# Introduction to Machine Learning

**Lecture 8 - Unsupervised Learning 1**

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## Unsupervised Learning

- Introduction to unsupervised learning.
- Introduction to clustering.
- K-means algorithm





## What is Unsupervised Learning

- It is one of three categories of machine learning.
- It is about to find underlying patterns in data and is often used in exploratory data analysis.
- The data used in unsupervised learning have no labels, only X. $D = \{(x_i,)\}_{i=1}^{N}$.
- It focuses on the data's features.
- The goal of the unsupervised learning is to find relationships or patterns within the data;
- Then group or cluster data points based on the input data alone.
- Not like the Supervised learning which makes predictions, the unsupervised learning has no prediction tasks but has tasks to discover patterns or group data into clusters.





## Examples of Unsupervised Learning Applications

- Examples of unsupervised learning application
  - Image segmentation
  - Data compression
  - Data mining -- discovery of association rules
  - Density estimation (e.g. texture synthesis), image compression
  - level set estimation
  - clustering/mode finding e.g. spike sorting; algorithm Mixture of Gaussians
  - metric learning e.g. 3D visualization; algorithm multidimensional scaling
  - feature extraction - or representation learning, e.g. whitening; algorithm principle component analysis.

# Unsupervised Learning : Clustering

- Clustering is the most common applications of unsupervised learning.
- It is a technique for finding similarity groups in data, called clusters. For instance,
  - Grouping data points that are similar to (close to) each other in one cluster;
  - Splitting (un-grouping) data points that are very different (far away) from each other into different clusters.
  - Clustering is an unsupervised learning task as no class values are given, unlike the case in supervised learning.
  - Association rule mining is also unsupervised.

 


# Unsupervised Learning : Clustering

- An illustration

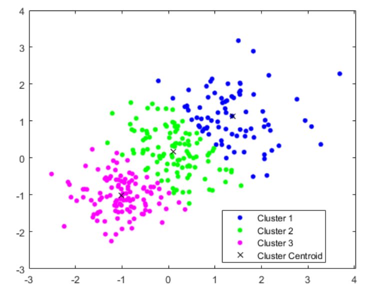


Image copied from https://www.mathworks.com/

 


# Unsupervised Learning : Clustering

- What is clustering useful in real-life?
- For example:
  - groups people of similar sizes together to make “small”, “medium” and “large” T-Shirts.
  - personalize tailor-made is very expensive and the amount of clothes is very limit.
  - Another example in marketing business, segment customers according to their similarities to do targeted marketing, etc.
  - Another example, like building topic hierarchy for organizing a collection of text documents, like libraries, etc.
  - Recommendation systems, such as giving you better Amazon suggestions

 


# Unsupervised Learning : Clustering

- Categories of clustering
  - A clustering algorithm
    - Partitional clustering — each data point in a dataset can only belong to one cluster
    - Hierarchical clustering — clusters within clusters
- A distance (similarity, or dissimilarity) function
- Clustering quality
  - Inter-clusters distance ⇒ maximized
  - Intra-clusters distance ⇒ minimized
- The quality of a clustering result depends on the algorithm, the distance function, and the application.

 

# Unsupervised Learning : Clustering

- The theorem of clustering is;
  - data points that are in the same group should have similar properties and/or features, while those in different groups should have highly dissimilar properties and/or features. The similarity between points is usually quantified by a distance metric based on some sort of feature variable set.

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# Clustering: K-means

- K-means is a partition clustering algorithm
- In k-means clustering, the goal is to partition, or divide, the data into a predetermined value for K, the number of clusters.
- Each data point will fall into only one cluster of the K clusters, and therefore the clusters will not overlap like they would in hierarchical clustering.
- Given a set of data points in N samples as: $\{x_1, x_2, \ldots, x_n\}$,
  - where $x_{i1}, \ldots x_{iD}$ is a D-dimensional vector in a real-valued space $X \in R^D$.
- The k-means algorithm partitions the given data into k clusters.
  - Each cluster has a cluster center, called centroid, or cluster prototype $\mu_k$.
  - k is known.

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# Clustering: K-means Algorithm

- Define a binary indicator variable, use 1-of-K coding scheme
  - $r_{nk} \in \{0,1\}$
  - $r_{nk} = 1, \;\; r_{nj} = 0 \;\; \forall j \neq k$
  - Distortion measure (objective function): $J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} || x_n - \mu_k ||^2$
- Given k, the k-means algorithm works as follows:
  1. Randomly choose k data points (seeds) to be the initial centroids, cluster centres
  2. Assign each data point to the closest centroid
  3. Re-compute the centroids using the current cluster memberships
  4. If a convergence criterion is not met, go to 2).

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# K-means Clustering: Expectation Maximization

- Find values for $\{r_{nk}\}$ and $\{\mu_k\}$ to minimize:
  - $J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} || x_n - \mu_k ||^2$
- Iterative procedure:
  - E-step:
    - Minimize J w.r.t. $r_{nk}$, keep $\mu_k$ fixed.
    - $r_{nk} = 1 \;$ if $\; k = \text{argmin}_j || x_n - \mu_k ||^2$ or, $r_{nk} = 0 \;$ otherwise
  - M-step:
    - minimize J w.r.t. $\mu_k$, keep $r_{nk}$ fixed
    - $2 \sum_{n=1}^{N} r_{nk}(x_n - \mu_k) = 0$, then $\mu_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$

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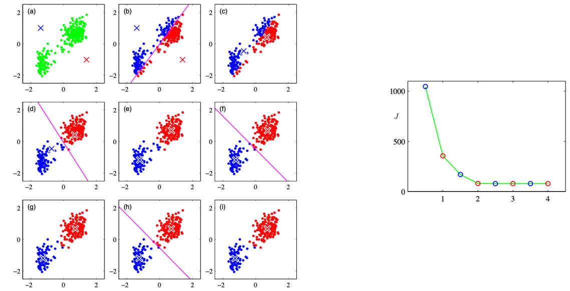
# K-means Clustering: Expectation Maximization

- Stopping/convergence criterion
  - no (or minimum) re-assignments of data points to different clusters,
  - no (or minimum) change of centroids, or
  - minimum decrease in the sum of squared error (SSE) — J function,
    - $J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \mathrm{dist}(x_n - \mu_k)$
  - $k_j$ is the jth cluster, $\mu_k$ is the centroid of cluster $k_j$ (the mean vector of all the data points in $k_j$), and $\mathrm{dist}(x_n, \mu_k)$is the distance between data point x and centroid $\mu_k$.





# K-means Clustering: Example



K-means clustering example in OldFaithful data

- Each E or M step reduces the value of the objective function J
- Convergence to a global or local maximum





**K-means clustering**

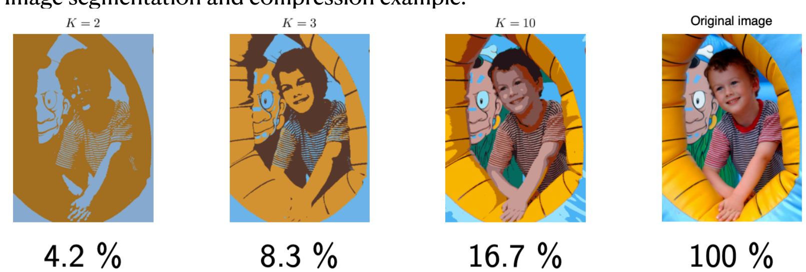
- Direct implementation of K-means can be slow.
- Online version: $\mu_k^{new} = \mu_k^{old} + \eta(x_n - \mu_k^{old})$.
- K-mediods, general distortion measure: $\tilde{J} = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} V(x_n, \mu_k)$,
  - where $v(\,.\,,\,.\,)$ is any kind of dissimilarity measure.





**Examples of K-means clustering applications**

- Image segmentation and compression example:




Cited from the book: Christopher M. Bishop, Pattern Recognition and Machine Learning, 2006

## An example distance function

- In the **Euclidean space**, the mean of a cluster is computed with:
  - $\mu_j = \frac{1}{|K_j|} \sum_{x_i \in K_j} x_i,$
  - where $|K_j|$ is the number of data points in cluster $K_j$
  - The distance from one data point $x_i$ to a mean (centroid) $\mu_j$ is computed with
    - $\text{dist}(x_i, \mu_j) = ||x_i - \mu_j|| = \sqrt{(x_{i1} - \mu_{j1})^2 + (x_{i2} - \mu_{j2})^2 + \ldots + (x_{iD} - \mu_{jD})^2}$



## K-means Clustering: Strengths

- Simple: easy to understand and to implement
- Efficient: Time complexity: O(tkn),
  - where n is the number of data points,
  - k is the number of clusters, and
  - t is the number of iterations.
- Since both k and t are small. k-means is considered a linear algorithm.
- K-means is the most popular clustering algorithm.
- Note that: it terminates at a local optimum if SSE is used. The global optimum is hard to find due to complexity.



## K-means Clustering: Weaknesses

- The algorithm is only applicable if the mean is defined.
- For categorical data, k-mode - the centroid is represented by most frequent values.
- The user needs to specify k.
- The algorithm is sensitive to outliers
- Outliers are data points that are very far away from other data points.
- Outliers could be errors in the data recording or some special data points with very different values.



## K-means Clustering: Weaknesses

- To deal with outliers
  - Remove some data points in the clustering process that are much further away from the centroids than other data points.
  - Perform random sampling. In sampling the chance of selecting an outlier is very small because of a small set of data points be selected.
  - Assign the rest of the data points to the clusters by distance or similarity comparison, or classification

# Clustering: Represent clusters

- Use the centroid of each cluster to represent the cluster.
  - compute the radius and
  - standard deviation of the cluster to determine its spread in each dimension
  - the centroid representation alone works well if the clusters are of the hyper-spherical shape.
  - if clusters are elongated or are of other shapes, centroids are not sufficient

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# Clustering: Represent clusters

- Use frequent values to represent cluster
  - This method is mainly for clustering of categorical data (e.g., k-modes clustering).
  - Main method used in text clustering, where a small set of frequent words in each cluster is selected to represent the cluster.

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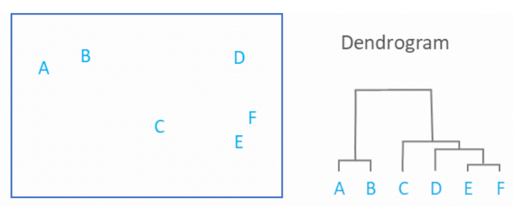
# Hierarchical Clustering

- Hierarchical clustering finds clusters within clusters by a system of hierarchies.
- Not like the partition clustering, every data points can belong to multiple clusters, some clusters will contain smaller clusters within it.
- This hierarchy system can be organized as a tree diagram.




Hierarchical Clustering Dendrogram —copied from displayr.com

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# Hierarchical Clustering

- This hierarchy system can be organized as a tree diagram.
  - Agglomerative algorithms find clusters with a bottom-up approach. These algorithms start with each data point as a cluster, then progressively “zoom out” and combine smaller clusters into larger clusters.
  - Divisive algorithms take the opposite approach: top-down. Divisive algorithms start out by looking at the entire dataset as one cluster, then “zooming in” to divide the dataset into smaller clusters.
- Unlike k-means clustering, with hierarchical clustering, the number of clusters in unknown beforehand.

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# Measure the distance of two clusters

- A few ways to measure distances of two clusters. Results in different variations of the algorithm.
  1. **Single link** -- The distance between two clusters is the distance between two closest data points in the two clusters, one data point from each cluster
  2. **Complete link** -- The distance between two clusters is the distance of two furthest data points in the two clusters. It is sensitive to outliers because they are far away
  3. **Average link** -- A compromise between single and complete link. The distance between two clusters is the average distance of all pairwise distances between the data points in two cluster
  4. **Centroids** -- In this method, the distance between two clusters is the distance between their centroids





# Distance Functions

- For Key to clustering. “similarity” and “dissimilarity” can also be commonly used terms.
- There are numerous distance functions for
  - Different types of data
    - Numeric data
    - Nominal data
  - Different specific applications





## Distance functions for numeric attributes

- Most commonly used functions are
  - Euclidean distance and
  - Manhattan (city block) distance
- We denote distance with: $\text{dist}(x_i, x_j)$, where $x_i$ and $x_j$ are data points (vectors)
- They are special cases of Minkowski distance. h is positive integer.
- $\text{dist}(x_i, x_j) = ((x_{i1} - x_{j1})^h + (x_{i2} - x_{j2})^h + \ldots + (x_{iD} - x_{jD})^h)^{1/h}$





## **Euclidean distance** and **Manhattan distance**

- If h = 2, it is the Euclidean distance:
  - $\text{dist}(x_i, x_j) = \sqrt{((x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \ldots + (x_{iD} - x_{jD})^2)},$
- If h = 1, it is the Manhattan distance:
  - $\text{dist}(x_i, x_j) = |(x_{i1} - x_{j1})| + |(x_{i2} - x_{j2})| + \ldots + |(x_{iD} - x_{jD})|$
- Weighted Euclidean distance
  - $\text{dist}(x_i, x_j) = \sqrt{w_1((x_{i1} - x_{j1})^2 + w_2(x_{i2} - x_{j2})^2 + \ldots + w_D(x_{iD} - x_{jD})^2)}$

### Squared distance and Chebyshev distance

- Squared distance and Chebyshev distance
  - Squared Euclidean distance: to place progressively greater weight on data points that are further apar
  - $\text{dist}(x_i, x_j) = ((x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \ldots + (x_{iD} - x_{jD})^2)$
  - Chebyshev distance: one wants to define two data points as "different" if they are different on any one of the attributes.
  - $\text{dist}(x_i, x_j) = max(|(x_{i1} - x_{j1})| + |(x_{i2} - x_{j2})| + \ldots + |(x_{iD} - x_{jD})|)$





### Distance function for binary and nominal attributes

- Use Binary attribute: has two values or states but no ordering relationships, e.g., Gender: male and female.
- We use a confusion matrix to introduce the distance functions/measures.
- Let the ith and jth data points be xi and xj (vectors)
- Symmetric binary attributes
- A binary attribute is symmetric if both of its states (0 and 1) have equal importance, and carry the same weights, e.g., male and female of the attribute Gender
- Distance function: Simple Matching Coefficient, proportion of mismatches of their values
  - $\text{dist}(x_i, x_j) = \dfrac{b + c}{a + b + c + d}$





### Distance function for binary and nominal attributes

- Nominal attributes: with more than two states or values.
- the commonly used distance measure is also based on the simple matching method.
- Given two data points xi and xj, let the number of attributes be r, and the number of values that match in xi and xj be q.
  - $\text{dist}(x_i, x_j) = \dfrac{r - q}{r}$





### Recap

- Unsupervised learning is one of three categories of machine learning
- Clustering is the main focus of the unsupervised learning.
- Data mining is another technique of the unsupervised learning.
- Clustering is has along history and still active
  - There are a huge number of clustering algorithms
  - More are still coming every year.
- We only introduced several main algorithms.
  - partitional-clustering and hierarchical clustering
  - K-means is a partitional-clustering

## Recap

- The There are many others, e.g.,
  - density based algorithm, sub-space clustering, scale-up methods, neural networks based methods, fuzzy clustering, co-clustering, etc.
- Clustering is hard to evaluate, but very useful in practice. This partially explains why there are still a large number of clustering algorithms being devised every year.
- Clustering is highly application dependent and to some extent subjective.

 





## Questions?

Datasets can be used in your project:
UCI Machine Learning Repository
https://archive.ics.uci.edu/ml/datasets.php





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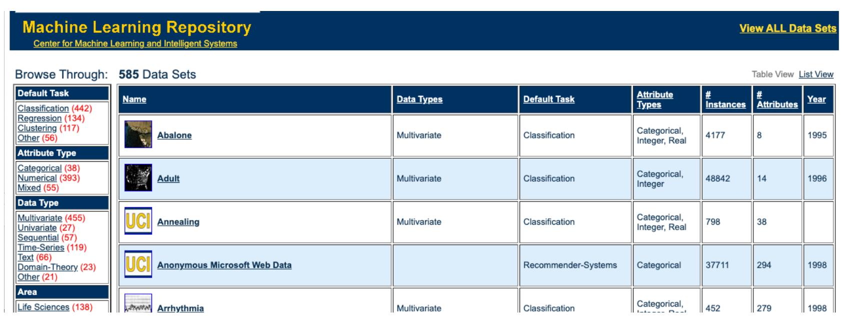

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Default Task
Classification (442)
Regression (134)
Clustering (117)
Other (56)
Attribute Type
Categorical (38)
Numerical (393)
Mixed (55)
Data Type
Multivariate (455)
Univariate (27)
Sequential (57)
Time-Series (119)
Text (66)
Domain-Theory (23)
Other (21)
Area
Life Sciences (138)

| Name | Data Types | Default Task | Attribute Types | # Instances | # Attributes | Year |
|---|---|---|---|---|---|---|
| Abalone | Multivariate | Classification | Categorical, Integer, Real | 4177 | 8 | 1995 |
| Adult | Multivariate | Classification | Categorical, Integer | 48842 | 14 | 1996 |
| Annealing | Multivariate | Classification | Categorical, Integer, Real | 798 | 38 | |
| Anonymous Microsoft Web Data | | Recommender-Systems | Categorical | 37711 | 294 | 1998 |
| Arrhythmia | Multivariate | Classification | Categorical, [illegible] | 452 | 279 | 1998 |

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