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Engineering®**

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# ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING ((IS353IA)

## Unit 5

## Unsupervised Learning- Overview, What Is Cluster Analysis, Different Types of Clustering's, Different Types of Clusters

**K-means**-The Basic K-means Algorithm, Additional Issues, Bisecting K-means, K-means and Different Types of Clusters, Strengths and Weaknesses, K-means as an Optimization Problem

**Cluster Evaluation**-Overview, Unsupervised Cluster Evaluation Using Cohesion and Separation, Unsupervised Cluster Evaluation Using the Proximity Matrix, Determining the Correct Number of Clusters, Supervised Measures of Cluster Validity, Assessing the Significance of Cluster Validity Measures, Choosing a Cluster Validity Measure

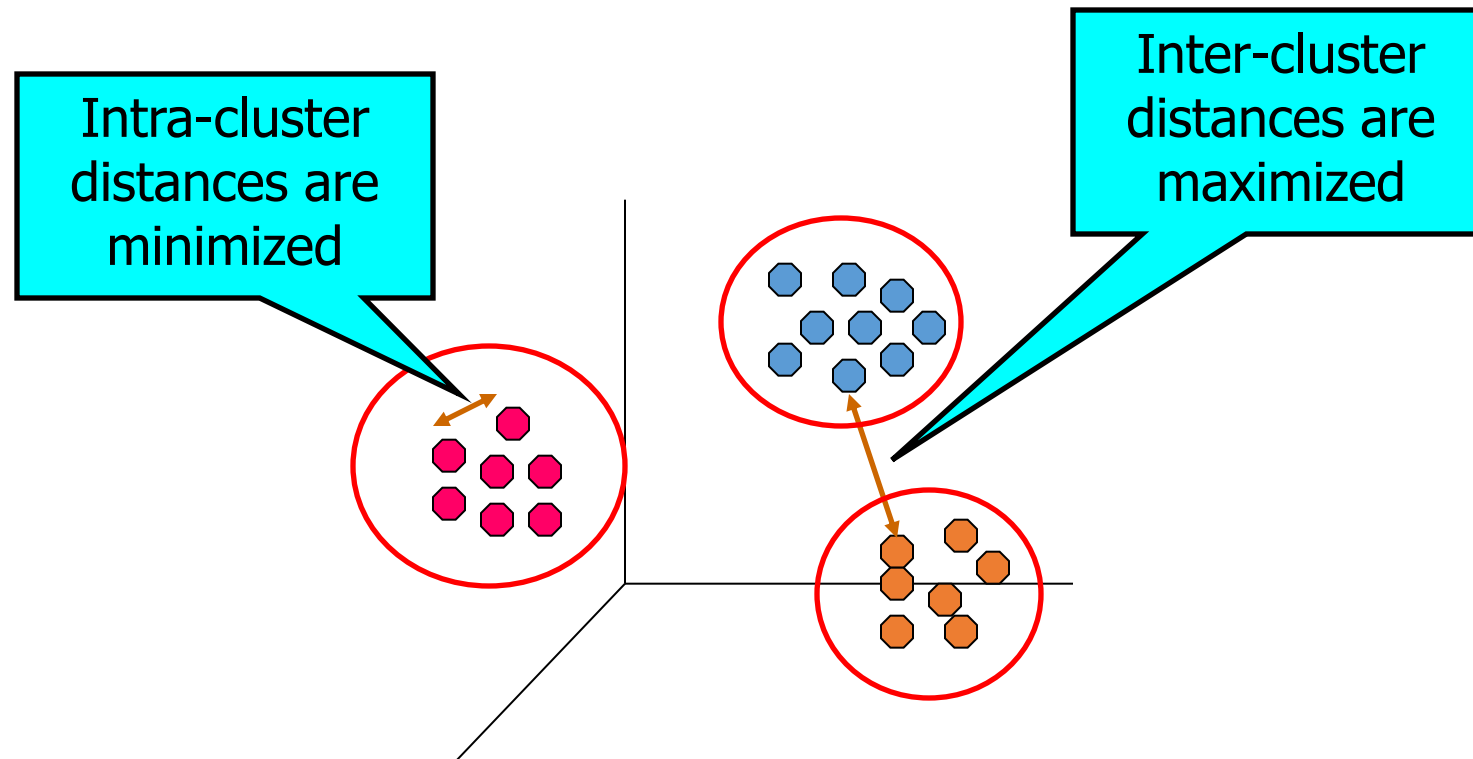
# What is Cluster Analysis?

- Cluster: A collection of data objects
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering*, *data segmentation*, ...)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- **Unsupervised learning**: no predefined classes (i.e., *learning by observations* vs. learning by examples: supervised)
- Typical applications
  - As a **stand-alone tool** to get insight into data distribution
  - As a **preprocessing step** for other algorithms

- Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- Information retrieval: document clustering
- Land use: Identification of areas of similar land use in an earth observation database
- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earth quake epicenters should be clustered along continent faults
- Climate: understanding earth climate, find patterns of atmospheric and ocean
- Economic Science: market research

- Summarization:
  - Preprocessing for regression, PCA, classification, and association analysis
- Compression:
  - Image processing: vector quantization
- Finding K-nearest Neighbors
  - Localizing search to one or a small number of clusters
- Outlier detection
  - Outliers are often viewed as those “far away” from any cluster

- 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



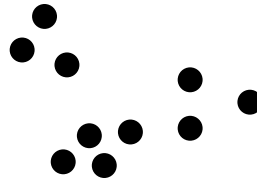
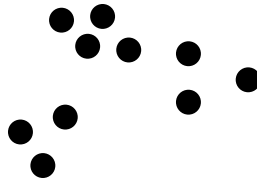
- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

# Measure the Quality of Clustering

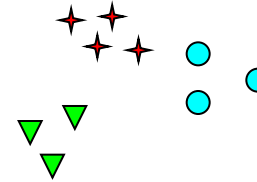
- **Dissimilarity/Similarity metric:** Similarity is expressed in terms of a distance function, typically metric:  $d(i, j)$
- There is a separate “quality” function that measures the “goodness” of a cluster.
- The definitions of **distance functions** are usually very different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables.
- Weights should be associated with different variables based on applications and data semantics.
- It is hard to define “similar enough” or “good enough”
  - the answer is typically highly subjective.



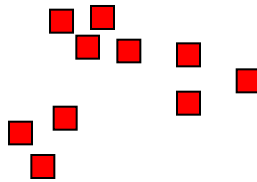
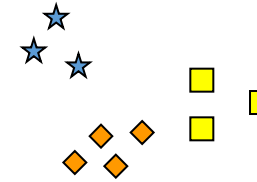
# Notion of a Cluster can be Ambiguous



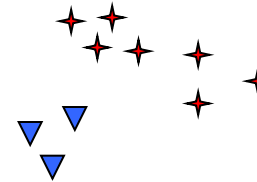
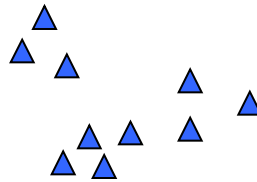
How many clusters?



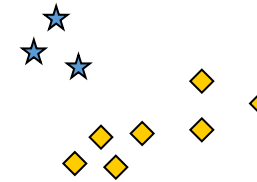
Six Clusters



Two Clusters



Four Clusters



# TYPES OF DATA IN CLUSTER ANALYSIS

- Data matrix
  - (two modes)
- Dissimilarity matrix
  - (one mode)

$$\begin{bmatrix} x_{11} & \dots & x_{1f} & \dots & x_{1p} \\ \dots & \dots & \dots & \dots & \dots \\ x_{i1} & \dots & x_{if} & \dots & x_{ip} \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1} & \dots & x_{nf} & \dots & x_{np} \end{bmatrix}$$

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \dots & \dots & 0 \end{bmatrix}$$

- Interval-scaled variables
- Binary variables
- Nominal, ordinal, and ratio variables
- Variables of mixed types

- Standardize data
  - Calculate the mean absolute deviation:

$$s_f = \frac{1}{n} (|x_{1f} - m_f| + |x_{2f} - m_f| + \dots + |x_{nf} - m_f|)$$

where  $m_f = \frac{1}{n}(x_{1f} + x_{2f} + \dots + x_{nf})$ .

- Calculate the standardized measurement (z-score)

$$z_{if} = \frac{x_{if} - m_f}{s_f}$$

- Using mean absolute deviation is more robust than using standard deviation

- Distances are normally used to measure the similarity or dissimilarity between two data objects

- Some popular ones include: *Minkowski distance*

$$d(i, j) = \sqrt[q]{(|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \dots + |x_{ip} - x_{jp}|^q)}$$

where  $i = (x_{i1}, x_{i2}, \dots, x_{ip})$  and  $j = (x_{j1}, x_{j2}, \dots, x_{jp})$  are two  $p$ -dimensional data objects, and  $q$  is a positive integer

- If  $q = 1$ ,  $d$  is *Manhattan distance*

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

- If  $q = 2$ ,  $d$  is **Euclidean distance**

$$d(i, j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + \dots + |x_{i_p} - x_{j_p}|^2)}$$

- Properties
  - $d(i, j) \geq 0$
  - $d(i, i) = 0$
  - $d(i, j) = d(j, i)$
  - $d(i, j) \leq d(i, k) + d(k, j)$
- Also, one can use weighted distance, parametric Pearson product moment correlation, or other dissimilarity measures

- A contingency table for binary data

		Object $j$		
		1	0	$sum$
Object $i$	1	$a$	$b$	$a+b$
	0	$c$	$d$	$c+d$
$sum$		$a+c$	$b+d$	$p$

- Distance measure for symmetric binary variables:
- Distance measure for asymmetric binary variables:
- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables):

$$d(i, j) = \frac{b+c}{a+b+c+d}$$

$$d(i, j) = \frac{b+c}{a+b+c}$$

$$sim_{Jaccard}(i, j) = \frac{a}{a+b+c}$$



## • Example

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N

- gender is a symmetric attribute
- the remaining attributes are asymmetric binary
- let the values Y and P be set to 1, and the value N be set to 0

$$d(jack, mary) = \frac{0 + 1}{2 + 0 + 1} = 0.33$$

$$d(jack, jim) = \frac{1 + 1}{1 + 1 + 1} = 0.67$$

$$d(jim, mary) = \frac{1 + 2}{1 + 1 + 2} = 0.75$$

- A generalization of the binary variable in that it can take more than 2 states, e.g., red, yellow, blue, green
- Method 1: Simple matching
  - $m$ : # of matches,  $p$ : total # of variables

$$d(i, j) = \frac{p - m}{p}$$

- Method 2: use a large number of binary variables
  - creating a new binary variable for each of the  $M$  nominal states

# Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank
- Can be treated like interval-scaled
  - replace  $x_{if}$  by their rank  $r_{if} \in \{1, \dots, M_f\}$
  - map the range of each variable onto  $[0, 1]$  by replacing  $i$ -th object in the  $f$ -th variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

- compute the dissimilarity using methods for interval-scaled variables

- Ratio-scaled variable: a positive measurement on a nonlinear scale, approximately at exponential scale, such as  $Ae^{Bt}$  or  $Ae^{-Bt}$
- Methods:
  - treat them like interval-scaled variables—*not a good choice!*  
(why?—the scale can be distorted)
  - apply logarithmic transformation

$$y_{if} = \log(x_{if})$$

- treat them as continuous ordinal data treat their rank as interval-scaled

- A database may contain all the six types of variables
  - symmetric binary, asymmetric binary, nominal, ordinal, interval and ratio

- One may use a weighted formula to combine their effects

$$d(i, j) = \frac{\sum_{f=1}^P \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^P \delta_{ij}^{(f)}}$$

- $f$  is binary or nominal:

$$d_{ij}^{(f)} = 0 \text{ if } x_{if} = x_{jf}, \text{ or } d_{ij}^{(f)} = 1 \text{ otherwise}$$

- $f$  is interval-based: use the normalized distance
- $f$  is ordinal or ratio-scaled

- compute ranks  $r_{if}$  and  $z_{if} = \frac{r_{if} - 1}{M_f - 1}$
- and treat  $z_{if}$  as interval-scaled

- Vector objects: keywords in documents, gene features in micro-arrays, etc.
- Broad applications: information retrieval, biologic taxonomy, etc.
- Cosine measure  $s(\vec{x}, \vec{y}) = \frac{\vec{x}^t \vec{y}}{\|\vec{x}\| \|\vec{y}\|}$  ,
- A variant: Tanimoto coefficient

$$s(\vec{x}, \vec{y}) = \frac{\vec{x}^t \vec{y}}{\vec{x}^t \vec{x} + \vec{y}^t \vec{y} - \vec{x}^t \vec{y}}$$

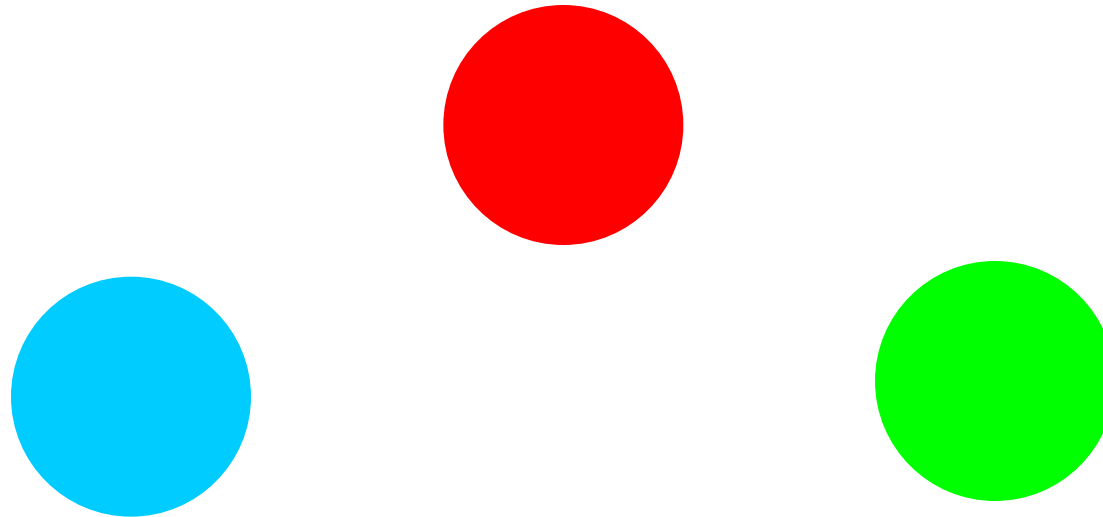
# Types of clusters

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



# Types of Clusters: Well-Separated

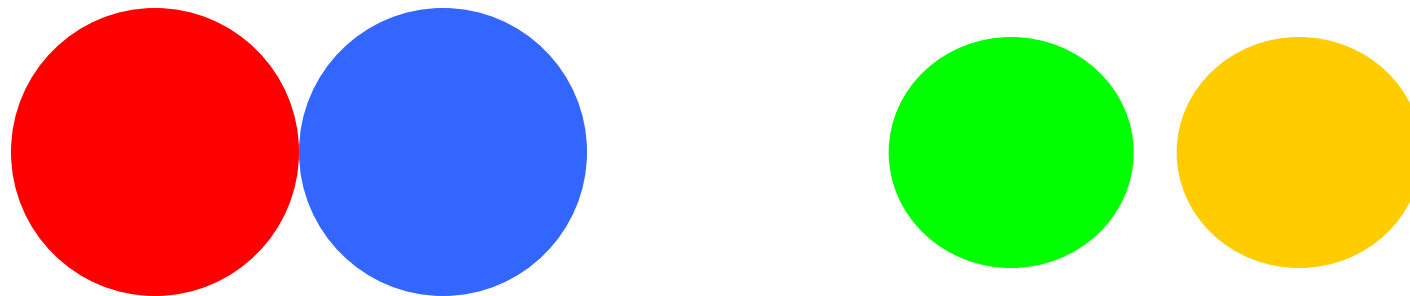
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

# Types of Clusters: Center-Based

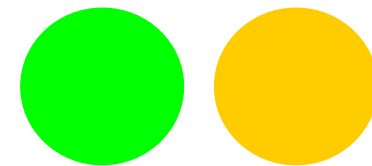
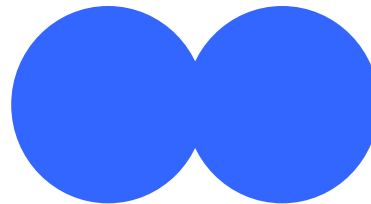
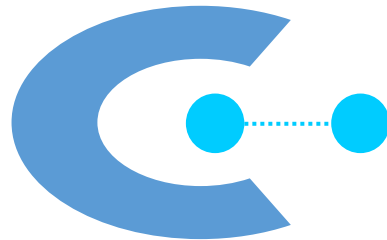
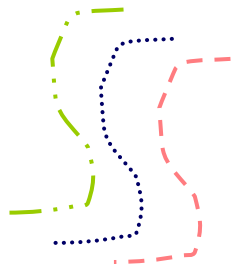
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
  - The center of a cluster is often a **centroid**, the average of all the points in the cluster, or a **medoid**, the most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



4 center-based clusters

# Types of Clusters: Contiguity-Based

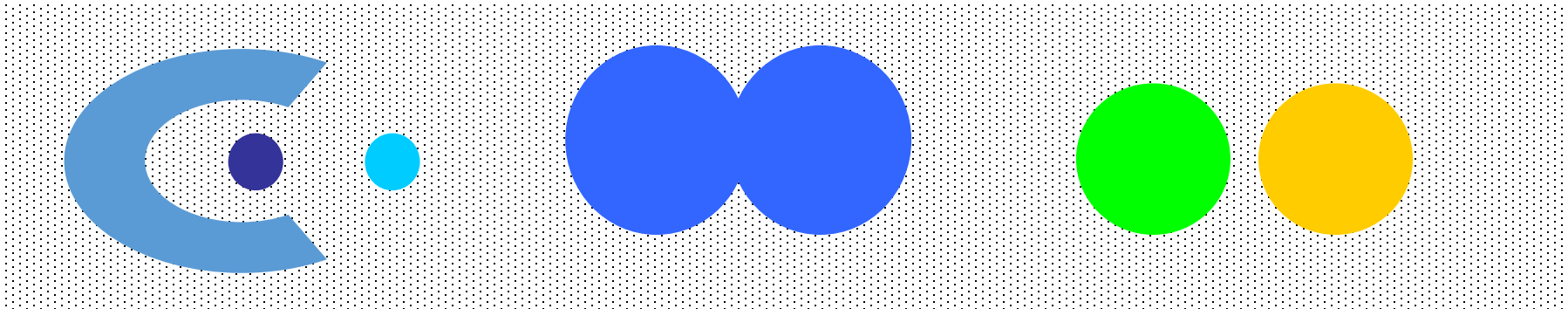
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

# Types of Clusters: Density-Based

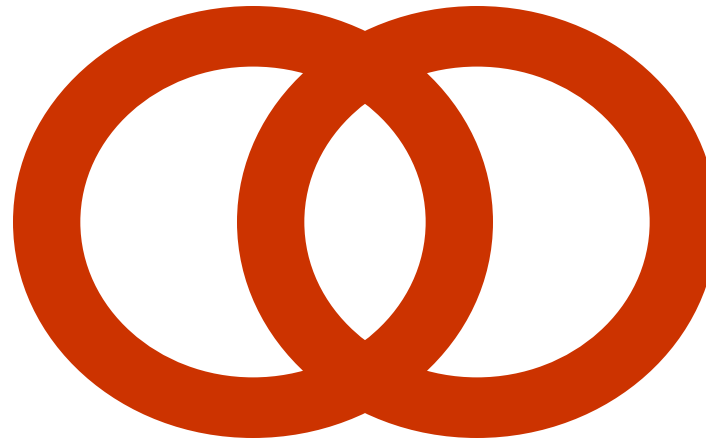
- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



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

## Types of Clusters: Objective Function ...

- Map the clustering problem to a different domain and solve a related problem in that domain
  - Proximity matrix defines a weighted graph, where the nodes are the points being clustered, and the weighted edges represent the proximities between points
  - Clustering is equivalent to breaking the graph into connected components, one for each cluster
  - Want to minimize the edge weight between clusters and maximize the edge weight within clusters

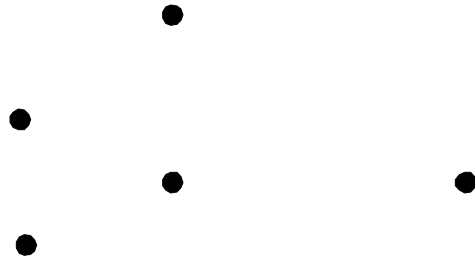
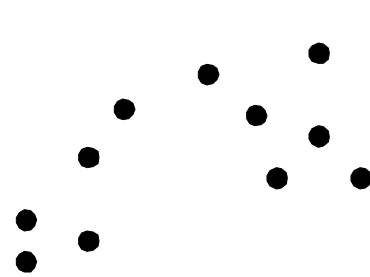
- Partitioning criteria
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable)
- Separation of clusters
  - Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class)
- Similarity measure
  - Distance-based (e.g., Euclidian, road network, vector) vs. connectivity-based (e.g., density or contiguity)
- Clustering space
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)



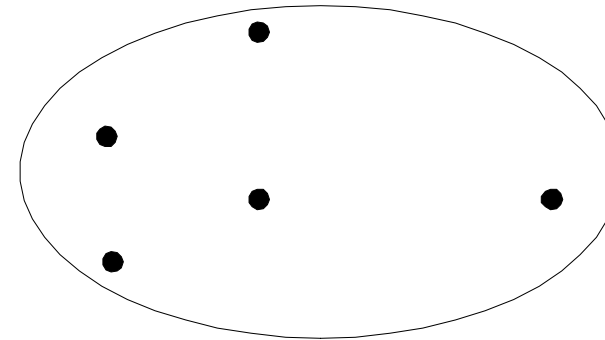
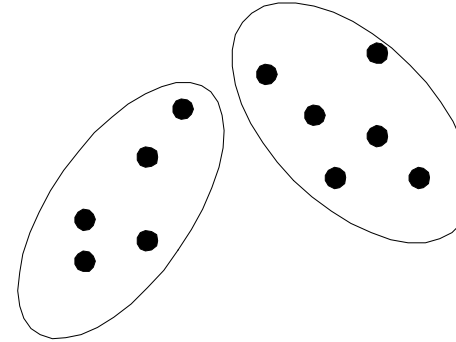
- Scalability
  - Clustering all the data instead of only on samples
- Ability to deal with different types of attributes
  - Numerical, binary, categorical, ordinal, linked, and mixture of these
- Constraint-based clustering
  - User may give inputs on constraints
  - Use domain knowledge to determine input parameters
- Interpretability and usability
- Others
  - Discovery of clusters with arbitrary shape
  - Ability to deal with noisy data
  - Incremental clustering and insensitivity to input order
  - High dimensionality

- Partitioning approach:
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  - Typical methods: k-means, k-medoids, CLARANS
- Hierarchical approach:
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Diana, Agnes, BIRCH, CAMELEON
- Density-based approach:
  - Based on connectivity and density functions
  - Typical methods: DBSCAN, OPTICS, DenClue
- Grid-based approach:
  - based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE

- Model-based:
  - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: EM, SOM, COBWEB
- Frequent pattern-based:
  - Based on the analysis of frequent patterns
  - Typical methods: p-Cluster
- User-guided or constraint-based:
  - Clustering by considering user-specified or application-specific constraints
  - Typical methods: COD (obstacles), constrained clustering
- Link-based clustering:
  - Objects are often linked together in various ways
  - Massive links can be used to cluster objects: SimRank, LinkClus

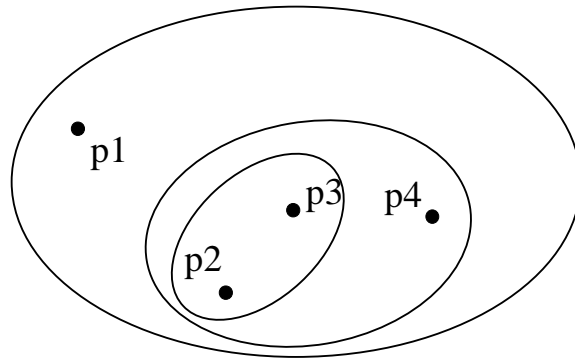


Original Points

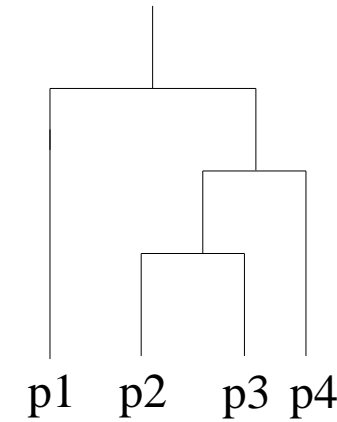


A Partitional Clustering

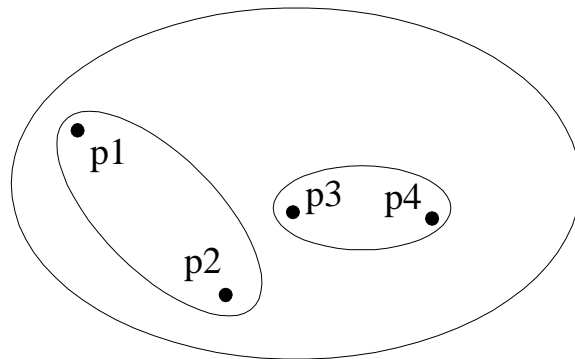
# Hierarchical Clustering



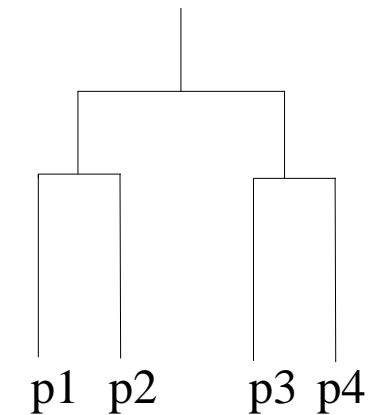
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering

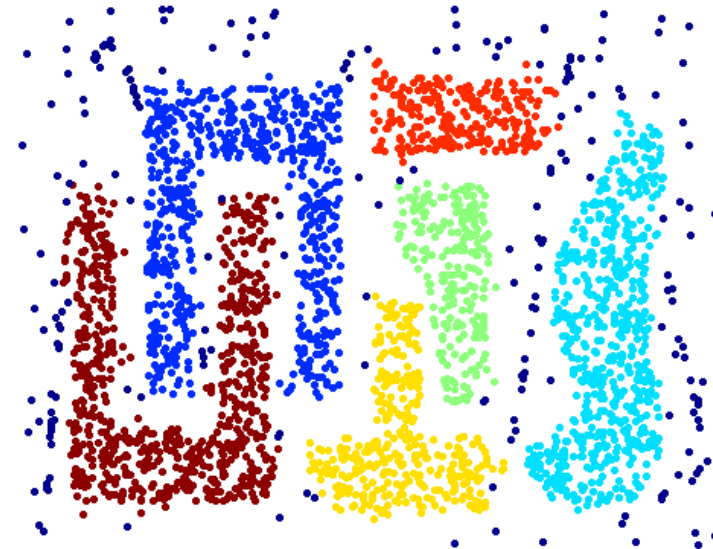


Non-traditional Dendrogram

# Density based Clustering



**Original Points**



**Clusters**