Cluster Analysis

Lecture 07

Taken from:

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Last Week

- Decision Tree
- Support Vector Machine

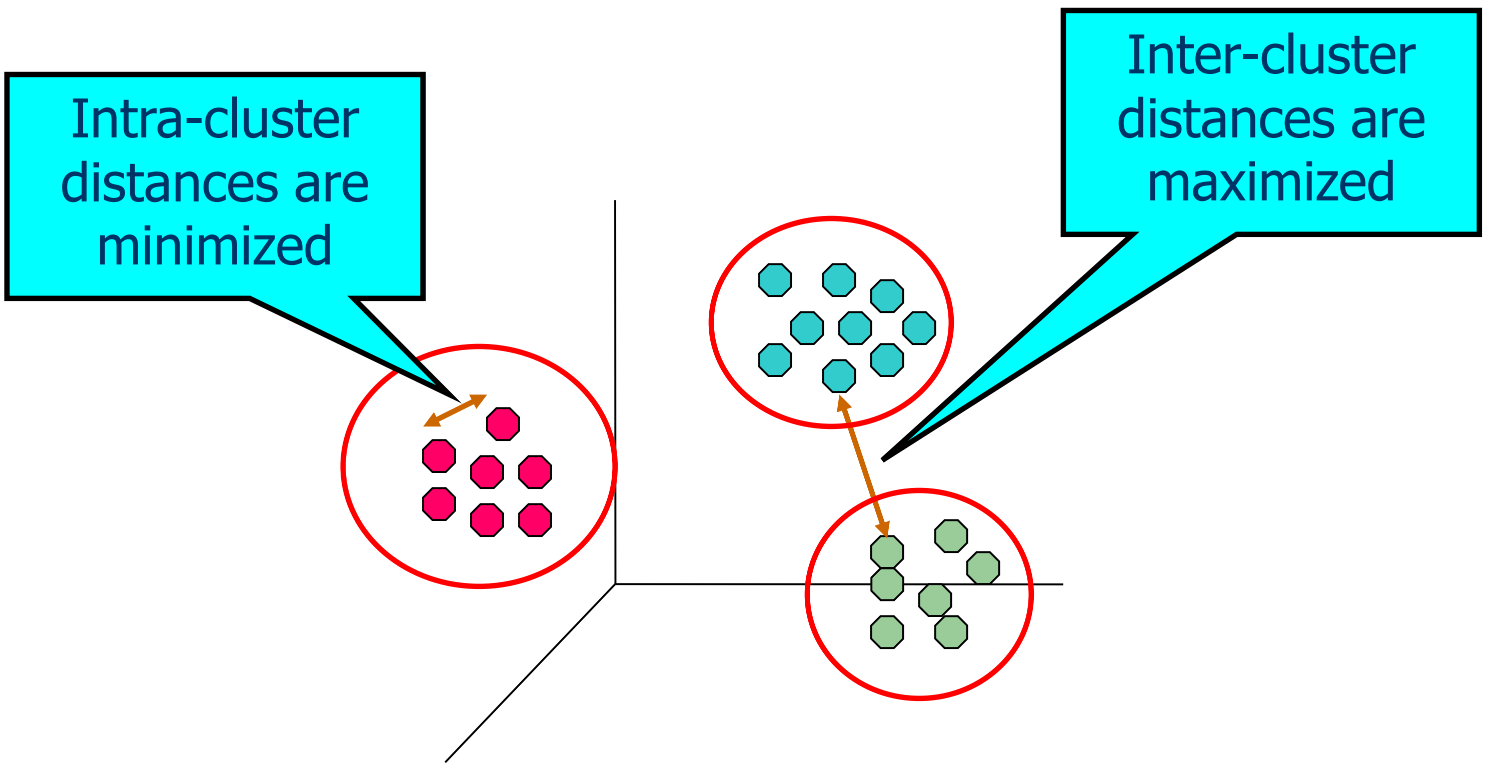
Content

[redacted]

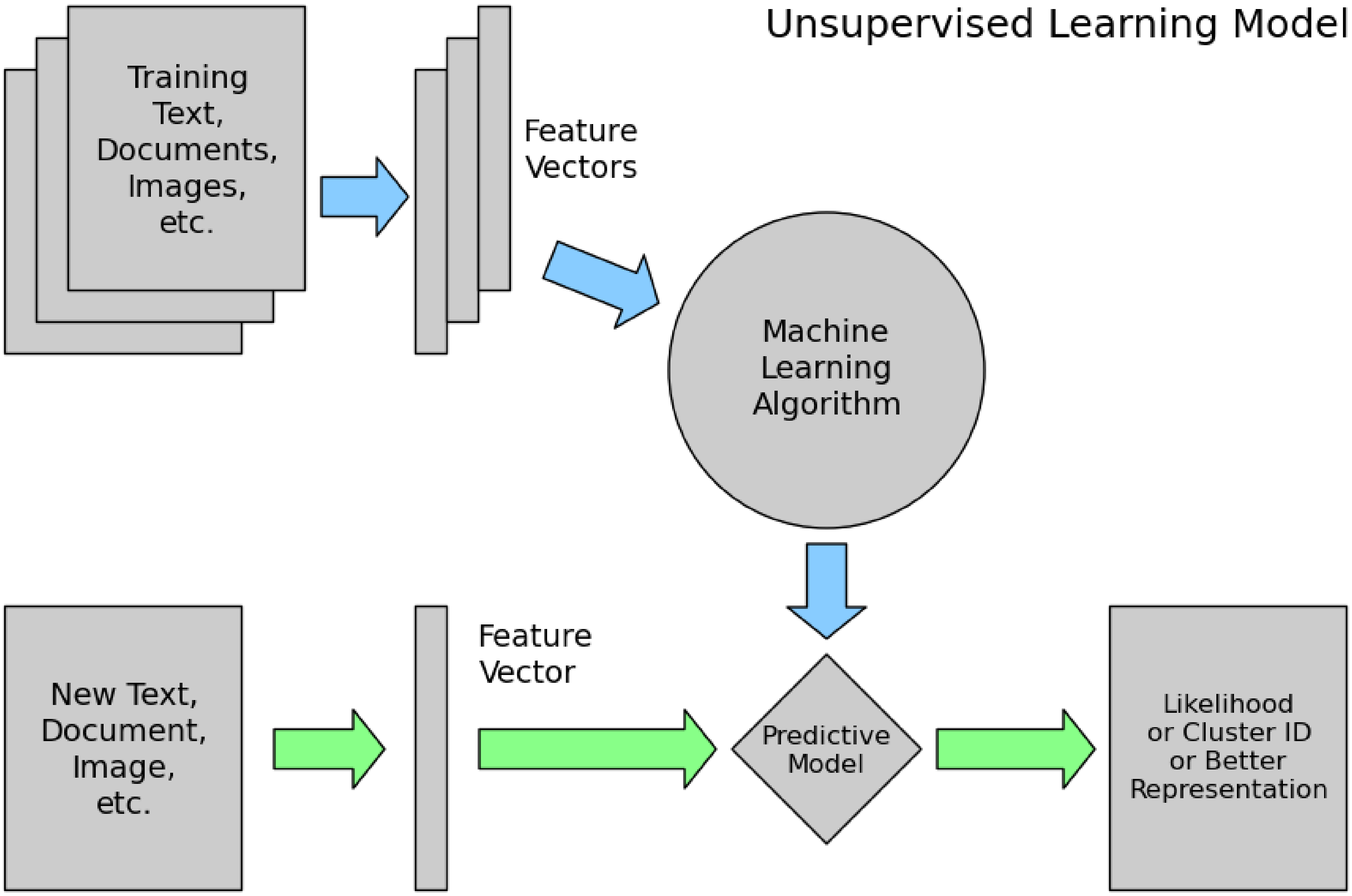
- Applications of Cluster
- Types of cluster
- Conclusions

What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will [redacted] (or unrelated to) the objects in other groups

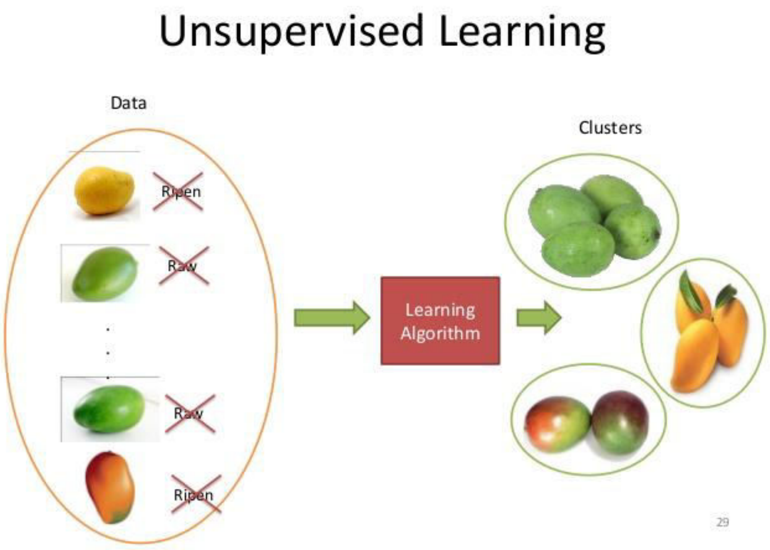


Unsupervised Learning



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

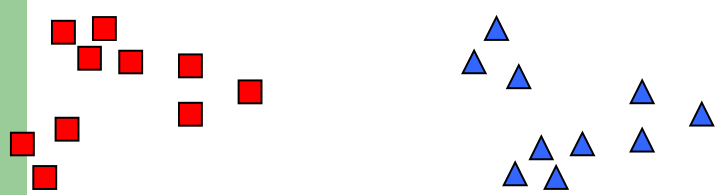


- **Summarization**
  - Reduce the size of large data sets

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters



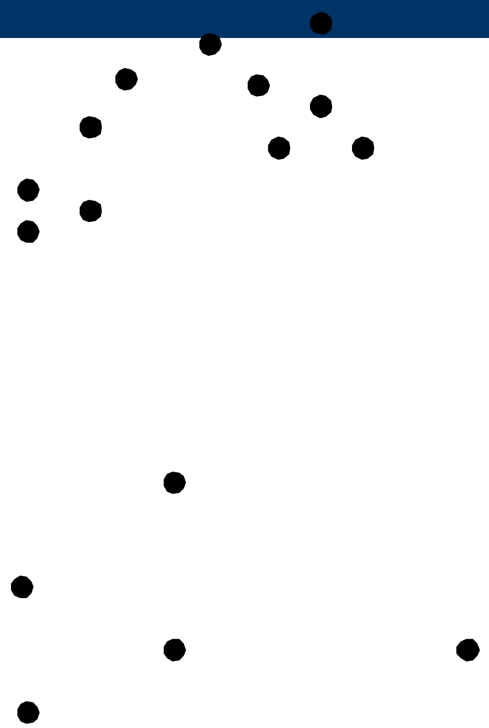
Two Clusters

Four Clusters

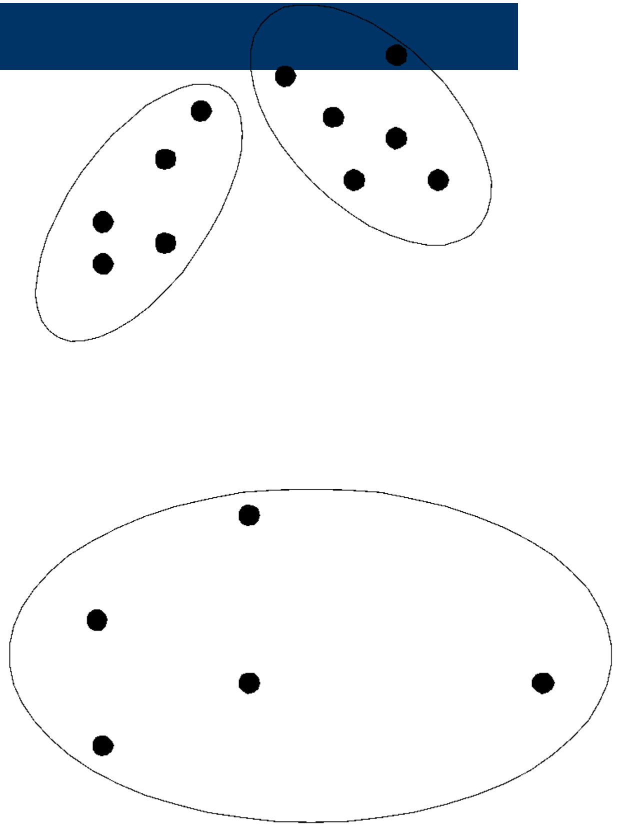
Types of Clusterings

- 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

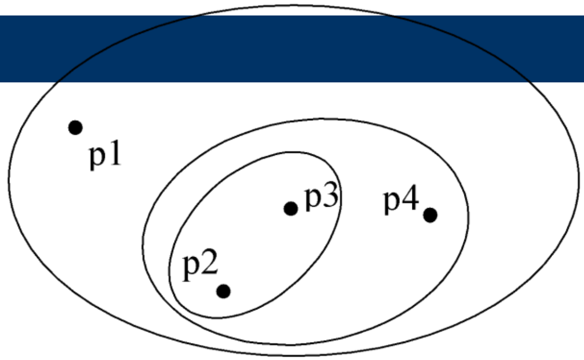


Original Points

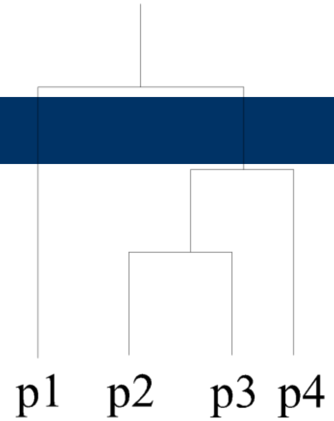


A Partitional Clustering

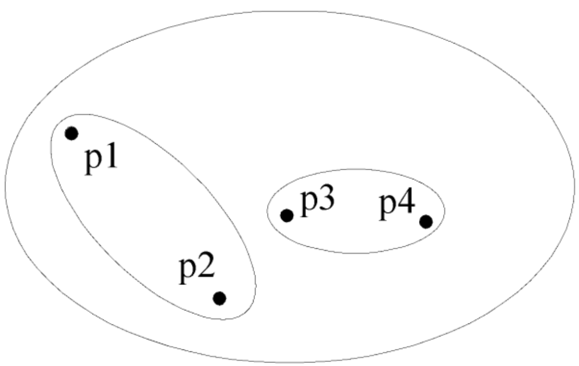
Hierarchical Clustering



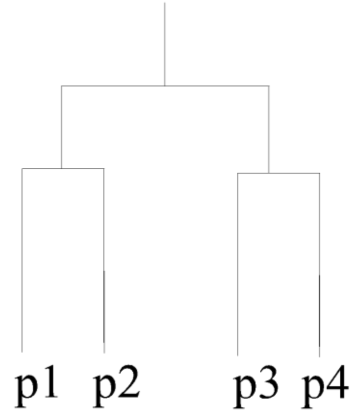
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

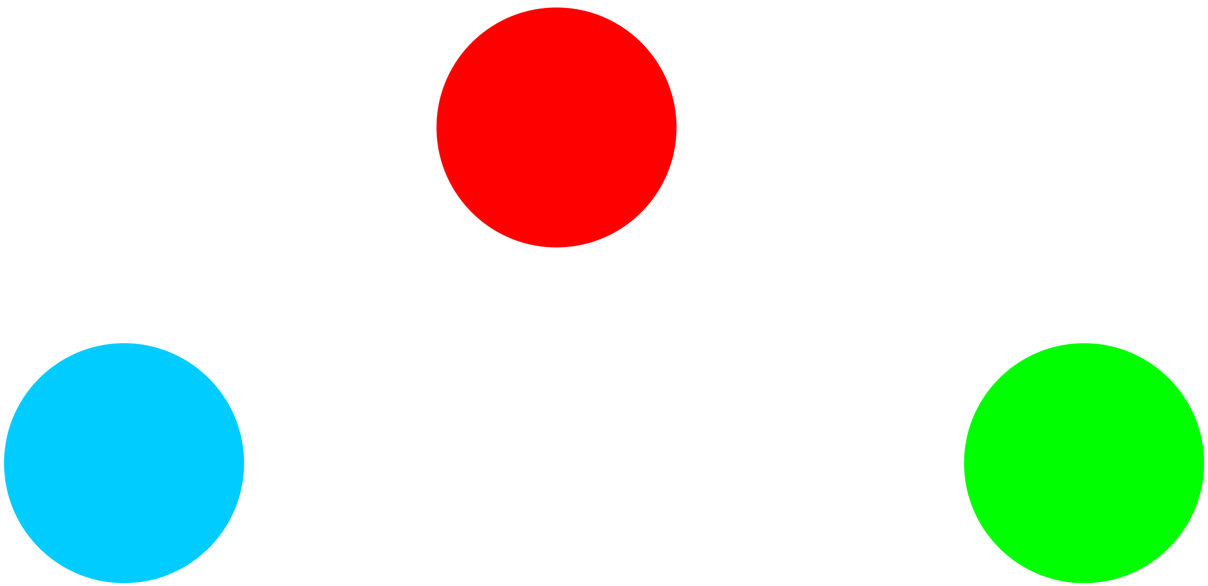
- Exclusive versus non-exclusive
  - In non-exclusive clusterings, points may belong to multiple clusters.
  - Can represent multiple classes or ‘border’ points
- Fuzzy versus non-fuzzy
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
  - Weights must sum to 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

- [redacted]
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
-

Types of Clusters: Well-Separated

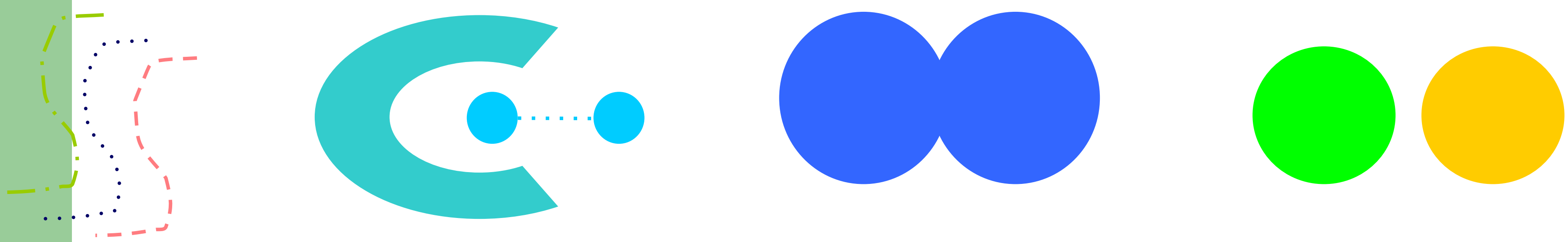
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Contiguity-Based

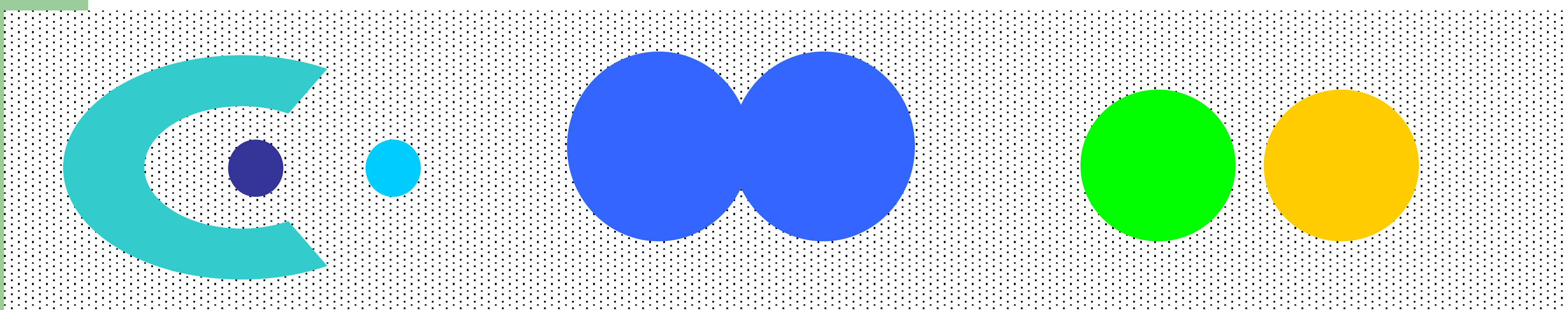
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Types of Clusters: Density-Based

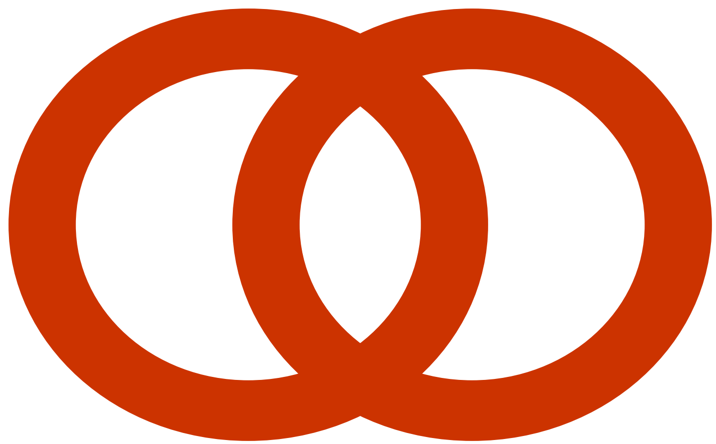
- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



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.
  - .

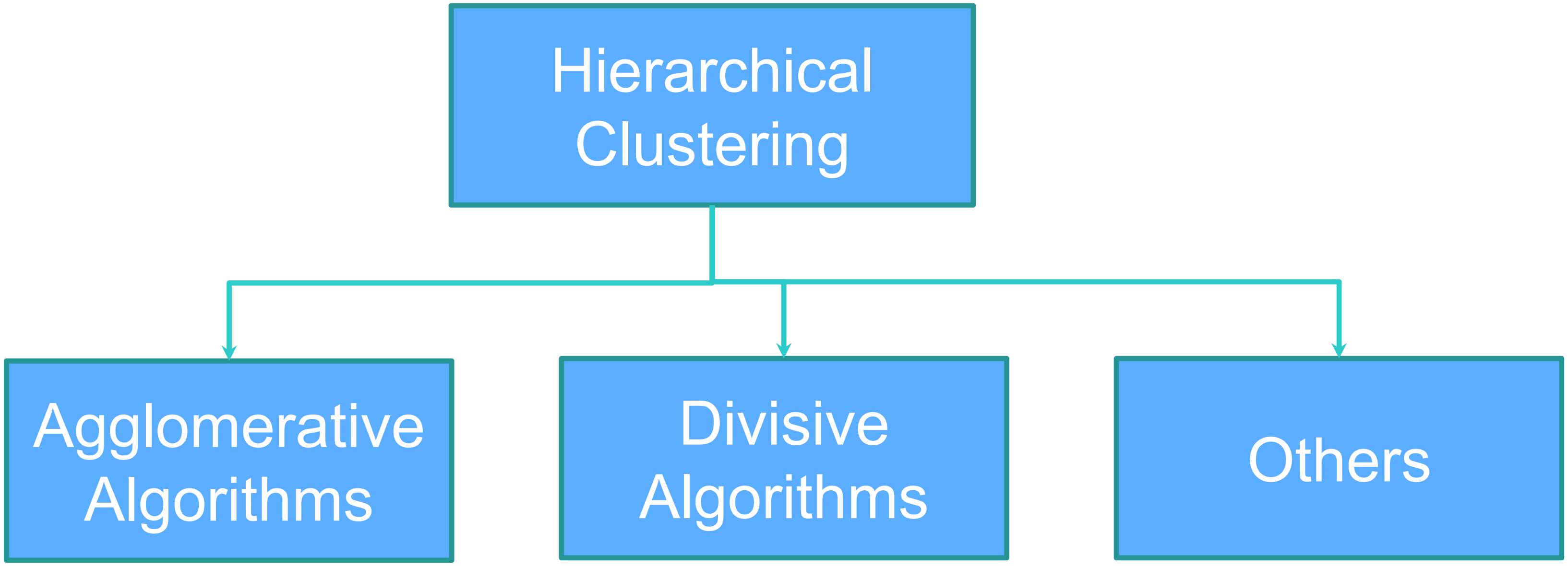


2 Overlapping Circles

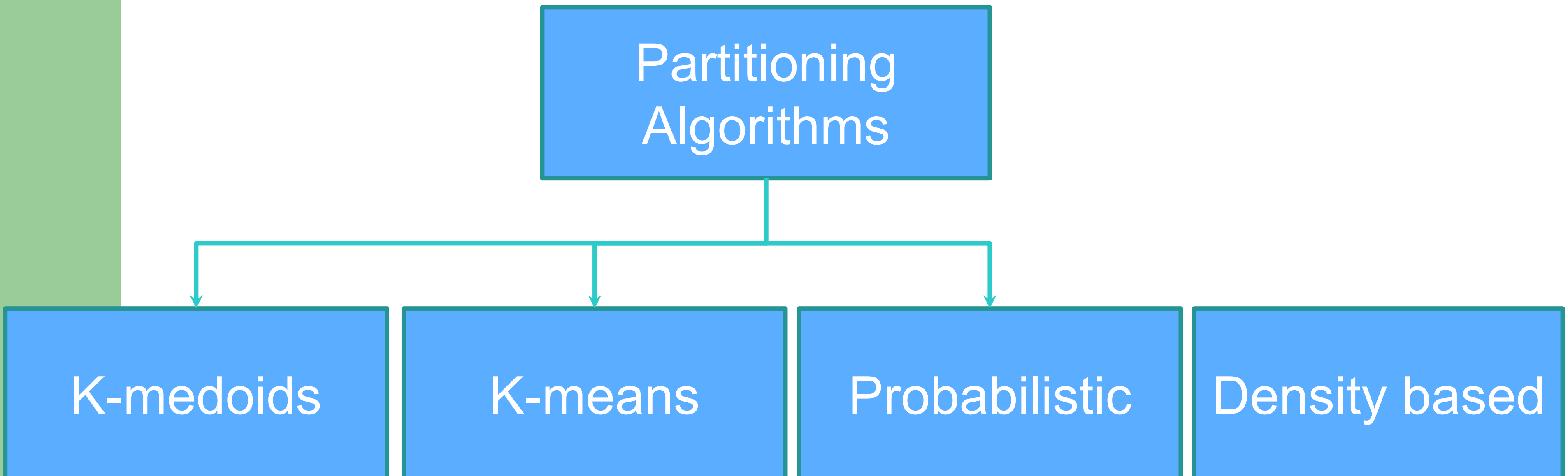
Types of Clusters: Objective Function

- 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.
    -

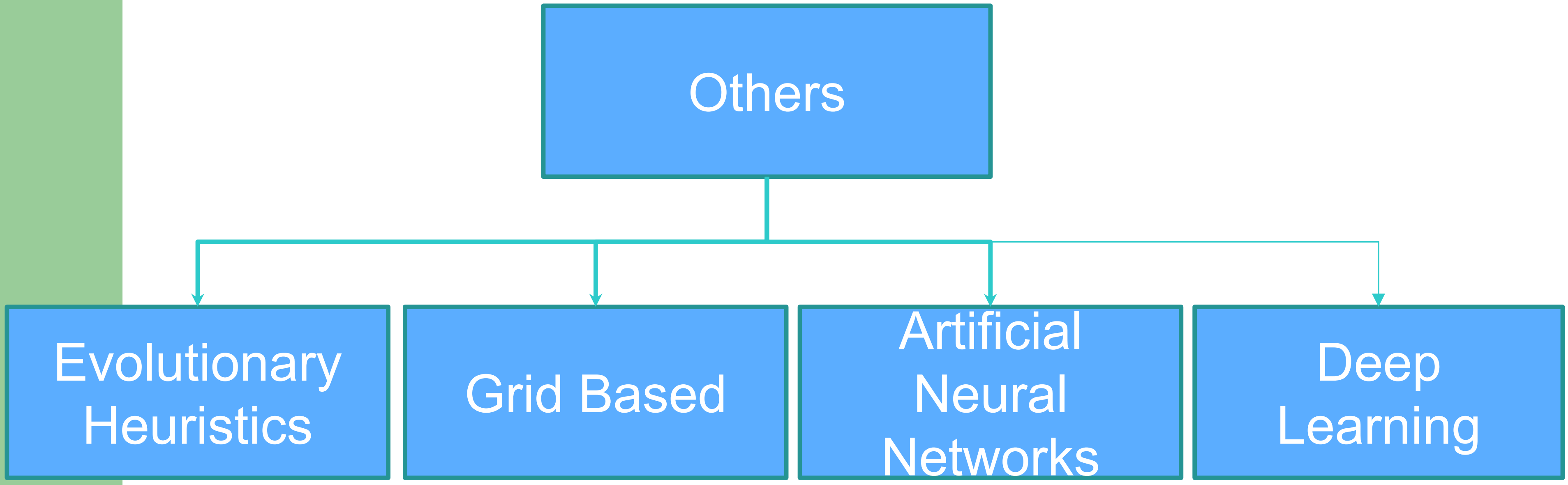
Clustering Algorithms



Clustering Algorithms



Clustering Algorithms



K-means Clustering

- Partitional clustering approach
- [redacted] centroid
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The basic algorithm is very simple

Algorithm 1 Basic K-means Algorithm.

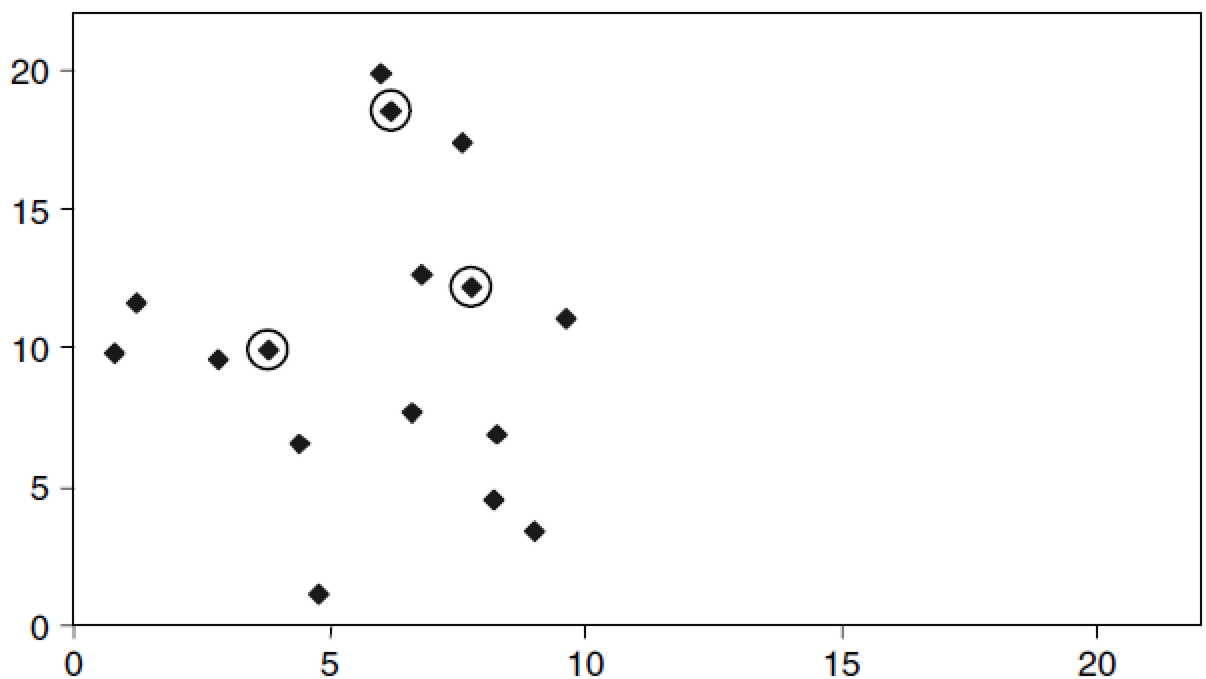
1: Select K points as the initial centroids.
2: **repeat**
3:     Form K clusters by assigning all points to the closest centroid.
4:     Recompute the centroid of each cluster.
5: **until** The centroids don't change

K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- [redacted]
- ‘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,

Example

[redacted] *to cluster the 16 objects* with two attributes *x and y*



x	y
6.8	12.6
0.8	9.8
1.2	11.6
2.8	9.6
3.8	9.9
4.4	6.5
4.8	1.1
6.0	19.9
6.2	18.5
7.6	17.4
7.8	12.2
6.6	7.7
8.2	4.5
8.4	6.9
9.0	3.4
9.6	11.1

- The columns headed *d1, d2 and d3 in Figure shows the Euclidean distance* of each of the 16 points from the three

- The column headed 'cluster' indicates the centroid closest to each point and thus the cluster to which it should be assigned.

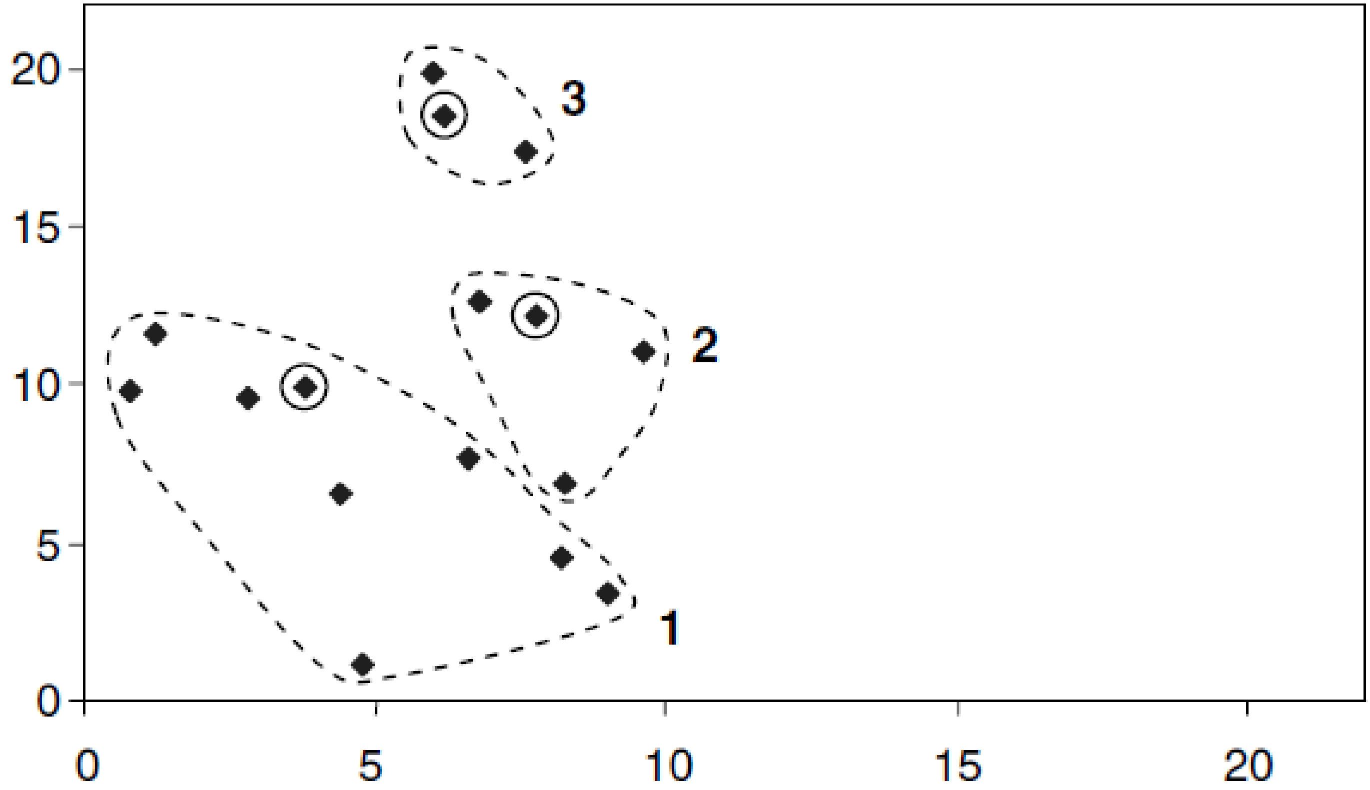
	Initial x	Initial y
Centroid 1	3.8	9.9
Centroid 2	7.8	12.2
Centroid 3	6.2	18.5

The distance of the first point (6.*8, 12.6) from the first centroid (3.8, 9.9) is simply*

$$\sqrt{(6.8-3.8)^2+(12.6-9.9)^2} = 4.0 \text{ (to one decimal place)}$$

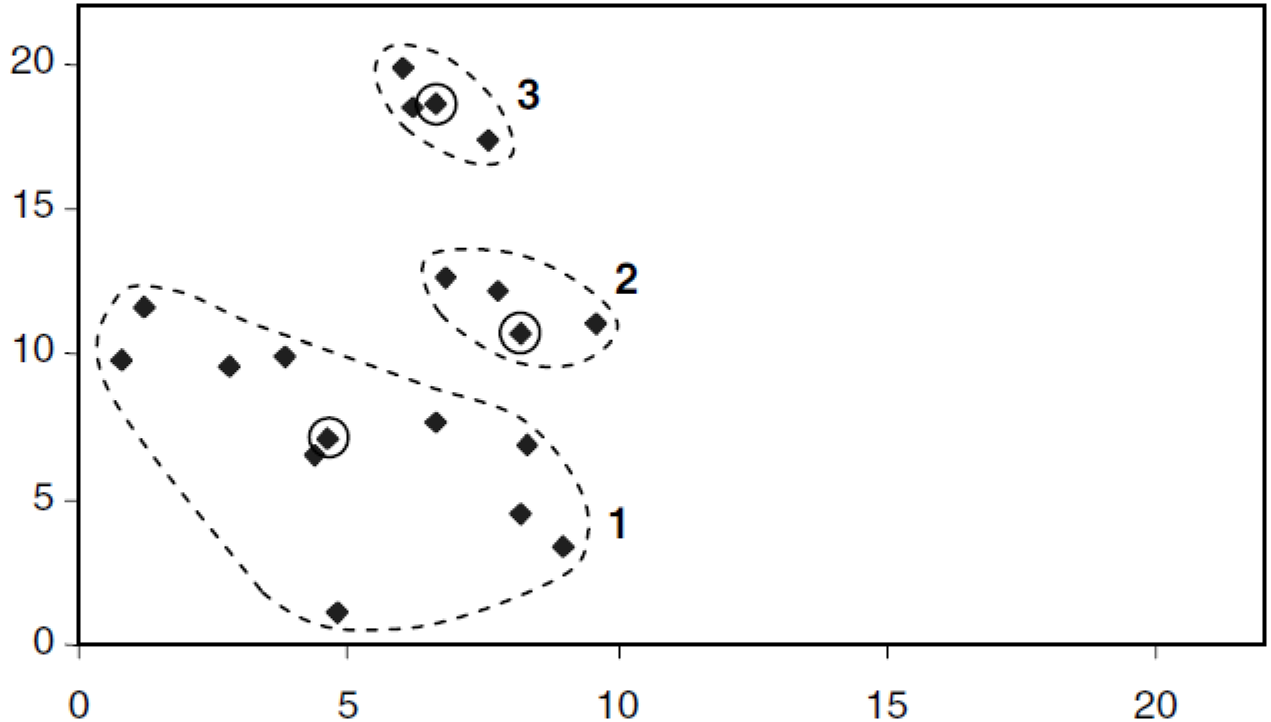
x	y	$d1$	$d2$	$d3$	cluster
6.8	12.6	4.0	1.1	5.9	2
0.8	9.8	3.0	7.4	10.2	1
1.2	11.6	3.1	6.6	8.5	1
2.8	9.6	1.0	5.6	9.5	1
3.8	9.9	0.0	4.6	8.9	1
4.4	6.5	3.5	6.6	12.1	1
4.8	1.1	8.9	11.5	17.5	1
6.0	19.9	10.2	7.9	1.4	3
6.2	18.5	8.9	6.5	0.0	3
7.6	17.4	8.4	5.2	1.8	3
7.8	12.2	4.6	0.0	6.5	2
6.6	7.7	3.6	4.7	10.8	1
8.2	4.5	7.0	7.7	14.1	1
8.4	6.9	5.5	5.3	11.8	2
9.0	3.4	8.3	8.9	15.4	1
9.6	11.1	5.9	2.1	8.1	2

The resulting clusters after 1st Iteration



Centroids after 1st Iteration and Revised Cluster

	Initial		After first iteration	
	x	y	x	y
Centroid 1	3.8	9.9	4.6	7.1
Centroid 2	7.8	12.2	8.2	10.7
Centroid 3	6.2	18.5	6.6	18.6

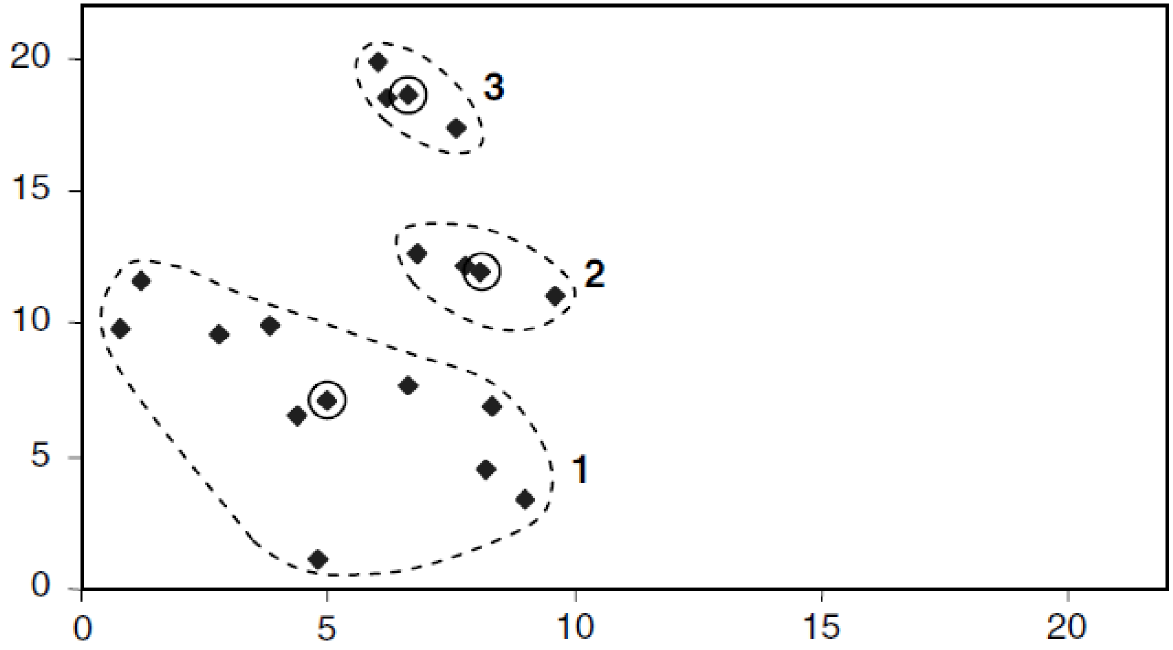


After 2nd Iteration and Third Set of Clusters

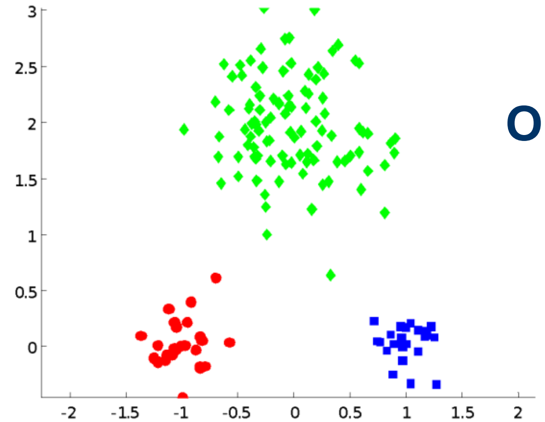
- These are the same clusters as before. Their centroids will be the same as those from which the clusters were generated.

- Hence the termination condition of the *k-means algorithm 'repeat ... until the centroids no longer move' has* been met and these are the final clusters produced by the algorithm for the initial choice of centroids made.

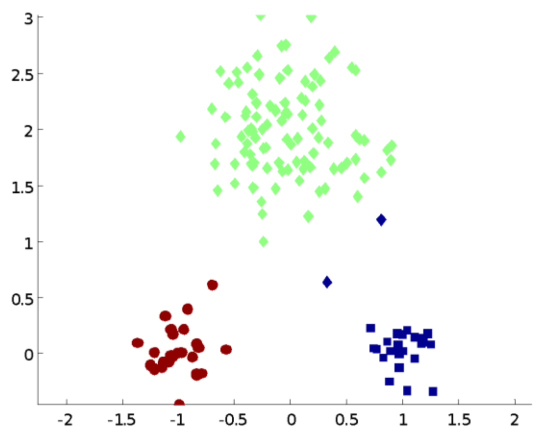
	Initial		After first iteration		After second iteration	
	x	y	x	y	x	y
Centroid 1	3.8	9.9	4.6	7.1	5.0	7.1
Centroid 2	7.8	12.2	8.2	10.7	8.1	12.0
Centroid 3	6.2	18.5	6.6	18.6	6.6	18.6



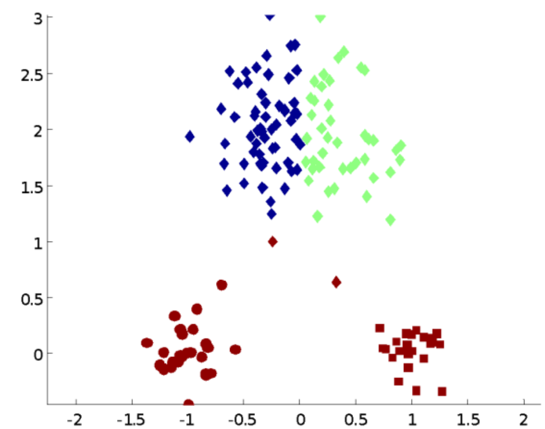
Two different K-means Clusterings



Orig[redacted]

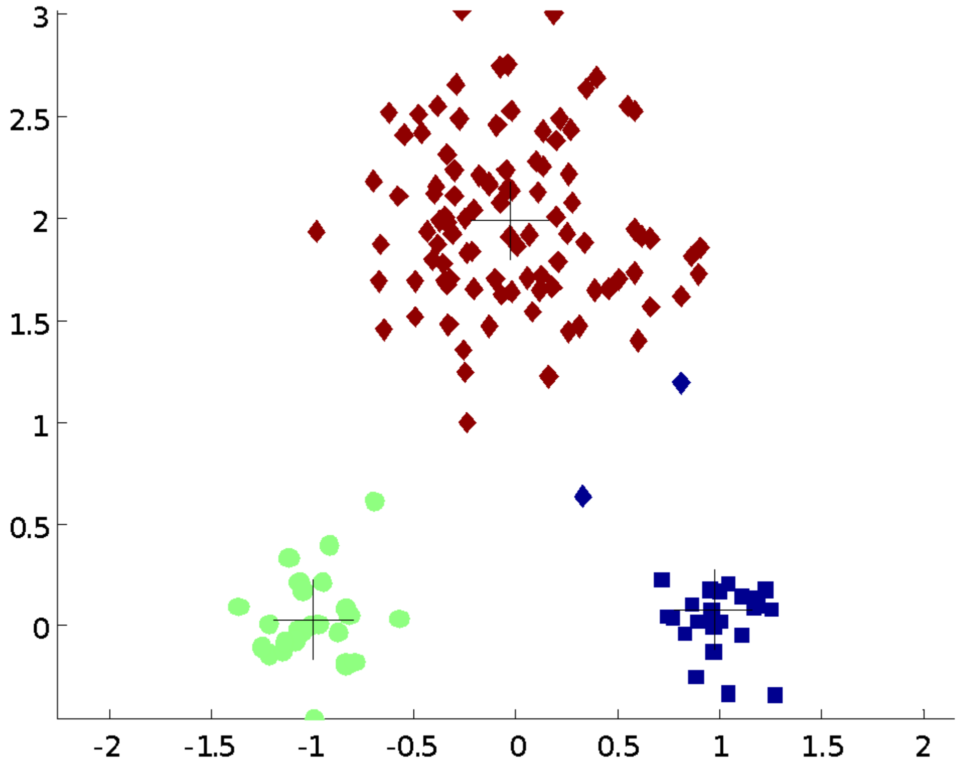


Optimal Clustering

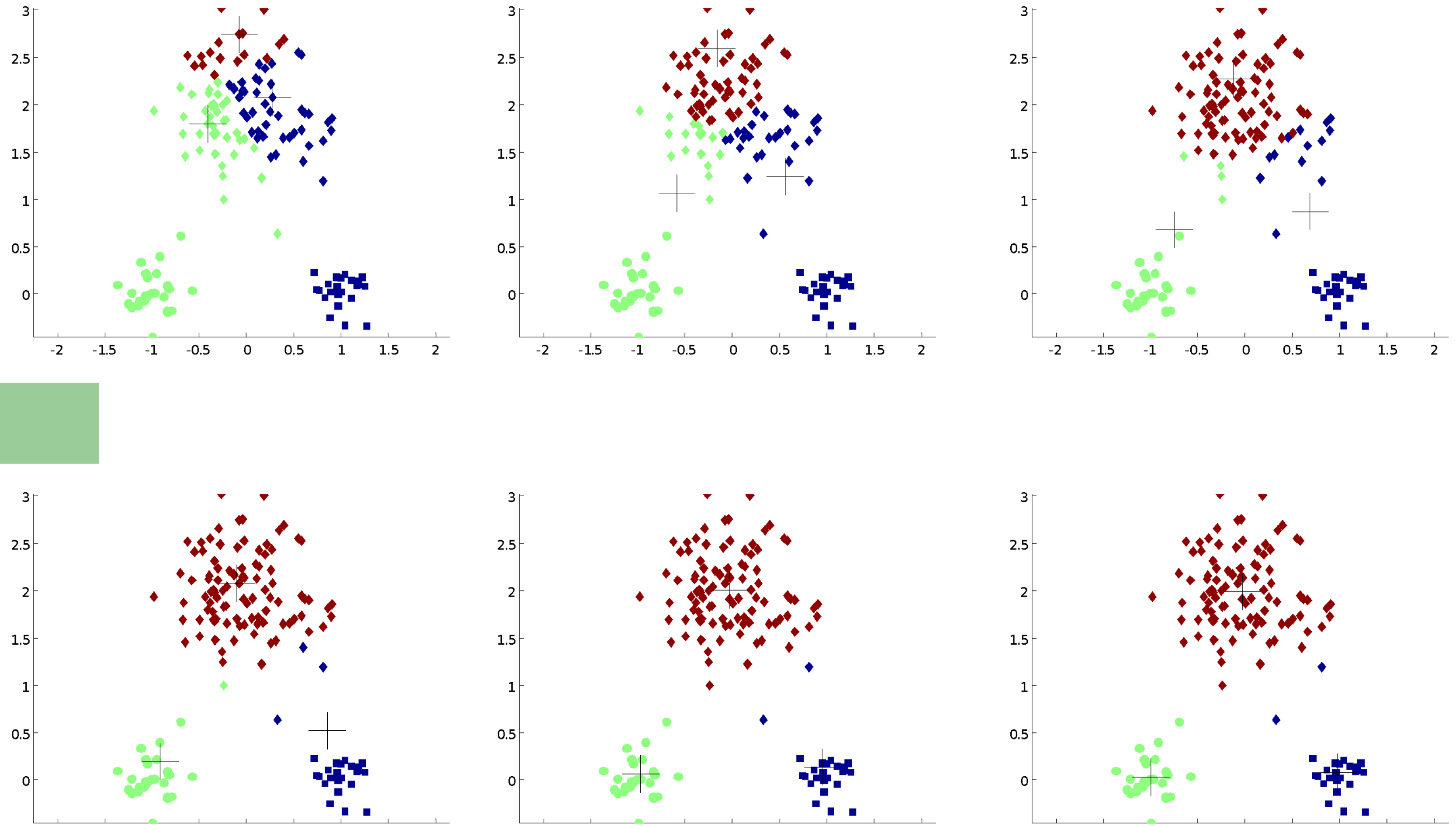


Sub-optimal Clustering

Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids



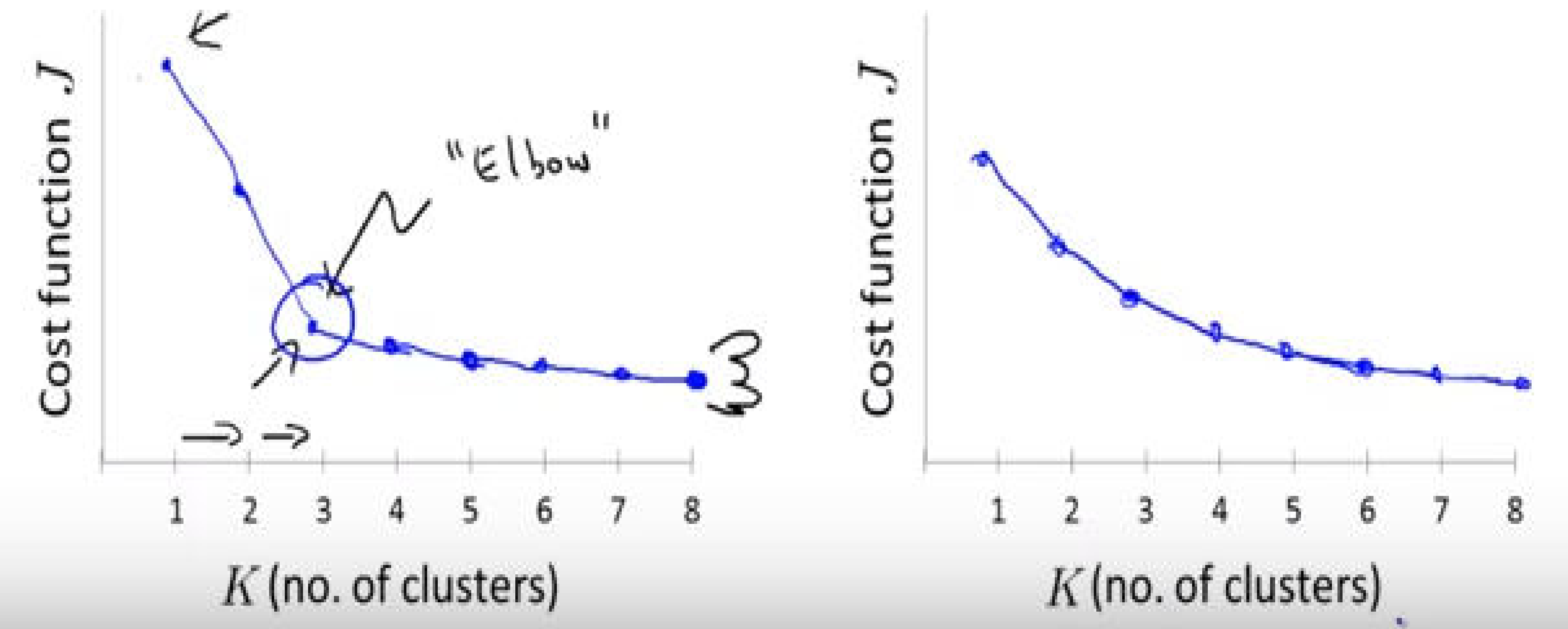
Evaluating K-means Clusters

- [redacted]E)
  - SSE is the sum of the squared differences between each observation and its group's mean. It can be used as a measure of variation within a cluster. If all cases within a cluster are identical the SSE would then be equal to 0.

$$SSE = \sum_{i=1}^{n} (x_i - \bar{x})^2$$

  - Where n is the number of observations, x_i is the value of the ith observation and $\bar{x}$ is the mean of all the observations. This can also be rearranged to be written as seen in J.H. Ward's paper.
  - Given two clusters, we can choose the one with the smallest error
  -

Elbow Method

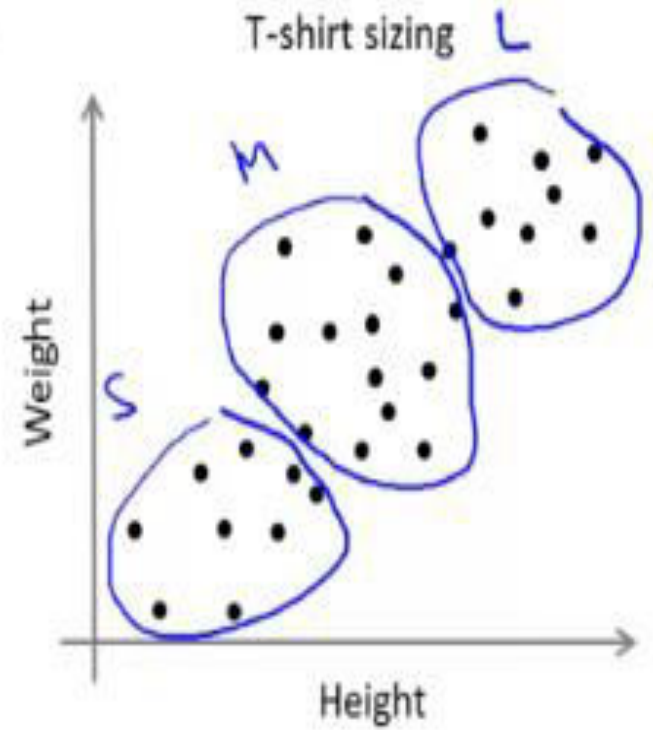


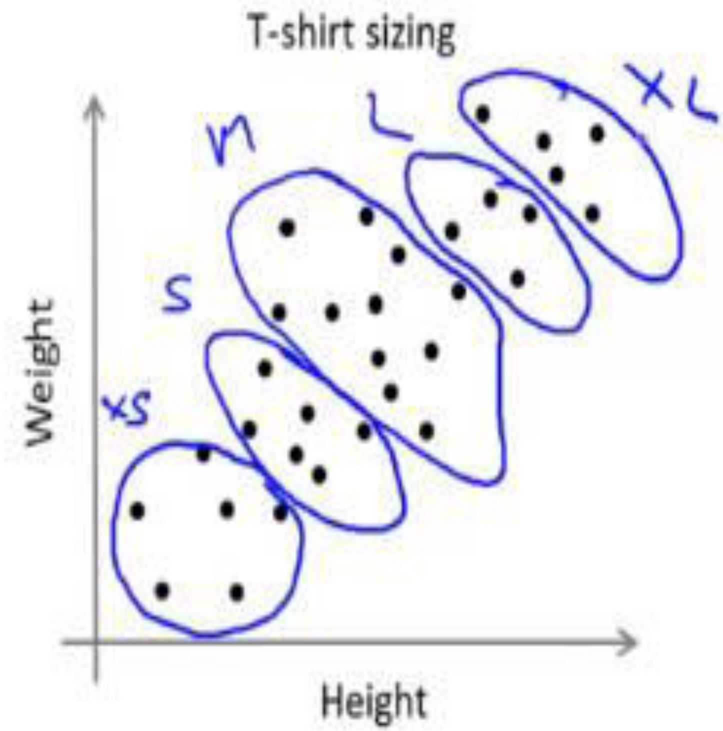
Choosing K based on a metric for how well it performs for the later purpose

k=3 S, M, L

k=5 XS, S, M, L, XL

E.g.





Solutions to Initial Centroids Problem

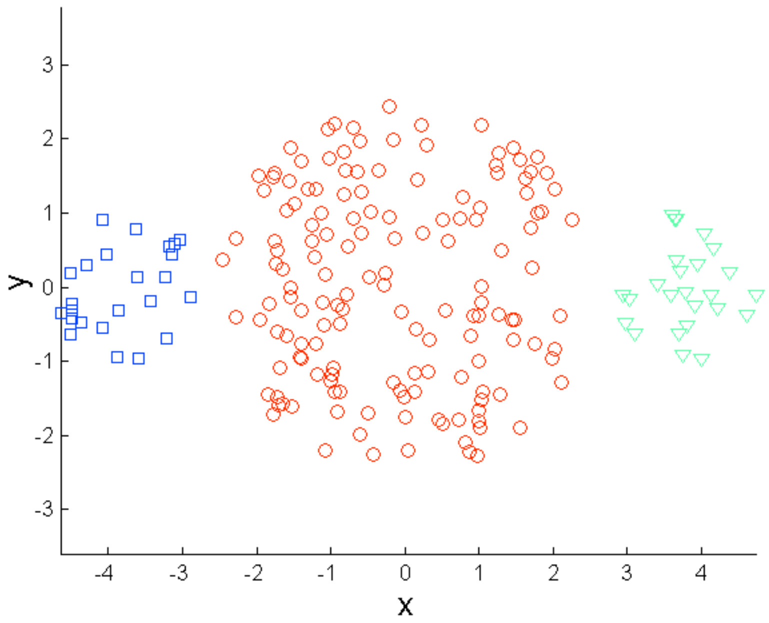
- [redacted]
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated

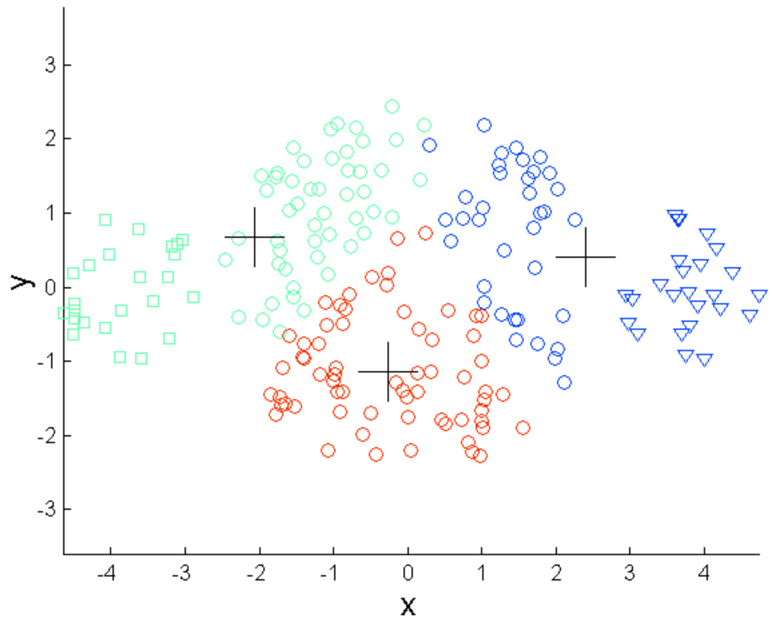
Limitations of K-means

- 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

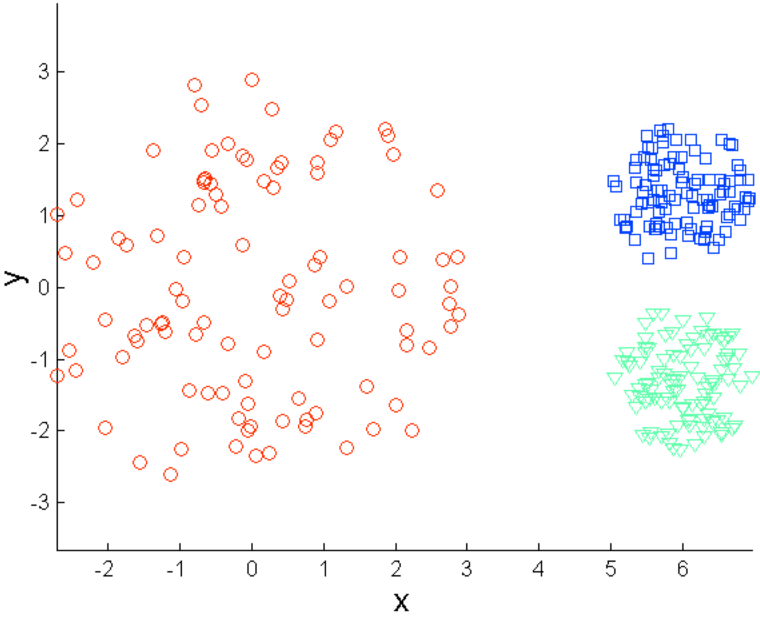


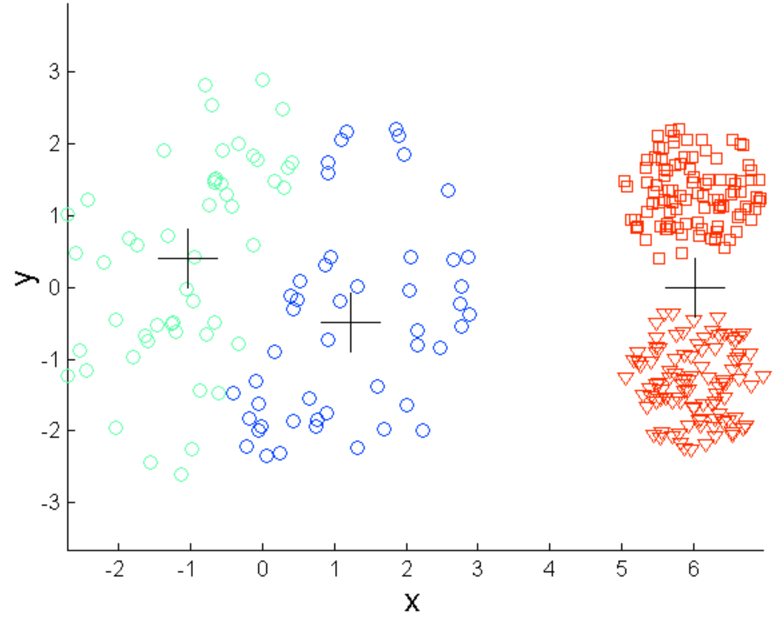


Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Density

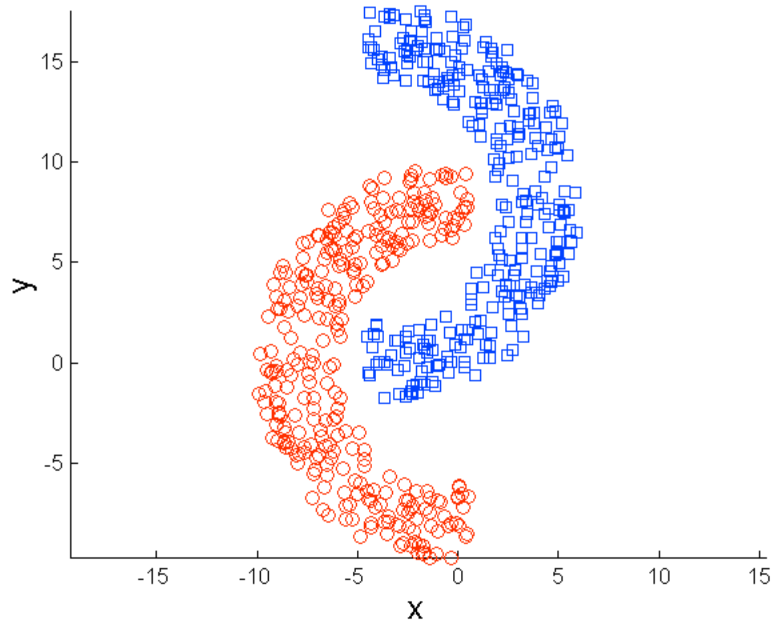


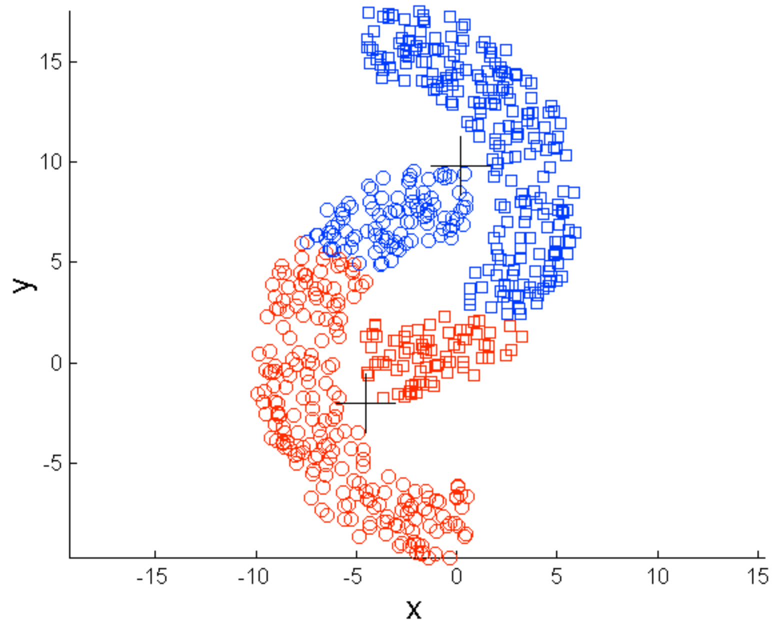


Original Points

K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



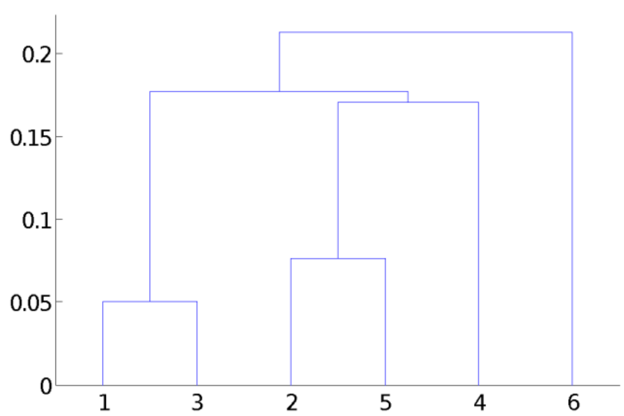


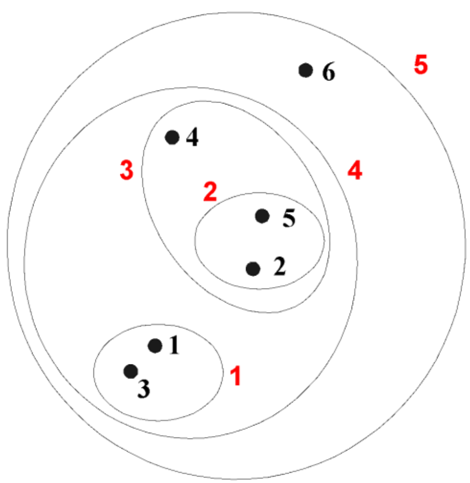
Original Points

K-means (2 Clusters)

Hierarchical Clustering

- [redacted]s a hierarchical tree
- Can be visualized as a dendrogram
  –





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 dendogram at the proper level

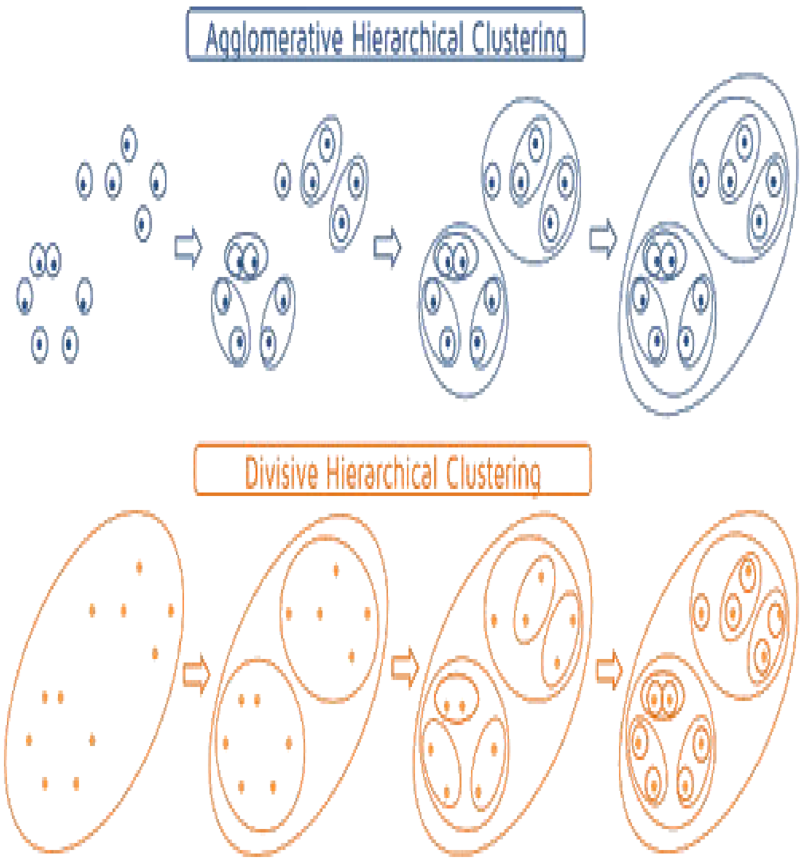
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Hierarchical Clustering

[redacted]
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)



Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique

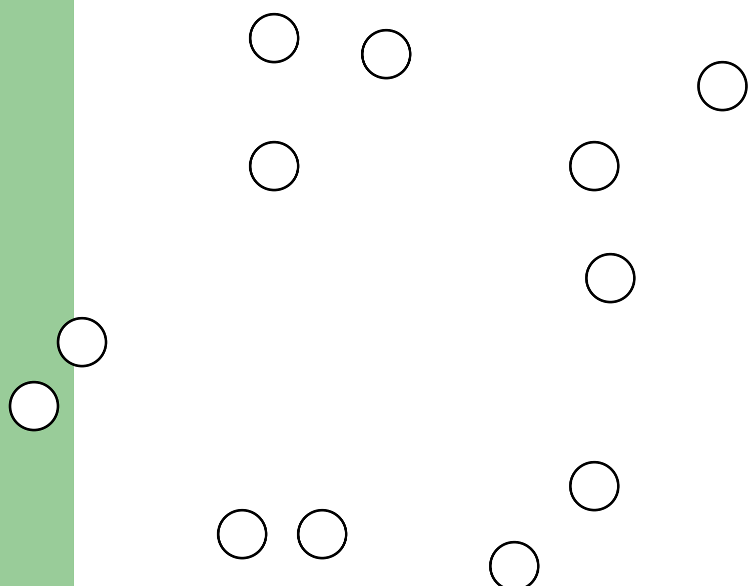
- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. **Repeat**
  4. Merge the two closest clusters
  5. Update the proximity matrix
  6. **Until** only a single cluster remains

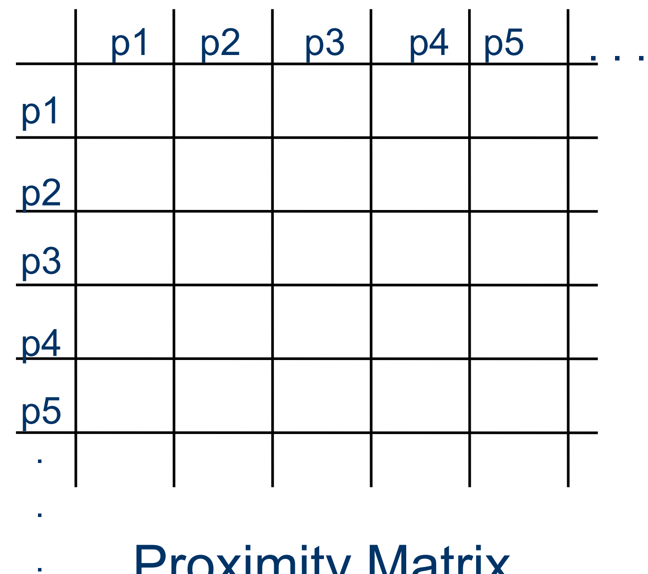
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance between clusters distinguish the different algorithms

Starting Situation

[redacted]

proximity matrix

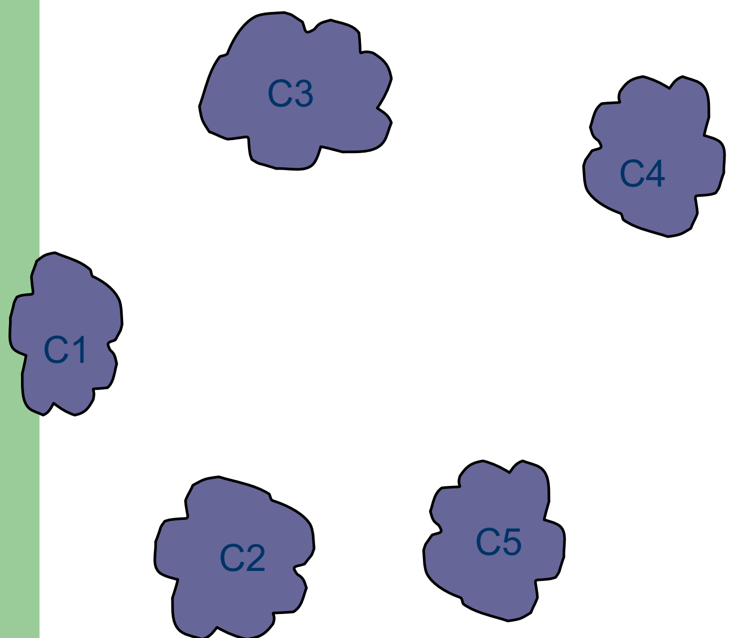




Proximity Matrix

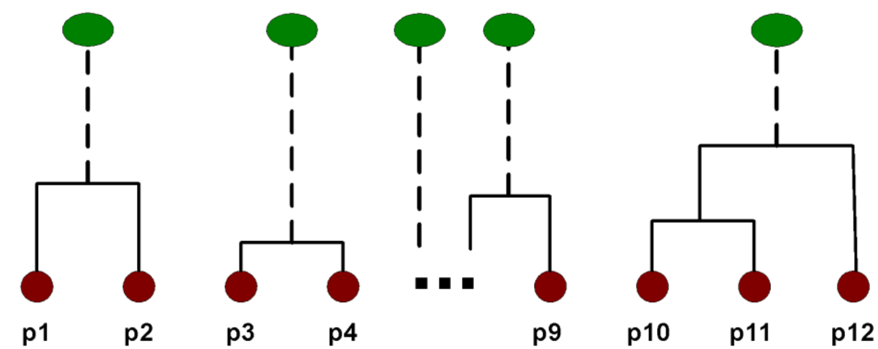
Intermediate Situation

- After some merging steps, we have some clusters



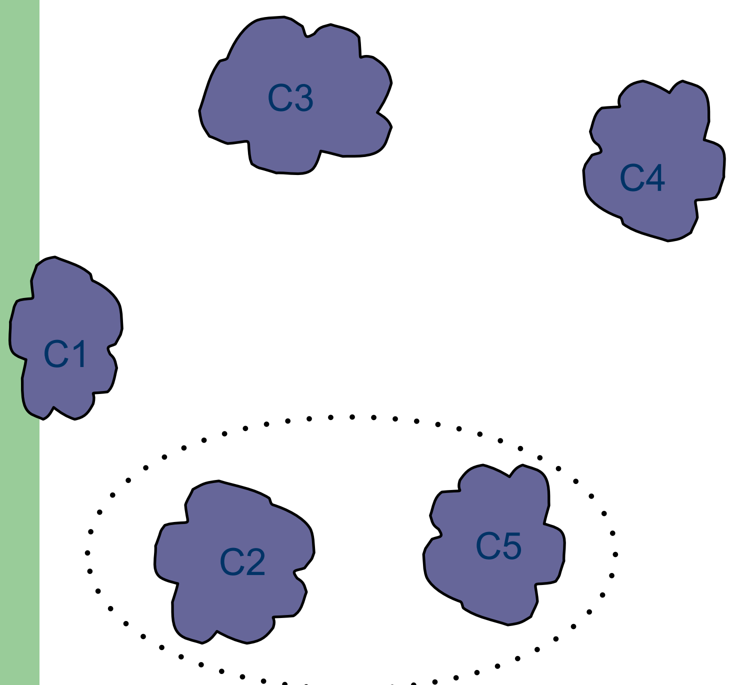
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

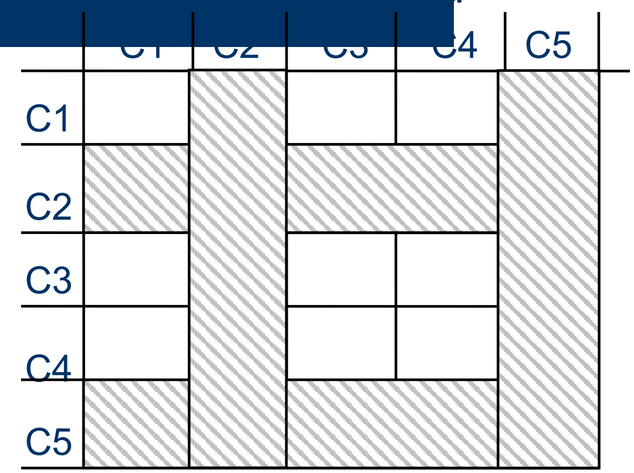
Proximity Matrix



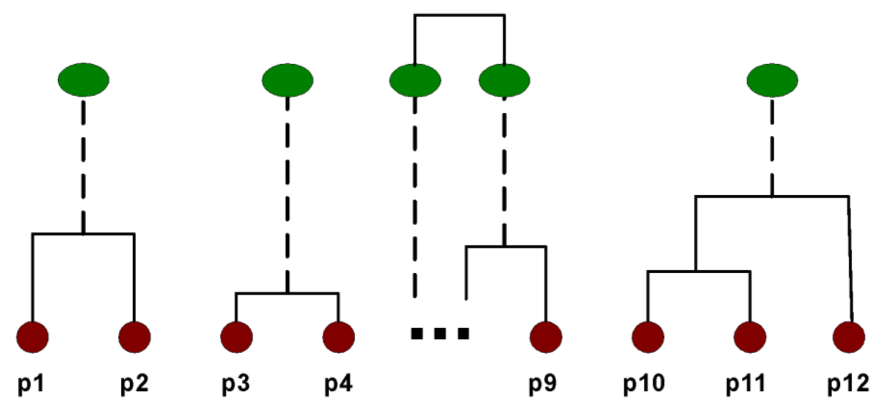
Intermediate Situation

- [redacted]



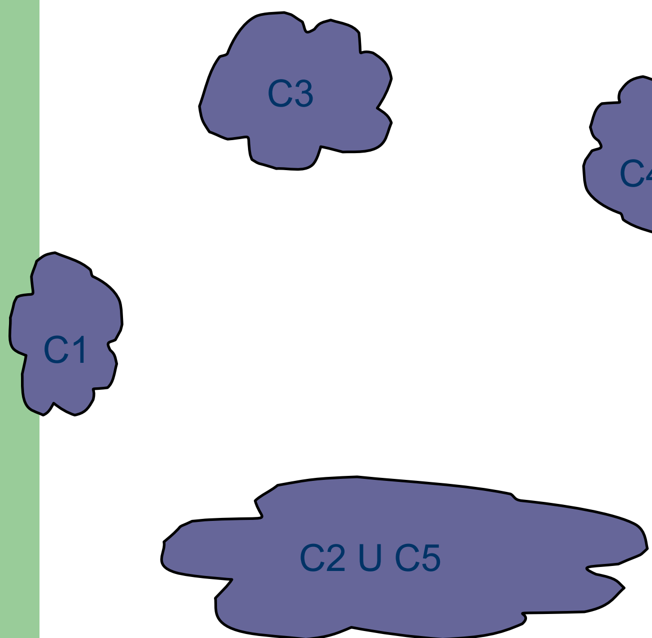


Proximity Matrix



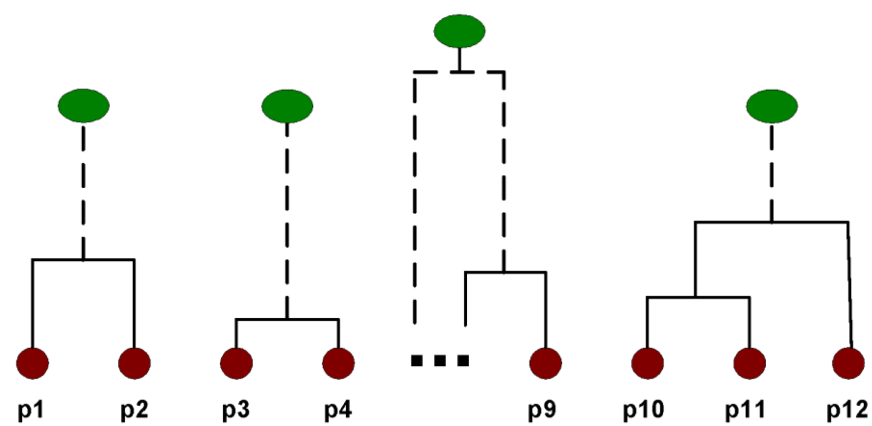
After Merging

- [redacted]

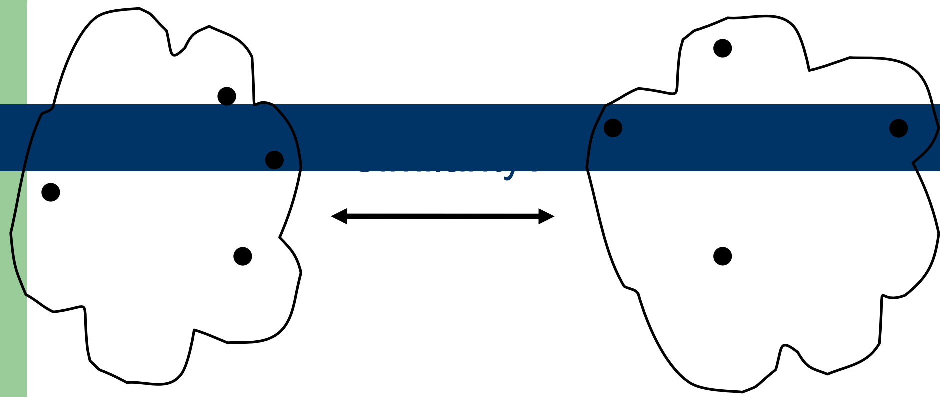


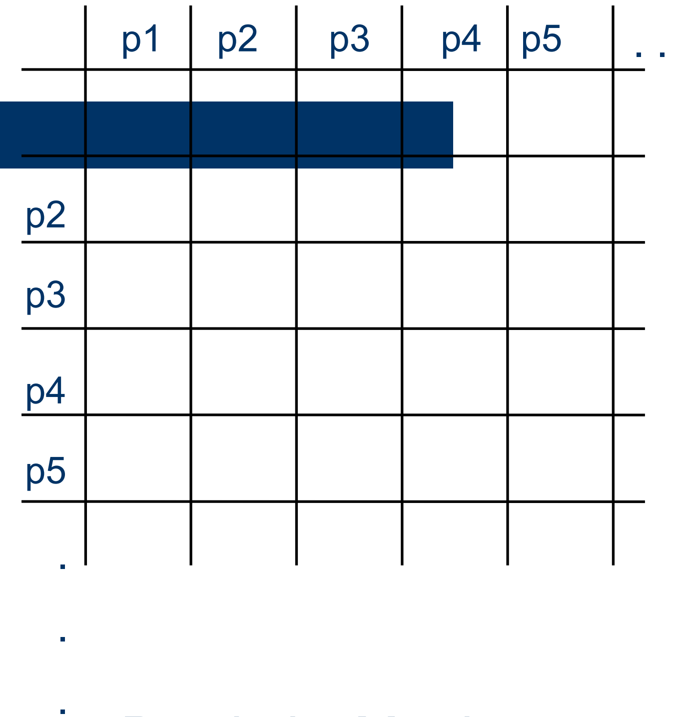
	C1	U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Similarity

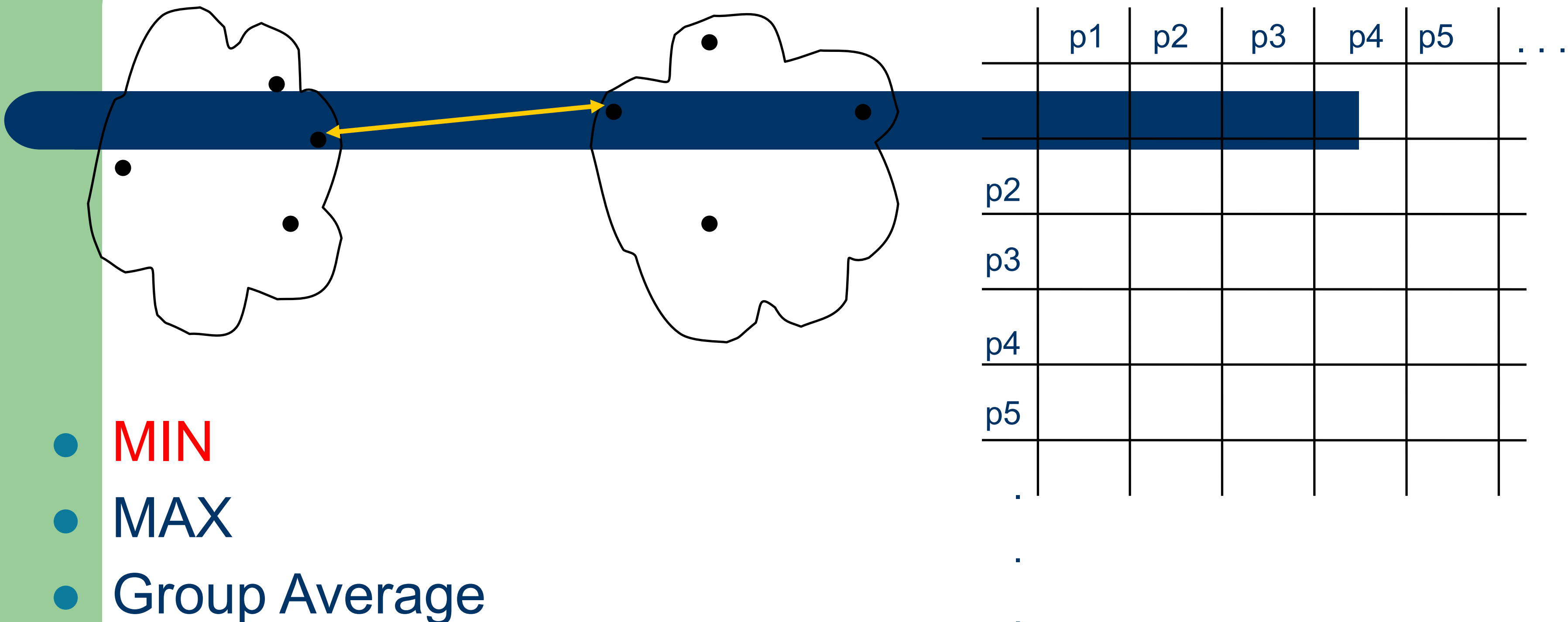




Proximity Matrix

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

How to Define Inter-Cluster Similarity



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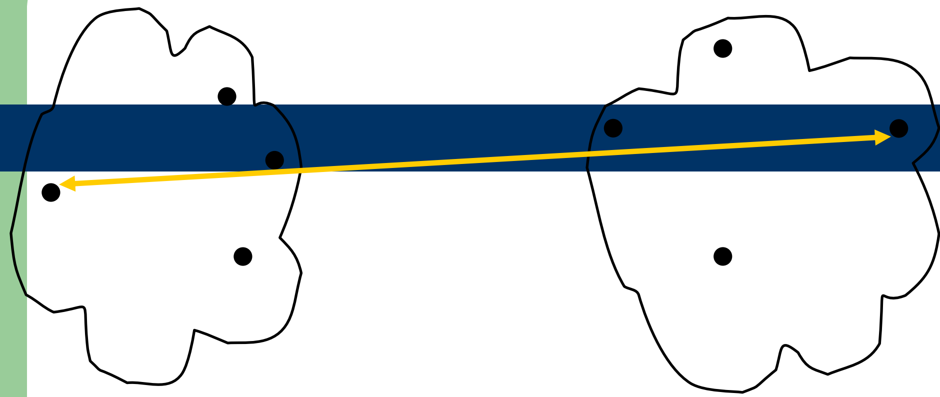

	p1	p2	p3	p4	p5	. . .
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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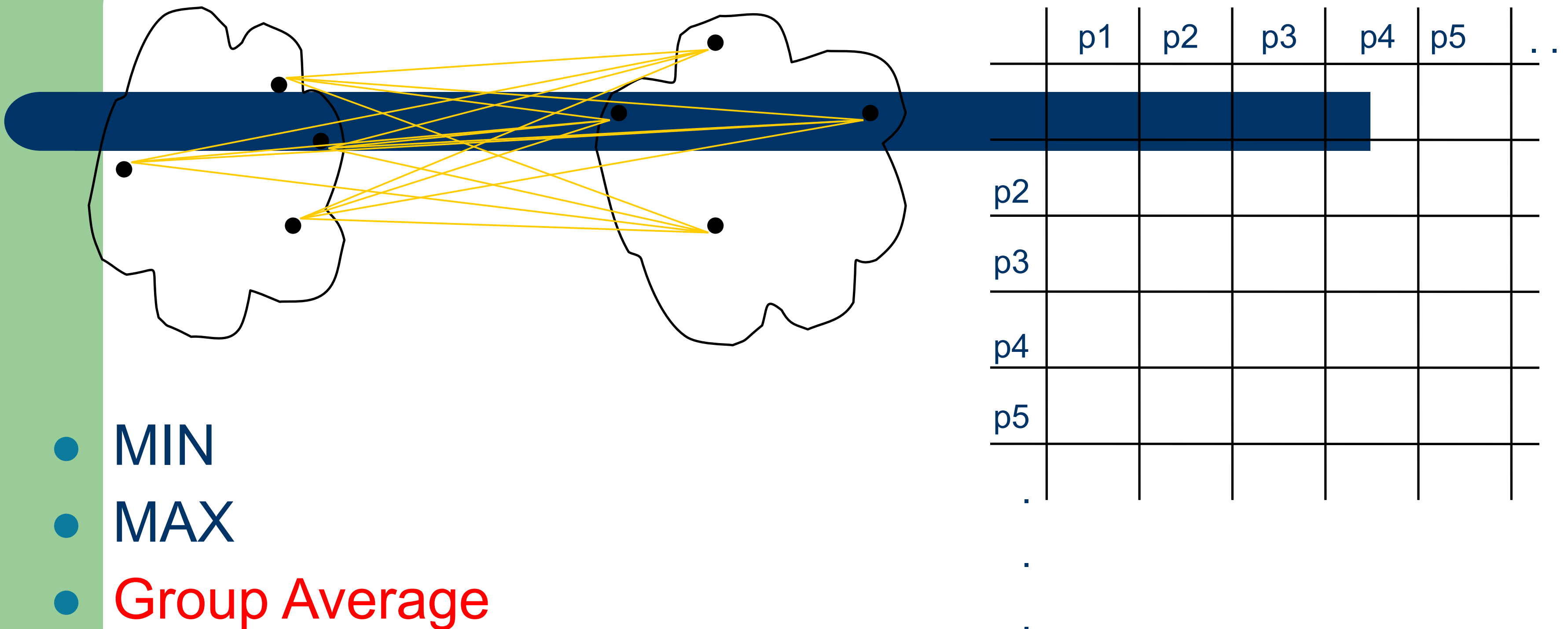

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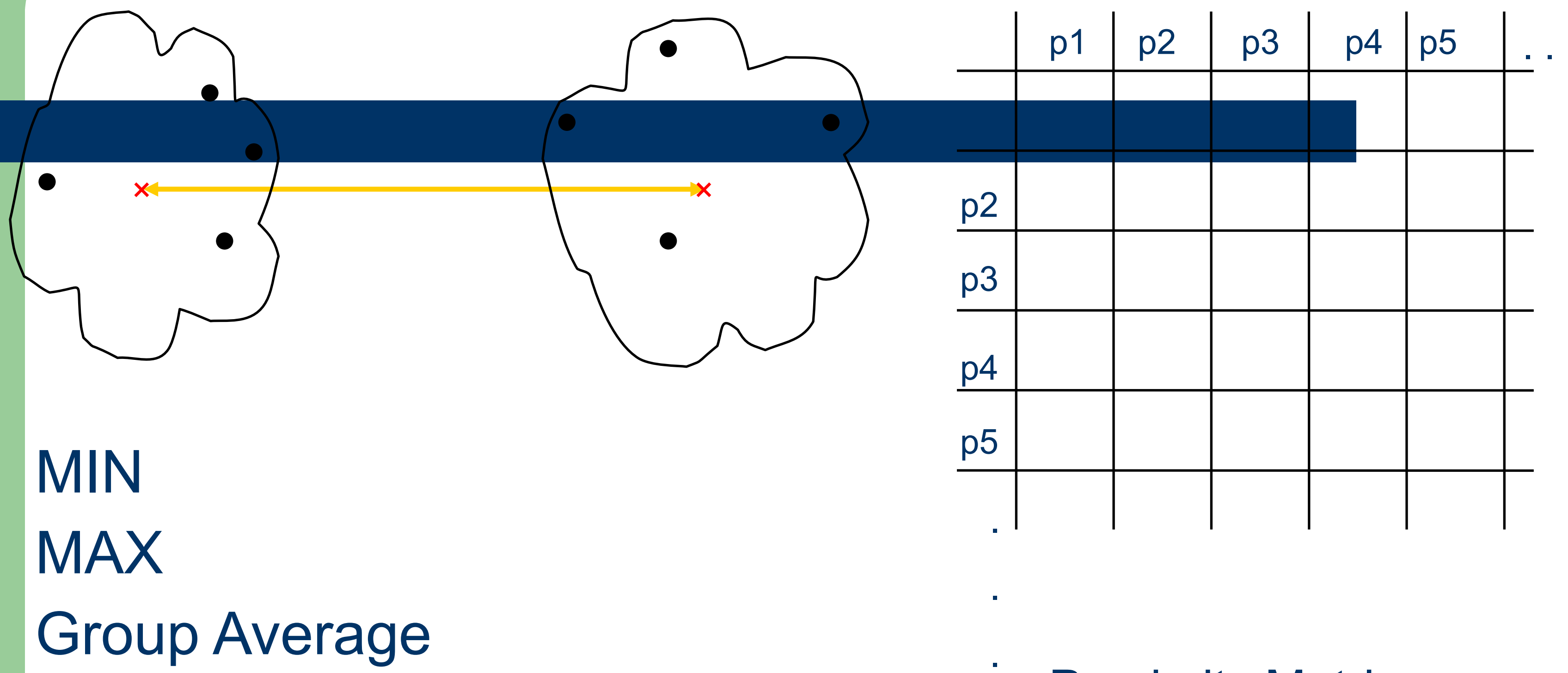


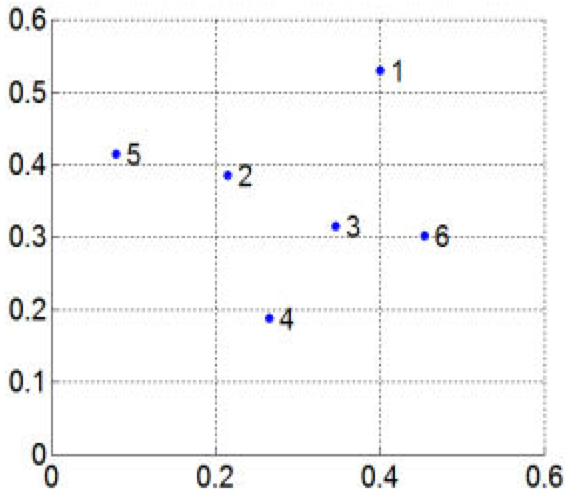
Proximity Matrix

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

Cluster Similarity: MIN or Single Link

most similar (closest) points in the different clusters

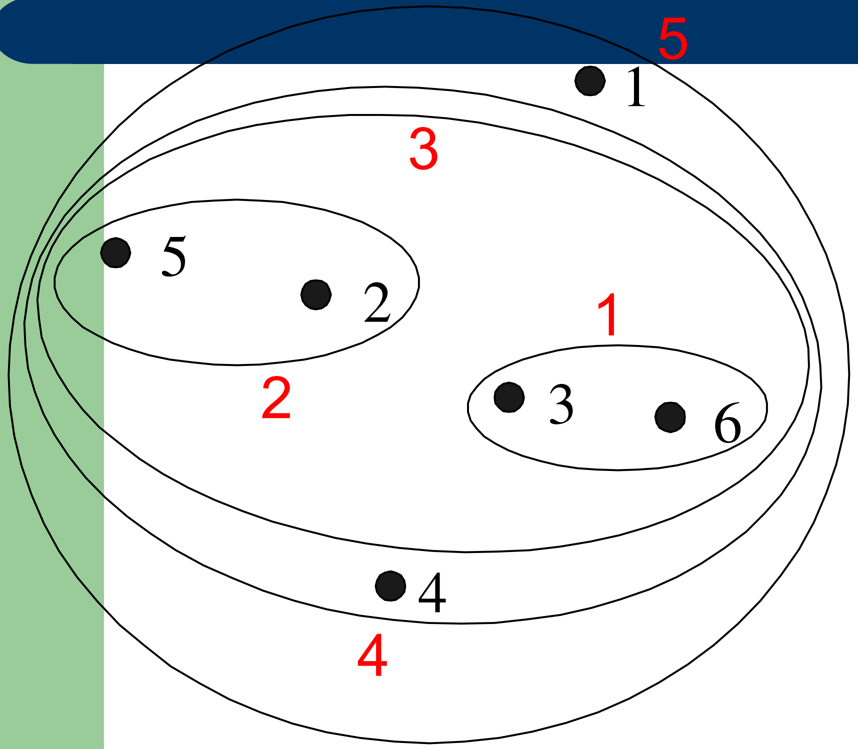
– Determined by one pair of points, i.e., by one link in the proximity graph.

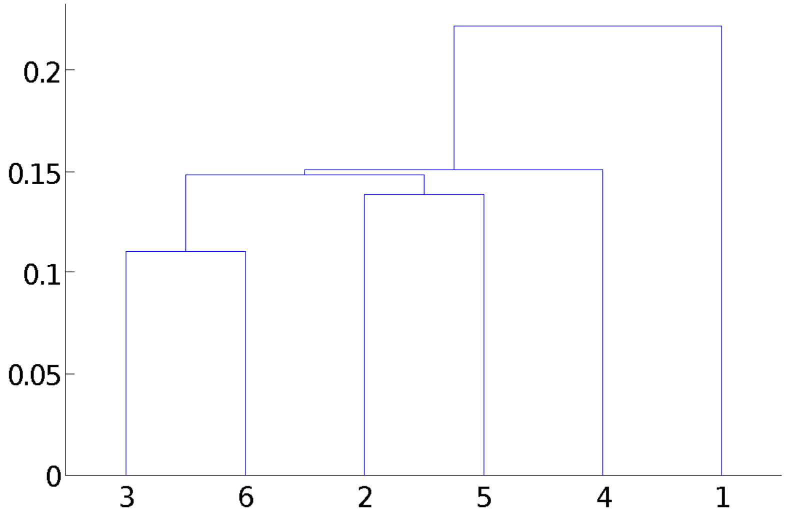


Distance Matrix:

	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

Hierarchical Clustering: MIN

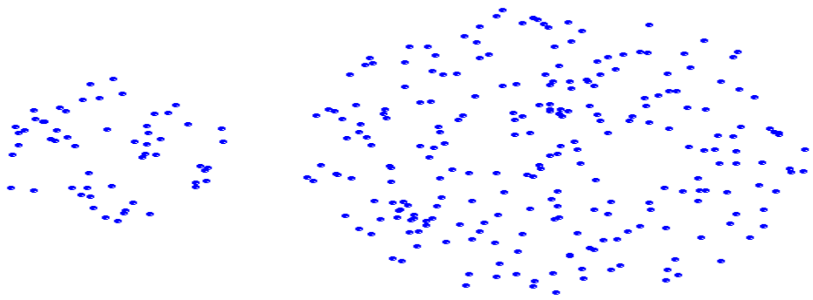




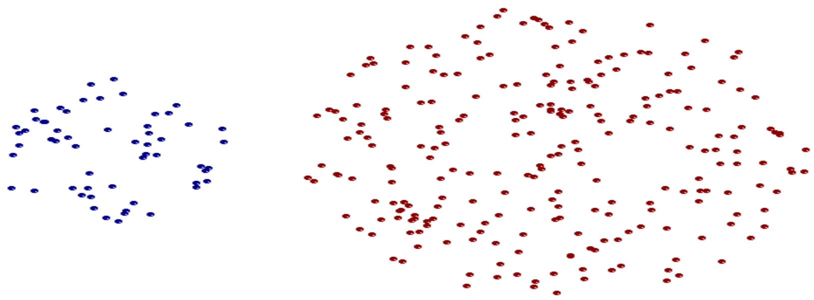
Nested Clusters

Dendrogram

Strength of MIN



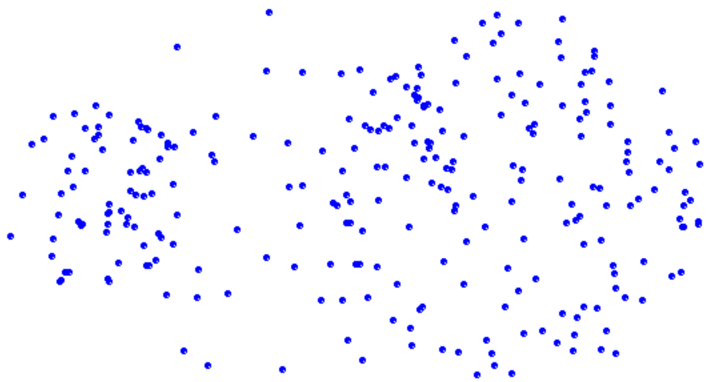
Original Points



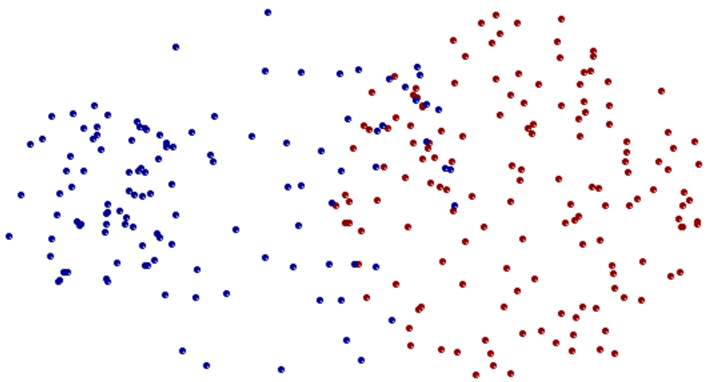
Two Clusters

- Can handle non-elliptical shapes

Limitations of MIN



Original Points

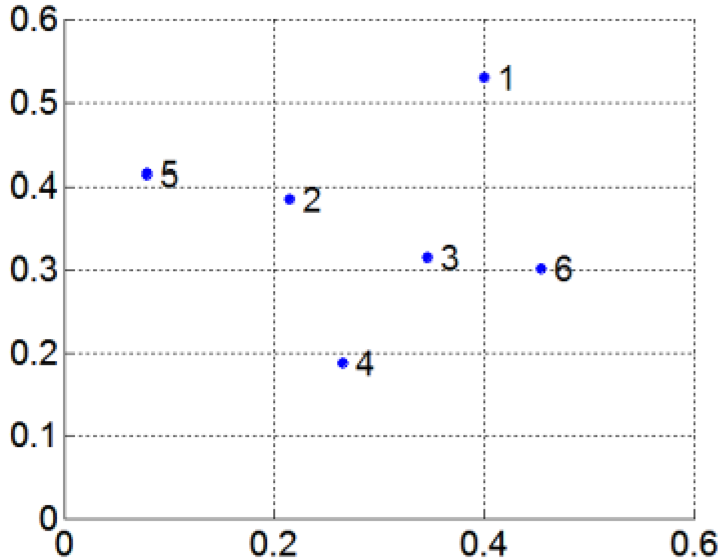


Two Clusters

- Sensitive to noise and outliers

Cluster Similarity: MAX or Complete Linkage

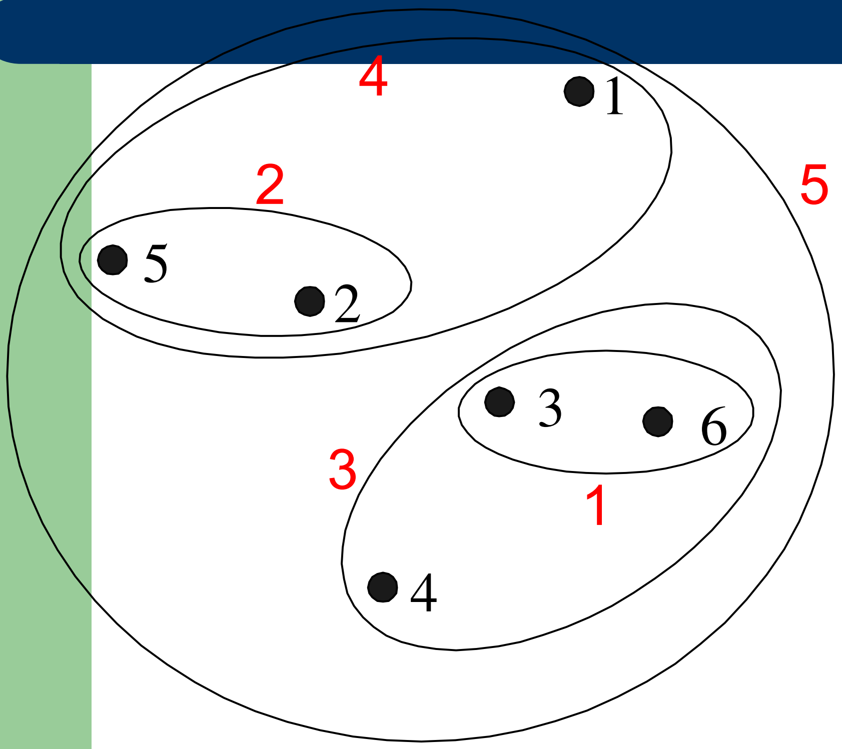
- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters



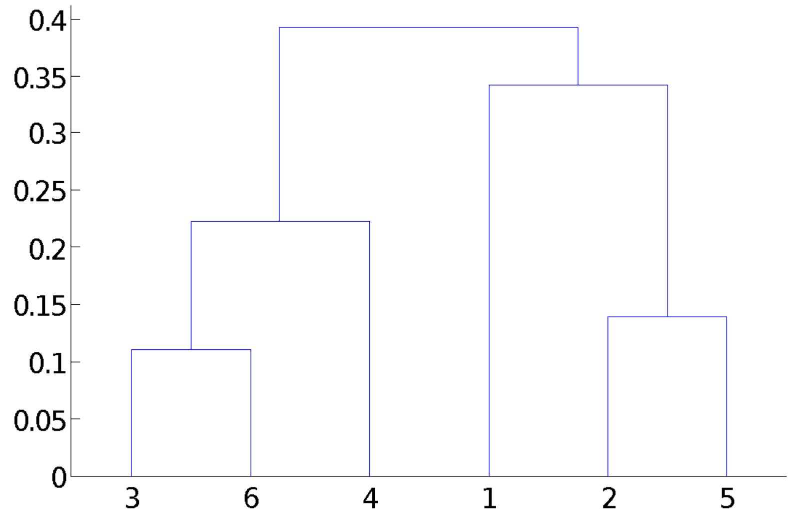
Distance Matrix:

	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

Hierarchical Clustering: MAX

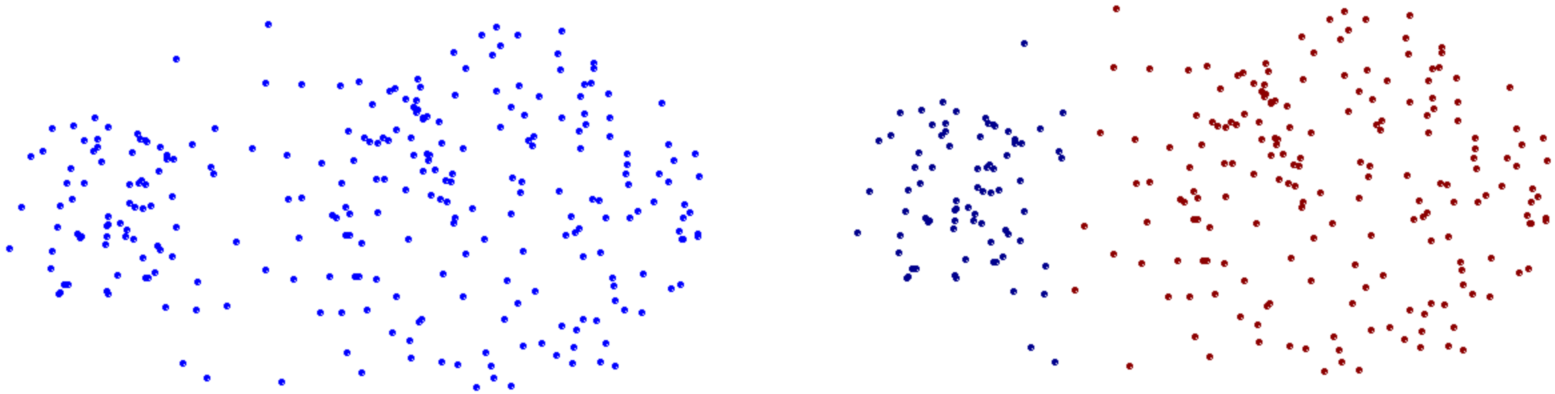


Nested Clusters



Dendrogram

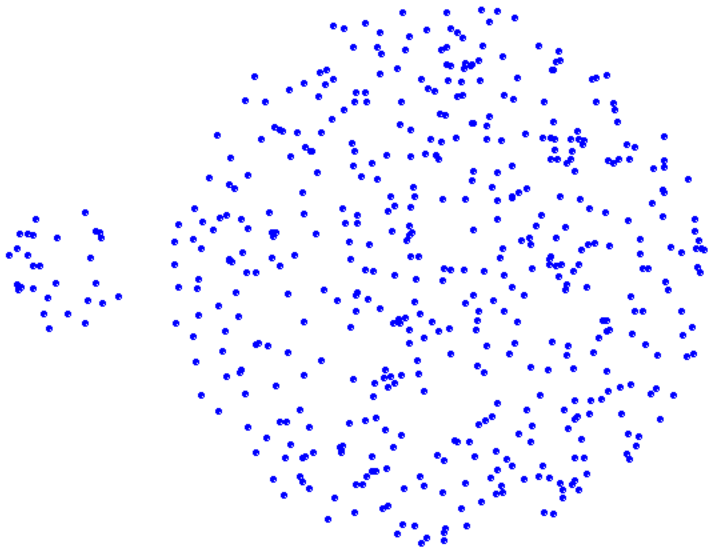
Strength of MAX



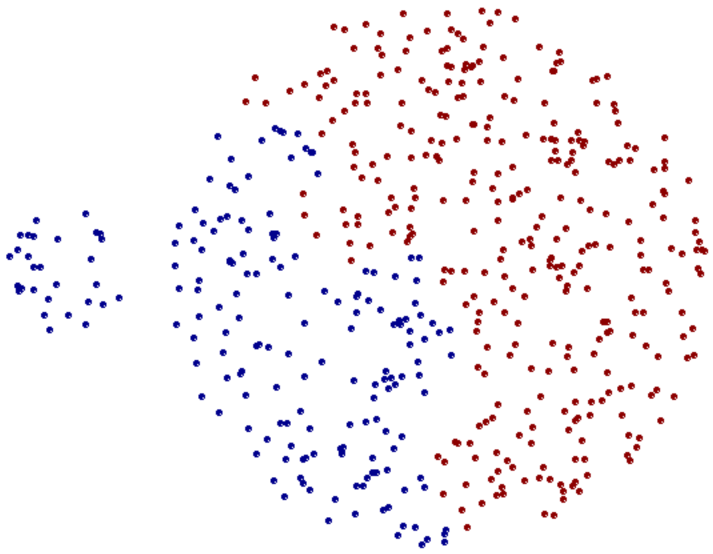
Original Points　　　　　Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

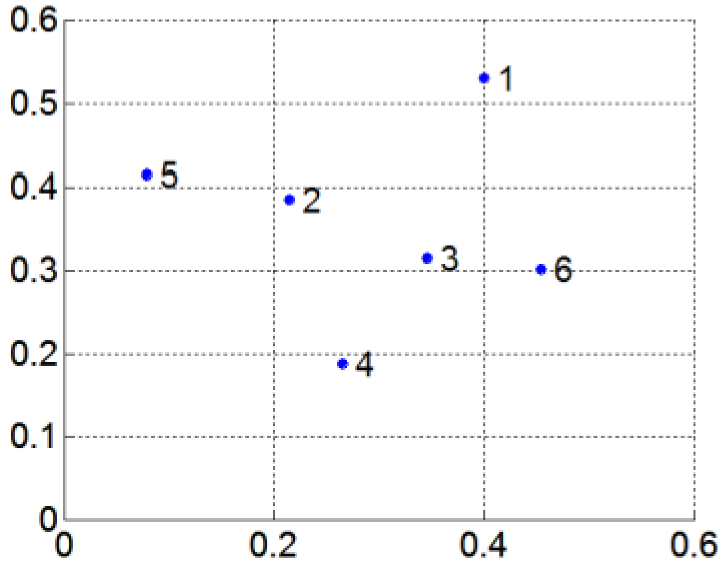
- Tends to break large clusters
- Biased towards globular clusters

Cluster Similarity: Group Average

- Proximity of two clusters is the average of pairwise proximity

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

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



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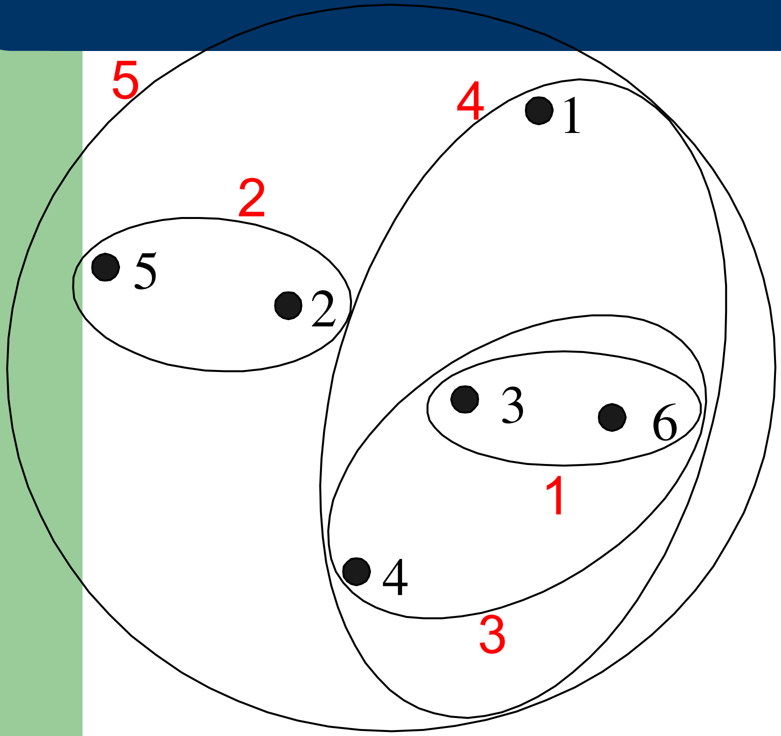
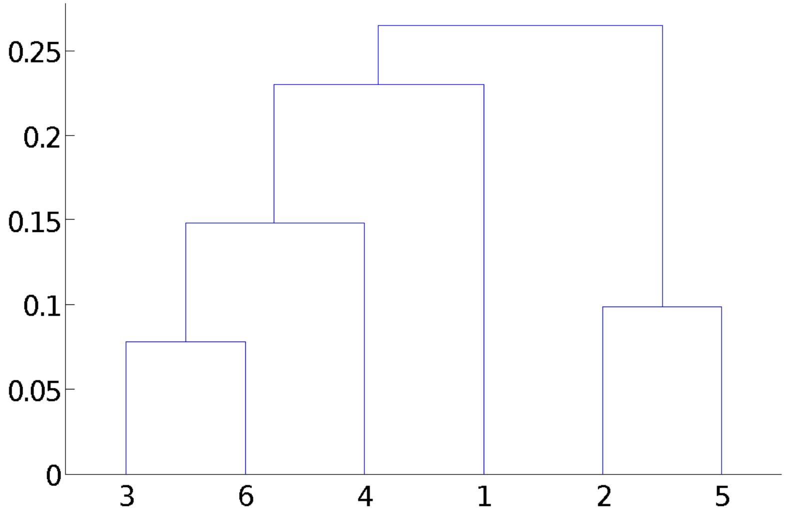
p6	0.23	0.25	0.11	0.22	0.39	0.00

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

- [redacted]ease 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

- [redacted]ters, 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

Programming Assignment

- Perform cluster validity task on your own choice of dataset:
  - Entropy and Purity of clusters
  - Cluster Cohesion and Separation
- Submission deadline: April 20, 2020

References

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

Questions!