Machine Learning (CE 40717)

Fall 2024

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November 16, 2025

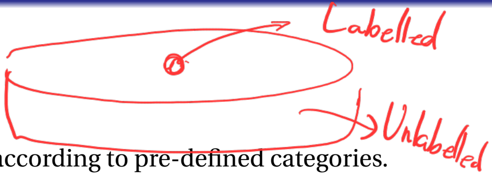
Supervised vs Unsupervised Learning

- **Supervised learning**: Given $(\mathbf{x}_i, y_i),\ i = 1, \ldots, n$, learn a function

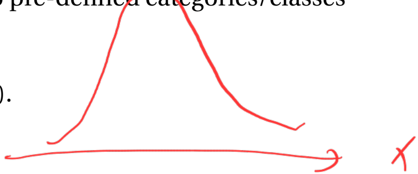
$$f : X \to Y.$$

  - Categorical Y: classification
  - Continuous Y: regression
- **Unsupervised learning**: Given only $(\mathbf{x}_i),\ i = 1, \ldots, n$, can we infer the underlying structure of X?
  - Involves analyzing unlabeled data to uncover hidden patterns or structures within the data.

Supervised vs Unsupervised Learning



- **Supervised Learning**
  - *Classification*: partition examples into groups according to pre-defined categories.
  - *Regression*: assign values to feature vectors.
  - Requires labeled data for training.
- **Unsupervised Learning**
  - خوشه‌بندی *Clustering*: partition examples into groups when no pre-defined categories/classes are available.
  - *Novelty detection*: find changes in data.
  - *Outlier detection*: find unusual events (e.g., hackers).
  - Requires only instances, with no labels.



~~Dimension Reduction~~ X

Some Common Tasks

- **Clustering**: grouping data points into clusters based on similarity.
- **Dimensionality Reduction**: reducing the number of features under consideration and keeping (perhaps approximately) the most informative ones.
- **Anomaly Detection**: identifying data points that deviate significantly from the norm (e.g., fraud detection).
- **Generative Modeling**: learning the distribution of data to generate new, similar instances.

Clustering

- Clustering organizes data points into groups of similar objects.
- Data points within a cluster are more similar to each other than to those in other clusters.
- The notion of similarity depends on the task at hand (e.g., purchase behavior in market segmentation).

Clustering

- **Goal:** automatically segment data into groups of similar points.
- **Question:** when and why would we want to do this?
- **Useful for:**
  - Automatically organizing data.
  - Understanding hidden structure in data.
  - Representing high-dimensional data in a low-dimensional space.
- **Some Applications of Clustering:**
  - Customer segmentation (marketing).
  - Image segmentation and object detection (computer vision).
  - Anomaly detection (cybersecurity, finance).
  - Genomics and bioinformatics.
  - Social network analysis and community detection.

Clustering Set-up

- Our data are

$$D = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}.$$

- Each data point is p-dimensional, i.e.,

$$\mathbf{x}_n = \langle x_{n,1}, \dots, x_{n,p} \rangle.$$

- Define a *distance function* between data,

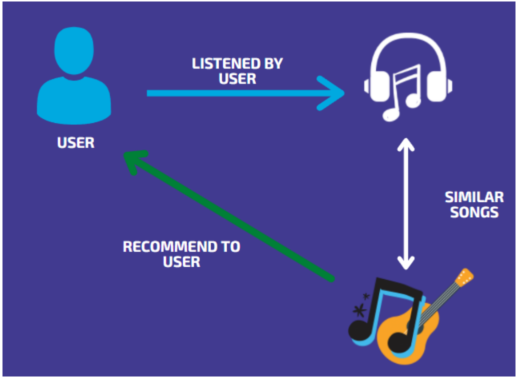
$$d(\mathbf{x}_n, \mathbf{x}_m).$$

- Goal: segment the data into K groups:

$$\{z_1, \dots, z_N\} \quad \text{where } z_i \in \{1, \dots, K\}.$$

Clustering in Action: Music Recommendation Systems

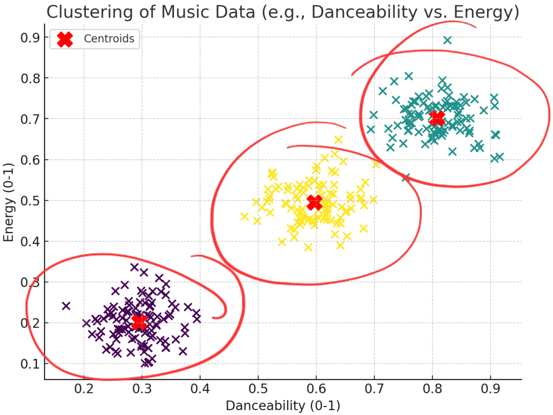
- Music recommendation systems cluster songs based on similarity.



Adopted from machinelearninggeek.com

Clustering in Action: Music Recommendation Systems

- When you like a song, the system suggests others from the same cluster.

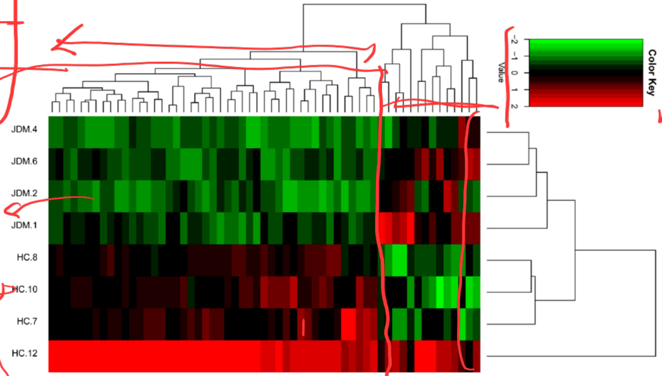


Clustering in Action: Gene Expression Clustering

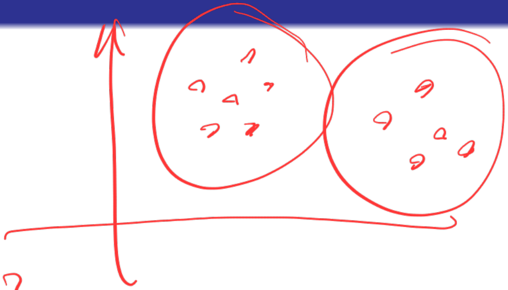
- Clustering can decipher hidden patterns in gene expression data, which can help in understanding disease mechanisms or genetic variations.

۵	-۱	۶
۳	۲۸	۸
۷	۳	۹
۱۲	۱۸	۱۴

مقیاس عددی



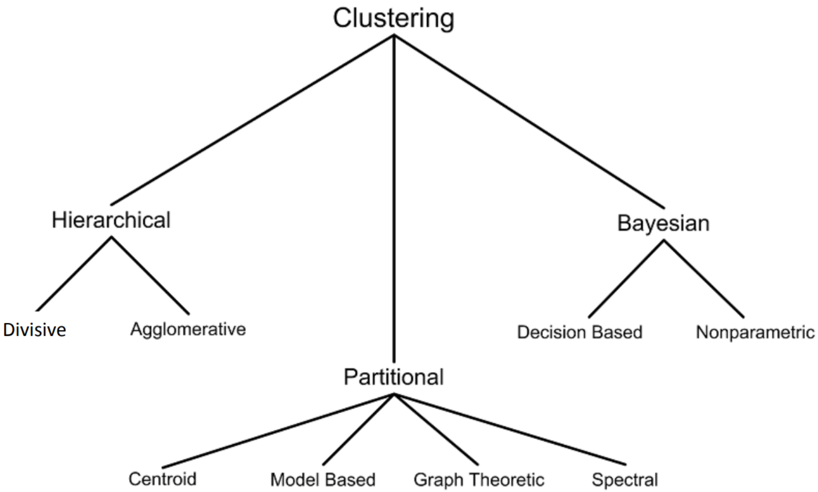
Two Beginning Questions



- How do we create good clusters?
- How many clusters do we need? → K ?

k = ۲

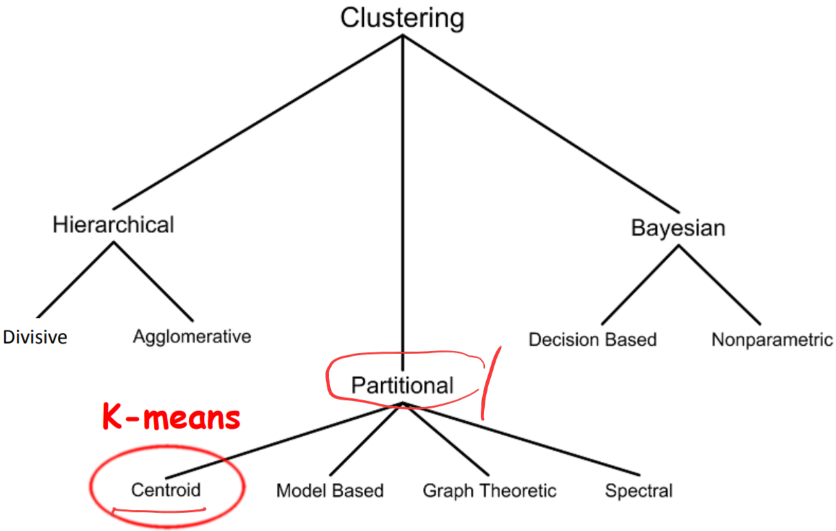
Clustering Techniques



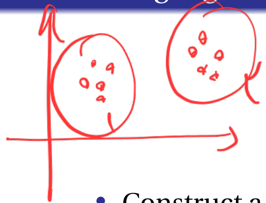
Clustering Techniques

- **Partitional** algorithms typically determine all clusters at once, but can also be used as divisive algorithms in hierarchical clustering.
- **Hierarchical** algorithms find successive clusters using previously established clusters. These algorithms can be either **agglomerative** (bottomup) or **divisive** (topdown):
  - **Agglomerative algorithms** begin with each element as a separate cluster and merge them into successively larger clusters.
  - **Divisive algorithms** begin with the whole set and proceed to divide it into successively smaller clusters.
- **Bayesian** algorithms try to generate an *a posteriori distribution* over the collection of all partitions of the data.

Clustering Techniques



Partitioning Algorithms: Basic Concept

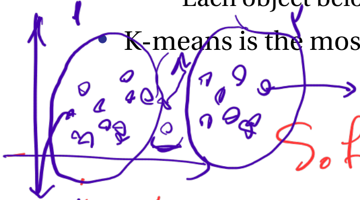


Hard Clustering : هر x به یک cluster تعلق دارد

$z_{ij} \in \{0, 1\}$

$\forall i : \sum_{j=1}^{K} z_{ij} = 1$

- Construct a partition of a set of *N* objects into a set of K clusters:
  - The number of clusters K is given in advance.
  - Each object belongs to **exactly one** cluster in hard clustering methods.
- K-means is the most popular partitioning algorithm.



$z_{i,1} \sim 0$

$z_{i,2} = 1$

Soft Clustering :

نمونه i $\in$ خوشه j

$z_{i,1}$ احتمال تعلق نمونه i به خوشه j

$z_{i,1} \sim 0$

$0 \leq z_{ij} \leq 1$

$\forall i : \sum_{j=1}^{K} z_{ij} = 1$

Objective Based Clustering

- **Input:** a set of N points, and a distance/dissimilarity measure.
- **Output:** a partition of the data.

- **K-median:** find center points $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_K$ to minimize

$$\sum_{i=1}^{N} \min_{j \in \{1,\ldots,K\}} d(\mathbf{x}^{(i)}, \mathbf{c}_j)$$

- **K-means:** find center points $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_K$ to minimize

$$\sum_{i=1}^{N} \min_{j \in \{1,\ldots,K\}} d^2(\mathbf{x}^{(i)}, \mathbf{c}_j)$$

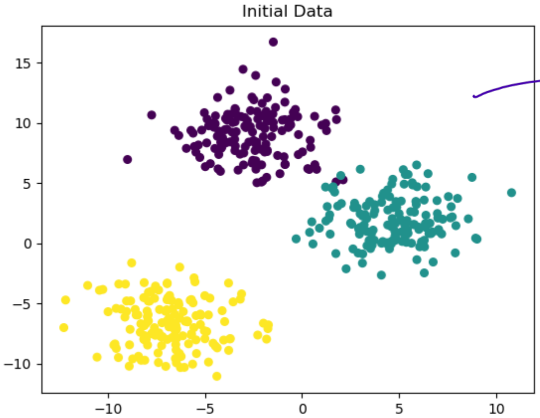
- **K-center:** find a partition that minimizes the maximum radius.

K-Means Overview

- The most widely used clustering algorithm.
- Partitions data into K distinct groups based on feature similarity.
- It works by **iteratively** assigning data points to the nearest centroid (mean of the group) and then recalculating the centroids based on the new group memberships.
- The K-means algorithm is a **heuristic**.
- It requires initial centroids, and the choice is important.
- The process repeats until the assignments no longer change.

K-Means in Action

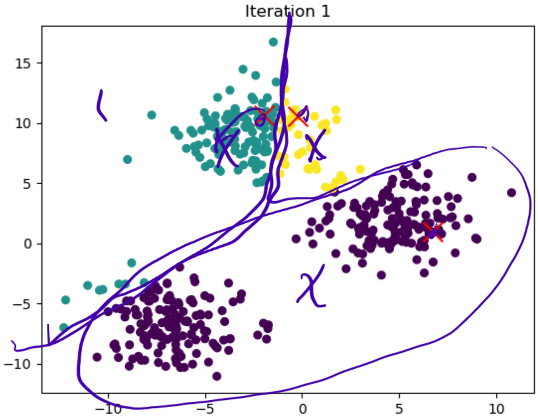
$K = ۳$



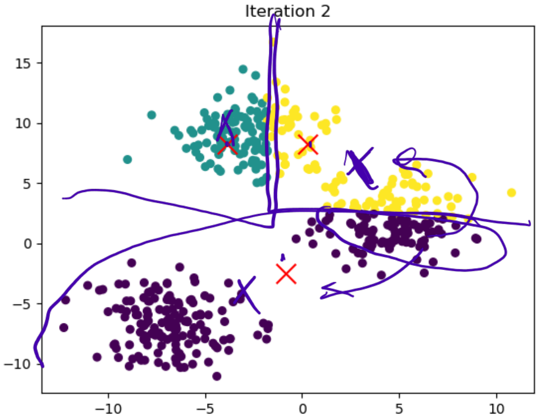
Unlabelled

[illegible]

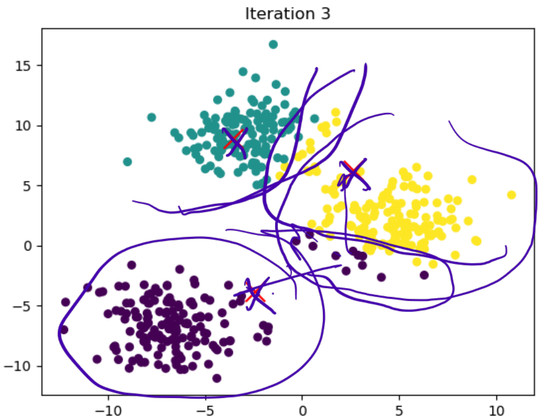
K-Means in Action



K-Means in Action



K-Means in Action

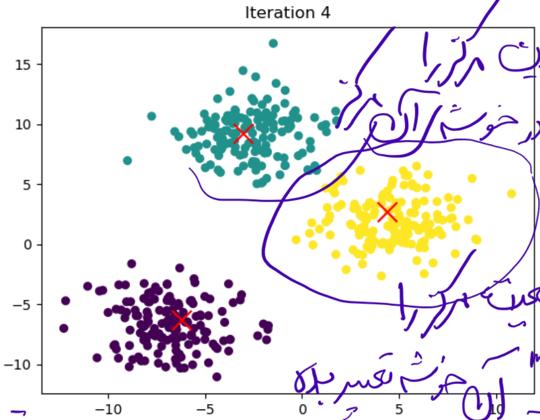


K-Means in Action

while true:

مرحله ۱

به ازای هر نقطه، نزدیک‌ترین مرکز را
پیدا کن و آن نقطه را در خوشه آن مرکز
قرار بده



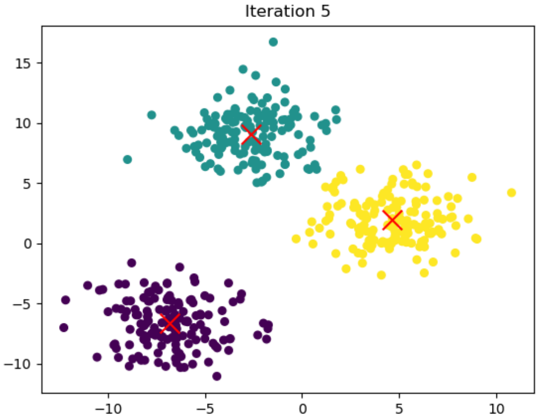
به ازای هر خوشه موقعیت مرکز را
به میانگین، mean
آن خوشه تغییر بده

median

center

اگر خوشه‌ها نسبت به بار قبل تغییر نکرد خارج شو

K-Means in Action



Problem Definition

- Formally: we have

$$X_{\text{train}} = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N)}\} \subseteq \mathbb{R}^d.$$

- K is the number of clusters.
- We are learning:
  - A function or mapping

Z عضو خوشه‌ها

$$f : \mathbb{R}^d \to \{1, 2, \ldots, K\}$$

    that assigns a cluster to each data point.
  - A set of K prototypes

$$\boldsymbol{\mu} = \{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K\} \subseteq \mathbb{R}^d$$

    as the cluster representatives, called **centroids**.

Center

Algorithm

Algorithm 1 K-means Clustering

Input: K (number of clusters), $D = \{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}\}$ (data points)
Initialize: Select K random points as centroids $\{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K\}$ تصادفی
repeat
  Assign each point $\boldsymbol{x}^{(i)}$ to nearest centroid $f(\boldsymbol{x}^{(i)}) = \arg\min_j \|\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j\|$
  For each $1 \le j \le K$ set $C_j = \{x^{(i)} | f(x^{(i)}) = j\}$
  Update centroids $\boxed{\boldsymbol{\mu}_j} = \frac{1}{|C_j|} \sum_{\boldsymbol{x}^{(i)} \in C_j} \boldsymbol{x}^{(i)}$
until Centroids do not change
Output: Final clusters $\{C_1, C_2, \ldots, C_K\}$

Objective Function

- We want samples in the same cluster to be similar.
- In K-means, this is expressed as:

$$J = \sum_{j=1}^{K} \sum_{\mathbf{x}^{(i)} \in C_j} \|\mathbf{x}^{(i)} - \boldsymbol{\mu}_j\|^2$$

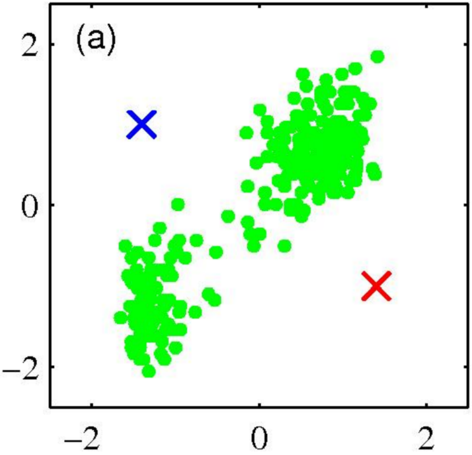
- Choose f and

$$\boldsymbol{\mu} = \{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K\}$$

  to minimize this.
- This problem is NP-hard. K-means is a heuristic solution, which is **not** guaranteed to find an optimal solution.

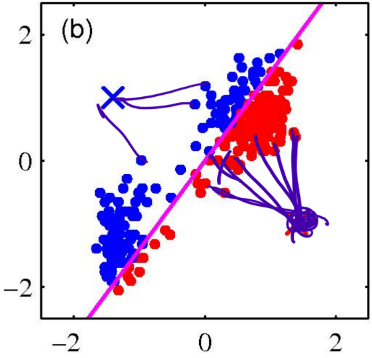
K-Means Process Example

- Pick K random points as cluster centers (means).
- Shown here for $K = 2$.



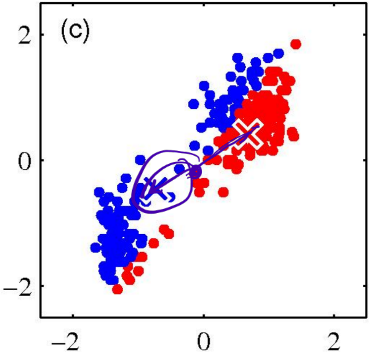
K-Means Process Example

Assignment Step (E-step)



Iterative Step 1: assign data points to the closest cluster center.

Update Step (M-step)

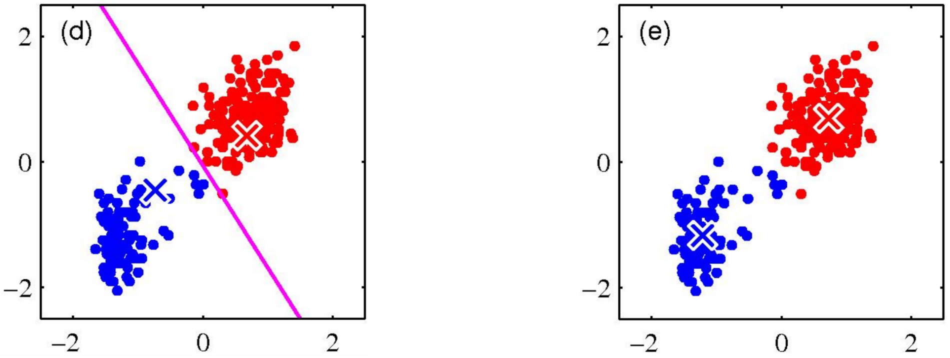


Iterative Step 2: update the cluster center to the average of the assigned points.

K-Means Process Example

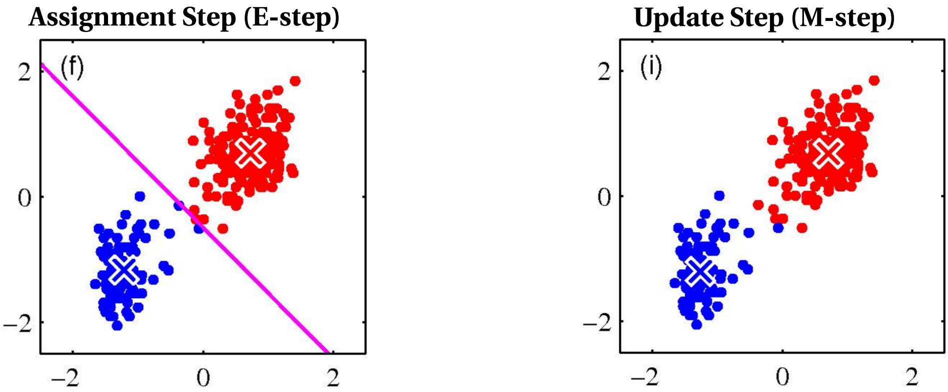
- Repeat until convergence.

Assignment Step (E-step) **Update Step (M-step)**



K-Means Process Example

- Repeat until convergence.



Convergence

- How do we know K-means will converge in a finite number of steps?
- First, we show that in each step J will decrease as long as we have not converged.

Convergence

- We initially assign each sample to the nearest centroid:

$$f(\mathbf{x}) := \arg\min_j \|\mathbf{x} - \boldsymbol{\mu}_j\|^2. \quad = J$$

- Keep each sample's assignment fixed until a closer centroid is found.
- Each time a sample is reassigned, the total distance between samples and their centroids decreases.
- The number of possible sample-to-centroid assignments is finite.
- The algorithm terminates when no sample changes its assigned centroid.

Convergence

- In the updating step, with $f(\mathbf{x})$ fixed, J is a quadratic function of $\boldsymbol{\mu}_j$ (like SSE), and by taking the derivative we can minimize it as:

$J = \sum \left(x^{(i)} - \mu_{C_i} \right)$

$$\frac{\partial J}{\partial \boldsymbol{\mu}_j} = 0 \implies \sum_{\mathbf{x}^{(i)} \in C_j} 2\left(\mathbf{x}^{(i)} - \boldsymbol{\mu}_j\right) = 0.$$

خوشه اختصاص داده شده به $x^{(i)}$

عوض نمی‌کنیم

- This means we should **update** each $\boldsymbol{\mu}_j$ as the mean of cluster C_j:

$$\boldsymbol{\mu}_j = \frac{\sum_{\mathbf{x}^{(i)} \in C_j} \mathbf{x}^{(i)}}{|C_j|}.$$

Convergence

- For each cluster, the mean of its samples minimizes squared distances.
- For C_j, if $\boldsymbol{\mu}_j'$ was the old centroid, we have:

$$\sum_{\mathbf{x}^{(i)} \in C_j} \|\mathbf{x}^{(i)} - \boldsymbol{\mu}_j'\|^2 \geq \sum_{\mathbf{x}^{(i)} \in C_j} \|\mathbf{x}^{(i)} - \boldsymbol{\mu}_j\|^2.$$

So $J_{\text{new}} \leq J_{\text{old}}$.

Convergence

- J is non-negative, and there are a finite number of partitions, so there is a minimum for J and we cannot decrease J forever.
- Therefore, we must converge at some point.
- The convergence properties of the K-means algorithm were studied by MacQueen (1967).

Convergence

EM

Likelihood

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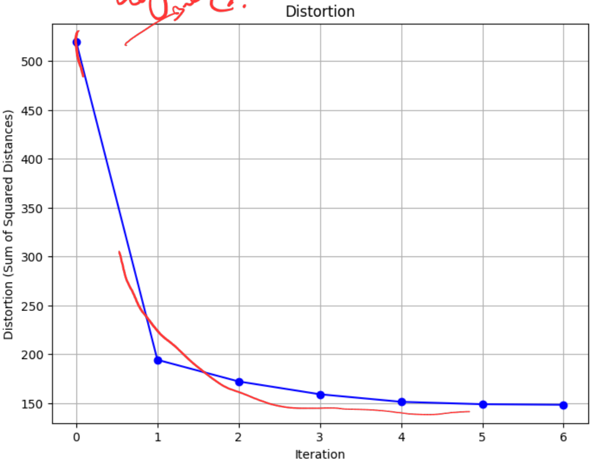
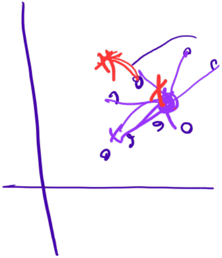
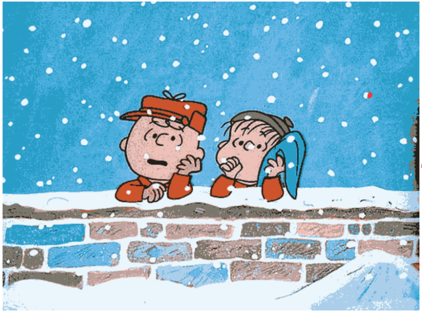


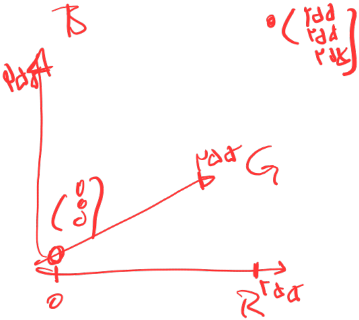


K-means Application: Compressing Images

- Each pixel is associated with a red, green, and blue value.
- A 1024×1024 image is a collection of 1048576 values $\langle x_1, x_2, x_3 \rangle$, represented as a vector $\mathbf{x}$, which requires 3M B of storage.
- How can we use K-means to compress this image?

Vector Quantization





- Replace each pixel $\mathbf{x}_n$ with its assignment $\mathbf{m}_{z_n}$ (paint by numbers).
- The K means are called the *codebook*.
- With $K = 100$, we need 7 bits per pixel plus 100×3 bytes ≈ 897K.

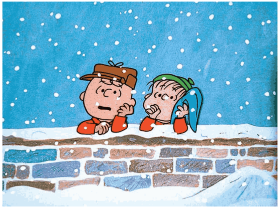
Vector Quantization

2 means

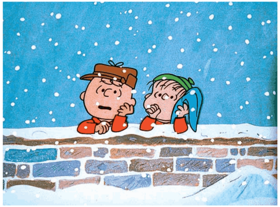
4 means

8 means

16 means



32 means



64 means

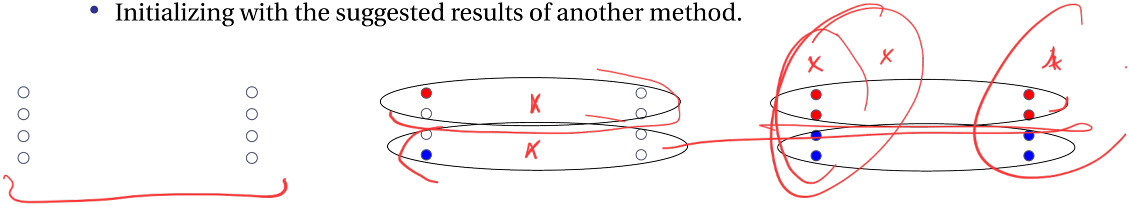
1. Clustering Overview
2. Partitional Clustering
3. **Challenges in K-means**
4. Hierarchical Clustering
5. Other Clustering Algorithms

Strengths

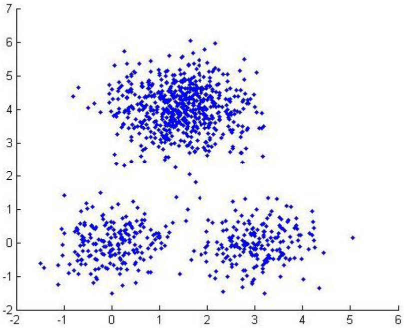
- **Simple:** easy to understand and implement.
- **Efficient:** time complexity $O(tKn)$, where
  - n is the number of data points,
  - K is the number of clusters, and
  - t is the number of iterations (it requires initial centroids, and the choice is important as it could affect t in $O(tkn)$).
- 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.

Local Optimum

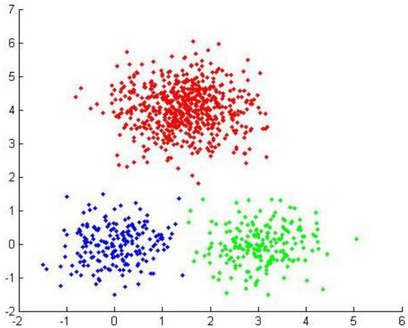
- The algorithm finds a local minimum, but there is no guarantee of finding the global minimum.
- Its result is highly affected by the initialization.
- Some suggestions are:
  - Multiple runs with random initial centroids, then select the best result.
  - Initialization heuristics (K-means++, Furthest Traversal).
  - Initializing with the suggested results of another method.



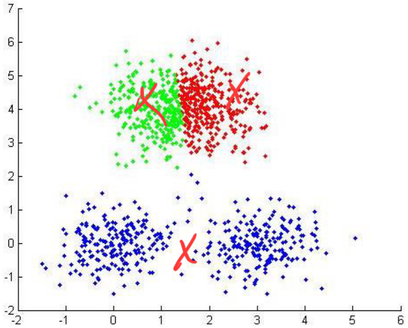
Local Optimum



Local Optimum



Optimal clustering



Possible clustering

Weaknesses of K-means

- The algorithm is only applicable if the **mean** is defined.
  - For categorical data, K-modes can be used — the centroid is represented by the 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 data recording or some special data points with very different values.

Definition of Mean

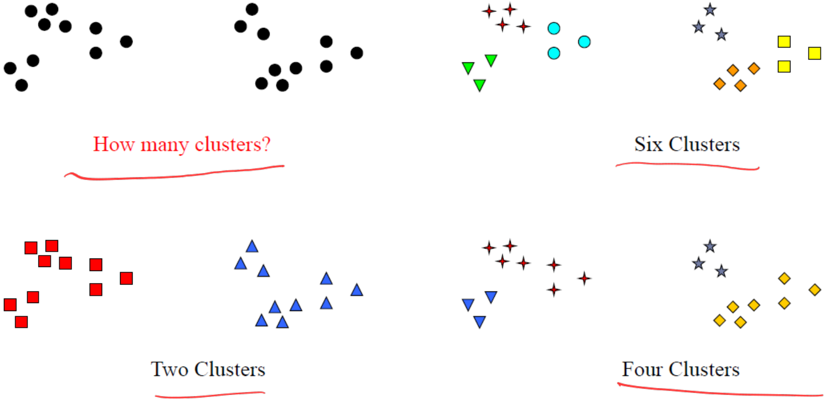
x

- We assume $\mathbf{x}^{(i)} \in \mathbb{R}^d$, which is not always the case. K-means requires a space where the sample **mean** is defined.

median

  - Categorical data.
  - A suggested solution: K-modes — the centroid is the most frequent category (the mode) in each cluster.
  - The closest centroid is found using the Hamming distance.

How many clusters?



Adopted from slides of Dr. Soleymani, Modern Information Retrieval Course, Sharif University of technology.

How Many Clusters?

- The number of clusters K is given in advance in the K-means algorithm.
  - However, finding the right number of clusters is itself part of the problem.
- There is a trade-off between having better focus within each cluster and having too many clusters.
- Hold-out validation / cross-validation on an auxiliary task (e.g., a supervised learning task).
- Optimization problem: penalize having many clusters.
  - Some criteria can be used to automatically estimate K.
  - Penalize the number of bits needed to describe the extra parameter.

$$J'(C) = J(C) + |C| \times \log N$$

- First, we need to know how we can evaluate a clustering.

Clustering Evaluation

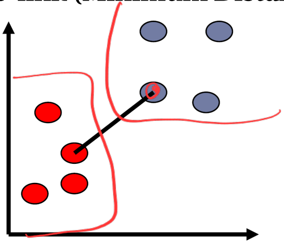
- Evaluating clusters involves two key aspects:
  - **Intra-cluster cohesion (compactness)**: how similar the data points are within a cluster.
    - Often measured by the within-cluster sum of squares (WCSS):

$$WCSS = \sum_{i=1}^{K} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$

  - **Inter-cluster separation (isolation)**: how different the data points are between clusters.

Inter-cluster Separation

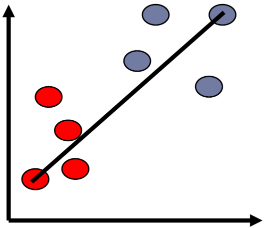
Single-link (Minimum Distance)



Measures the minimum distance between any two points from different clusters.

$$d_{\text{single}}(C_i, C_j) = \min_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$

Complete-link (Maximum Distance)

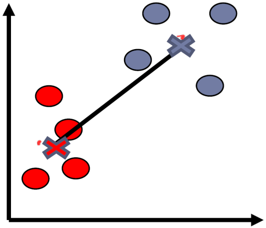


Measures the maximum distance between any two points from different clusters.

$$d_{\text{complete}}(C_i, C_j) = \max_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$

Inter-cluster Separation

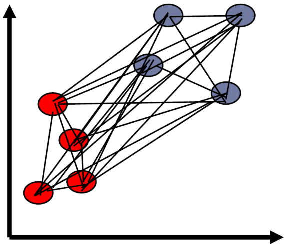
Centroid (Wards Method)



Measures the distance between the centroids of two clusters.

$$d_{\text{centroid}}(C_i, C_j) = d(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)$$

Average-link

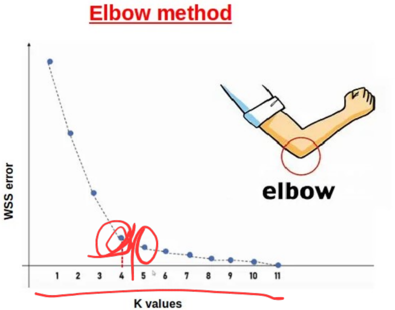


Measures the average distance between all pairs of points from different clusters.

$$d_{\text{average}}(C_i, C_j) = \frac{1}{|C_i| \cdot |C_j|} \sum_{\mathbf{x} \in C_i} \sum_{\mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$

Elbow Method for Optimal K

- Finds the optimal number of clusters K by minimizing the within-cluster sum of squares (WCSS).
- Elbow point:
  - Plot WCSS versus K.
  - The point where the rate of decrease sharply slows down (resembling an elbow) is considered the optimal K.



Silhouette Method for Cluster Evaluation

- Silhouette score for a single point i:

$$S(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

- where:
  - $a(i)$ is the average distance between i and all other points in the same cluster.
  - $b(i)$ is the average distance between i and points in the nearest neighboring cluster.
- Interpretation:
  - $S(i) \in [-1, 1]$
  - $S(i) \approx 1$: well-clustered.
  - $S(i) \approx 0$: on or near the decision boundary between clusters.
  - $S(i) \approx -1$: misclustered.

How Many Clusters?

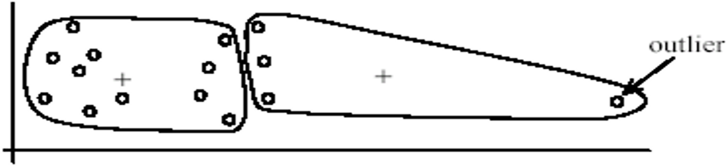
- There is a trade-off between having better focus within each cluster or having too many clusters.
- Don't want one-element clusters.
- **Optimization problem:** penalize having too many clusters

$$K^* = \arg\min_k \left(J(k) + \lambda k \right)$$

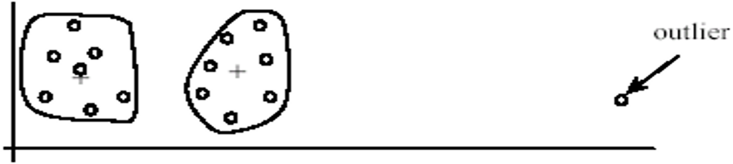
Outliers

- The algorithm is sensitive to outliers.
- Outliers are data points that are very far away from other data points.
- Outliers could be errors in data recording or unique data points with significantly different values.

Weaknesses of K-means: Problems with Outliers



Undesirable clusters

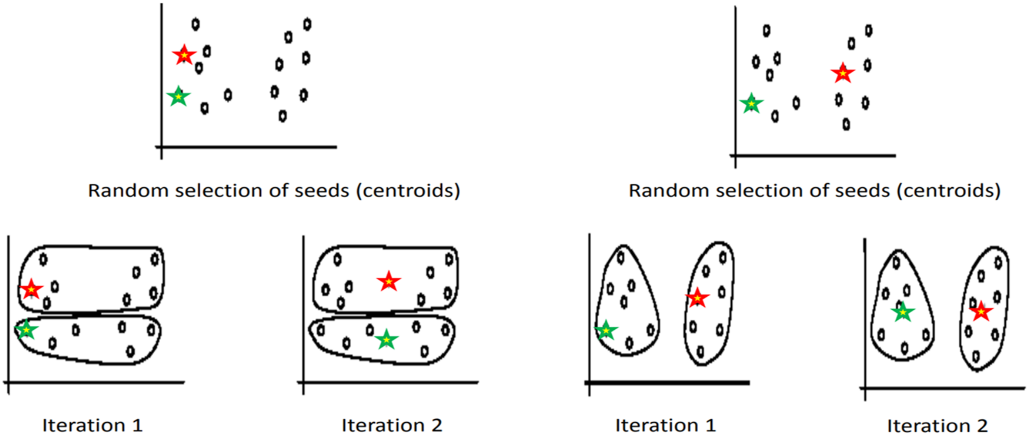


Ideal clusters

Dealing with Outliers

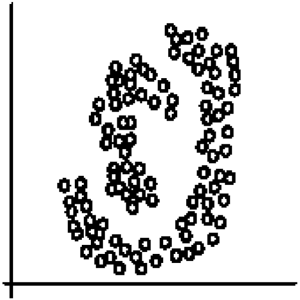
- Remove data points that are much farther away from the centroids than other data points.
  - To be safe, we may want to monitor these possible outliers over a few iterations and then decide whether to remove them.
- Perform random sampling: by choosing a small subset of the data points, the chance of selecting an outlier is much smaller.
  - Assign the rest of the data points to the clusters by distance or similarity comparison, or by classification.

Sensitivity to Initial Seeds

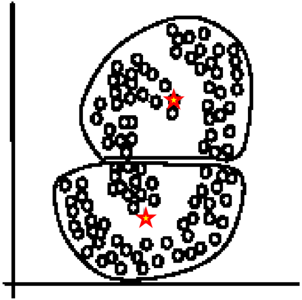


Special Data Structures

- The K-means algorithm is not suitable for discovering clusters that are not hyper-ellipsoids (or hyper-spheres).



Two natural clusters



K-means clusters

Data Distribution

- There is a problem with how K-means defines clusters.
- K-means assumes clusters are spherical and separated with equal variance, which limits its effectiveness on non-spherical or complex-shaped clusters.

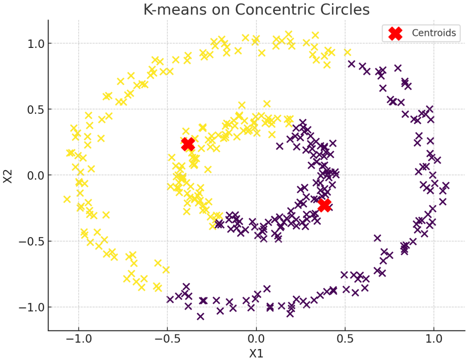
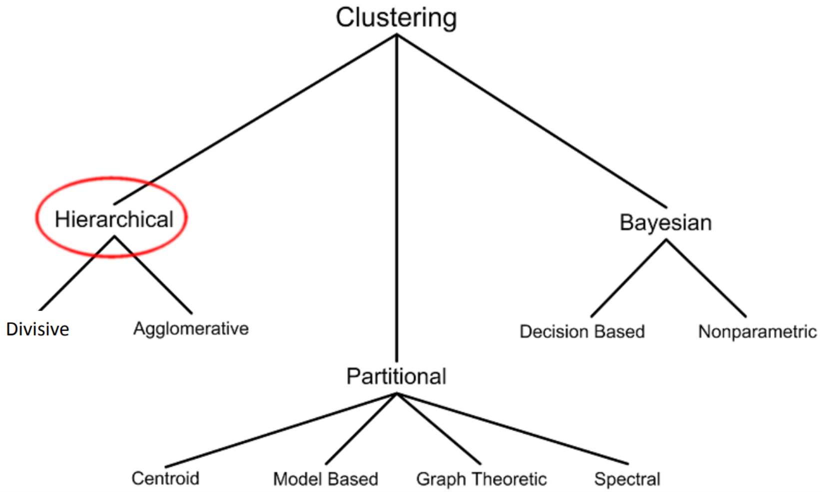


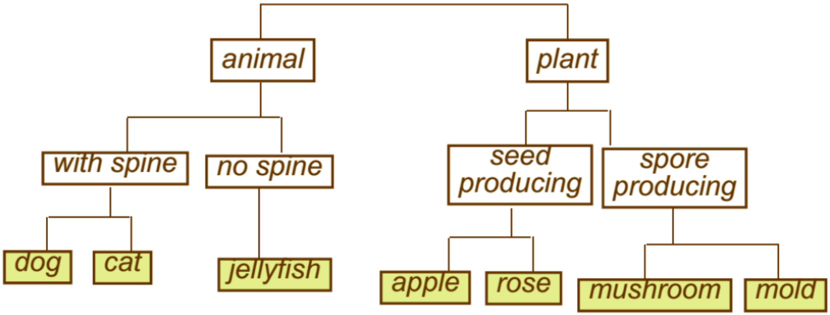
Figure 1: Example when K-means won't work

Hierarchical Algorithm

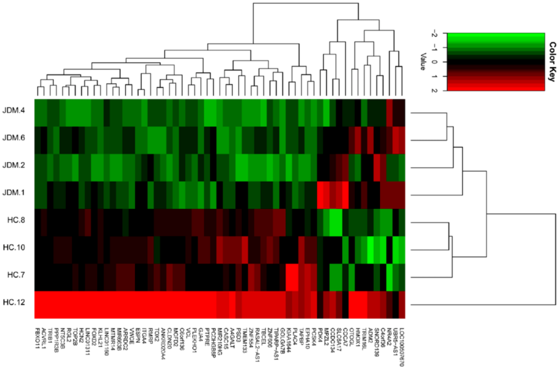


Hierarchical Clustering

- **Hierarchical** algorithms find successive clusters using previously established clusters. Two types:
  - **Agglomerative (bottom-up)**: start with individual points and merge clusters.
  - **Divisive (top-down)**: start with all points and split clusters.
- **Result:** a hierarchy of clusters represented by a dendrogram.



Dendrogram



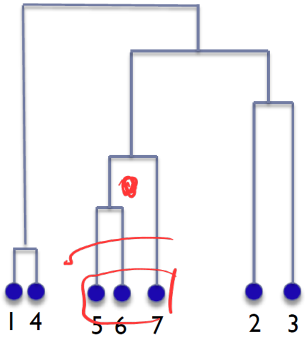
Types of Hierarchical Clustering

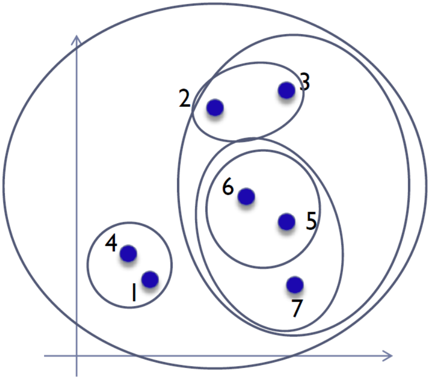
- **Agglomerative (bottom-up) clustering:** It builds the dendrogram (tree) from the bottom level.
  - Merges the most similar (or nearest) pair of clusters.
  - Stops when all data points are merged into a single cluster (i.e., the root cluster).
- **Divisive (top-down) clustering:** It starts with all data points in one cluster, the root.
  - Splits the root into a set of child clusters; each child cluster is recursively divided further.
  - Stops when only singleton clusters of individual data points remain (i.e., each cluster has only a single point).

Hierarchical Agglomerative Clustering (HAC)

- Start with each point as its own cluster.
- Merge the closest clusters.
- Repeat until one cluster remains or the desired number is reached.
- The closest clusters can be determined using inter-cluster separation measures.
- Basic algorithm:
    - Start with all instances in their own cluster.
    - Until there is only one cluster:
        - Among the current clusters, determine the two clusters, c_i and c_j, that are closest.
        - Replace c_i and c_j with a single cluster $c_i \cup c_j$.

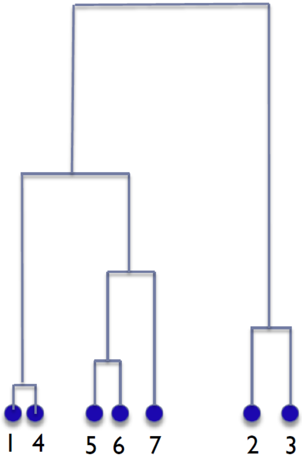
Single-Link

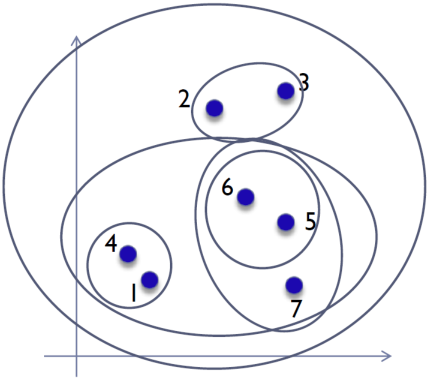




Keep the maximum bridge length as small as possible.

Complete Link

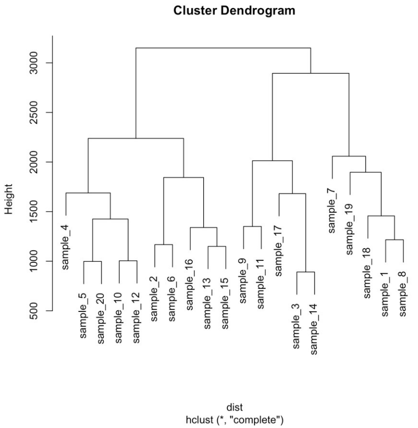




Keep the maximum diameter as small as possible.

Dendrogram and Cutting

- A dendrogram shows the hierarchy of merges.
- Cut the dendrogram at a desired level to form clusters.



Hierarchical Algorithms

- Advantages:
  - No need to specify the number of clusters.
  - Produces a dendrogram for visualization.
  - Works with arbitrary-shaped clusters.
- Disadvantages:
  - High computational cost.
  - Sensitive to noise and outliers.
  - Greedy: cannot undo merges.

Hard vs Soft Clustering

- **Hard Clustering (Partitional)**: Each data point belongs to exactly one cluster
    - More common and easier to use.
- **Soft Clustering (Bayesian)**:

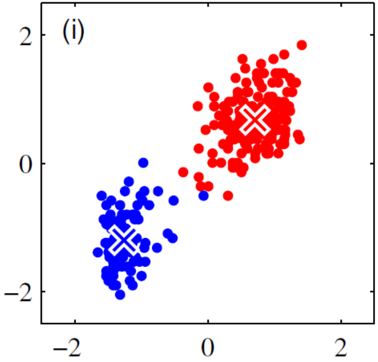


Figure adapted from Machine Learning and Pattern Recognition, Bishop

Hard vs Soft Clustering

- **Hard Clustering (Partitional)**
- **Soft Clustering (Bayesian)**: Each sample is assigned to different clusters with probabilities, rather than $\{0, 1\}$.
  - A data point belongs to each cluster with a probability.

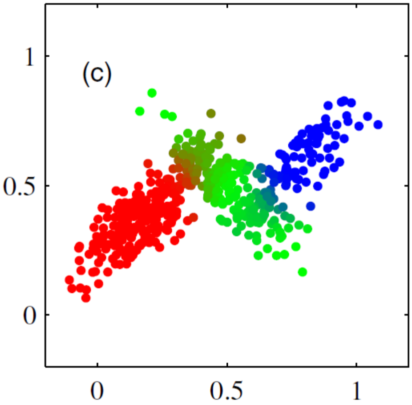


Figure adapted from Machine Learning and Pattern Recognition, Bishop

DBSCAN

DBSCAN (Density-Based Spatial Clustering of Applications with Noise):

- Groups points in high-density regions.
- Labels points in low-density regions as noise.
- Does not require specifying the number of clusters K.

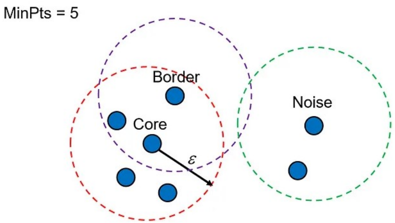
Parameters:

- ϵ (epsilon): Maximum distance for neighbors.
- `minPts`: Minimum number of points to form a dense region.

Core Concepts in DBSCAN

DBSCAN defines three types of points:

- **Core Point**: A point with at least `minPts` neighbors within distance ϵ.
- **Border Point**: A point within ϵ of a core point but with fewer than `minPts` neighbors.
- **Noise**: Points that are neither core points nor border points.



Adopted from ai.plainenglish.io

Core Concepts in DBSCAN

Definitions:

- A point x_i is a core point if:

$$|\{x_j : d(x_i, x_j) \leq \epsilon\}| \geq \texttt{minPts}$$

- A point is a border point if it is within distance ϵ of a core point but is not itself a core point.

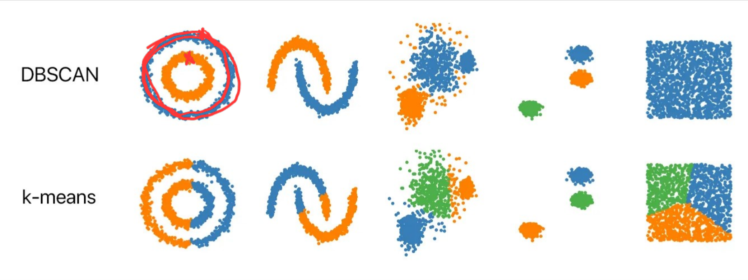
DBSCAN Algorithm Steps

Algorithm Steps:

- For each unvisited point x_i:
  - Mark x_i as visited.
  - Find all points within distance ϵ (neighborhood).
- If x_i is a core point:
  - Create a new cluster and expand it by recursively adding all reachable core and border points.
- If x_i is not a core point:
  - Label it as noise if it does not belong to any cluster.

Advantages of DBSCAN

- Can find clusters of arbitrary shape (non-spherical).
- Does not require specifying the number of clusters K in advance.
- Robust to noise and outliers.
- Works well with large datasets.



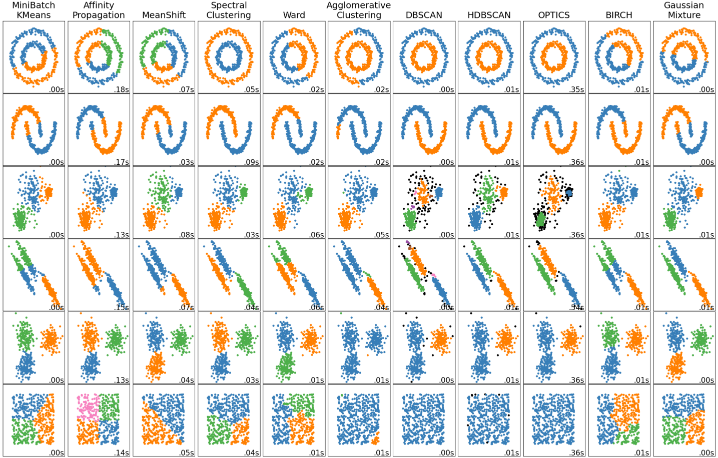
Adopted from mrinalyadav7.medium.com

Limitations of DBSCAN

- DBSCAN struggles with datasets of varying densities.
- Sensitive to the selection of parameters ϵ and `minPts`.
- Does not perform well with high-dimensional data.

Clustering Algorithms

- Each algorithm is suited for different kinds of patterns and information in data.



Contributions

- **This slide has been prepared thanks to:**
  - Hooman Zolfaghari
  - Mahdi Aghaei

[1] M. Soleymani Baghshah, “Machine learning.” Lecture slides.

[2] B. Póczos, “Advanced introduction to machine learning.” Lecture slides. CMU-10715.

[3] M. Gormley, “Introduction to machine learning.” Lecture slides. 10-701.

[4] M. Gormley, “Introduction to machine learning.” Lecture slides. 10-301/10-601.

[5] F. Seyyedsalehi, “Machine learning and theory of machine learning.” Lecture slides. CE-477/CS-828.

[6] G. Strang, “Linear algebra and its applications,” 2000.