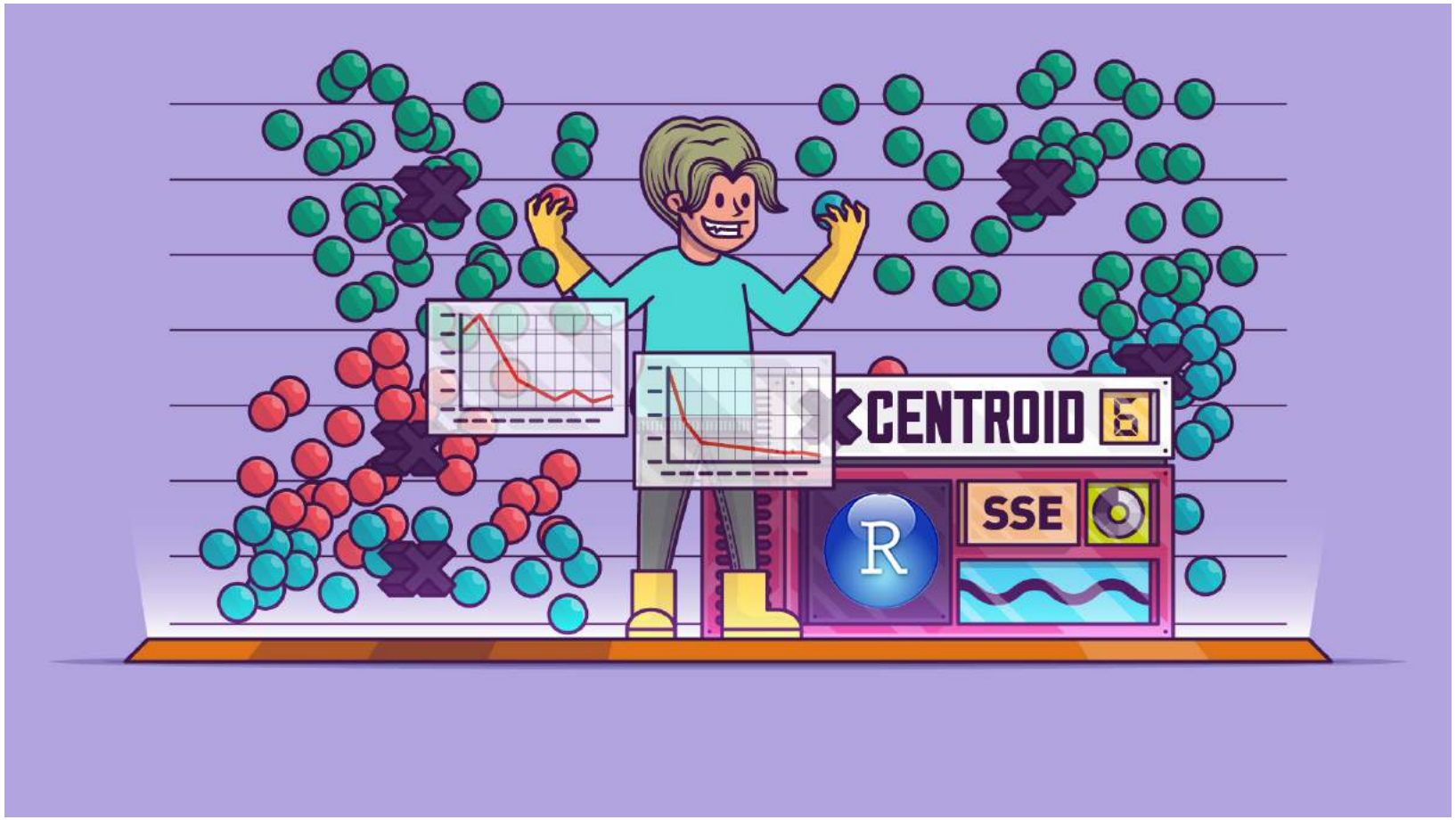


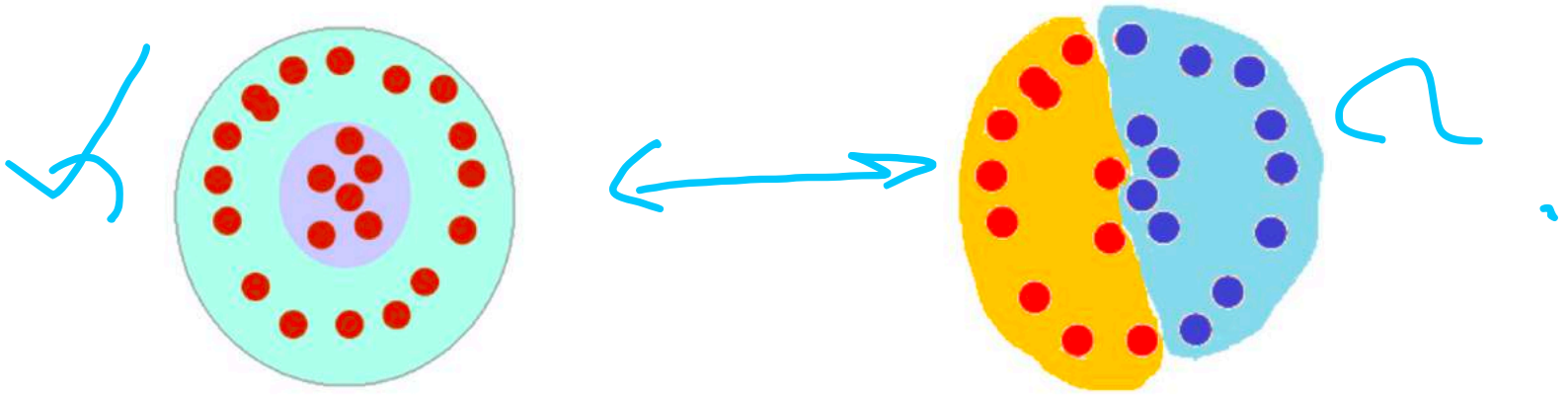
Clustering Analysis

Day 1 : February 25, 2021

What is clustering?

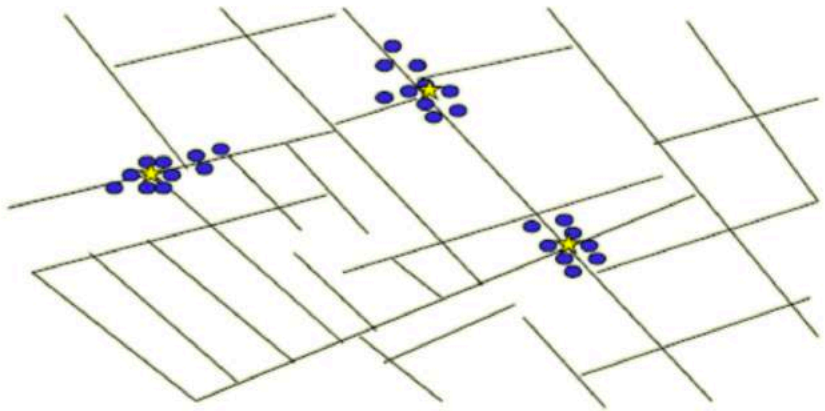
What is clustering?

- The organization of unlabeled data into similarity groups called clusters.
- A cluster is a collection of data items which are “similar” between them, and “dissimilar” to data items in other clusters.



History of clustering

- John Snow, a London physician plotted the location of cholera deaths on a map during an outbreak in the 1850s.
- The locations indicated that cases were clustered around certain intersections where there were polluted wells -- thus exposing both the problem and the solution.

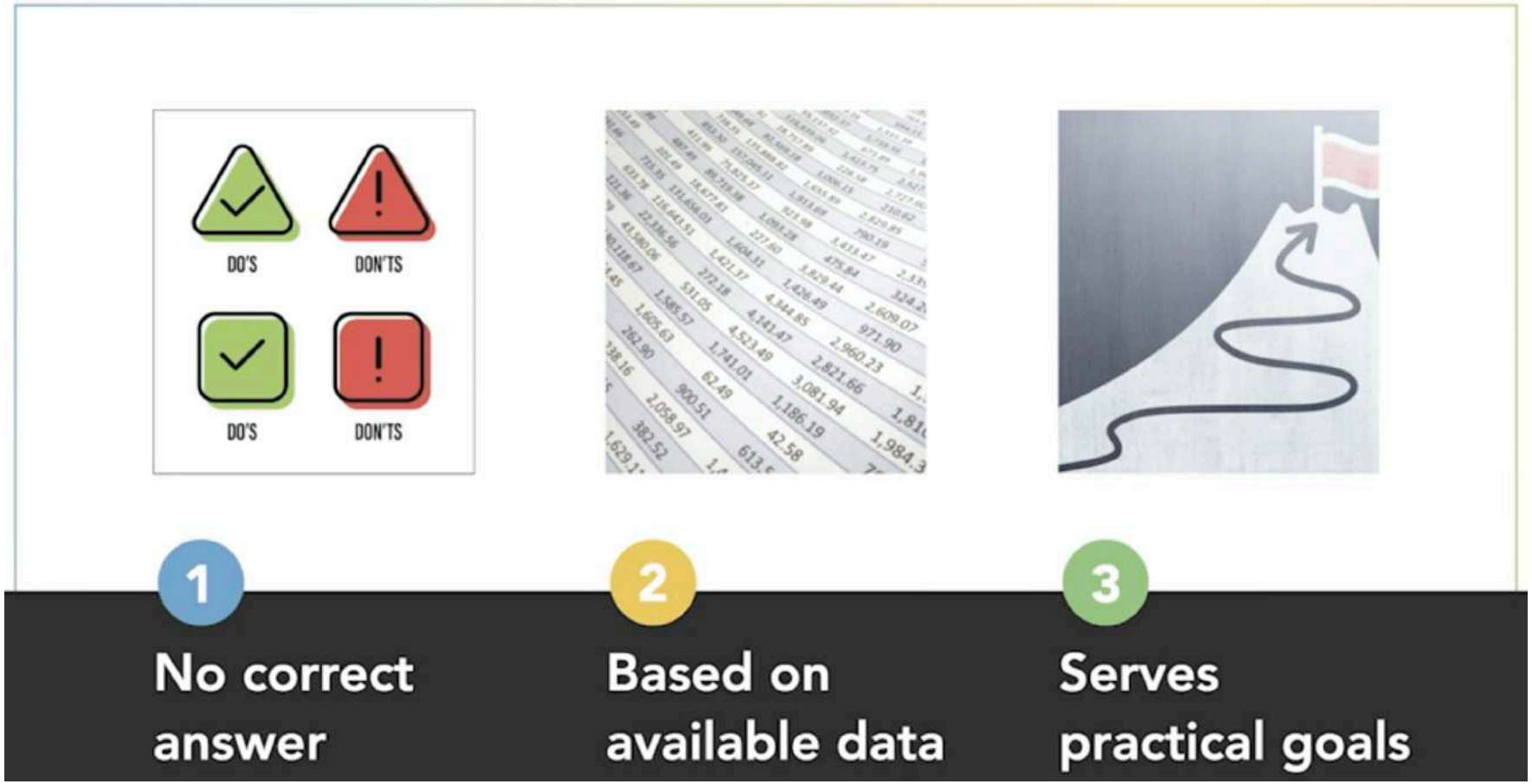


From: Nina Mishra HP Labs

Cluster Analysis

- **What is a cluster?**
  - A cluster is a collection of data objects which are
    - Similar (or related) to one another within the same group (i.e., cluster)
    - Dissimilar (or unrelated) to the objects in other groups (i.e., clusters)
- **Cluster analysis** (or ***clustering, data segmentation***, …)
  - Given a set of data points, partition them into a set of groups (i.e., clusters) which are as similar as possible
- Cluster analysis is **unsupervised learning** (i.e., no predefined classes)
  - This contrasts with *classification* (i.e., *supervised learning*)
- Typical ways to use/apply cluster analysis
  - As a stand-alone tool to get insight into data distribution, or
  - As a preprocessing (or intermediate) step for other algorithms

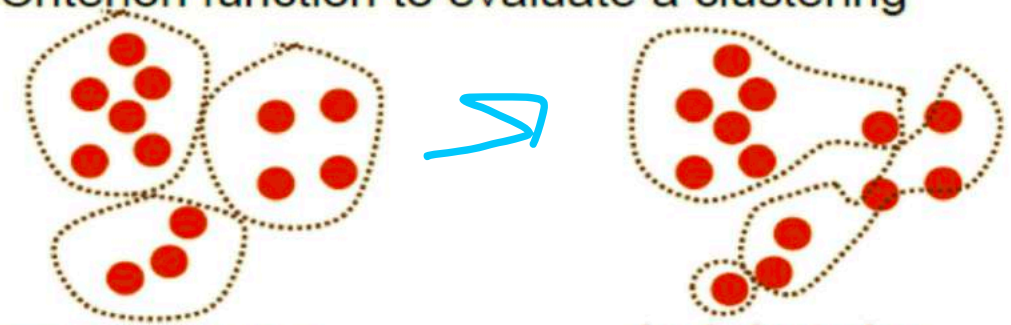
Reminder!


DO'S
DON'TS
DO'S
DON'TS
1
No correct answer
2
Based on available data
3
Serves practical goals

Elements of clustering

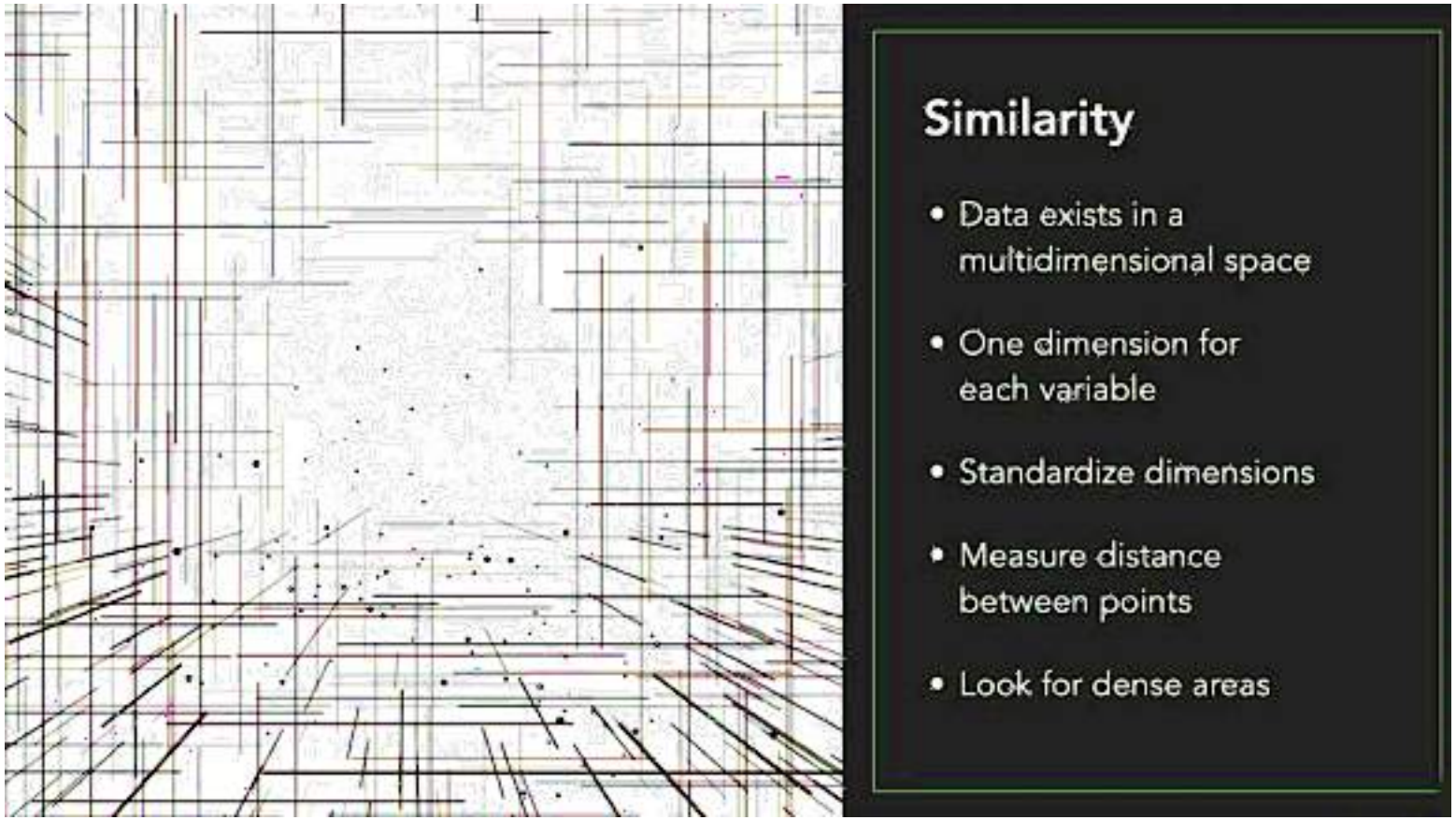
1. Proximity measure, *either*
   - similarity measure $s(x_i, x_k)$: large if x_i, x_k are similar
   - dissimilarity(or distance) measure $d(x_i, x_k)$: small if x_i, x_k are similar

2. Criterion function to evaluate a clustering



3. Algorithm to compute clustering
   - For example, by optimizing the criterion function

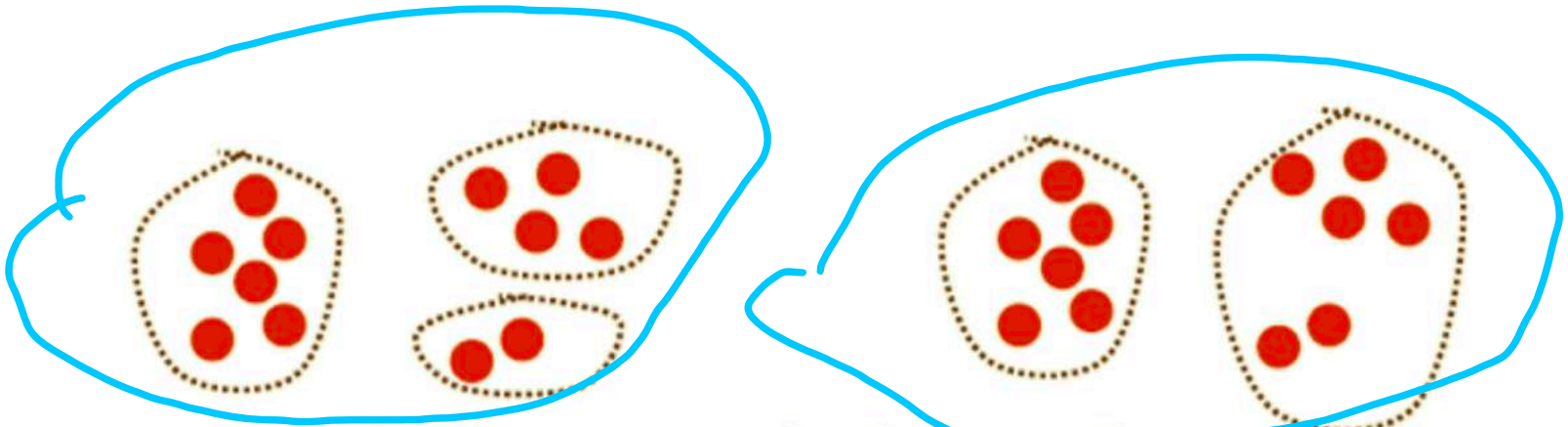
Similarity


Similarity
• Data exists in a multidimensional space
• One dimension for each variable
• Standardize dimensions
• Measure distance between points
• Look for dense areas

Cluster evaluation

- **Intra-cluster cohesion** (compactness):
  - Cohesion measures how near the data points in a cluster are to the cluster centroid.
  - Sum of squared error (SSE) is a commonly used measure.
- **Inter-cluster separation** (isolation):
  - Separation means that different cluster centroids should be far away from one another.
- In most applications, expert judgments are still the key

Number of clustering



- Possible approaches
  1. fix the number of clusters to ***k***
  2. find the best clustering according to the criterion function (number of clusters may vary)

Cluster analysis applications

- A key intermediate step for other data mining tasks
  - Generating a compact summary of data for classification, pattern discovery, hypothesis generation and testing, etc.
  - Outlier detection: Outliers—those "far away" from any cluster
- Data summarization, compression, and reduction
  - Ex. Image processing: Vector quantization
- Collaborative filtering, recommendation systems, or customer segmentation
  - Find like-minded users or similar products
- Dynamic trend detection
  - Clustering stream data and detecting trends and patterns
- Multimedia data analysis, biological data analysis and social network analysis
  - Ex. Clustering images or video/audio clips, gene/protein sequences, etc.

Elements and Types of Clustering

Requirements and Challenges

- **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., Euclidean, 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)

Requirements and Challenges

- **Quality**
  - Ability to deal with different types of attributes: Numerical, categorical, text, multimedia, networks, and mixture of multiple types
  - Discovery of clusters with arbitrary shape
  - Ability to deal with noisy data
- **Scalability**
  - Clustering all the data instead of only on samples
  - High dimensionality
  - Incremental or stream clustering and insensitivity to input order
- **Constraint-based clustering**
  - User-given preferences or constraints; domain knowledge; user queries
- **Interpretability and usability**

A Multi-Dimensional Categorization

- **Technique-Centered**
  - Distance-based methods
  - Density-based and grid-based methods
  - Probabilistic and generative models
  - Leveraging dimensionality reduction methods
  - High-dimensional clustering
  - Scalable techniques for cluster analysis
- **Data Type-Centered**
  - Clustering numerical data, categorical data, text data, multimedia data, time-series data, sequences, stream data, networked data, uncertain data
- **Additional Insight-Centered**
  - Visual insights, semi-supervised, ensemble-based, validation-based

Typical Clustering Methodologies

- **Distance-based methods**
  - Partitioning algorithms: K-Means, K-Medians, K-Medoids
  - Hierarchical algorithms: Agglomerative vs. divisive methods
- **Density-based and grid-based methods**
  - Density-based: Data space is explored at a high-level of granularity and then post-processing to put together dense regions into an arbitrary shape
  - Grid-based: Individual regions of the data space are formed into a grid-like structure
- **Probabilistic and generative models:** Modeling data from a generative process
  - Assume a specific form of the generative model (e.g., mixture of Gaussians)
  - Model parameters are estimated with the Expectation-Maximization (EM) algorithm (using the available dataset, for a maximum likelihood fit)
  - Then estimate the generative probability of the underlying data points

Typical Clustering Methodologies

- High Dimensional Clustering
  - Subspace clustering: clustering on various subspaces
    - Bottom-up, top-down, correlation-based methods vs. δ-cluster method
  - Dimensionality reduction: a vertical form of clustering
    - Probabilistic latent semantic indexing (PLSI) then LDA: topic modeling of text data
    - Non-negative matrix factorization (NMF) clustering (an example of co-clustering)
    - Spectral clustering: use the spectrum of the similarity matrix of the data to perform dimensionality reduction for clustering in fewer dimensions

Clustering Different Types of Data

- **Numerical data**
  - Most earliest clustering algorithms were designed for numerical data
- **Categorical data** (including binary data)
  - Discrete data, no natural order (e.g., sex, race, zip-code, and market-basket)
- **Text data**: Popular in social media, Web, and social networks
  - Features: High-dimensional, sparse, value corresponding to word frequencies
  - Methods: Combination of k-means and agglomerative; topic modeling; co-clustering
- **Multimedia data**: Image, audio, video (e.g., on Flickr, YouTube)
  - Multi-modal (often combined with text data)
  - Contextual: Containing both behavioral and contextual attributes

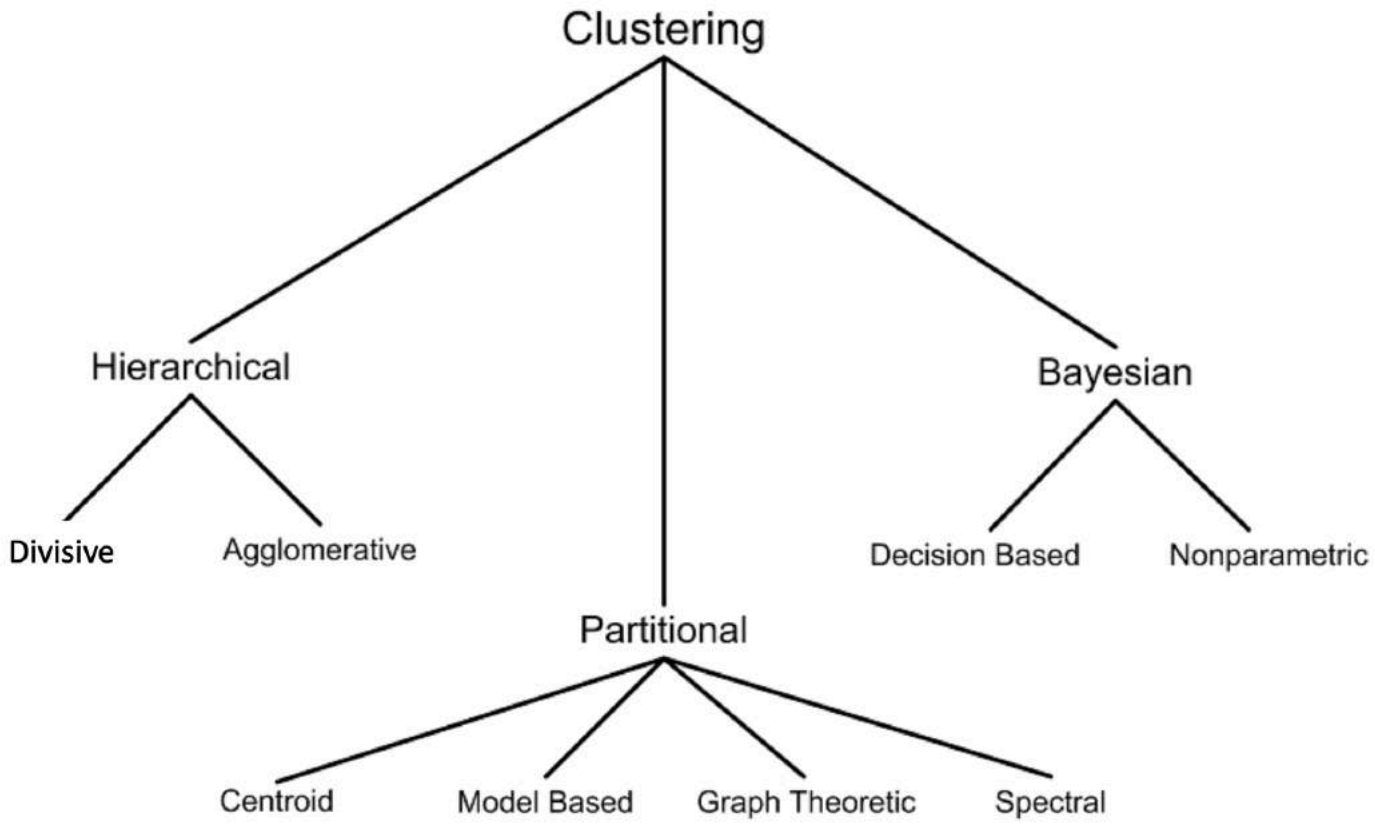
Clustering Different Types of Data

- **Time series data:** Sensor data, stock markets, temporal tracking, forecasting, etc.
- **Sequence data:** Weblogs, biological sequences, system command sequences
- **Stream data:** Real-time data

User Insights and Clustering

- **Visual insights**: One picture is worth a thousand words
  - Human eyes: High-speed processor linking with a rich knowledge-base
  - A human can provide intuitive insights; HD-eye: visualizing HD clusters
- **Semi-supervised insights**: Passing user's insights or intention to system
  - User-seeding: A user provides a number of labeled examples, approximately representing categories of interest
- **Multi-view and ensemble-based insights**
  - Multi-view clustering: Multiple clusterings represent different perspectives
  - Multiple clustering results can be ensembled to provide a more robust solution
- **Validation-based insights**: Evaluation of the quality of clusters generated
  - May use case studies, specific measures, or pre-existing labels

Clustering techniques



Recommended readings

- Major Reference Books on Cluster Analysis
  - Jiawei Han, Micheline Kamber, and Jian Pei. Data Mining: Concepts and Techniques. Morgan Kaufmann, 3rd ed. , 2011 (Chapters 10 & 11)
  - Charu Aggarwal and Chandran K. Reddy (eds.). Data Clustering: Algorithms and Applications. CRC Press, 2014
  - Mohammed J. Zaki and Wagner Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge University Press, 2014
- Reference paper for this lecture
  - Charu Aggarwal. An Introduction to Clustering Analysis. *in* Aggarwal and Reddy (eds.). Data Clustering: Algorithms and Applications (Chapter 1). CRC Press, 2014

Similarity Measures for Clustering

Good clustering

- A good clustering method will produce high quality clusters which should have
  - **High intra-class similarity:** Cohesive within clusters
  - **Low inter-class similarity:** Distinctive between clusters
- **Quality function**
  - There is usually a separate "quality" function that measures the "goodness" of a cluster
  - It is hard to define "similar enough" or "good enough"
    - The answer is typically highly subjective
- There exist many similarity measures and/or functions for different applications
- Similarity measure is critical for cluster analysis

Similarity, Dissimilarity, and Proximity

- **Similarity measure** or **similarity function**
  - A real-valued function that quantifies the similarity between two objects
  - Measure how two data objects are alike: The higher value, the more alike
  - Often falls in the range [0,1]: 0: no similarity; 1: completely similar
- **Dissimilarity** (or **distance**) measure
  - Numerical measure of how different two data objects are
  - In some sense, the inverse of similarity: The lower, the more alike
  - Minimum dissimilarity is often 0 (i.e., completely similar)
  - Range [0, 1] or [0, ∞) , depending on the definition
- **Proximity** usually refers to either similarity or dissimilarity

Data and Dissimilarity Matrices

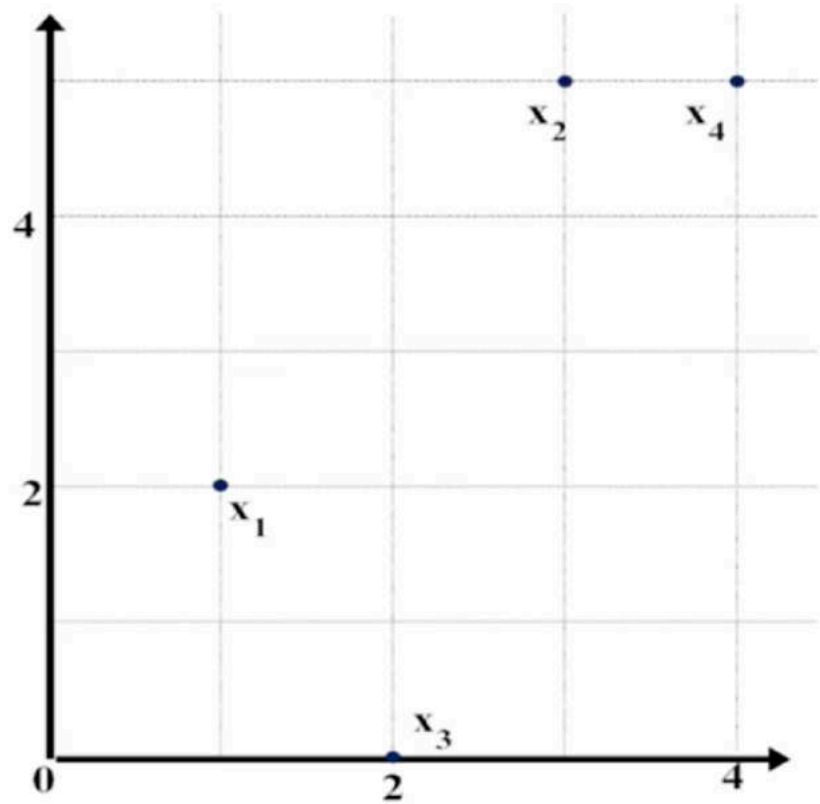
- Data matrix
  - A data matrix of n data points with *l* dimensions

$$D = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1l} \\ x_{21} & x_{22} & \dots & x_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nl} \end{pmatrix}$$

- Dissimilarity (distance) matrix
  - n data points, but registers only the distance $d(i, j)$ (typically metric)
  - Usually symmetric, thus a triangular matrix
  - Distance functions are usually different for real, boolean, categorical, ordinal, ratio, and vector variables
  - Weights can be associated with different variables based on applications and data semantics

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

Example



Data Matrix

point	attribute1	attribute2
x1	1	2
x2	3	5
x3	2	0
x4	4	5

Dissimilarity Matrix (by Euclidean Distance)

	x1	*x2*	*x3*	*x4*
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Numeric Data: Minkowski Distance

- Minkowski distance: A popular distance measure

$$d(i, j) = \sqrt[p]{| x_{i1} - x_{j1} |^p + | x_{i2} - x_{j2} |^p + \cdots + | x_{il} - x_{jl} |^p}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{il})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jl})$ are two l-dimensional data objects, and p is the order (the distance so defined is also called L-p norm)

- Properties
  - d(i, j) > 0 if i ≠ j, and d(i, i) = 0 (Positivity)
  - d(i, j) = d(j, i) (Symmetry)
  - d(i, j) ≤ d(i, k) + d(k, j) (Triangle Inequality)
- A distance that satisfies these properties is a metric
- Note: There are nonmetric dissimilarities, e.g., set differences

Minkowski Distance

- p = 1: (L_1 norm) Manhattan (or city block) distance
  - E.g., the Hamming distance: the number of bits that are different between two binary vectors

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{il} - x_{jl}|$$

- p = 2: (L_2 norm) Euclidean distance

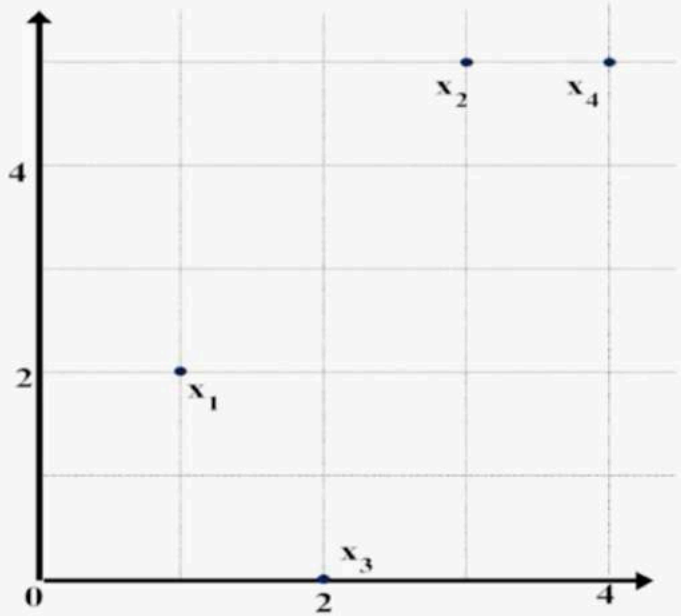
$$d(i, j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \cdots + |x_{il} - x_{jl}|^2}$$

- $p \to \infty$: (L_{max} norm, L_∞ norm) "supremum" distance
  - The maximum difference between any component (attribute) of the vectors

$$d(i, j) = \lim_{p \to \infty} \sqrt[p]{|x_{i1} - x_{j1}|^p + |x_{i2} - x_{j2}|^p + \cdots + |x_{il} - x_{jl}|^p} = \max_{f=1}^{l} |x_{if} - x_{jf}|$$

Example

point	attribute 1	attribute 2
x1	1	2
x2	3	5
x3	2	0
x4	4	5



Manhattan (L_1)

L	x1	x2	x3	x4
x1	0			
x2	5	0		
x3	3	6	0	
x4	6	1	7	0

Euclidean (L_2)

L2	x1	x2	x3	x4
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Supremum (L_∞)

L_∞	x1	x2	x3	x4
x1	0			
x2	3	0		
x3	2	5	0	
x4	3	1	5	0

Proximity Measure for Binary Attributes

- A contingency table for binary data

Object *i* \ Object *j*	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

- Distance measure for symmetric binary variables: $$d(i,j) = \frac{r+s}{q+r+s+t}$$
- Distance measure for asymmetric binary variables: $$d(i,j) = \frac{r+s}{q+r+s}$$
- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables): $$sim_{Jaccard}(i,j) = \frac{q}{q+r+s}$$
- Note: Jaccard coefficient is the same as "coherence": (a concept discussed in Pattern Discovery)

$$coherence(i,j) = \frac{sup(i,j)}{sup(i)+sup(j)-sup(i,j)} = \frac{q}{(q+r)+(q+s)-q}$$

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 (not counted in)
- The remaining attributes are asymmetric binary
- Let the values Y and P be 1, and the value N be 0
- Distance: $d(i, j) = \frac{r + s}{q + r + s}$

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

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

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

Mary

Jack	1	0	$\sum_{row}$
1	2	0	2
0	1	3	4
$\sum_{col}$	3	3	6

Jim

Jack	1	0	$\sum_{row}$
1	1	1	2
0	1	3	4
$\sum_{col}$	2	4	6

Mary

Jim	1	0	$\sum_{row}$
1	1	1	2
0	2	2	4
$\sum_{col}$	3	3	6

Proximity Measure for Categorical Attributes

- Categorical data, also called nominal attributes
  - Example: Color (red, yellow, blue, green), profession, etc.
- 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 attributes
  - Creating a new binary attribute for each of the *M* nominal states

Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank (e.g., freshman, sophomore, junior, senior)
- Can be treated like interval-scaled
  - Replace *an ordinal variable value* by its rank: $r_{if} \in \{1, \ldots, M_f\}$
  - Map the range of each variable onto [0, 1] by replacing *i*-th object in the *f*-th variable by

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

    - Example: freshman: 0; sophomore: 1/3; junior: 2/3; senior 1
      - Then distance: d(freshman, senior) = 1, d(junior, senior) = 1/3
  - Compute the dissimilarity using methods for interval-scaled variables

Attributes of Mixed Type

- A dataset may contain all attribute types
  - Nominal, symmetric binary, asymmetric binary, numeric, and ordinal
- One may use a weighted formula to combine their effects:

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

  - If f is numeric: Use the normalized distance
  - If f is binary or nominal: $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$; or $d_{ij}^{(f)} = 1$ otherwise
  - If f is ordinal
    - Compute ranks z_{if} (where $z_{if} = \frac{r_{if} - 1}{M_f - 1}$)
    - Treat z_{if} as interval-scaled

Cosine Similarity of Two Vectors

- A **document** can be represented by a bag of terms or a long vector, with each attribute recording the *frequency* of a particular term (such as word, keyword, or phrase) in the document

Document	*team*	*coach*	*hockey*	*baseball*	*soccer*	*penalty*	*score*	*win*	*loss*	*season*
Document1	5	0	3	0	2	0	0	2	0	0
Document2	3	0	2	0	1	1	0	1	0	1
Document3	0	7	0	2	1	0	0	3	0	0
Document4	0	1	0	0	1	2	2	0	3	0

- Other vector objects: Gene features in micro-arrays
- Applications: Information retrieval, biologic taxonomy, gene feature mapping, etc.
- Cosine measure: If d_1 and d_2 are two vectors (e.g., term-frequency vectors), then

$$cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\| d_1 \| \times \| d_2 \|}$$

where $\bullet$ indicates vector dot product, $||d||$: the length of vector d

Recommended Readings

- L. Kaufman and P. J. Rousseeuw, Finding Groups in Data: An Introduction to Cluster Analysis, John Wiley & Sons, 1990
- Mohammed J. Zaki and Wagner Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge University Press, 2014
- Jiawei Han, Micheline Kamber, and Jian Pei. Data Mining: Concepts and Techniques. Morgan Kaufmann, 3rd ed. , 2011
- Charu Aggarwal and Chandran K. Reddy (eds.). Data Clustering: Algorithms and Applications. CRC Press, 2014

Partitioning-Based Clustering Methods

Partitioning Algorithms: Basic Concepts

- Partitioning method: Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions
- *K*-partitioning method: Partitioning a dataset ***D*** of ***n*** objects into a set of ***K*** clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where c_k is the centroid or medoid of cluster C_k)
  - A typical objective function: **Sum of Squared Errors** (**SSE**)

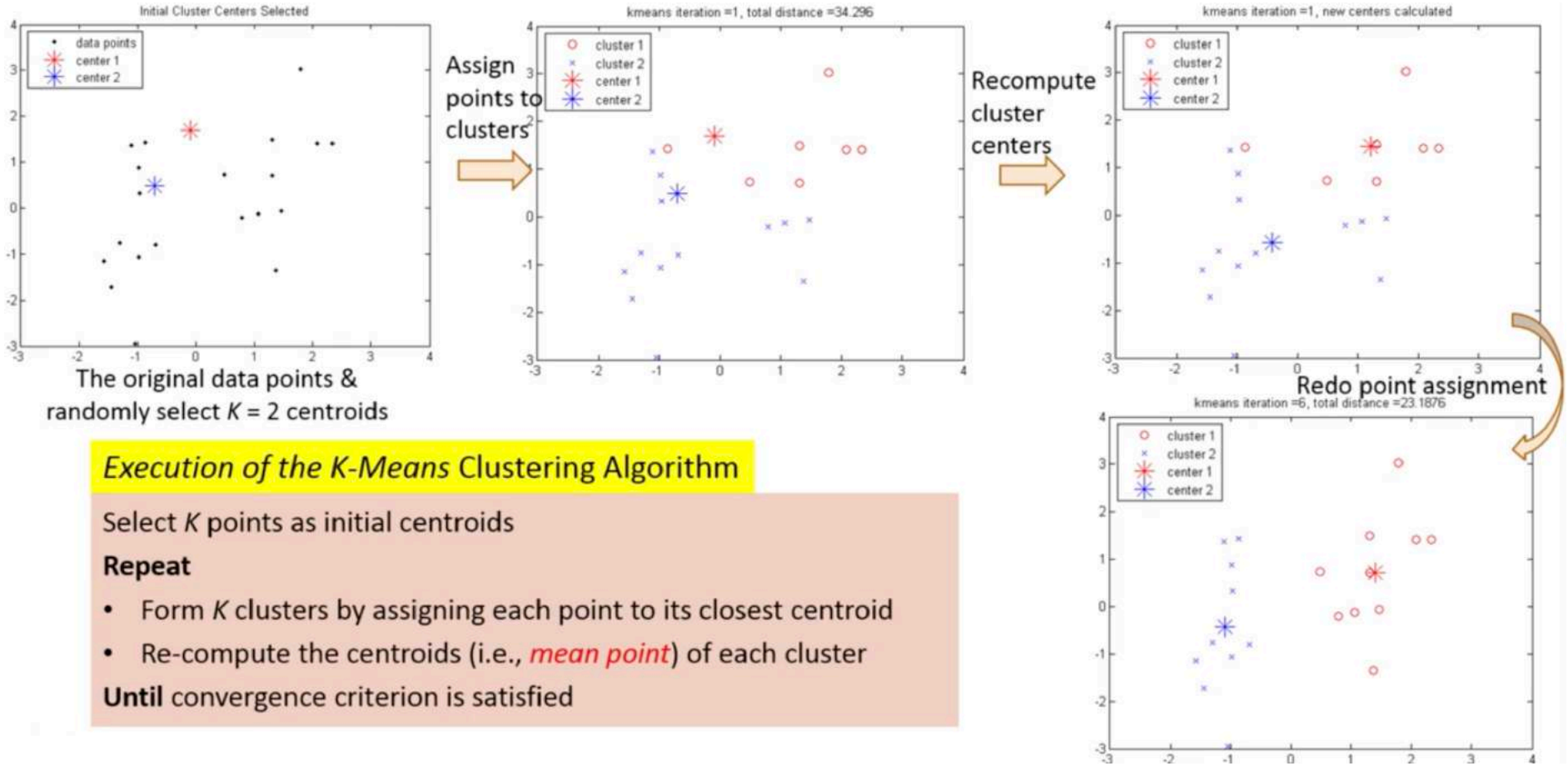
$$SSE(C) = \sum_{k=1}^{K} \sum_{x_{ie}c_k} || x_i - c_k ||^2$$

- Problem definition: Given *K*, find a partition of *K clusters* that optimizes the chosen partitioning criterion
  - Global optimal: Needs to exhaustively enumerate all partitions
  - Heuristic methods (i.e., greedy algorithms): *K-Means*, *K-Medians*, *K-Medoids*, etc.

K-Means Clustering

- *K-Means* (MacQueen'67, Lloyd'57/'82)
  - Each cluster is represented by the center of the cluster
- Given K, the number of clusters, the *K-Means* clustering algorithm is outlined as follows
  - Select *K* points as initial centroids
  - **Repeat**
    - Form *K* clusters by assigning each point to its closest centroid
    - Re-compute the centroids (i.e., *mean point*) of each cluster
  - **Until** convergence criterion is satisfied
- Different kinds of measures can be used
  - Manhattan distance (L_1 norm), Euclidean distance (L_2 norm), Cosine similarity

Example



Execution of the K-Means Clustering Algorithm

Select *K* points as initial centroids

Repeat

- Form *K* clusters by assigning each point to its closest centroid
- Re-compute the centroids (i.e., *mean point*) of each cluster

Until convergence criterion is satisfied

K-Means Discussion

- **Efficiency**: $O(tKn)$ where n: # of objects, K: # of clusters, and t: # of iterations
  - Normally, $K, t << n$; thus, an efficient method
- K-means clustering often ***terminates at* a *local optimal***
  - Initialization can be important to find high-quality clusters
- **Need to specify *K*,** the *number* of clusters, in advance
  - There are ways to automatically determine the "*best*" *K*
  - In practice, one often runs a range of values and selected the "*best*" *K* value
- **Sensitive to noisy data and *outliers***
  - Variations: Using K-medians, K-medoids, etc.
- K-means is applicable only to objects in a continuous n-dimensional space
  - Using the K-modes for ***categorical data***
- Not suitable to discover clusters with ***non-convex shapes***
  - Using density-based clustering, kernel *K*-means, etc.

Variations of K-Means Clustering

- There are many variants of the *K-Means* method, varying in different aspects
  - Choosing better initial centroid estimates
    - *K-means++, Intelligent K-Means, Genetic K-Means*
  - Choosing different representative prototypes for the clusters
    - *K-Medoids, K-Medians, K-Modes*
  - Applying feature transformation techniques
    - *Weighted K-Means, Kernel K-Means*

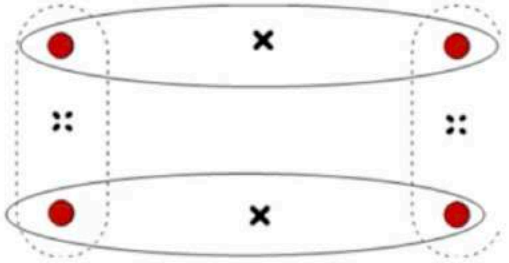
To be discussed later

To be discussed later

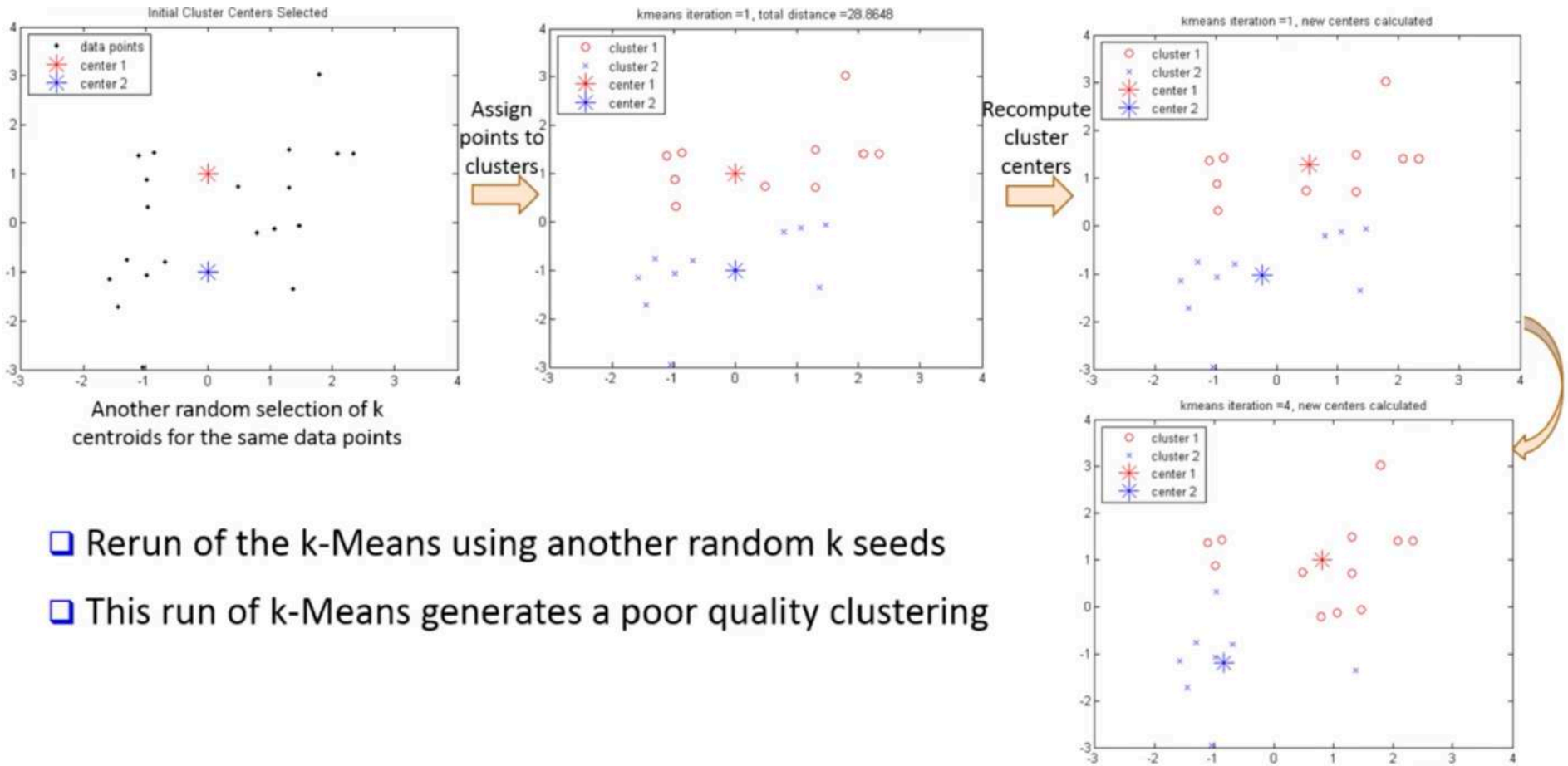
To be discussed later

Initialization of K-Means

- Different initializations may generate rather different clustering results (some could be far from optimal)
- Original proposal (MacQueen'67): Select k seeds randomly
  - Need to run the algorithm multiple times using different seeds
- There are many methods proposed for better initialization of *k* seeds
  - **K-Means++** (Arthur & Vassilvitskii'07):
    - The first centroid is selected at random
    - The next centroid selected is the one that is farthest from the currently selected (selection is based on a weighted probability score)
    - The selection continues until *k* centroids are obtained



Example

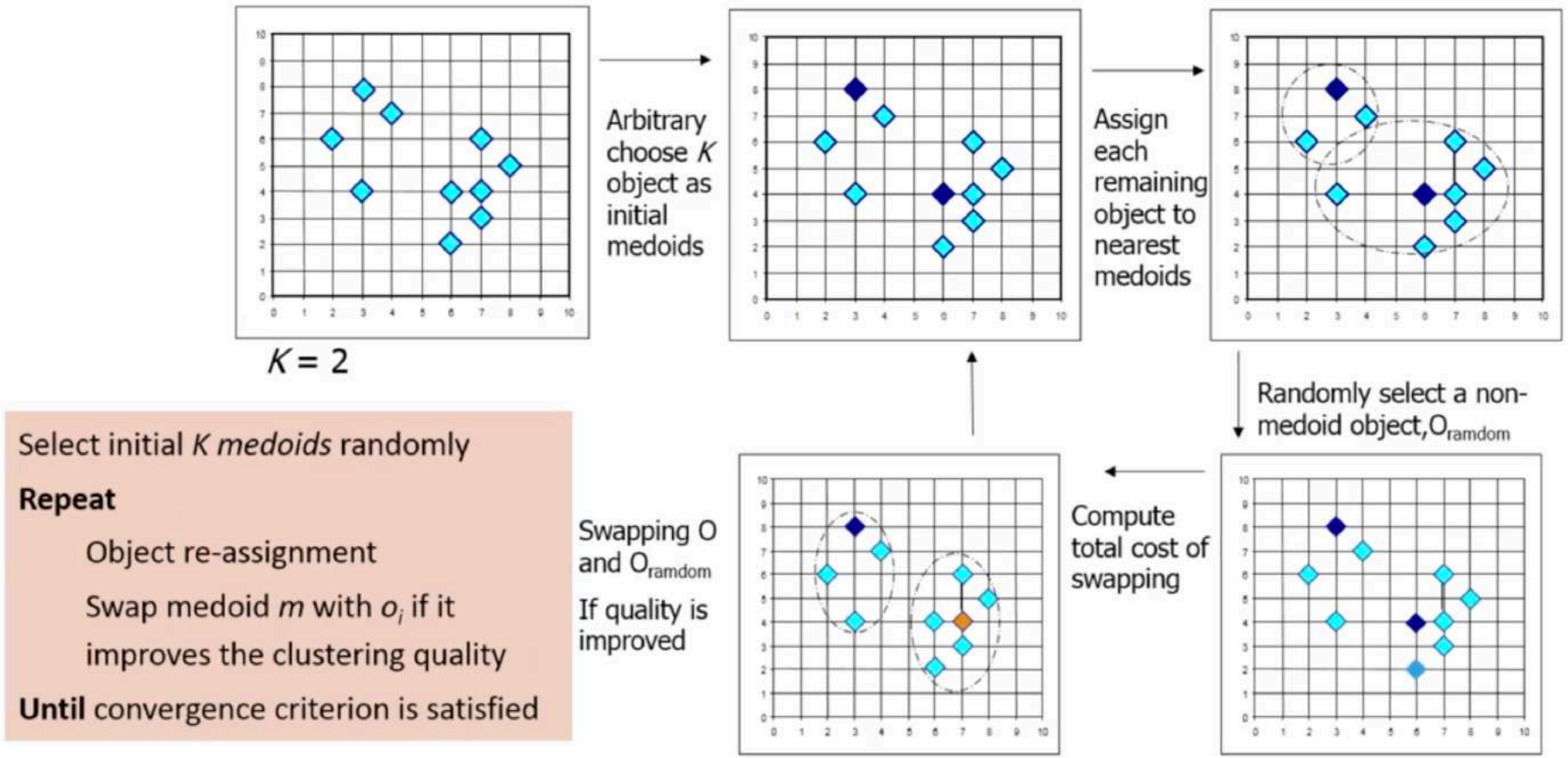


- Rerun of the k-Means using another random k seeds
- This run of k-Means generates a poor quality clustering

Outliers: From K-Means to K-Medoids

- The *K-Means* algorithm is sensitive to outliers!—since an object with an extremely large value may substantially distort the distribution of the data
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster
- The *K-Medoids* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K-medoids*)
  - **Repeat**
    - Assigning each point to the cluster with the closest medoid
    - Randomly select a non-representative object o_i
    - Compute the total cost S of swapping the medoid m with o_i
    - If $S < 0$, then swap m with o_i to form the new set of medoids
  - **Until** convergence criterion is satisfied

Partitioning Around Medoids (PAM)



K-Medoids Discussion

- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
- *PAM* (Partitioning Around Medoids: Kaufmann & Rousseeuw 1987)
  - Starts from an initial set of medoids, and
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) of the resulting clustering
  - *PAM* works effectively for small data sets but does not scale well for large data sets (due to the computational complexity)
  - Computational complexity: PAM: $O(K(n-K)^2)$ (quite expensive!)
- Efficiency improvements on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990):
    - PAM on samples; $O(Ks^2 + K(n-K))$, s is the sample size
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality

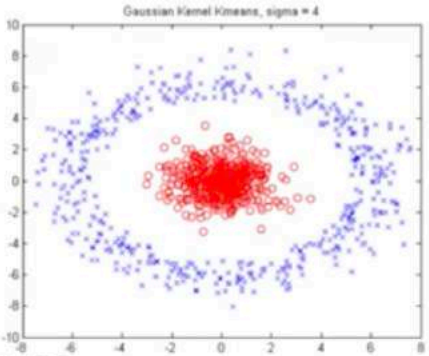
K-Medians & Outliers

- Medians are less sensitive to outliers than means
  - Think of the median salary vs. mean salary of a large firm when adding a few top executives!
- ***K-Medians***: Instead of taking the **mean** value of the object in a cluster as a reference point, **medians** are used (L_1-norm as the distance measure)
- The criterion function for the *K-Medians* algorithm: $S = \sum_{k=1}^{K} \sum_{x_{i \in C_k}} | x_{ij} - med_{kj} |$
- The *K-Medians* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K medians*)
  - **Repeat**
    - Assign every point to its nearest median
    - Re-compute the median using the median of each individual feature
  - **Until** convergence criterion is satisfied

K-Modes: Clustering Categorical Data

- *K-Means* cannot handle non-numerical (categorical) data
  - Mapping categorical value to 1/0 cannot generate quality clusters for high-dimensional data
- ***K-Modes***: An extension to *K-Means* by replacing means of clusters with ***modes***
- Dissimilarity measure between object X and the center of a cluster Z
  - $\Phi(x_j, z_j) = 1 - n_j^r/n_l$ when $x_j = z_j$; 1 when $x_j \neq z_j$
    - where z_j is the categorical value of attribute j in Z_l, n_l is the number of objects in cluster *l*, and n_j^r is the number of objects whose attribute value is r
- This dissimilarity measure (distance function) is **frequency-based**
- Algorithm is still based on iterative *object cluster assignment* and *centroid update*
- A ***fuzzy K-Modes*** method is proposed to calculate a ***fuzzy cluster membership value*** for each object to each cluster
- A mixture of categorical and numerical data: Using a ***K-Prototype*** method

Kernel K-Means Clustering



- *Kernel K-Means* can be used to detect non-convex clusters
  - *K-Means* can only detect clusters that are linearly separable
- Idea: Project data onto the high-dimensional kernel space, and then perform *K-Means* clustering
  - Map data points in the input space onto a high-dimensional feature space using the kernel function
  - Perform *K-Means* on the mapped feature space
- Computational complexity is higher than K-Means
  - Need to compute and store n x n kernel matrix generated from the kernel function on the original data
- The widely studied spectral clustering can be considered as a variant of Kernel K-Means clustering

Kernel Functions and Kernel K-Means

- Typical kernel functions:
  - Polynomial kernel of degree h: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = (\boldsymbol{X}_i \cdot \boldsymbol{X}_j + 1)^h$
  - Gaussian radial basis function (RBF) kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$
  - Sigmoid kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \tanh(\kappa \boldsymbol{X}_i \cdot \boldsymbol{X}_j - \delta)$
- The formula for kernel matrix K for any two points $x_i, x_j \in C_k$ is $K_{x_i x_j} = \phi(x_i) \bullet \phi(x_j)$
- The SSE criterion of *kernel K-means*: $SSE(C) = \sum_{k=1}^{K} \sum_{x_i \in C_k} \| \phi(x_i) - c_k \|^2$
  - The formula for the cluster centroid: $c_k = \frac{\sum_{x_i \in C_k} \phi(x_i)}{|C_k|}$
- Clustering can be performed without the actual individual projections $\phi(x_i)$ and $\phi(x_j)$ for the data points $x_i, x_j \in C_k$

Example

- Gaussian radial basis function (RBF) kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$
- Suppose there are 5 original 2-dimensional points:
  - $x_1(0, 0)$, $x_2(4, 4)$, $x_3(-4, 4)$, $x_4(-4, -4)$, $x_5(4, -4)$
- If we set σ to 4, we will have the following points in the kernel space
  - E.g., $\left|\left|x_1 - x_2\right|\right|^2 = (0-4)^2 + (0-4)^2 = 32$, therefore, $K(x_1, x_2) = e^{-\frac{32}{2 \cdot 4^2}} = e^{-1}$

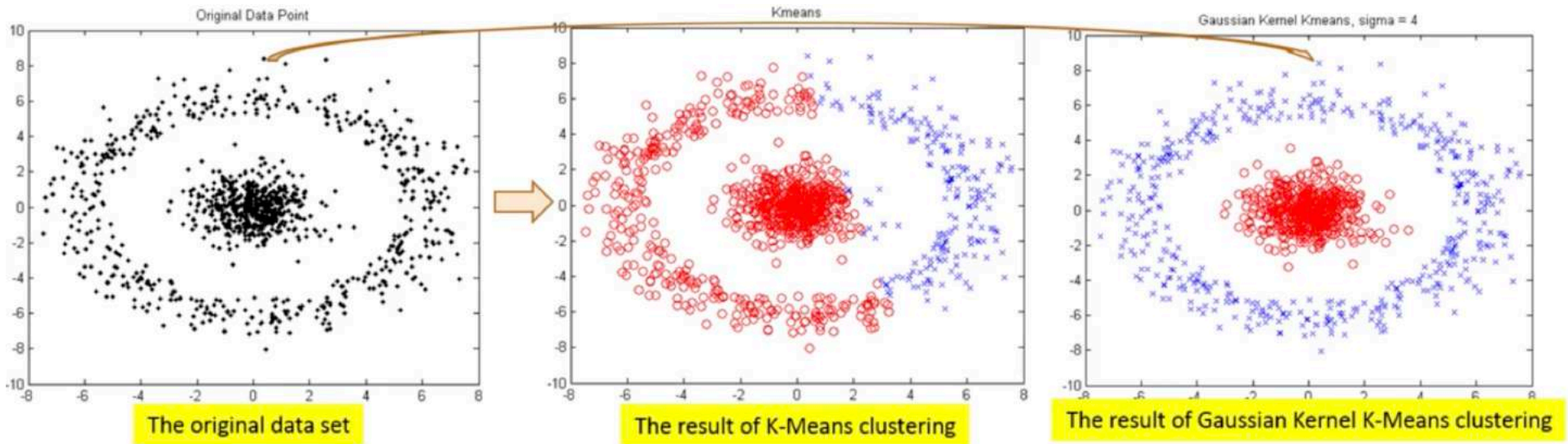
Original Space

	x	y
x_1	0	0
x_2	4	4
x_3	-4	4
x_4	-4	-4
x_5	4	-4

RBF Kernel Space ($\sigma = 4$)

$K(x_i, x_1)$	$K(x_i, x_2)$	$K(x_i, x_3)$	$K(x_i, x_4)$	$K(x_i, x_5)$
0	$e^{-\frac{4^2+4^2}{2 \cdot 4^2}} = e^{-1}$	e^{-1}	e^{-1}	e^{-1}
e^{-1}	0	e^{-2}	e^{-4}	e^{-2}
e^{-1}	e^{-2}	0	e^{-2}	e^{-4}
e^{-1}	e^{-4}	e^{-2}	0	e^{-2}
e^{-1}	e^{-2}	e^{-4}	e^{-2}	0

Example: Kernel K-Means Clustering



The original data set | The result of K-Means clustering | The result of Gaussian Kernel K-Means clustering

- The above data set cannot generate quality clusters by K-Means since it contains non-covex clusters
- Gaussian RBF Kernel transformation maps data to a kernel matrix K for any two points x_i, x_j: $K_{x_i x_j} = \phi(x_i) \bullet \phi(x_j)$ and Gaussian kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$
- K-Means clustering is conducted on the mapped data, generating quality clusters

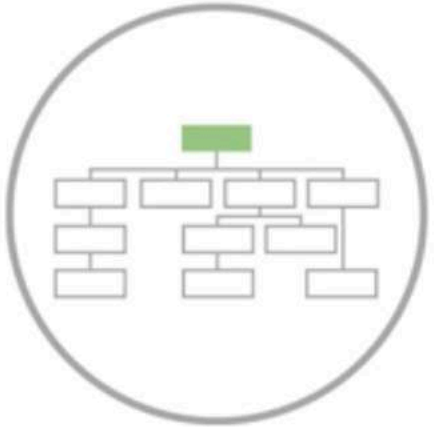
Recommended Readings

- J. MacQueen. Some Methods for Classification and Analysis of Multivariate Observations. In *Proc. of the 5th Berkeley Symp. on Mathematical Statistics and Probability*, 1967
- S. Lloyd. Least Squares Quantization in PCM. *IEEE Trans. on Information Theory*, 28(2), 1982
- A. K. Jain and R. C. Dubes. Algorithms for Clustering Data. Prentice Hall, 1988
- L. Kaufman and P. J. Rousseeuw. Finding Groups in Data: An Introduction to Cluster Analysis. John Wiley & Sons, 1990
- R. Ng and J. Han. Efficient and Effective Clustering Method for Spatial Data Mining. VLDB'94
- B. Schölkopf, A. Smola, and K. R. Müller. Nonlinear Component Analysis as a Kernel Eigenvalue Problem. *Neural computation*, 10(5):1299–1319, 1998
- I. S. Dhillon, Y. Guan, and B. Kulis. Kernel K-Means: Spectral Clustering and Normalized Cuts. *KDD*'04
- D. Arthur and S. Vassilvitskii. K-means++: The Advantages of Careful Seeding. SODA'07
- C. K. Reddy and B. Vinzamuri. A Survey of Partitional and Hierarchical Clustering Algorithms, in (Chap. 4) Aggarwal and Reddy (eds.), Data Clustering: Algorithms and Applications. CRC Press, 2014
- M. J. Zaki and W. Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge Univ. Press, 2014

Next session!

Hierarchical Clustering

- Agglomerative: all cases start separately, then similar cases are joined
- Divisive: all cases start in one category, then split
- Dendrogram shows all levels of splits



DBSCAN

DBSCAN

- Density-based spatial clustering of applications with noise
- Works on local density
- Finds nonconvex and nonlinearly separable clusters
- Points can also be classified as noise