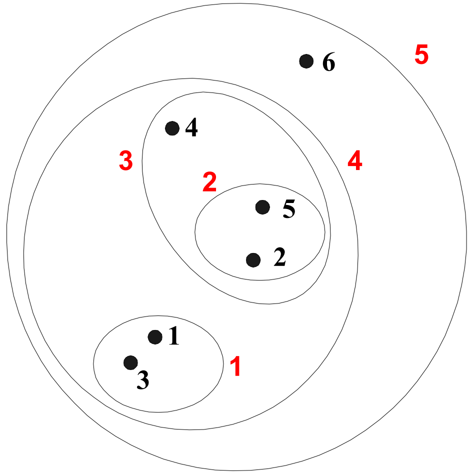
Hierarchical Clustering

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





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Strengths of Hierarchical Clustering

Do not have to assume any particular numbers of clusters

- Any desired number of clusters can be obtained by 'cutting' the dendrogram at the proper level

They may correspond to meaningful taxonomies

- Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

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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 an individual point (or there are k clusters)

Traditional hierarchical algorithms use a similarity or distance matrix

- Merge or split one cluster at a time

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Agglomerative Clustering Algorithm

Key Idea: Successively merge closest clusters

Basic algorithm

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

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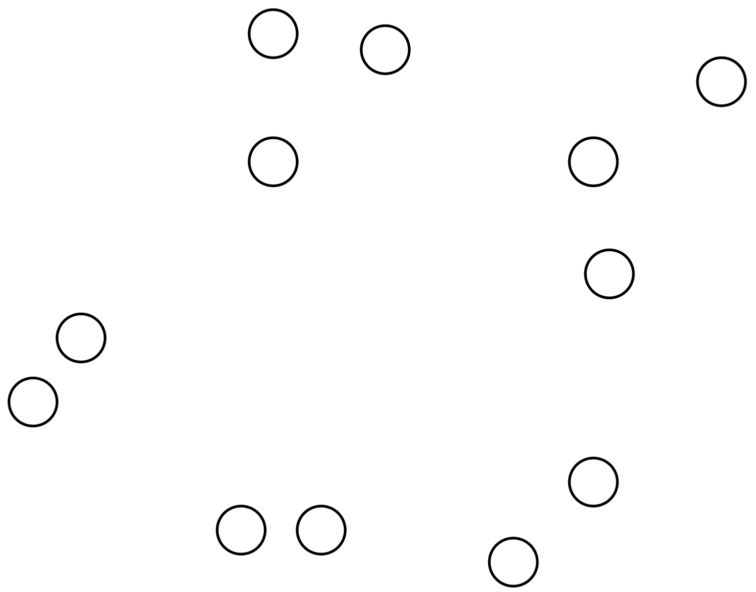
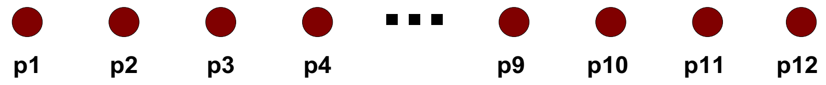
Steps 1 and 2

Start with clusters of individual points and a proximity matrix



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

Proximity Matrix



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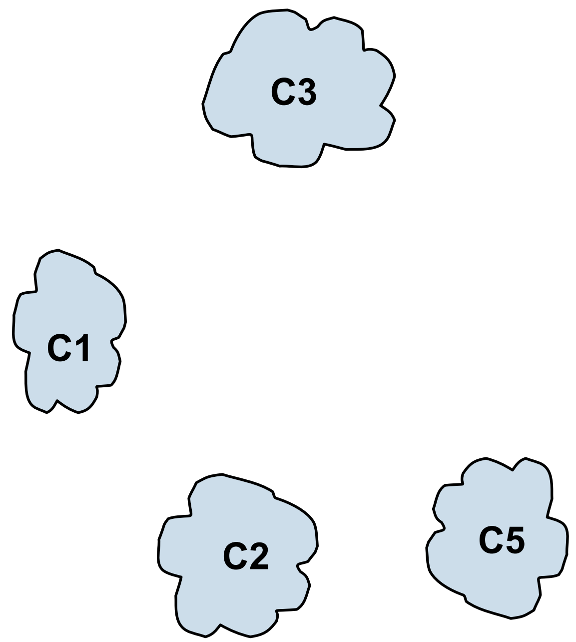
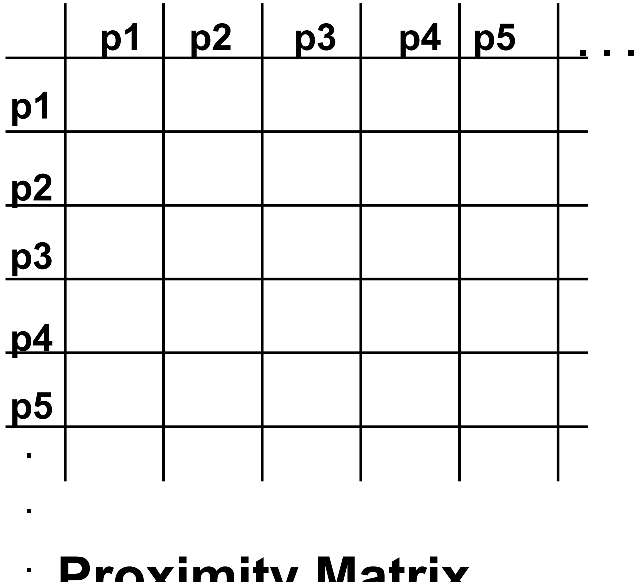
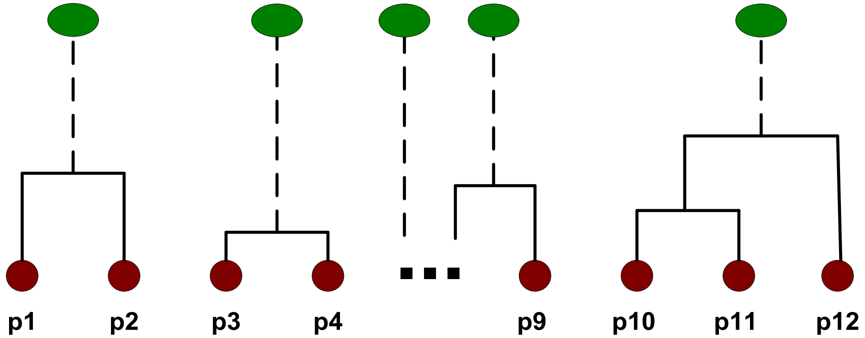
Intermediate Situation

After some merging steps, we have some clusters





Proximity Matrix



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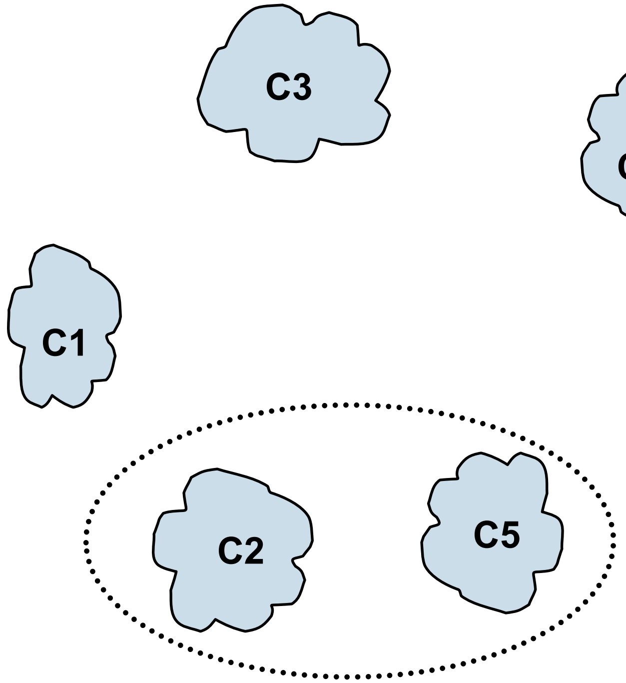
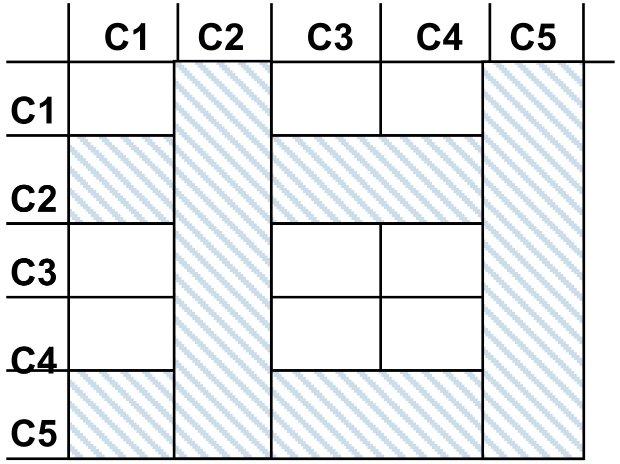
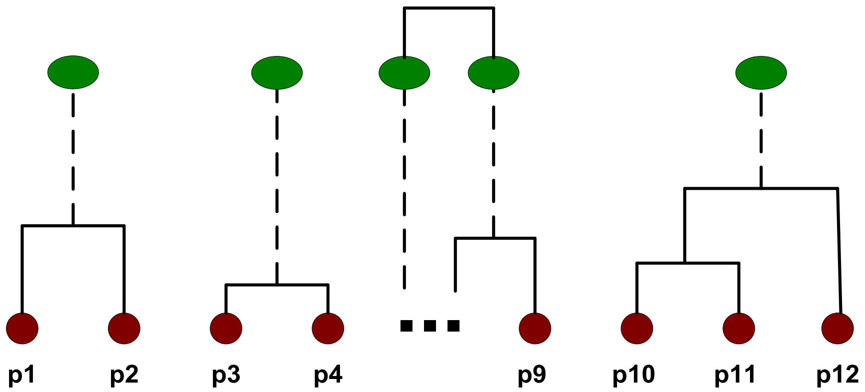
Step 4

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





Proximity Matrix



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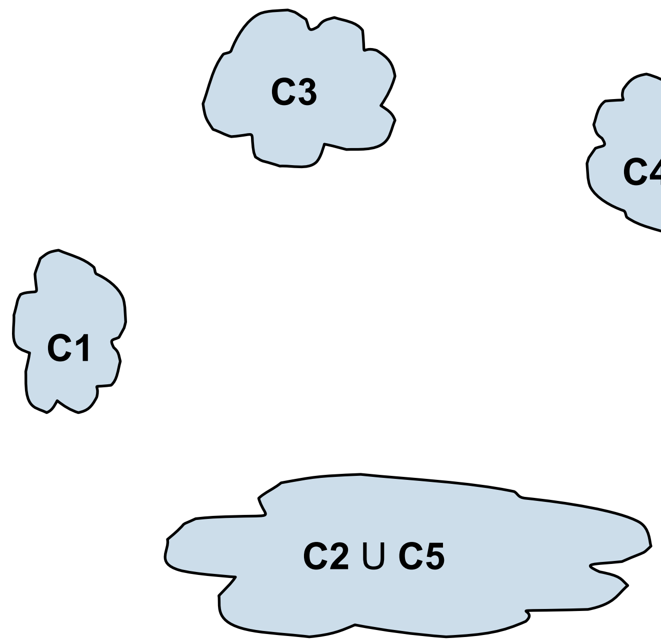
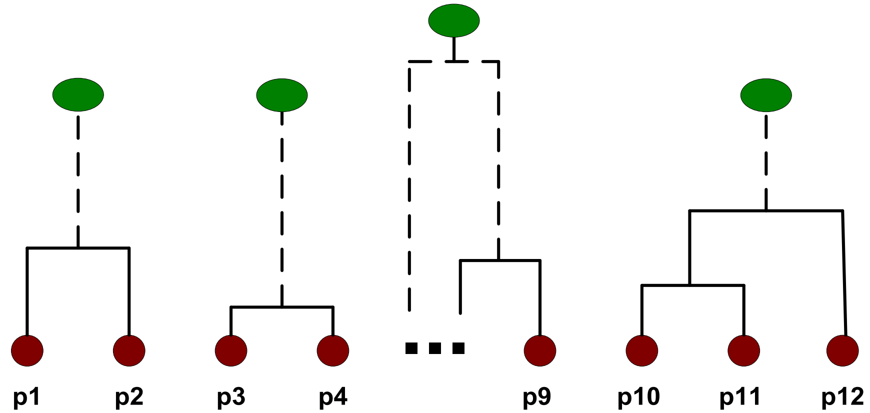
Step 5

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



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

Proximity Matrix



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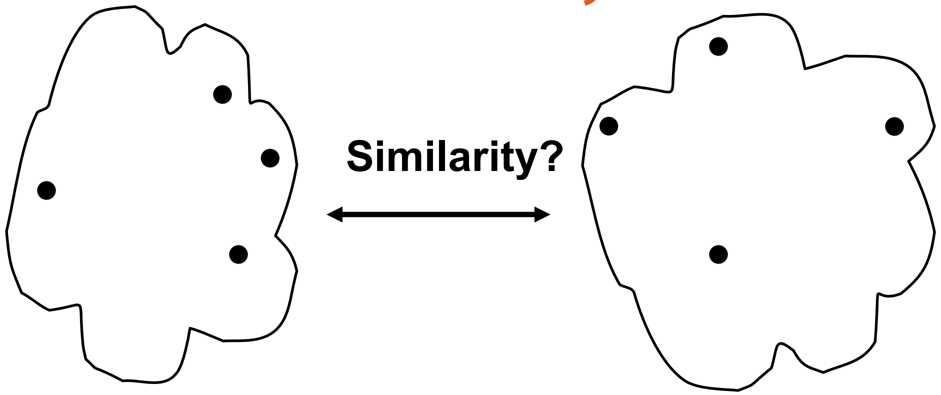
Defining Inter-Cluster Similarity



	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

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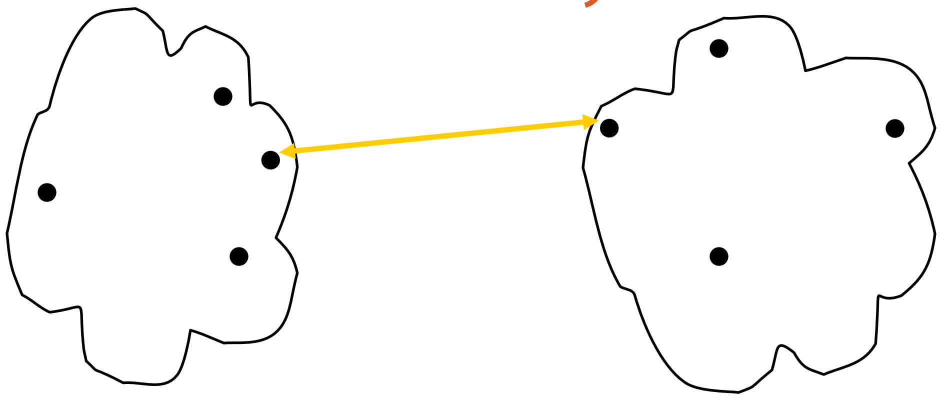

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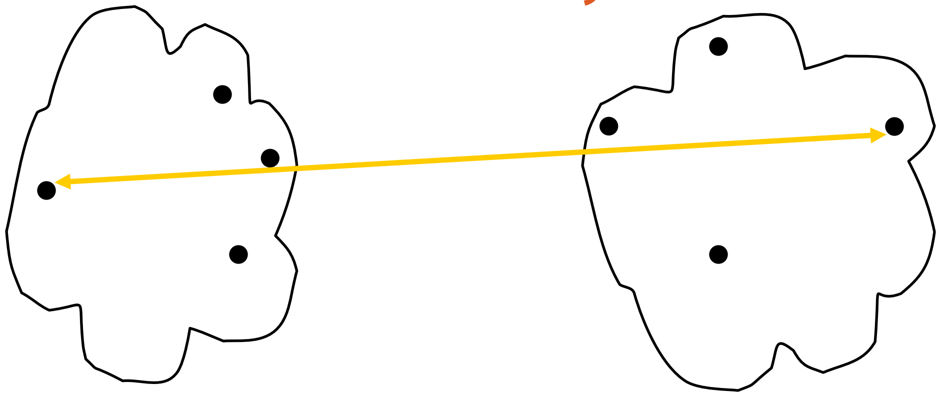

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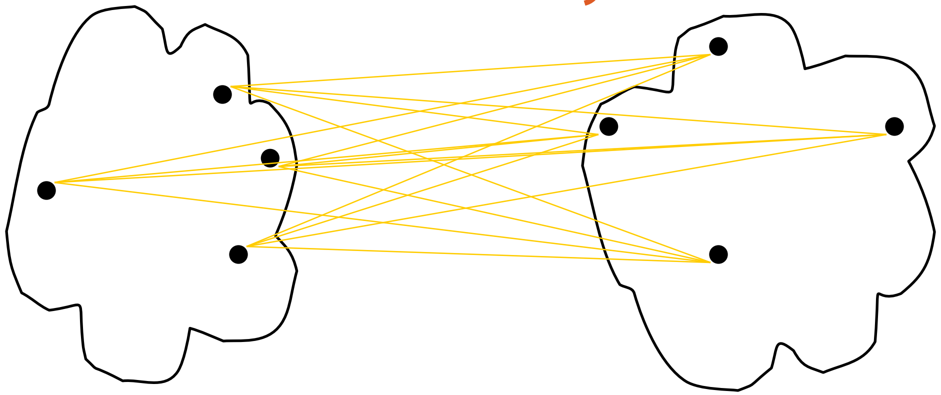

	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
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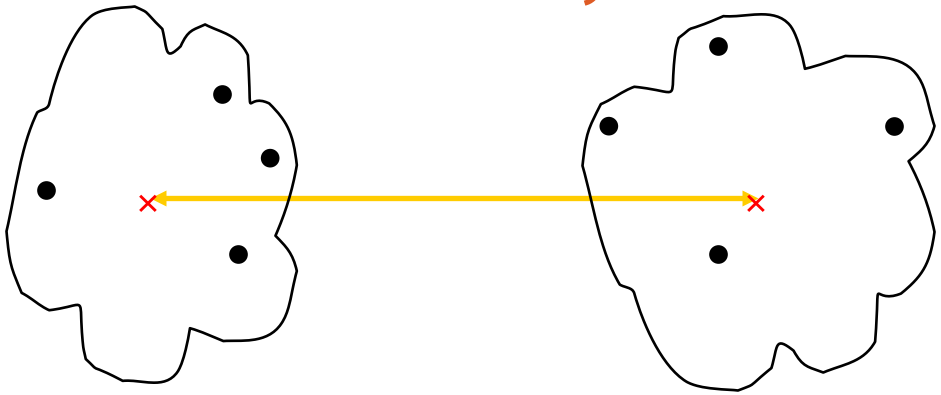
Defining Inter-Cluster Similarity



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p1						
p2						
p3						
p4						
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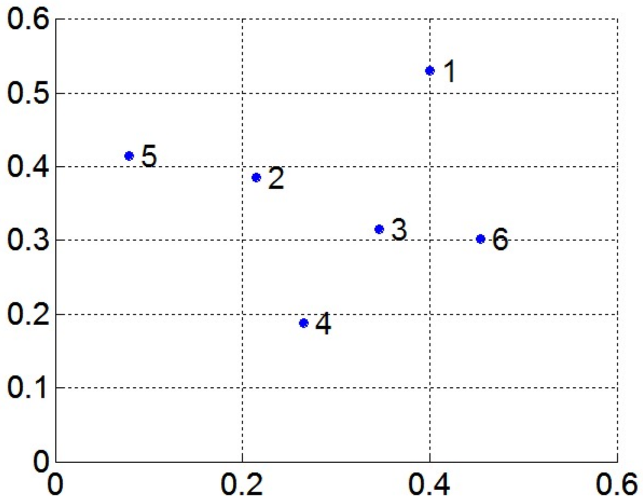
MIN or Single Link

Proximity of two clusters is based on the two closest points in the different clusters

- Determined by one pair of points, i.e., by one link in the proximity graph

Example:



Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

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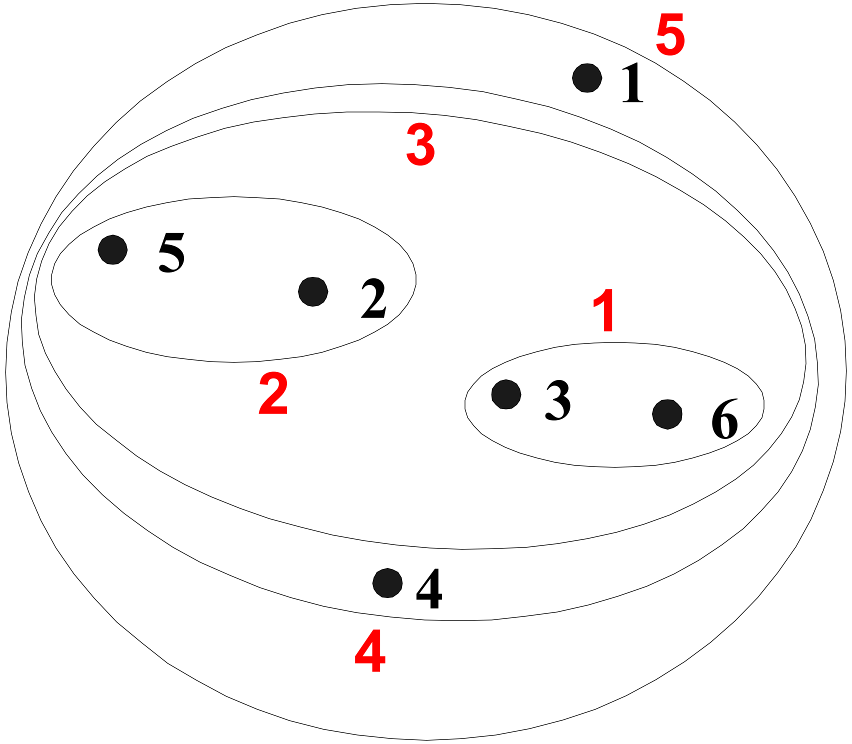
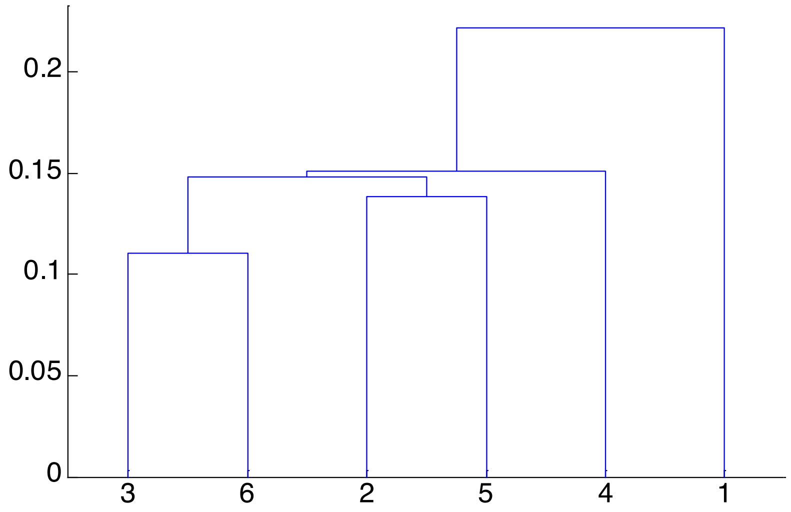
MIN or Single Link



Nested Clusters



Dendrogram

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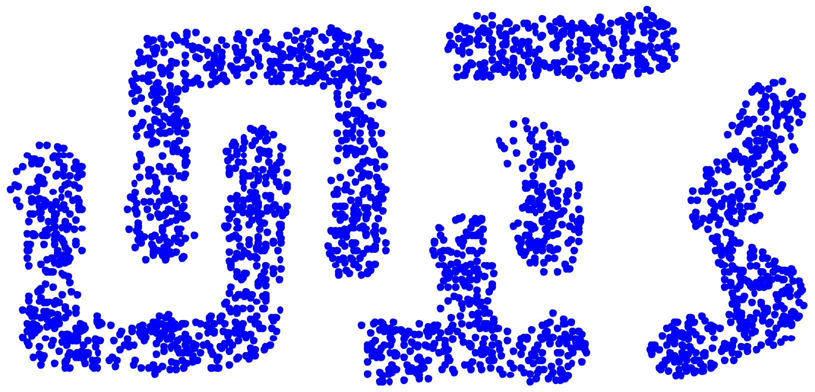
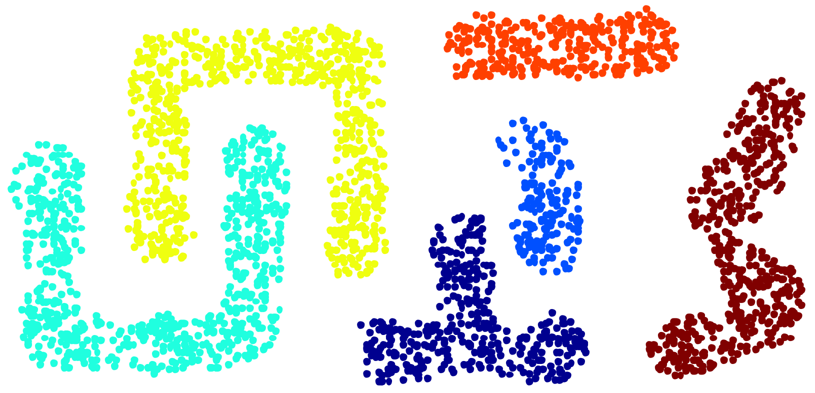
Strength of MIN



Original Points



Six Clusters

- **Can handle non-elliptical shapes**

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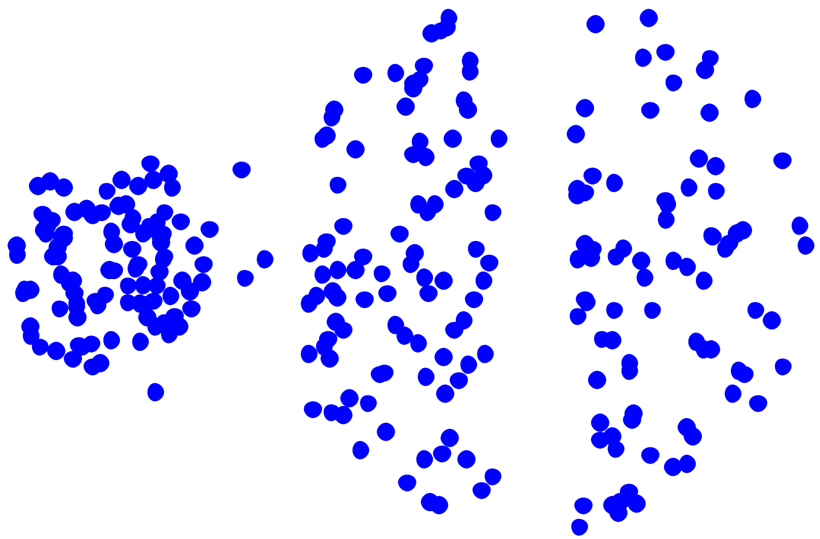
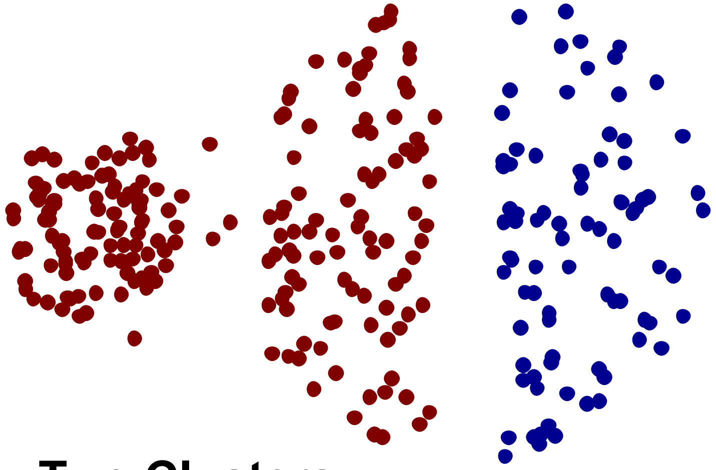
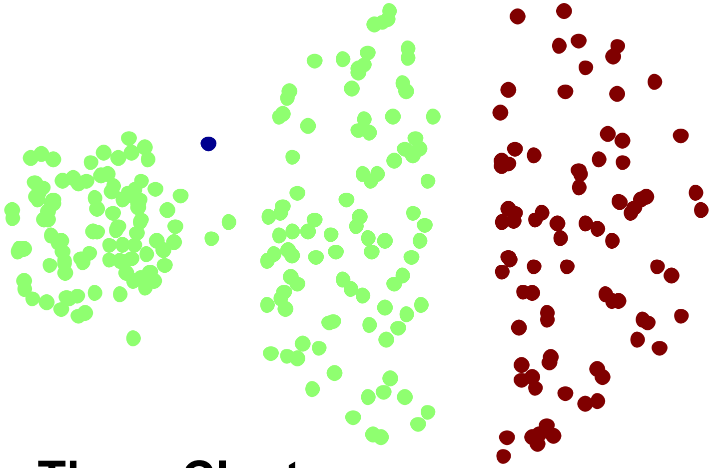
Limitations of MIN



Original Points



Two Clusters



Three Clusters

- **Sensitive to noise**

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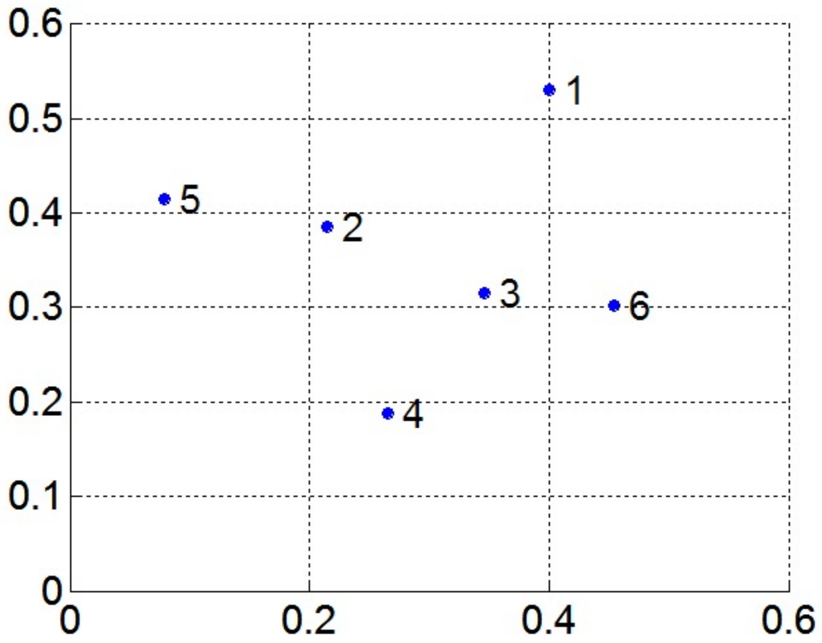
MAX or Complete Linkage

Proximity of two clusters is based on the two most distant points in the different clusters

- ints in the two clusters



Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

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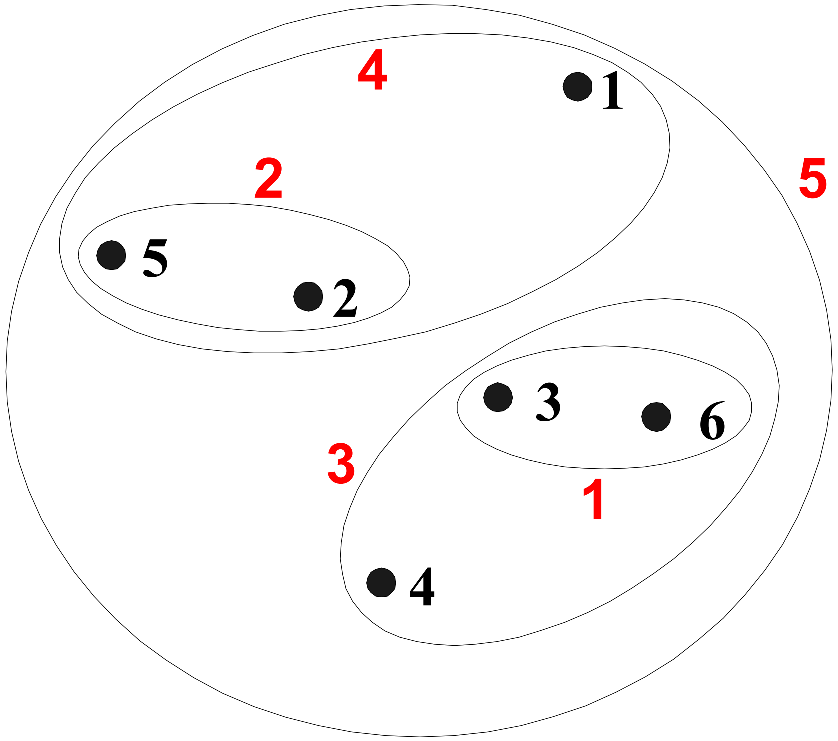
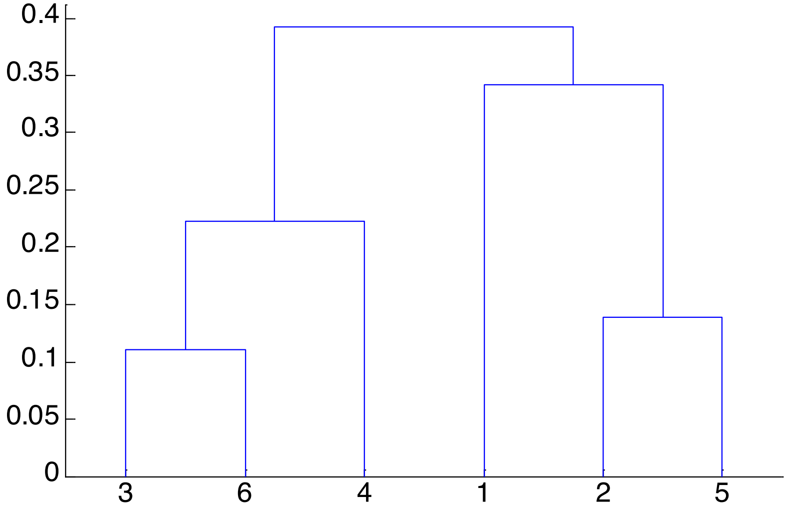
Hierarchical Clustering: MAX



Nested Clusters



Dendrogram

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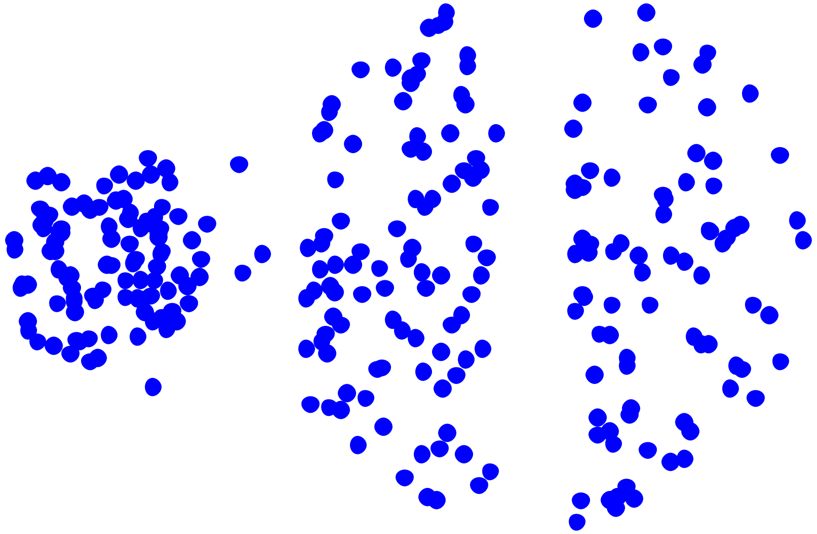
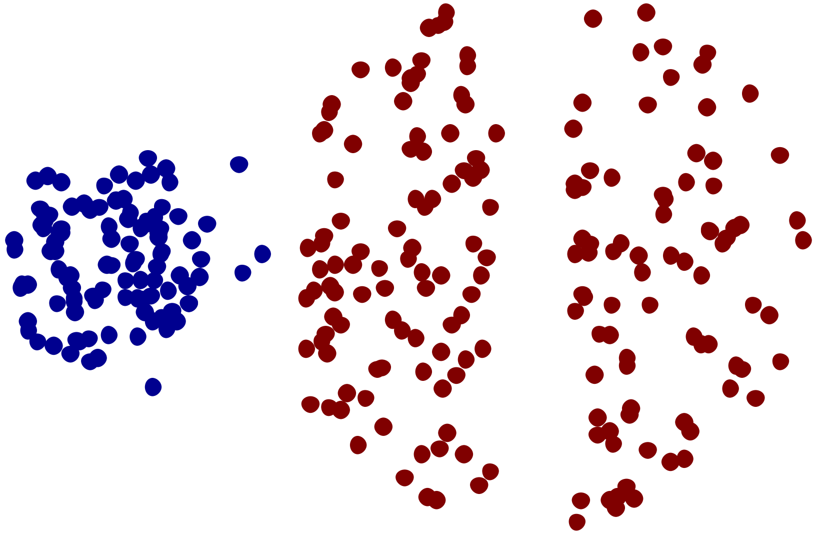
Strength of MAX



Original Points



Two Clusters

- **Less susceptible to noise**

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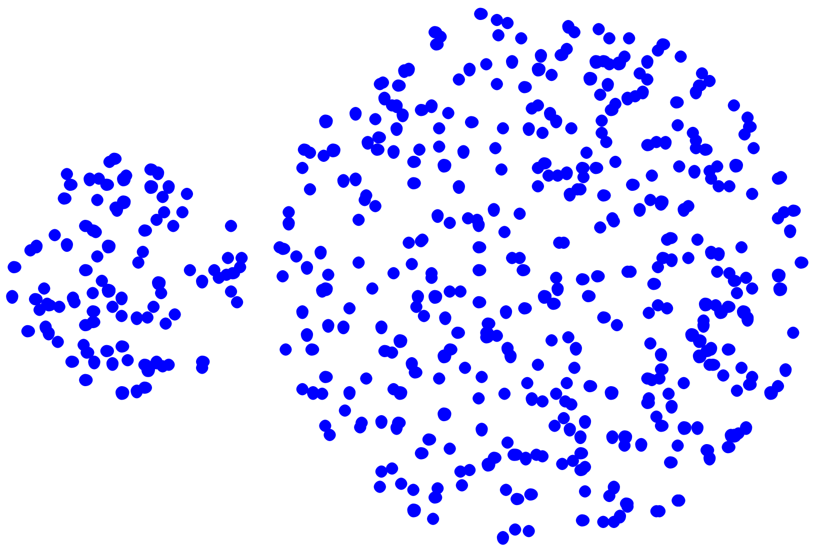
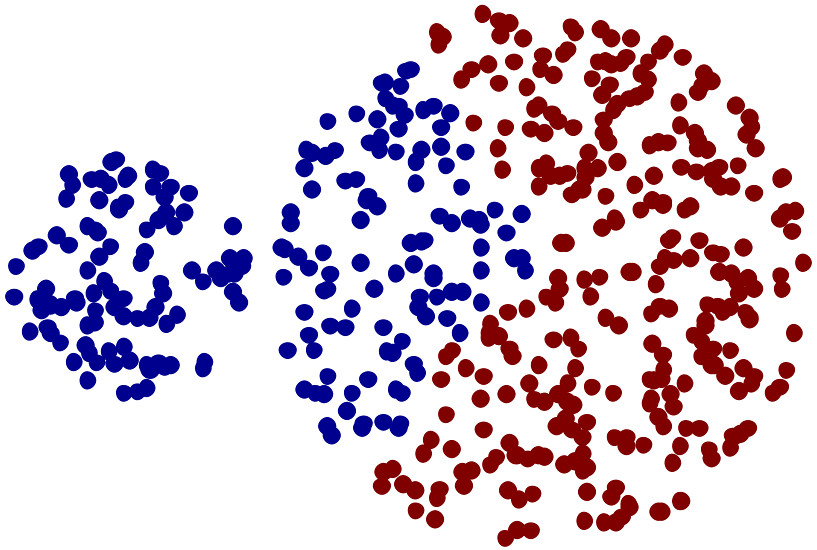
Limitations of MAX



Original Points



Two Clusters

- **Tends to break large clusters**
- **Biased towards globular clusters**

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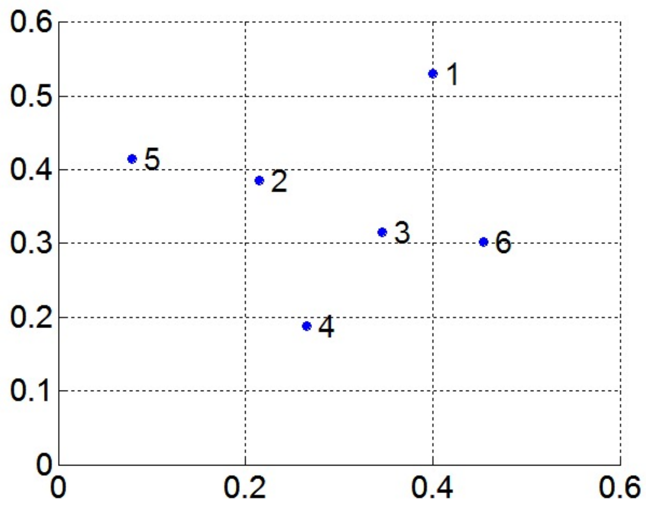
Group Average

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

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



Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
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p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

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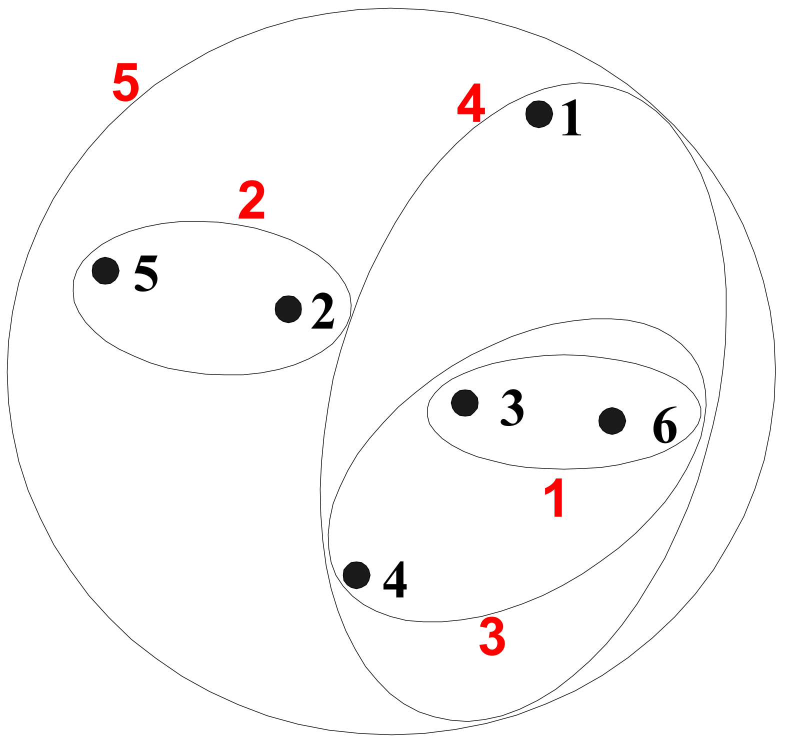
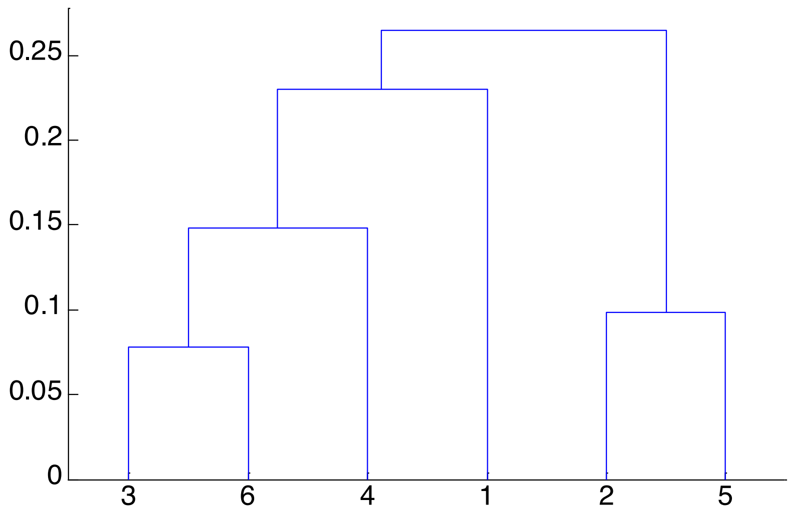
Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

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Hierarchical Clustering: Group Average

Compromise between Single and Complete Link

Strengths

- Less susceptible to noise

Limitations

- Biased towards globular clusters

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Cluster Similarity: Ward's Method

Similarity of two clusters is based on the increase in squared error when two clusters are merged

- Similar to group average if distance between points is distance squared

$$\Delta(A,B) = \sum_{i \in A \cup B} \left|\left|\vec{x} - \vec{m}_{A \cup B}\right|\right|^2 - \sum_{i \in A} \left|\left|\vec{x} - \vec{m}_{A}\right|\right|^2 - \sum_{i \in B} \left|\left|\vec{x} - \vec{m}_{B}\right|\right|^2$$

Less susceptible to noise

Biased towards globular clusters

Hierarchical analogue of K-means

- Can be used to initialize K-means

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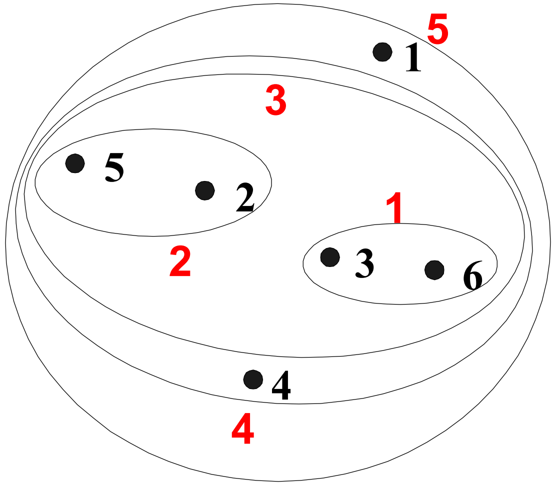
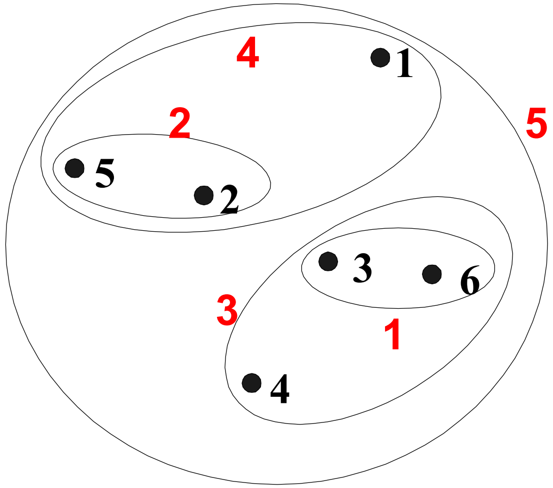
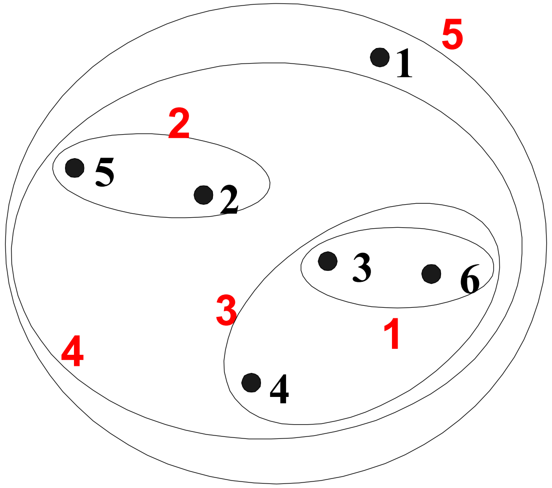
Hierarchical Clustering: Comparison



MIN

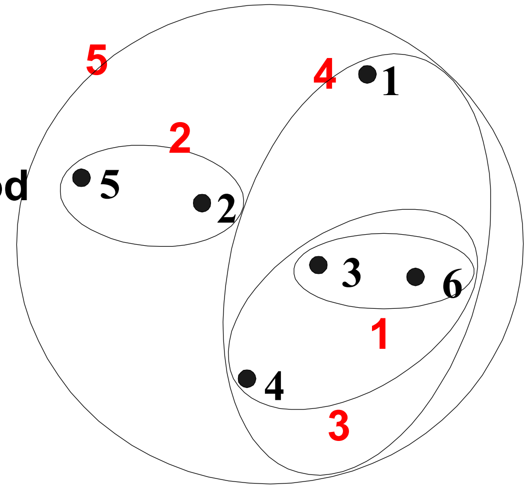
MAX





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 with some cleverness

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Hierarchical Clustering: Problems and Limitations

Once a decision is made to combine two clusters, it cannot be undone

No global objective function is directly minimized

Different schemes have problems with one or more of the following:

- Sensitivity to noise
- Difficulty handling clusters of different sizes and non-globular shapes
- Breaking large clusters

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Code Example

Performing Agglomerative Clustering and Drawing Dendrogram.

https://scikit-learn.org/stable/auto_examples/cluster/plot_agglomerative_dendrogram.html#sphx-glr-auto-examples-cluster-plot-agglomerative-dendrogram-py

Density-Based Clustering

Clusters are regions of high density that are separated from one another by regions on low density.

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DBSCAN

DBSCAN is a density-based algorithm.

- Density = number of points within a specified radius (Eps)
- A point is a core point if it has at least a specified number of points (MinPts) within Eps
  - These are points that are at the interior of a cluster
  - Counts the point itself
- A border point is not a core point, 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

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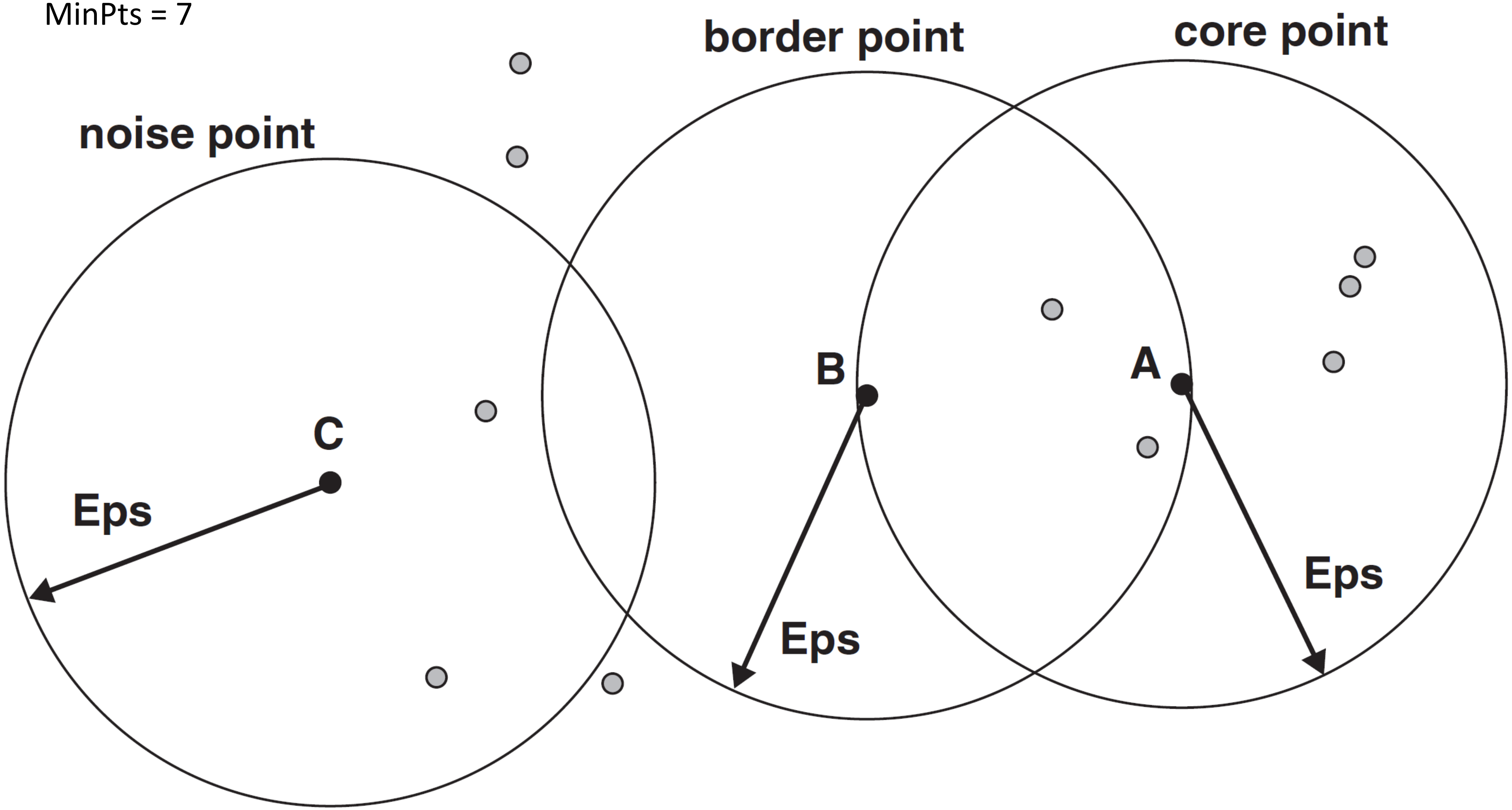
DBSCAN: Core, Border, and Noise Points

MinPts = 7



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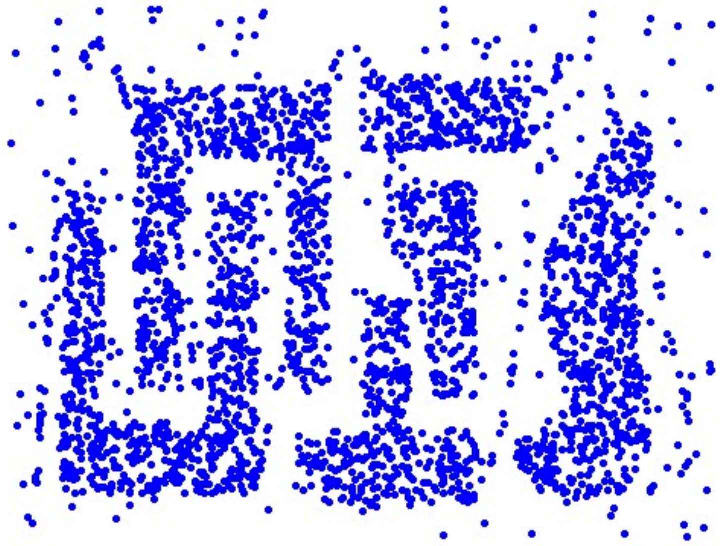
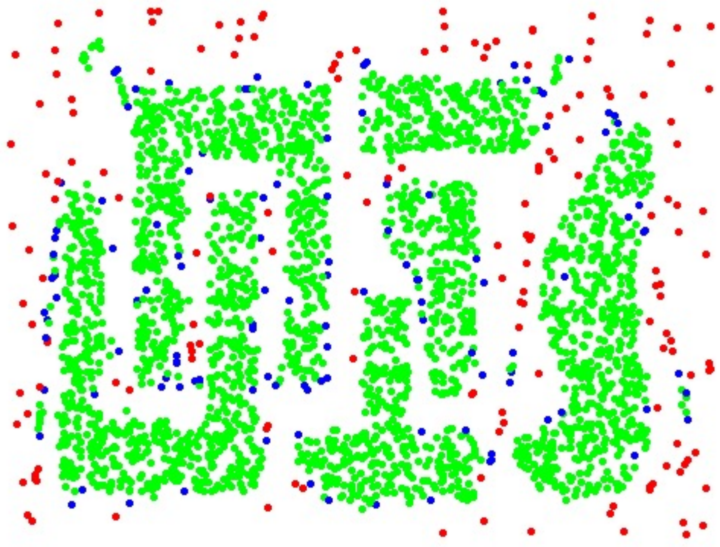
DBSCAN: Core, Border, and Noise Points



Original Points



Point types: core, border and noise

Eps = 10, MinPts = 4

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DBSCAN Algorithm

Form clusters using core points, and assign border points to one of its neighboring clusters

1: Label all points as core, border, or noise points.

2: Eliminate noise points.

3: Put an edge between all core points within a distance *Eps* of each other.

4: Make each group of connected core points into a separate cluster.

5: Assign each border point to one of the clusters of its associated core points

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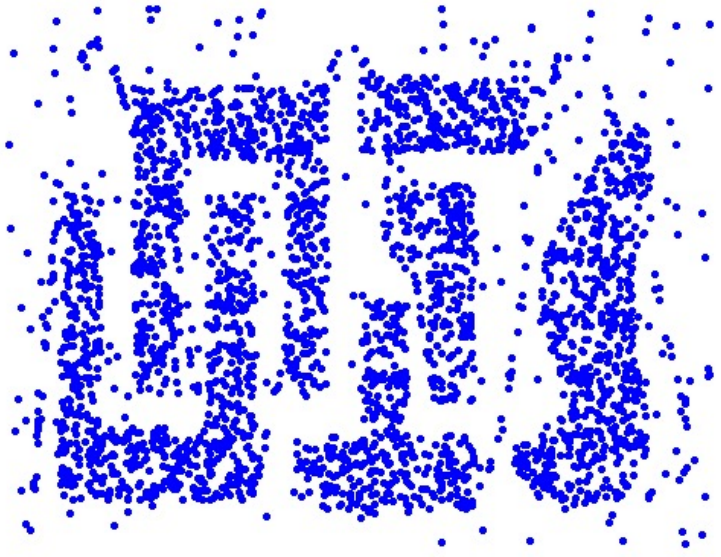
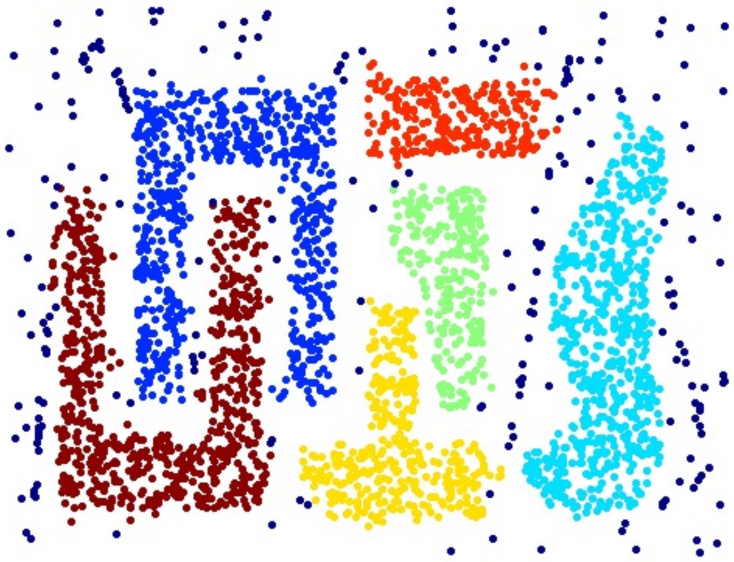
When DBSCAN Works Well



Original Points



Clusters (dark blue points indicate noise)

- **Can handle clusters of different shapes and sizes**
- **Resistant to noise**

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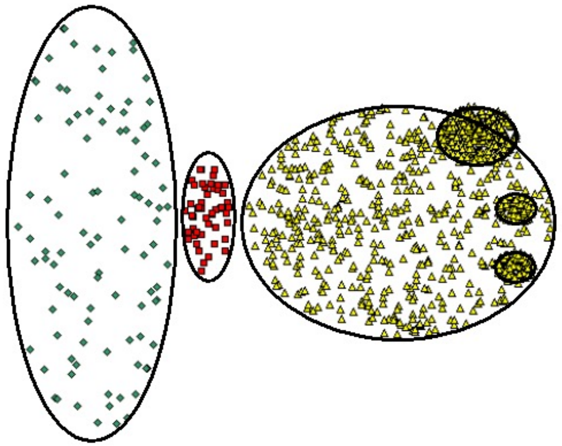
When DBSCAN Does NOT Work Well



Original Points

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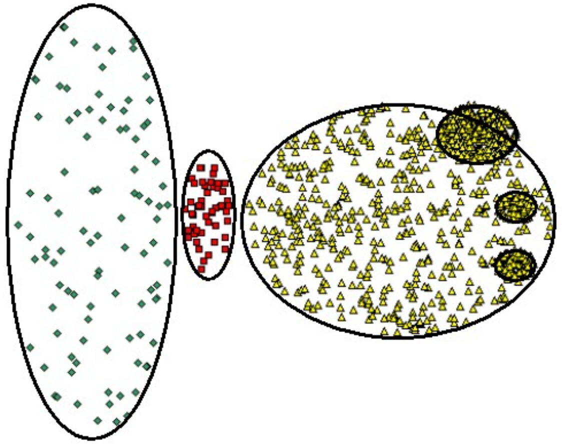
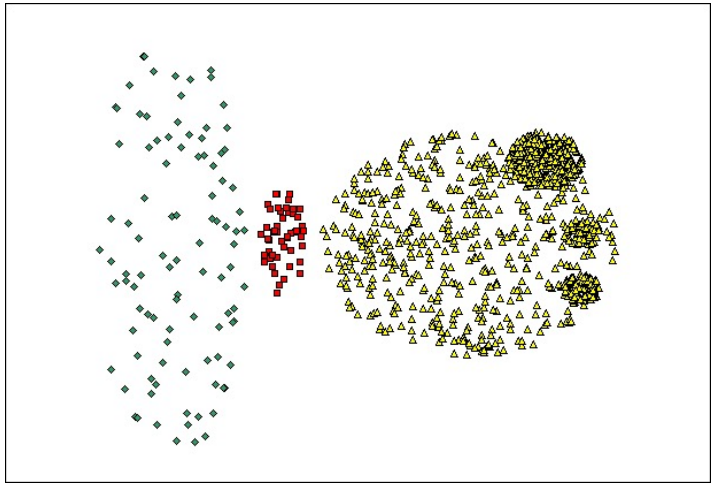
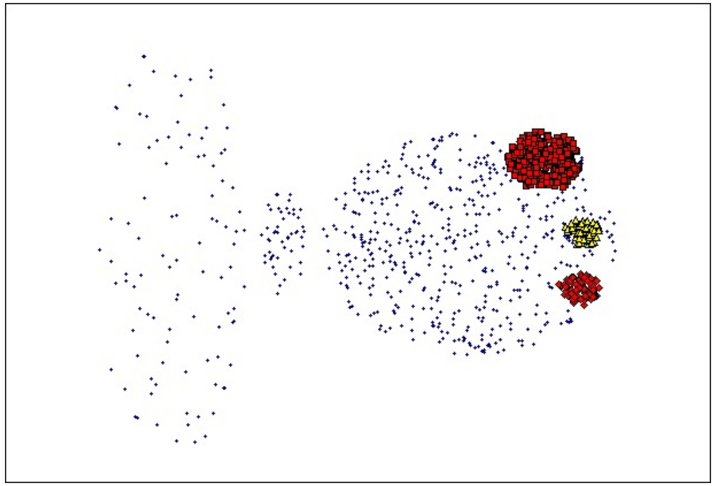
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.92).



(MinPts=4, Eps=9.75)

- **Varying densities**
- **High-dimensional data**

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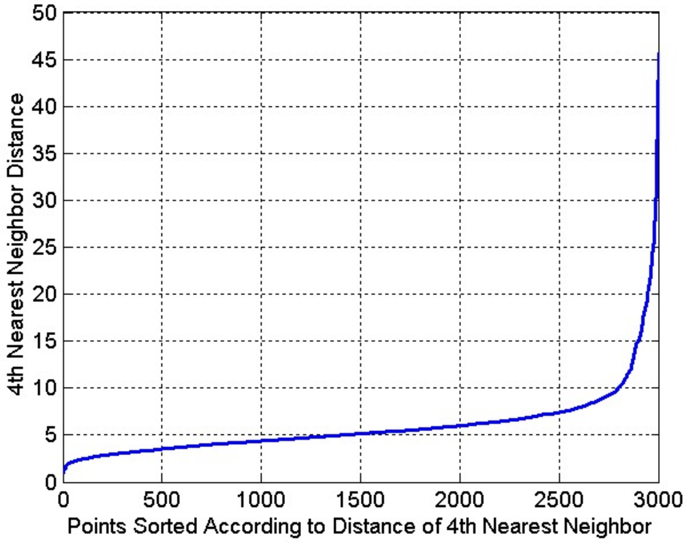
DBSCAN: Determining EPS and MinPts

Idea is that for points in a cluster, their k^{th} nearest neighbors are at close 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



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Code Example

DBSCAN and Coloring the Clusters

https://scikit-learn.org/stable/auto_examples/cluster/plot_dbscan.html#sphx-glr-auto-examples-cluster-plot-dbscan-py