

Cluster Analysis

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Last Week

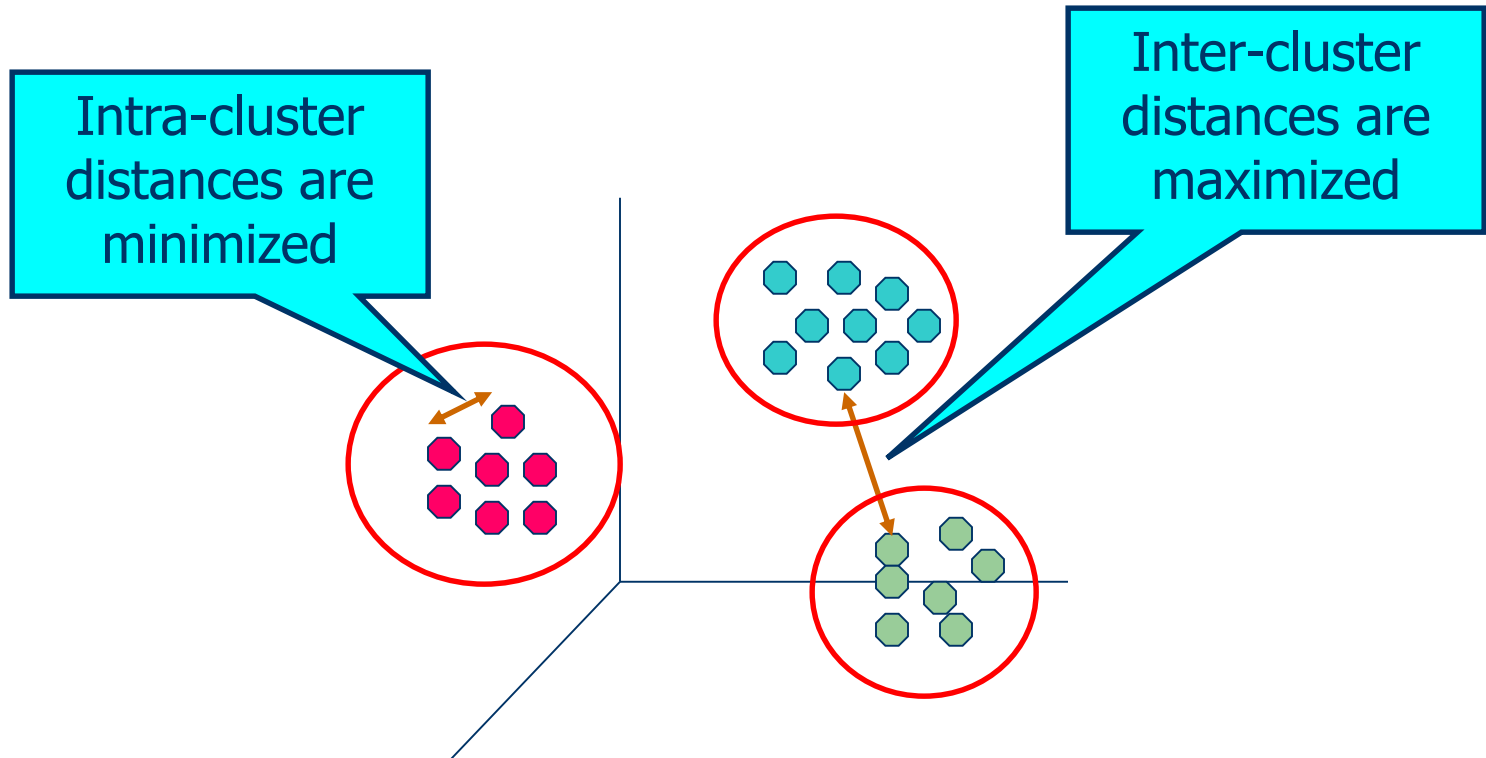
- Decision Tree
- Support Vector Machine

Content

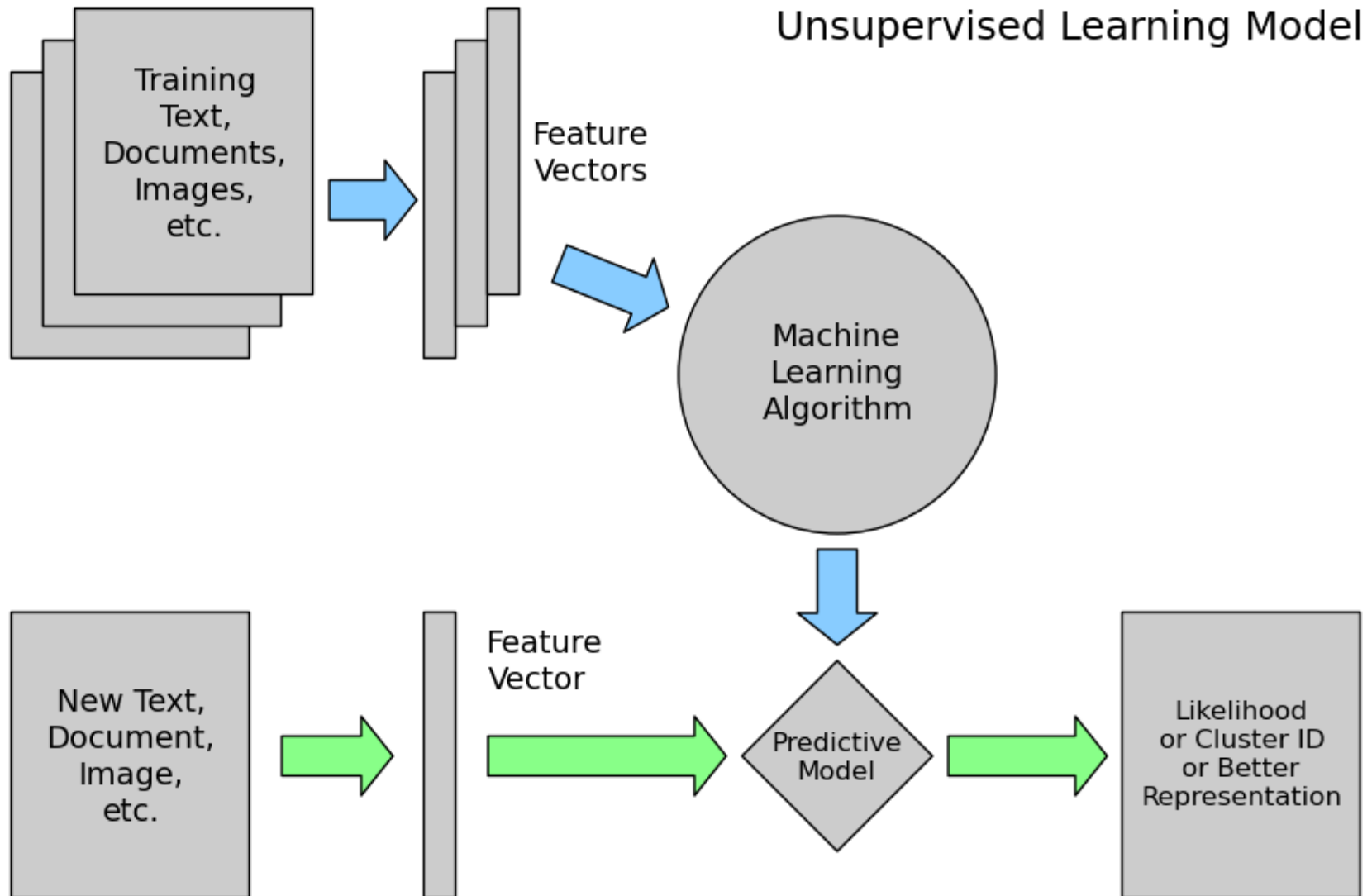
- What is cluster
- Applications of Cluster
- Types of cluster
- Conclusions

What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



Unsupervised Learning



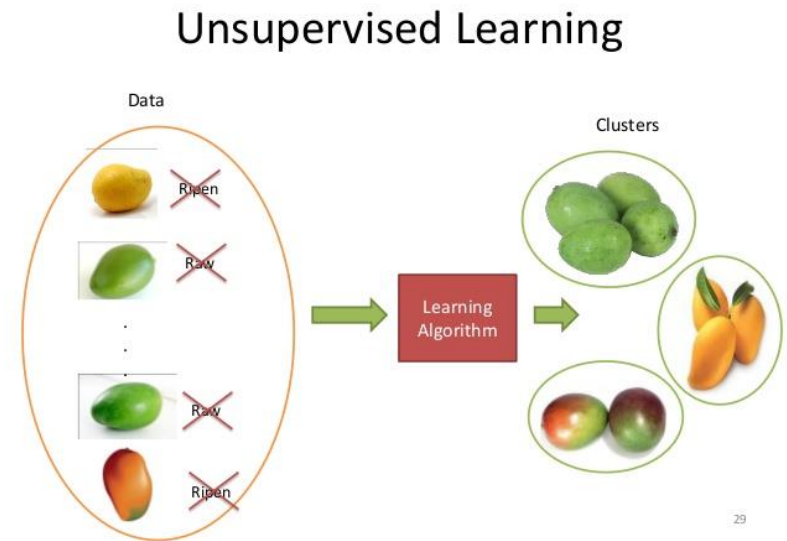
Applications of Cluster Analysis

- **Understanding**

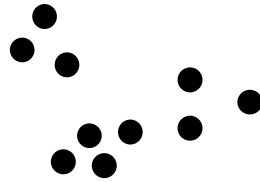
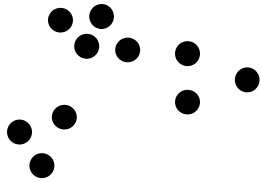
- Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

- **Summarization**

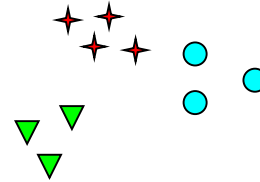
- Reduce the size of large data sets



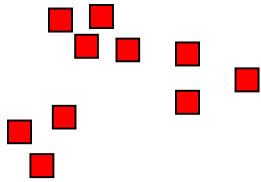
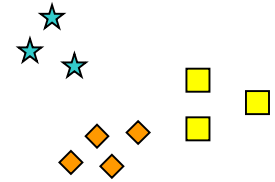
Notion of a Cluster can be Ambiguous



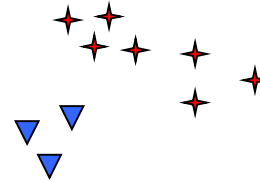
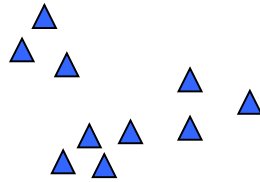
How many clusters?



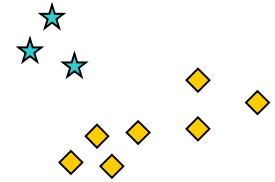
Six Clusters



Two Clusters



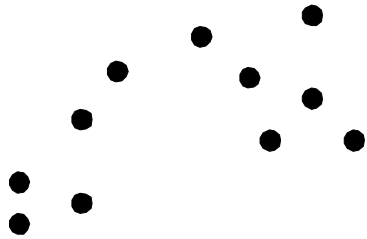
Four Clusters



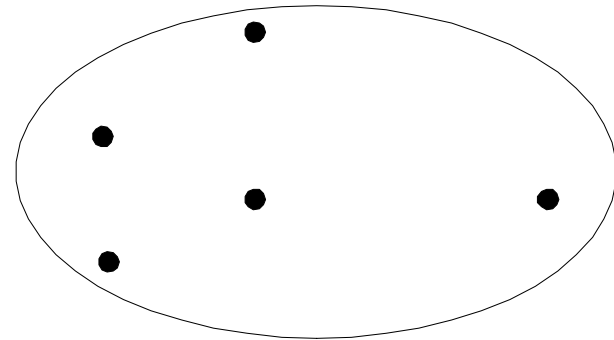
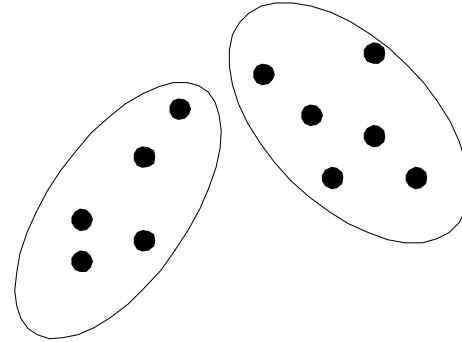
Types of Clusterings

- A **clustering** is a set of clusters
- Important distinction between **hierarchical** and **partitional** sets of clusters
- Partitional Clustering
 - A division data objects into non-overlapping 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

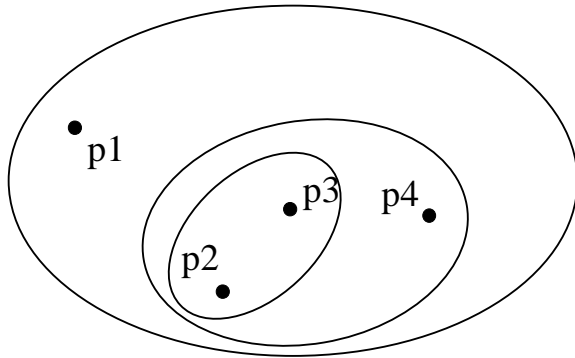


Original Points

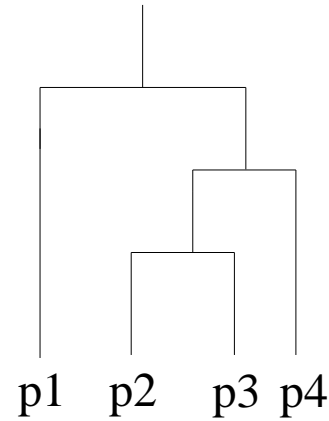


A Partitional Clustering

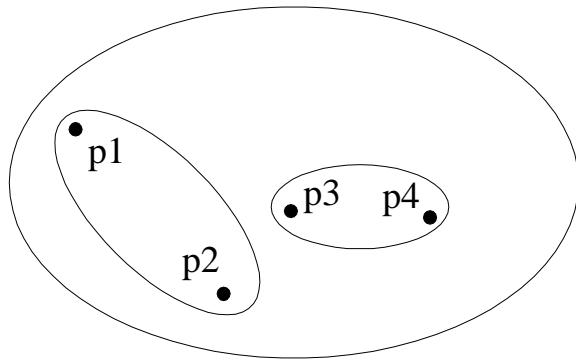
Hierarchical Clustering



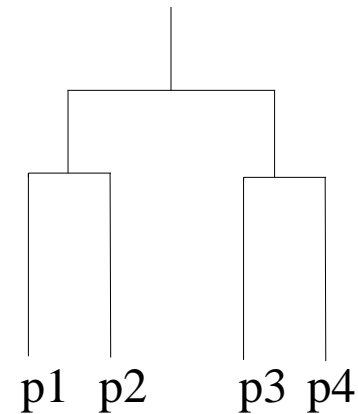
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

- **Exclusive versus non-exclusive**
 - In non-exclusive clusterings, points may belong to multiple clusters.
 - Can represent multiple classes or 'border' points
- **Fuzzy versus non-fuzzy**
 - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
 - Weights must sum to 1
 - Probabilistic clustering has similar characteristics
- **Partial versus complete**
 - In some cases, we only want to cluster some of the data
- **Heterogeneous versus homogeneous**
 - Cluster of widely different sizes, shapes, and densities

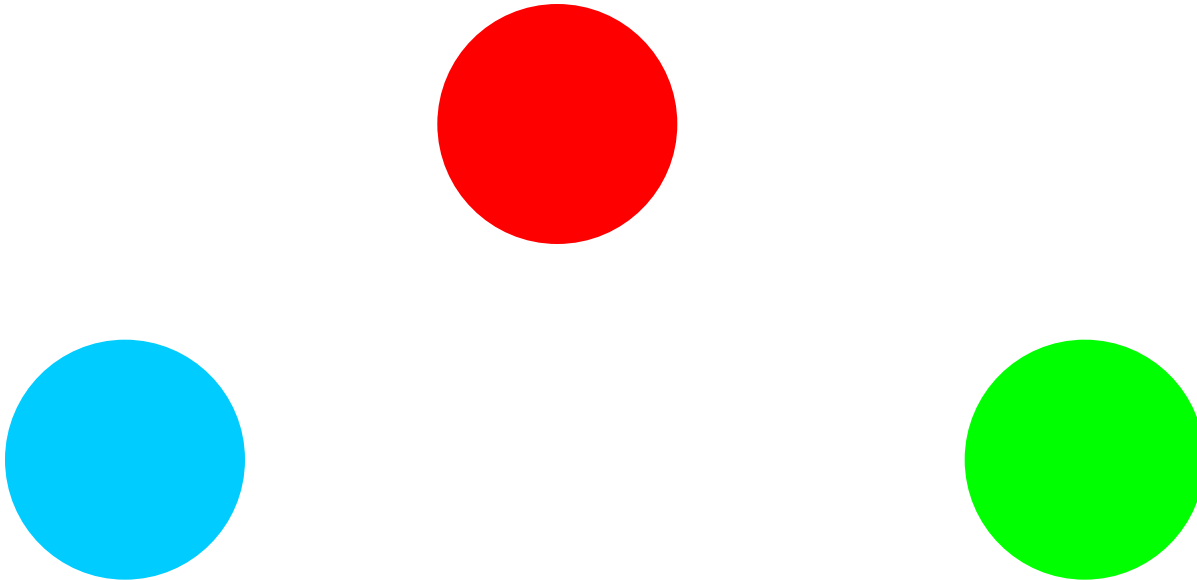
Types of Clusters

- Well-separated clusters
- Center-based clusters
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
- Described by an Objective Function

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.

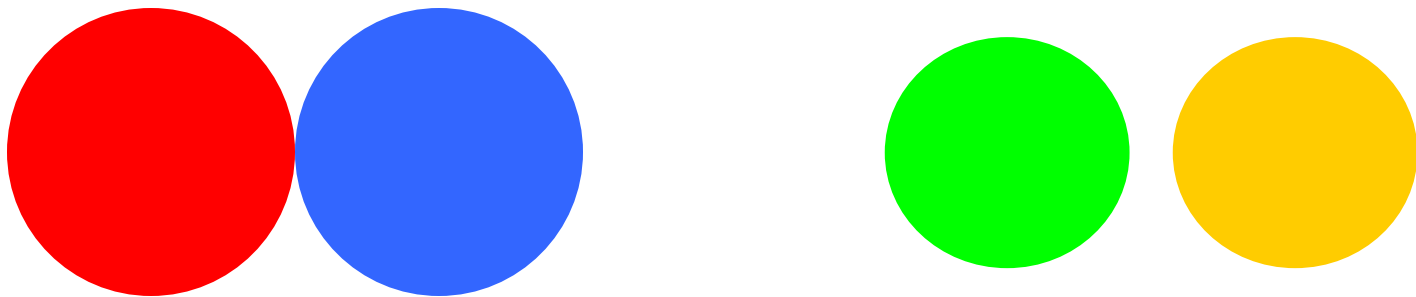


3 well-separated clusters

Types of Clusters: Center-Based

- Center-based

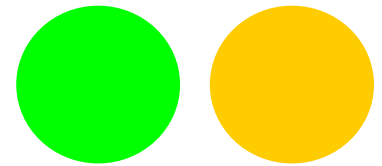
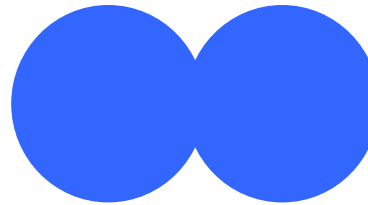
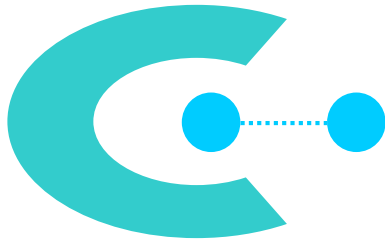
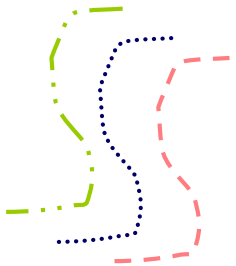
- A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
- The center of a cluster is often a **centroid**, the average of all the points in the cluster, or a **medoid**, the most “representative” point 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.

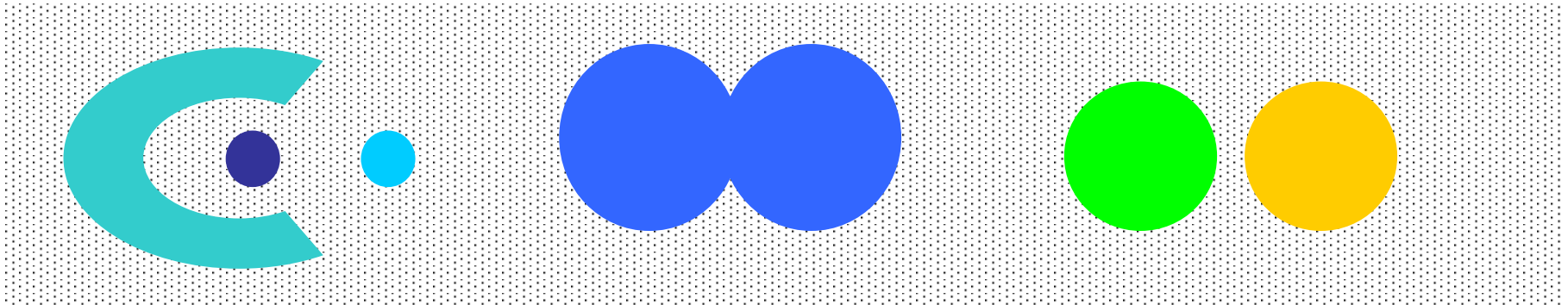


8 contiguous clusters

Types of Clusters: Density-Based

- Density-based

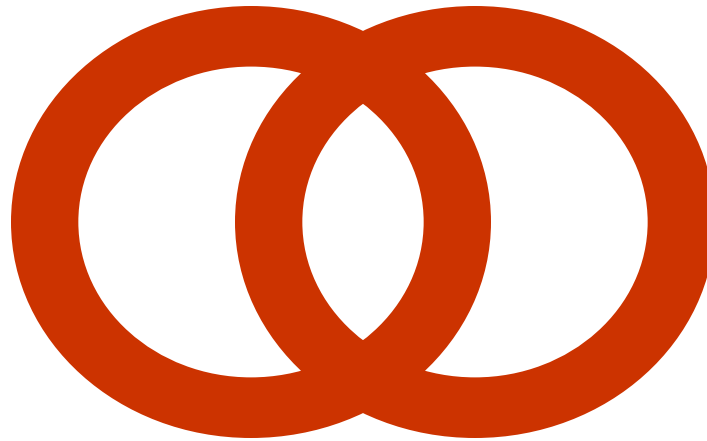
- A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
- Used when the clusters are irregular or intertwined, and when noise and outliers are present.



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.
 - .



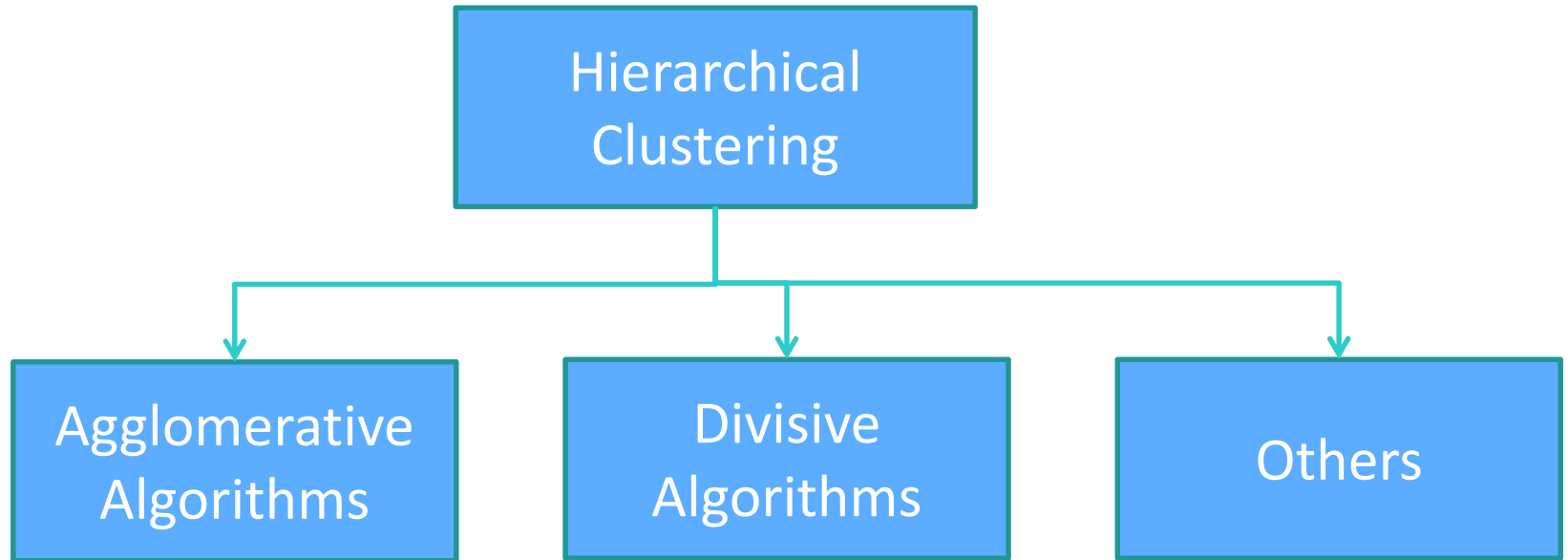
2 Overlapping Circles

Types of Clusters: Objective Function

- Clusters Defined by an Objective Function

- 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.
 - Parameters for the model are determined from the data.
 - Mixture models assume that the data is a 'mixture' of a number of statistical distributions.

Clustering Algorithms



Clustering Algorithms

Partitioning
Algorithms

```
graph TD; A[Partitioning Algorithms] --> B[K-medoids]; A --> C[K-means]; A --> D[Probabilistic]; E[Density based];
```

K-medoids

K-means

Probabilistic

Density based

Clustering Algorithms

Others

```
graph TD; Others[Others] --> Evolutionary[Evolutionary Heuristics]; Others --> Grid[Grid Based]; Others --> ANN[Artificial Neural Networks]; Others --> DL[Deep Learning];
```

Evolutionary
Heuristics

Grid Based

Artificial Neural
Networks

Deep Learning

K-means Clustering

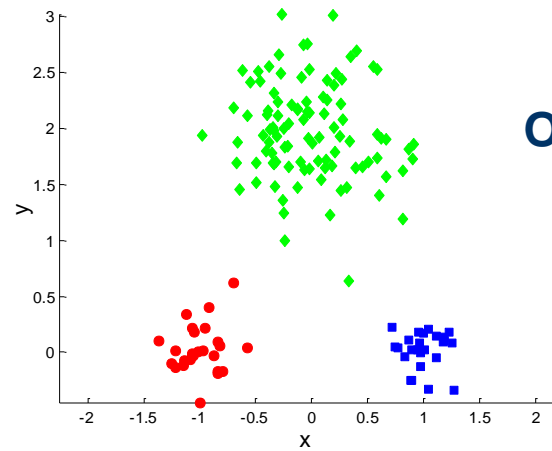
- Partitional clustering approach
- Each cluster is associated with a **centroid** (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K , must be specified
- The basic algorithm is very simple

-
- 1: Select K points as the initial centroids.
 - 2: **repeat**
 - 3: Form K clusters by assigning all points to the closest centroid.
 - 4: Recompute the centroid of each cluster.
 - 5: **until** The centroids don't change
-

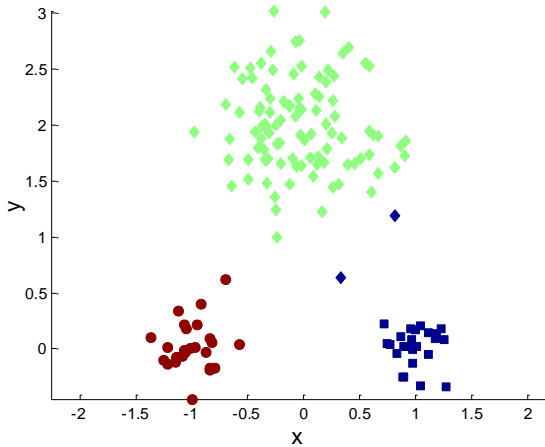
K-means Clustering – Details

- Initial centroids are often chosen randomly.
 - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- 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 = number of attributes

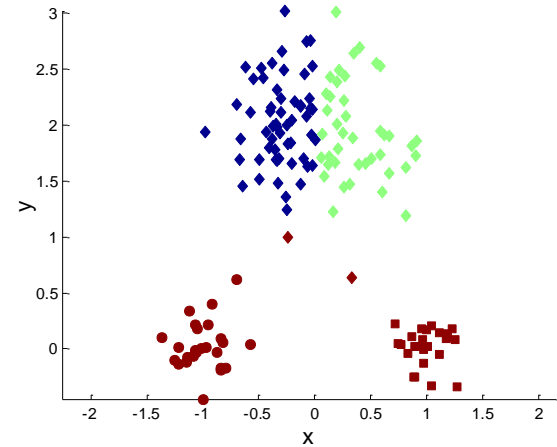
Two different K-means Clusterings



Original Points

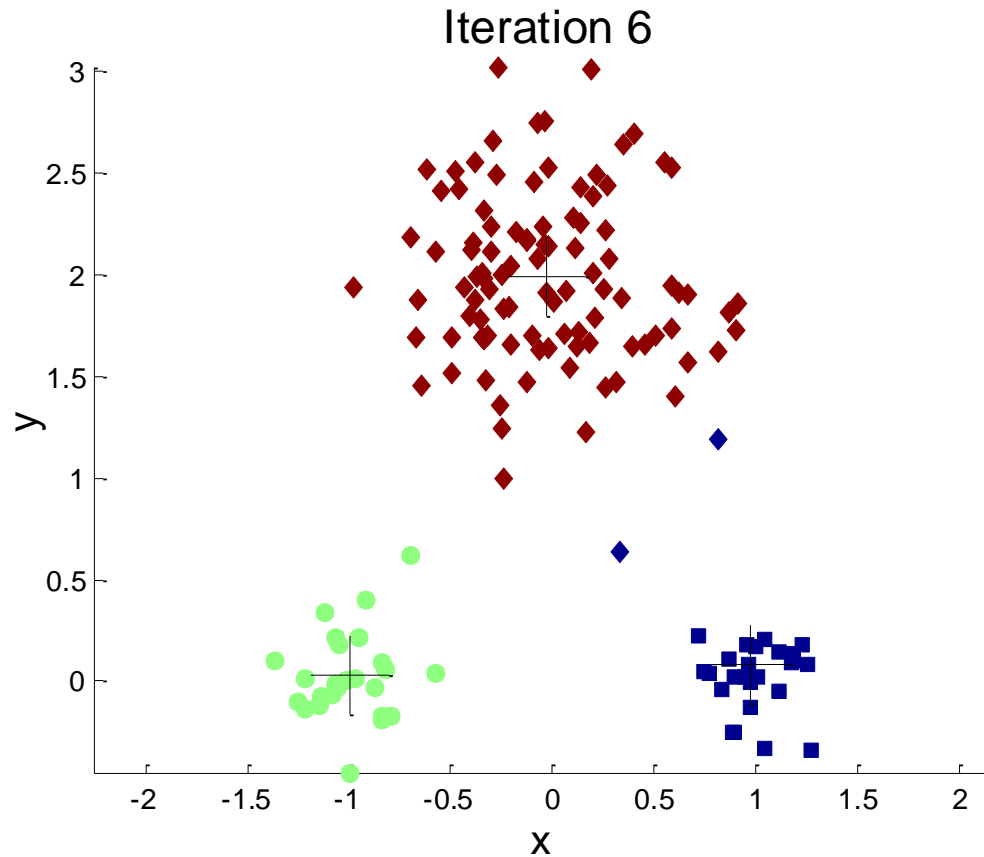


Optimal Clustering

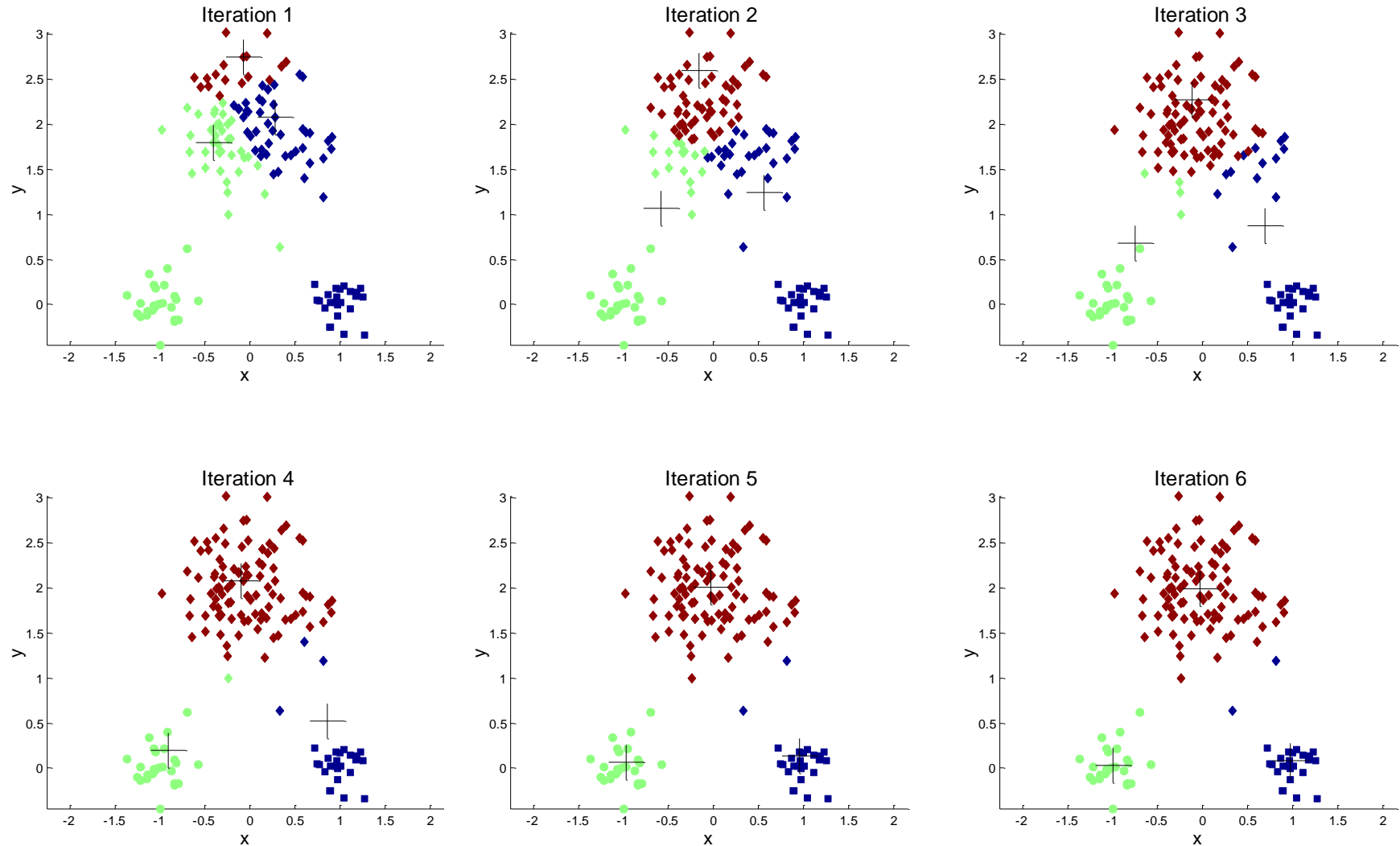


Sub-optimal Clustering

Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids



Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
 - For each point, the error is the distance to the nearest cluster
 - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^K \sum_{x \in C_i} dist^2(m_i, x)$$

- x is a data point in cluster C_i and m_i is the representative point for cluster C_i
 - can show that m_i corresponds to the center (mean) of the cluster
- Given two clusters, we can choose the one with the smallest error
- One easy way to reduce SSE is to increase K , the number of clusters
 - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

Problems with Selecting Initial Points

- If there are K 'real' clusters then the chance of selecting one centroid from each cluster is small.
 - Chance is relatively small when K is large
 - If clusters are the same size, n , then

$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

- For example, if $K = 10$, then probability = $10!/10^{10} = 0.00036$
- Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't

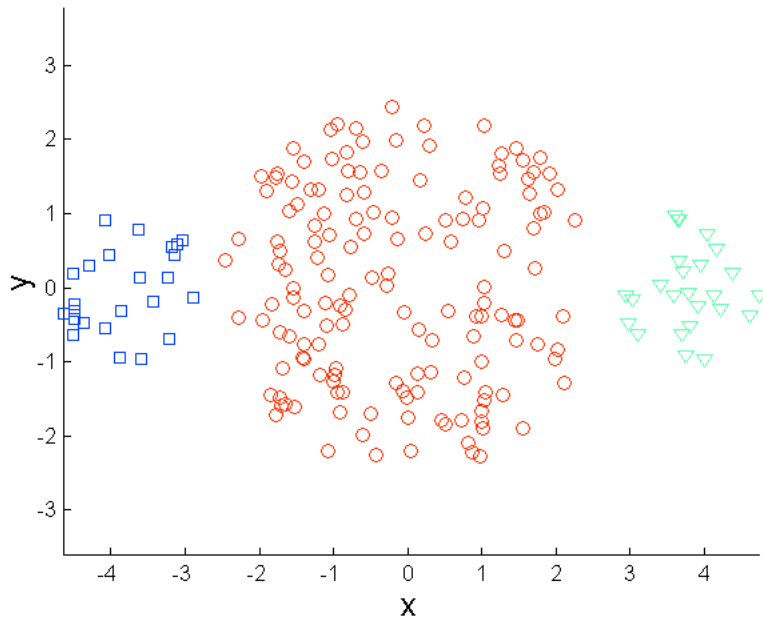
Solutions to Initial Centroids Problem

- Multiple runs
 - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
 - Select most widely separated

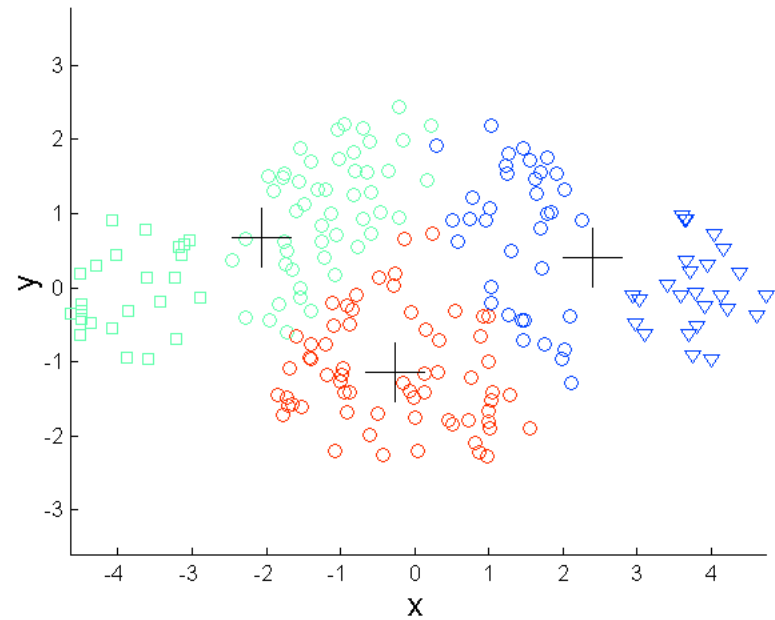
Limitations of K-means

- K-means has problems when clusters are of differing
 - Sizes
 - Densities
 - Non-globular shapes
- K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

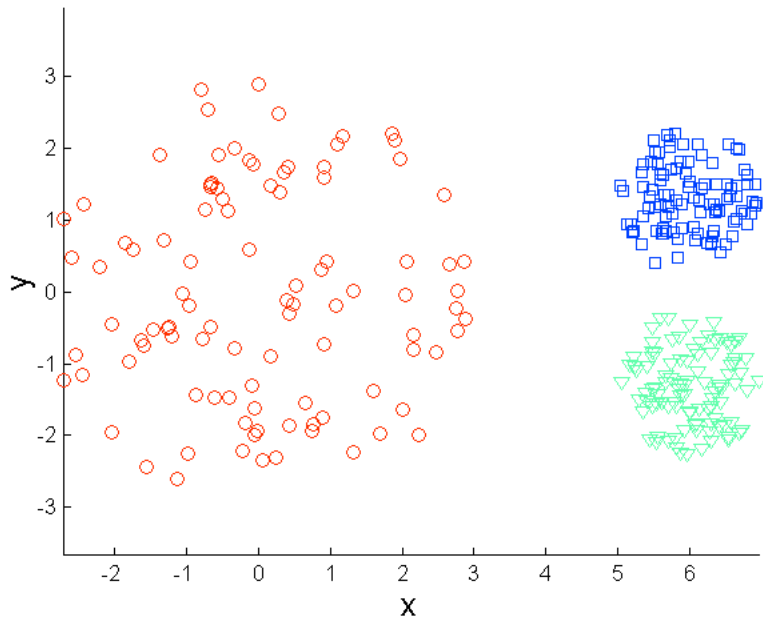


Original Points

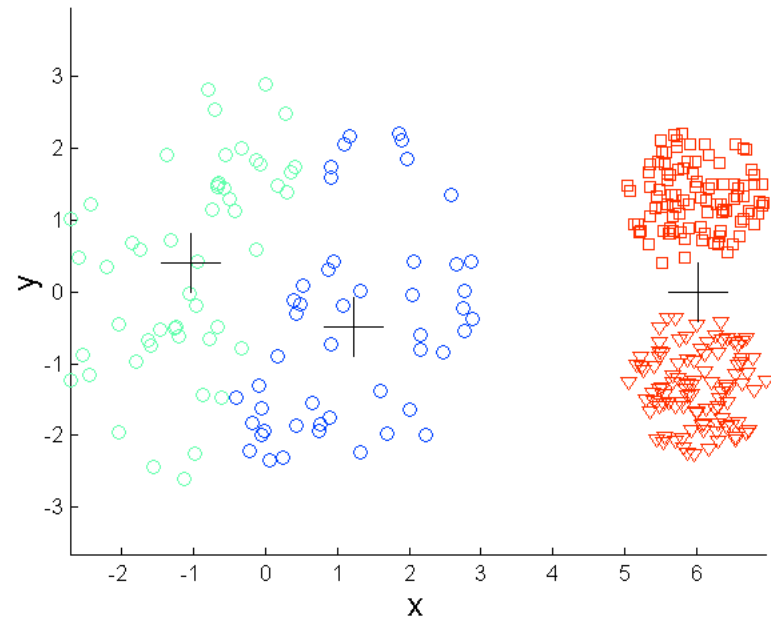


K-means (3 Clusters)

Limitations of K-means: Differing Density

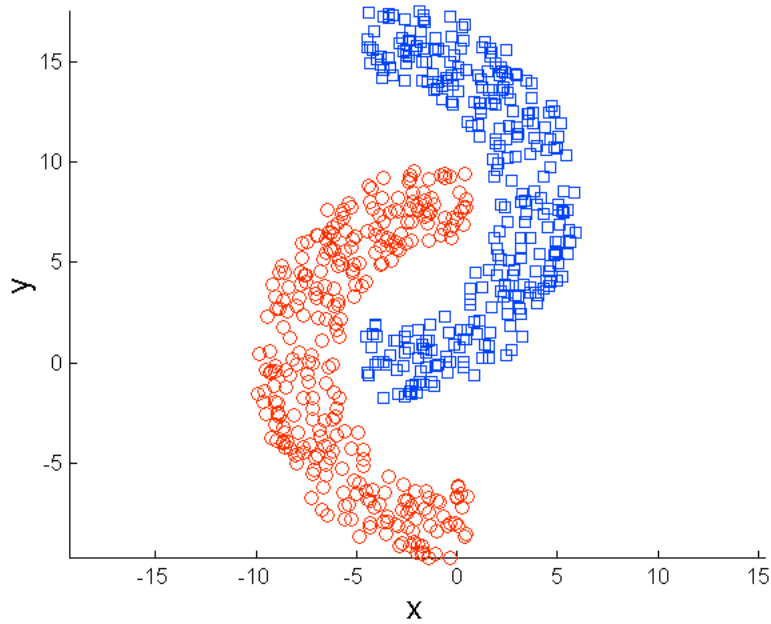


Original Points

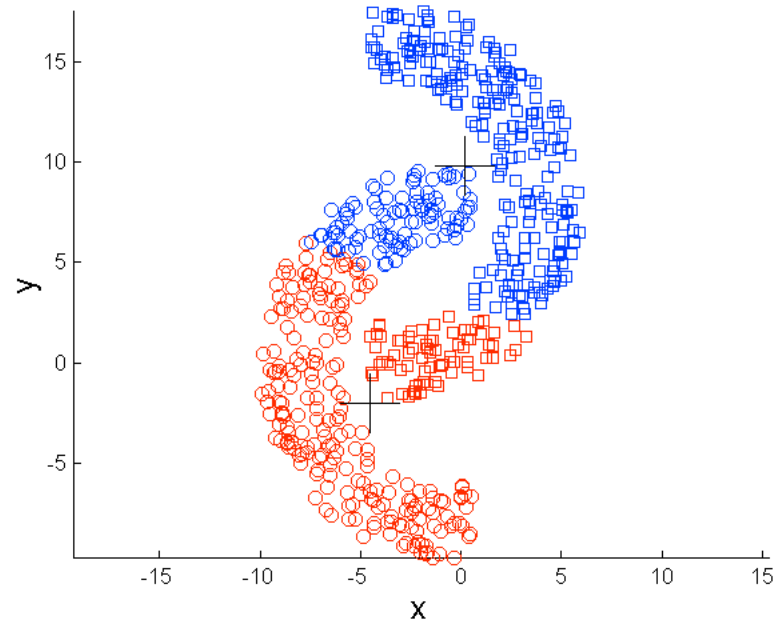


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



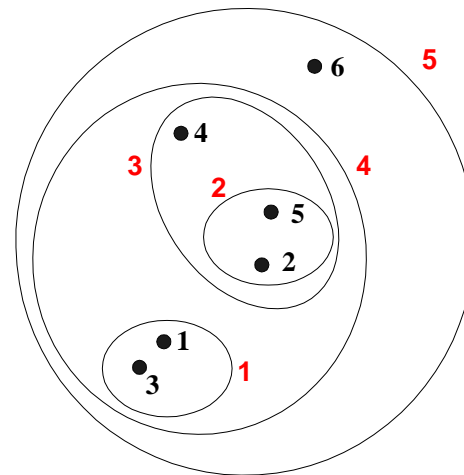
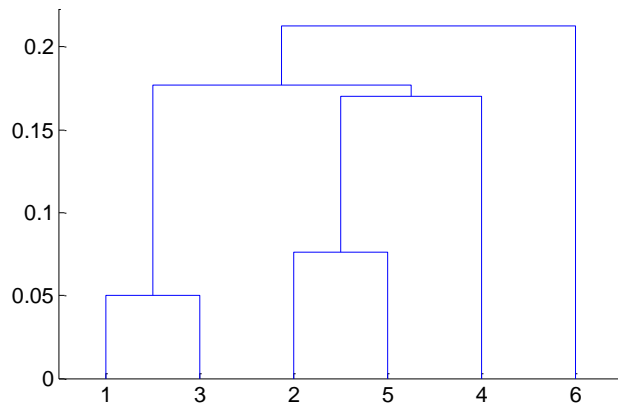
Original Points



K-means (2 Clusters)

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 dendrogram at the proper level
- They may correspond to meaningful taxonomies
 - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

Hierarchical Clustering

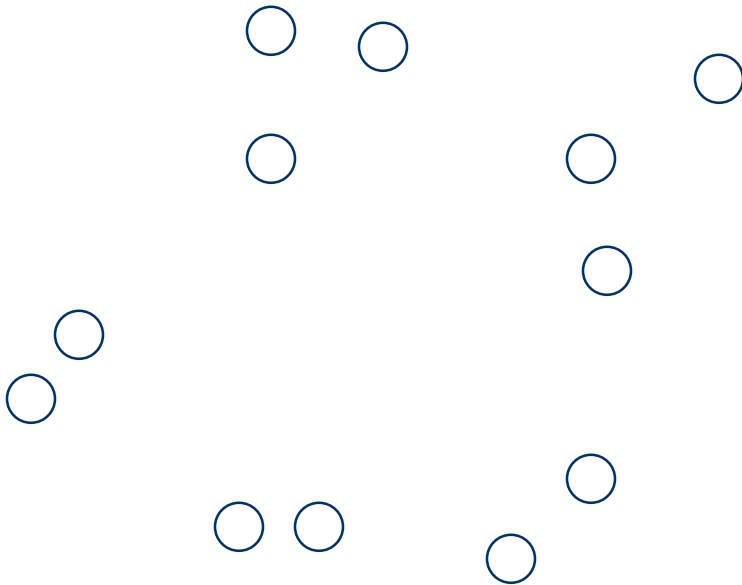
- Two main types of hierarchical clustering
 - Agglomerative:
 - Start with the points as individual clusters
 - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - Divisive:
 - Start with one, all-inclusive cluster
 - At each step, split a cluster until each 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

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



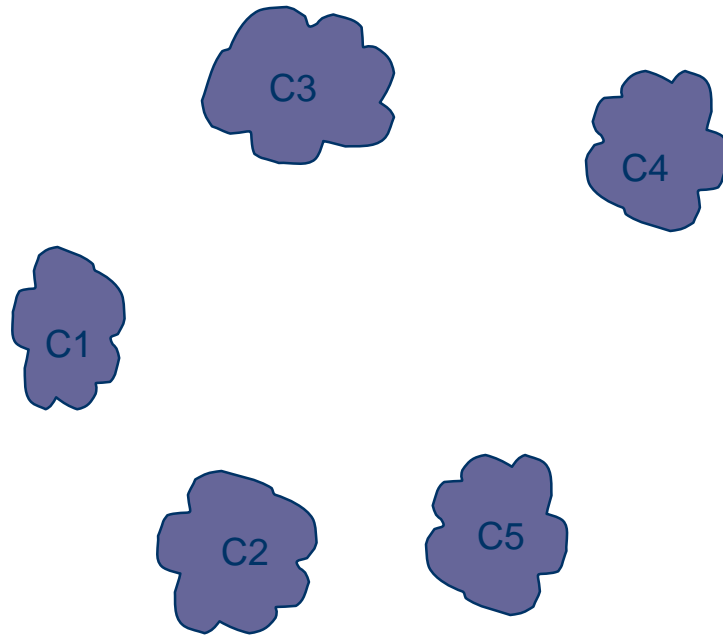
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



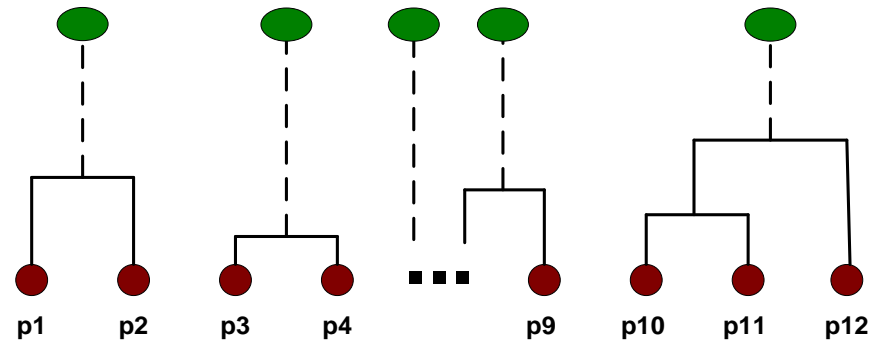
Intermediate Situation

- After some merging steps, we have some clusters



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix

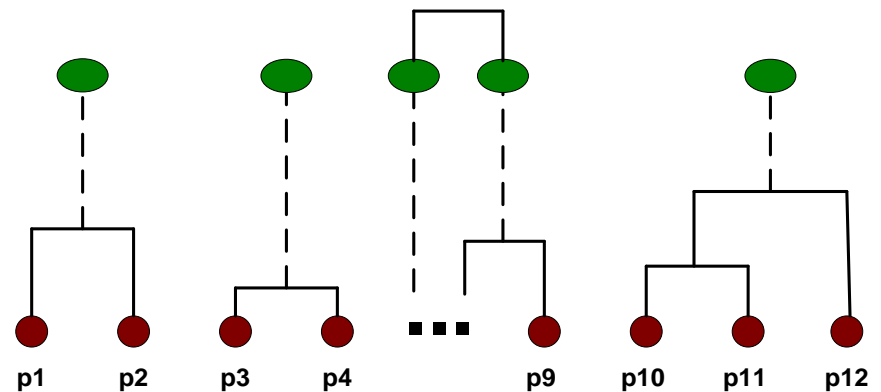
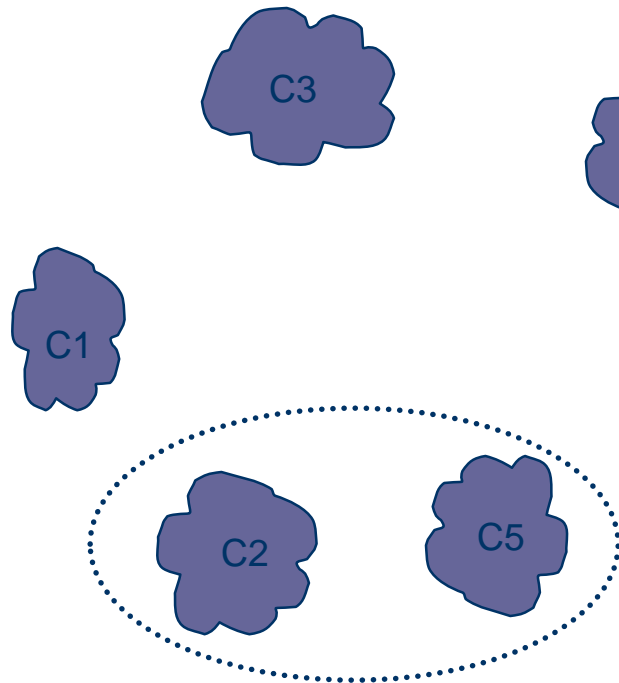


Intermediate Situation

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

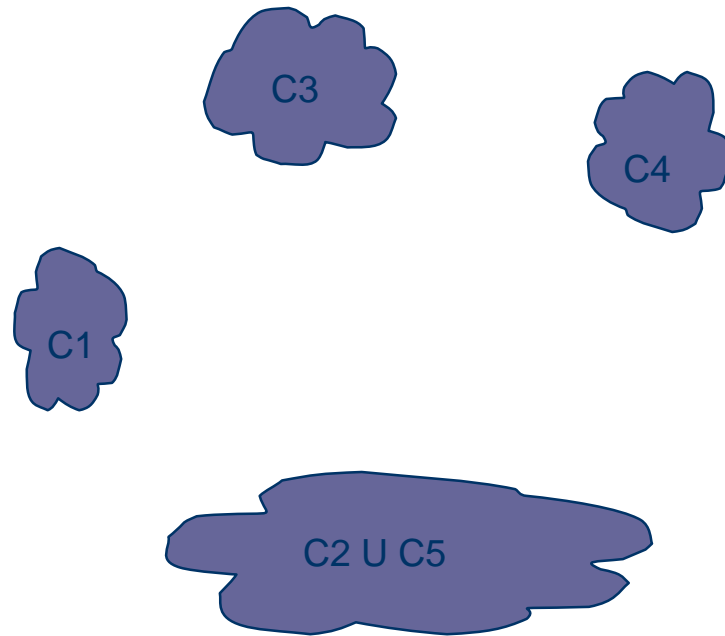
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



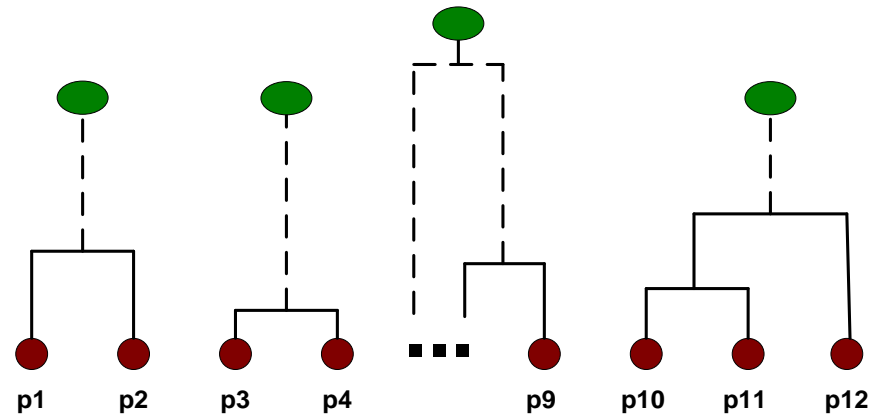
After Merging

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

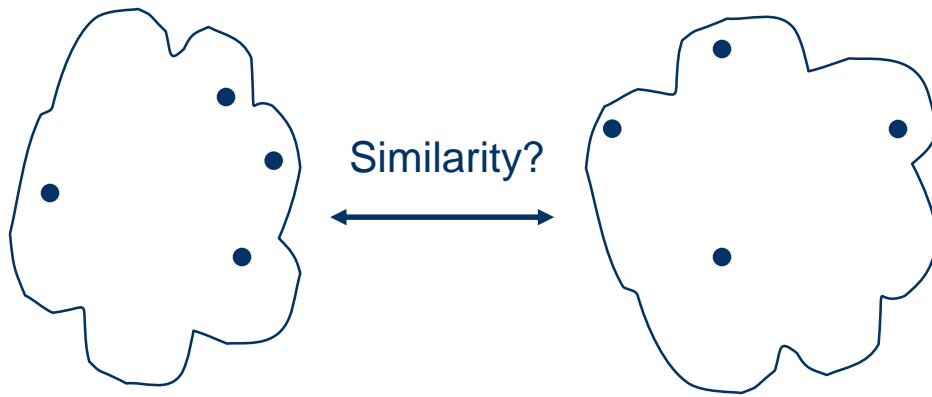


		C1	C2 U C5	C3	C4
C1			?		
C2 U C5		?	?	?	?
C3			?		
C4			?		

Proximity Matrix



How to Define Inter-Cluster Similarity

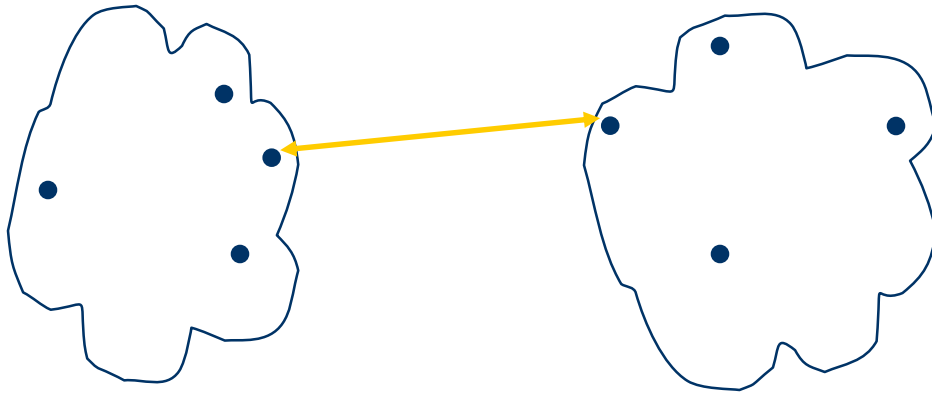


- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

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

· Proximity Matrix

How to Define Inter-Cluster Similarity

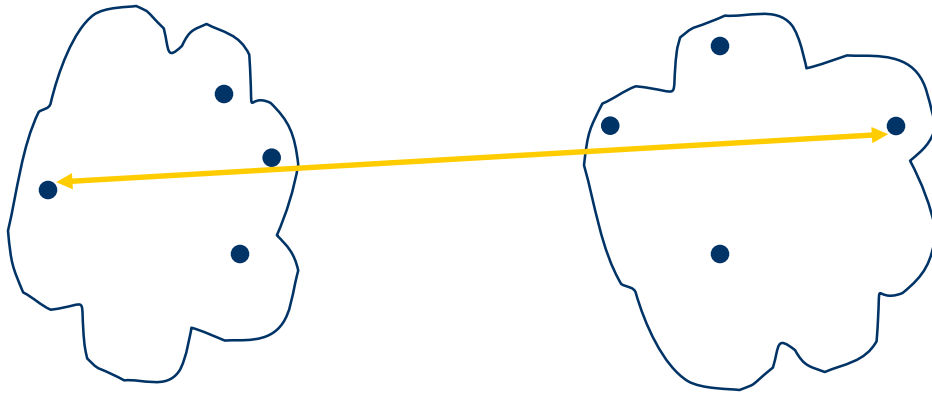


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	p1	p2	p3	p4	p5	...
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p2						
p3						
p4						
p5						
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Proximity Matrix

How to Define Inter-Cluster Similarity

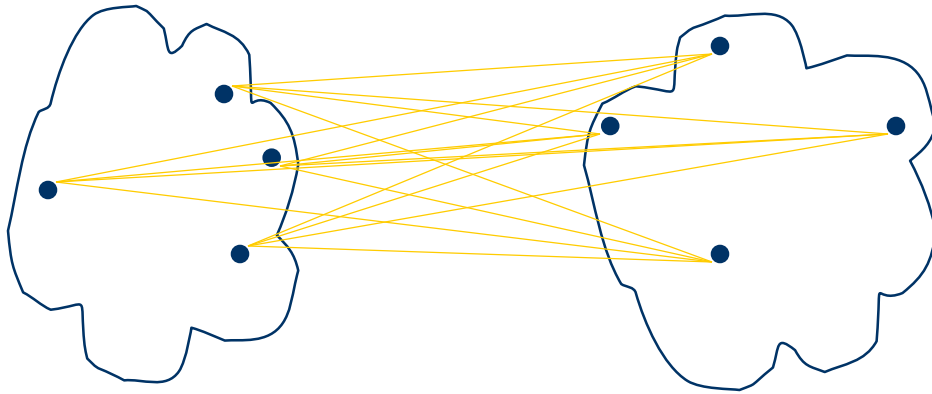


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p2						
p3						
p4						
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Proximity Matrix

How to Define Inter-Cluster Similarity

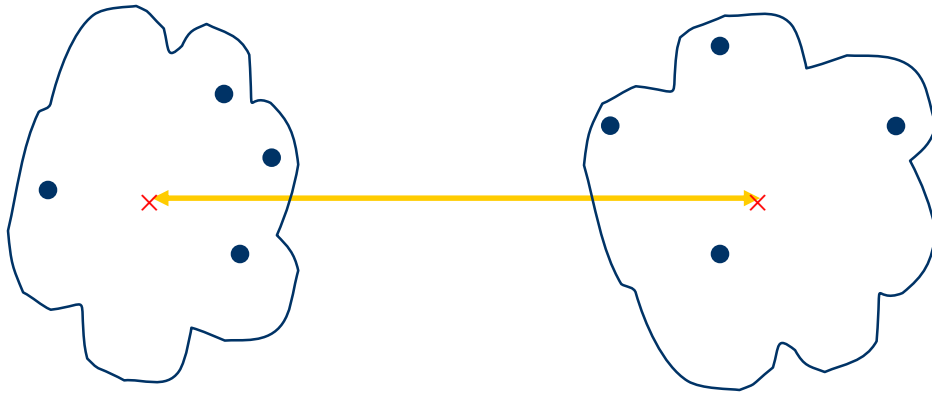


- MIN
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- **Group Average**
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	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
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Proximity Matrix

How to Define Inter-Cluster Similarity



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

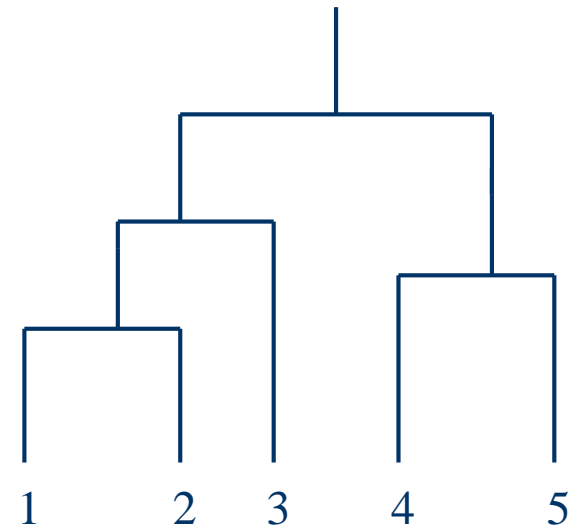
	p1	p2	p3	p4	p5	...
p1						
p2						
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Proximity Matrix

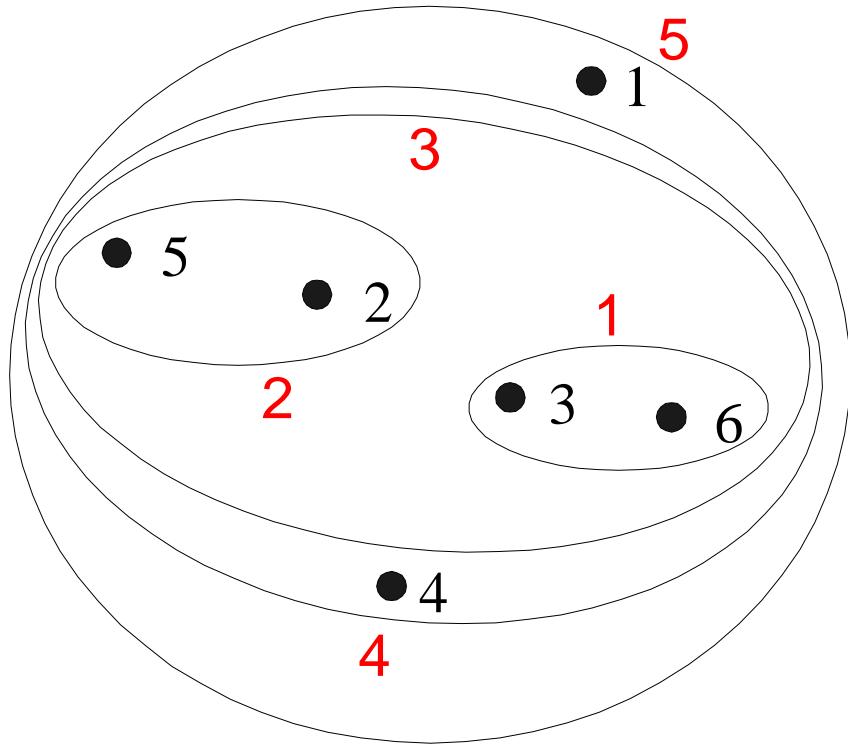
Cluster Similarity: MIN or Single Link

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
 - Determined by one pair of points, i.e., by one link in the proximity graph.

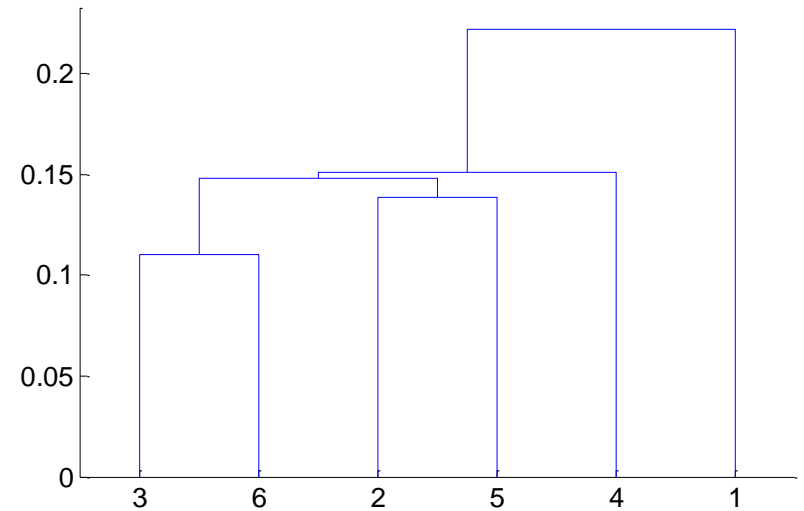
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: MIN

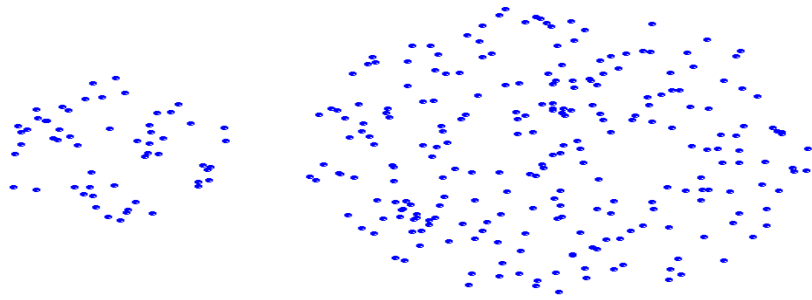


Nested Clusters

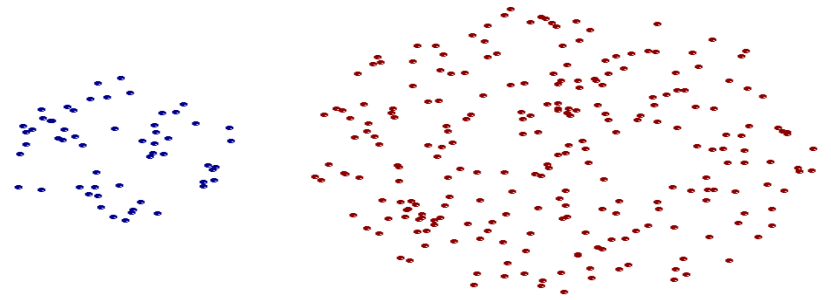


Dendrogram

Strength of MIN



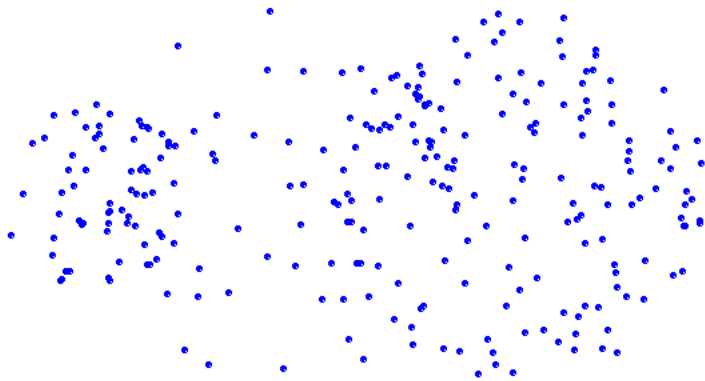
Original Points



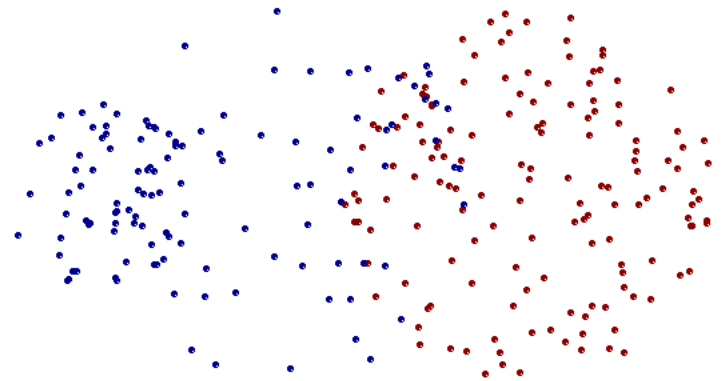
Two Clusters

- Can handle non-elliptical shapes

Limitations of MIN



Original Points



Two Clusters

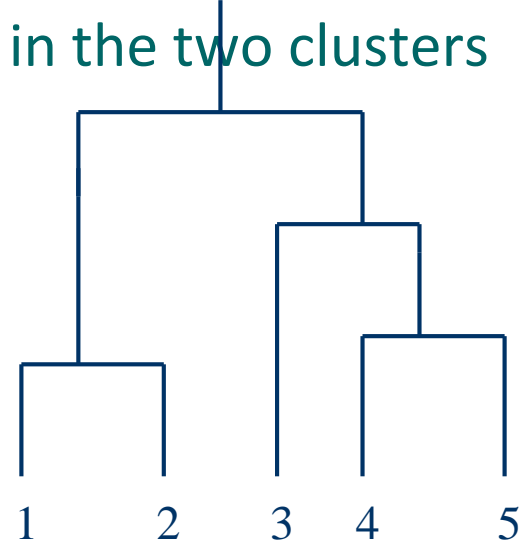
- Sensitive to noise and outliers

Cluster Similarity: MAX or Complete Linkage

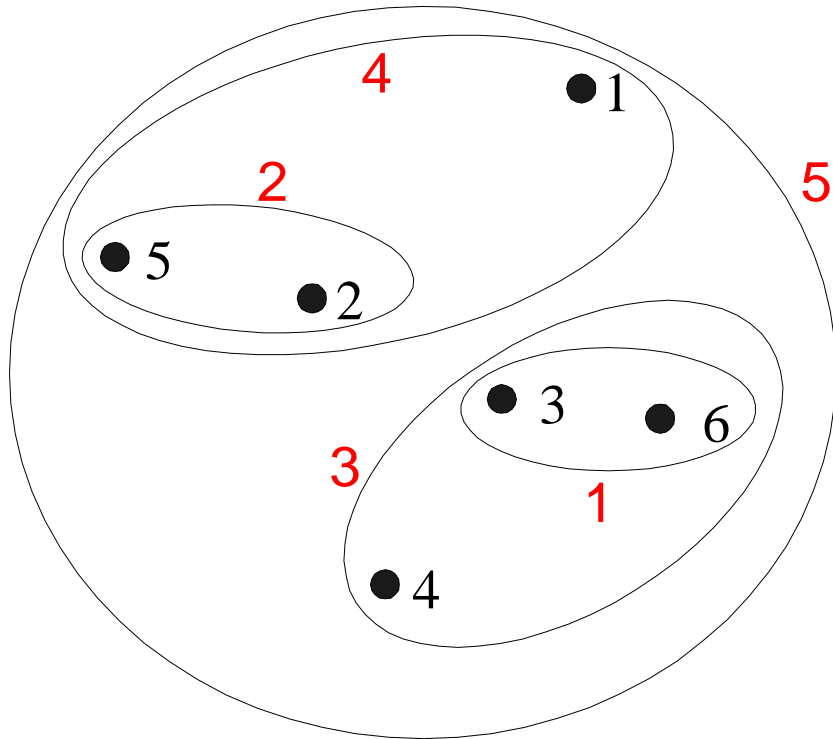
- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters

Determined by all pairs of points in the two clusters

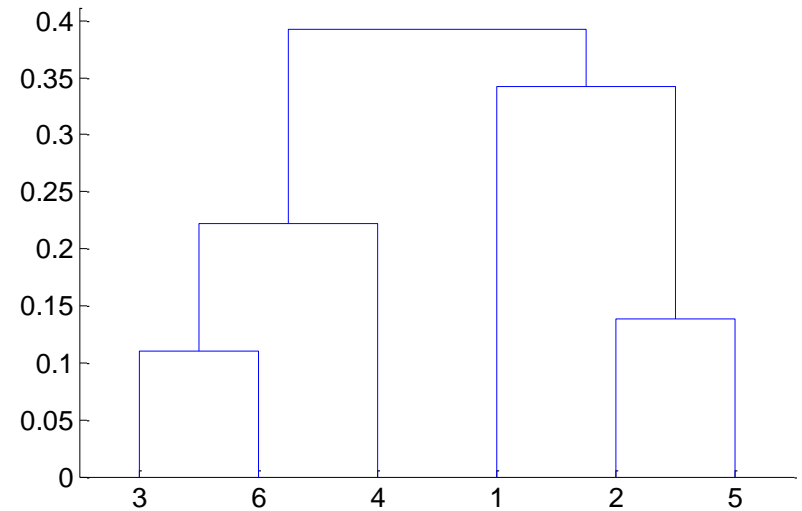
	11	12	13	14	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: MAX

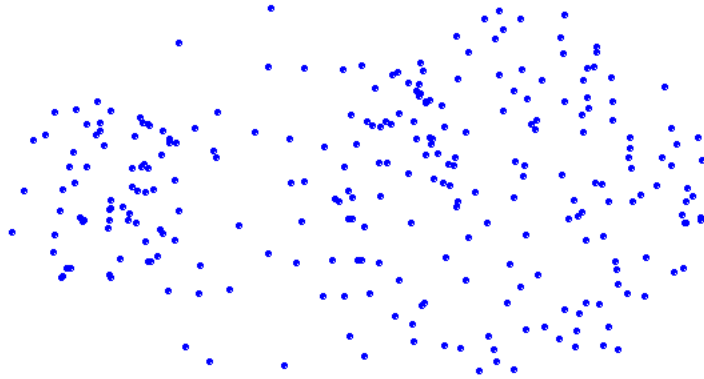


Nested Clusters

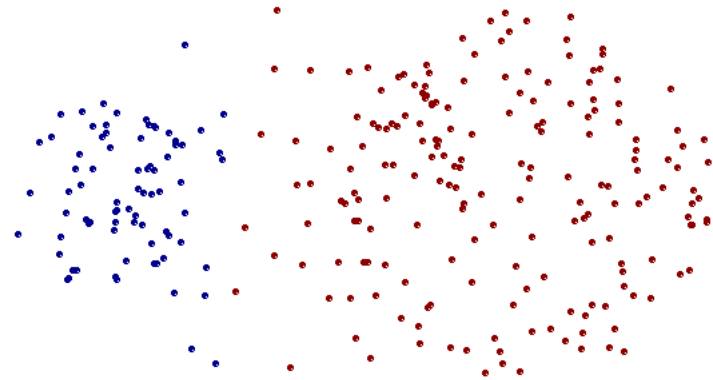


Dendrogram

Strength of MAX



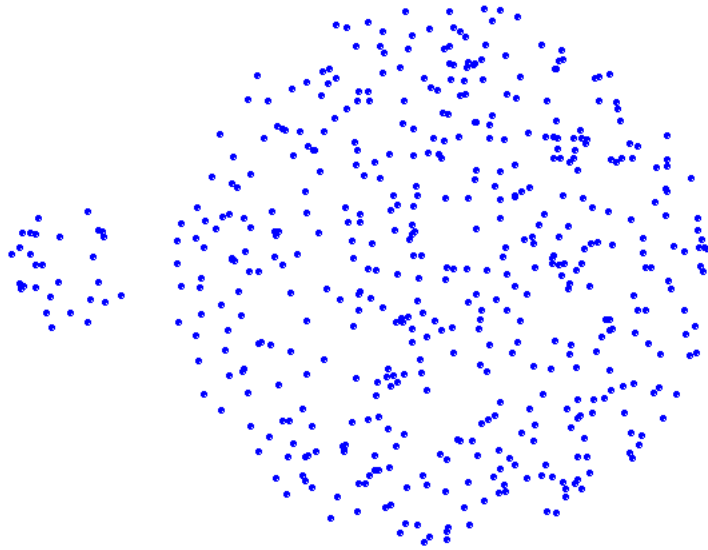
Original Points



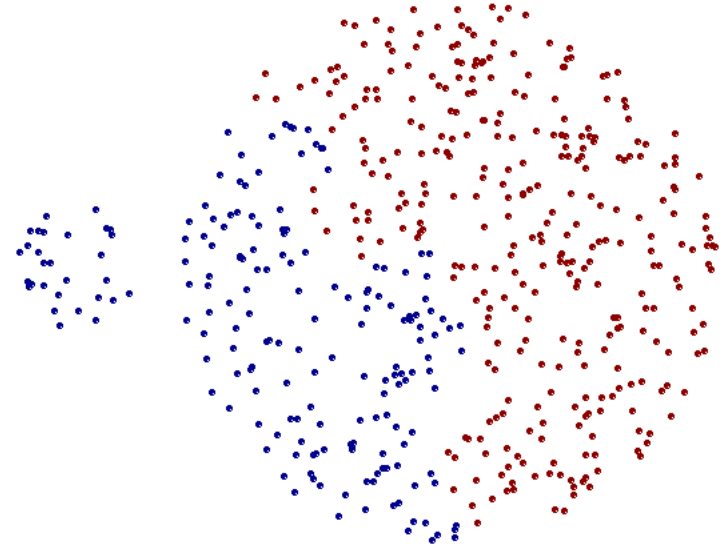
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

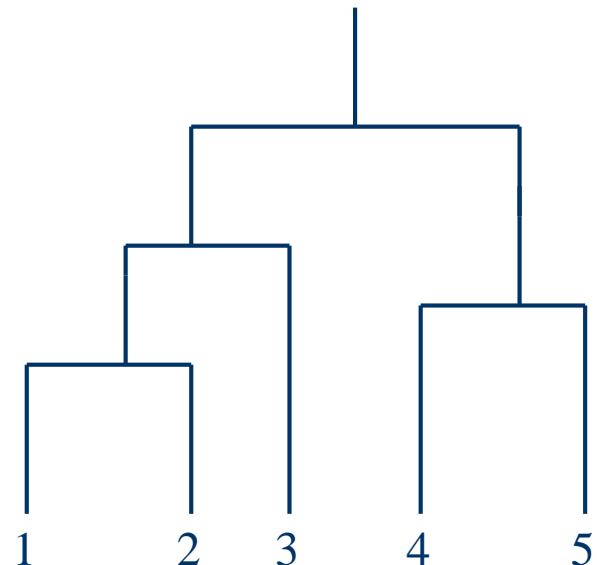
Cluster Similarity: Group Average

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

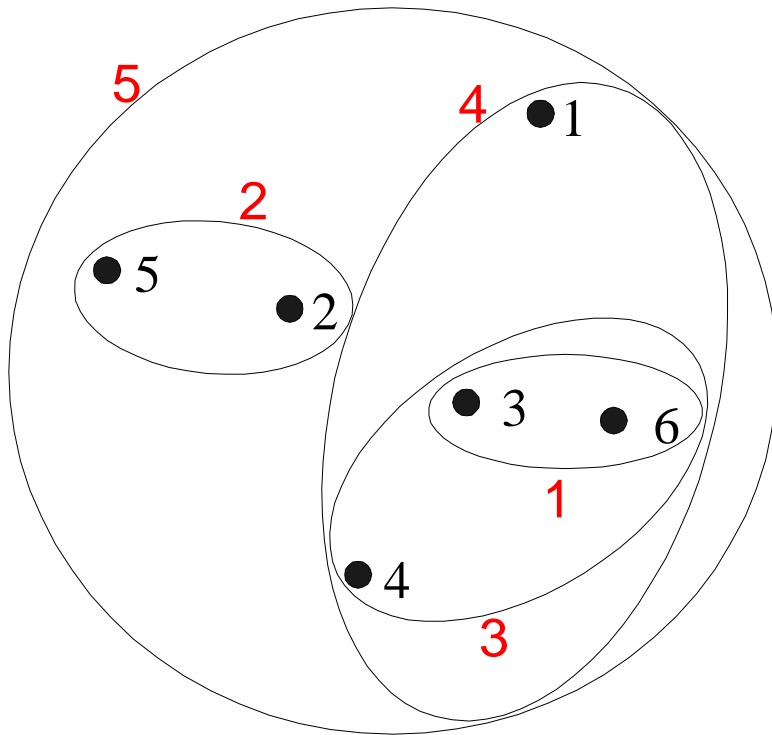
$$\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| * |\text{Cluster}_j|}$$

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

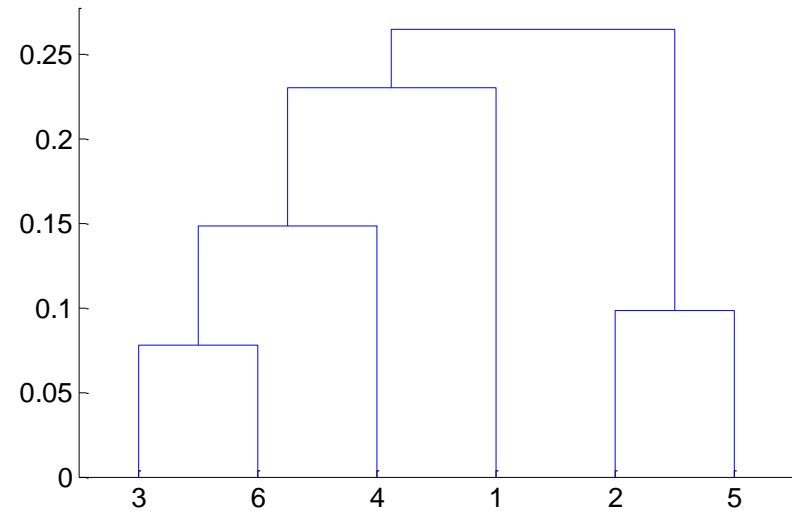
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: Group Average



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 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: 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

- 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

References

- Introduction to Data Mining by Tan, Steinbach, Kumar (Lecture Slides)
- <https://www.iula.upf.edu/materials/040701wanner.pdf>

Questions!