Big Data Computing

Master's Degree in Computer Science

2025-2026

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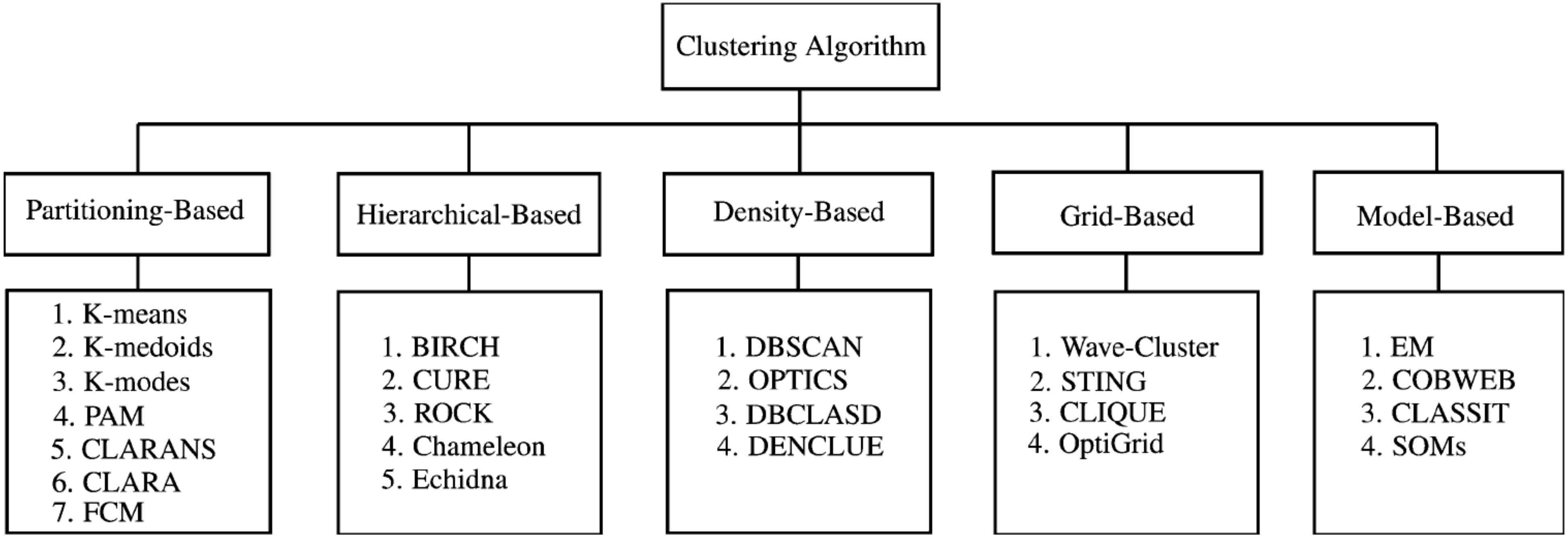
Recap from Last Lecture(s)

- Clustering is an unsupervised learning technique to group "similar" data objects together
- Depends on:
  - **object representation**
  - **similarity measure**
- Harder when data dimensionality gets large (**curse of dimensionality**)
- Number of output clusters is part of the problem itself!

Clustering Algorithms

Clustering Algorithms: Taxonomy



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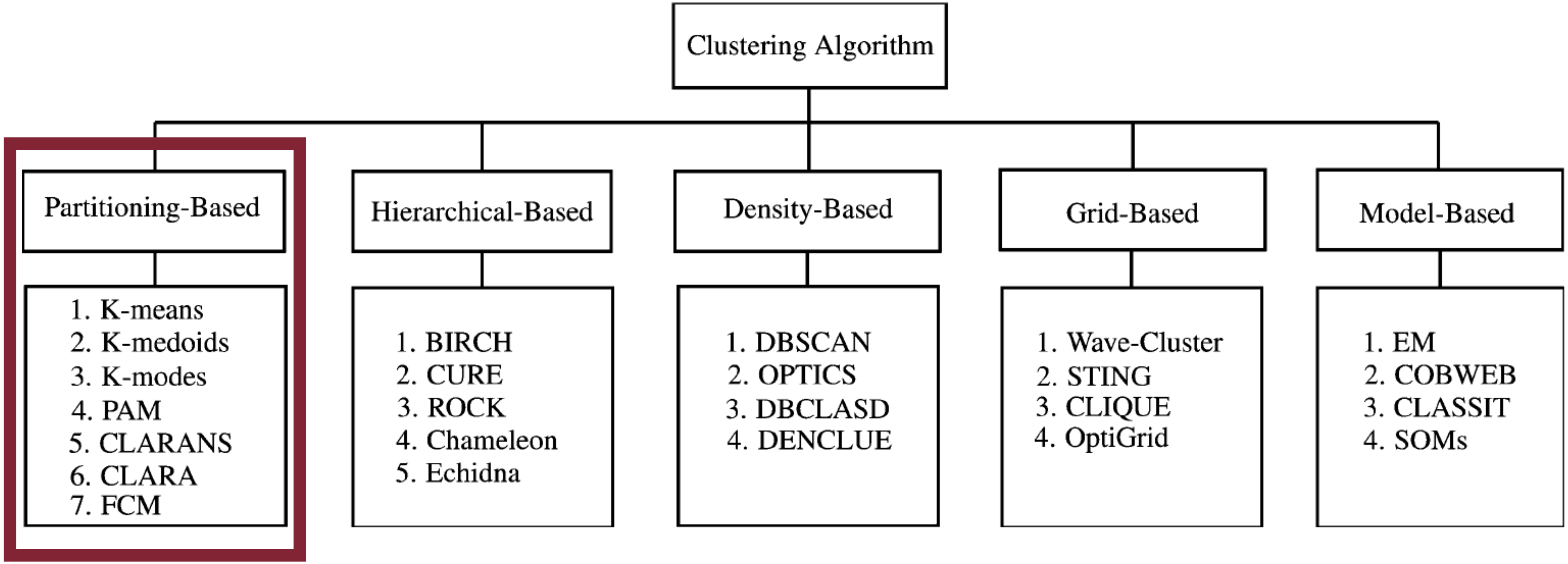

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Partitioning: Hard Clustering

- **Input:** A set of N data points and a number K (K < N)

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- **Output:** A partition of the N data points into K clusters
- **Goal:** Find the partition which optimizes a certain criterion

Partitioning: Intuition

Let K=2 for simplicity

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Here is a possible assignment (i.e., clustering output):

	0	1	2			…				N-1
C	0	1	1	…	0	0	1	…	0	1

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Roughly, 2^N; More generally, K^N

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{0..K-1}	{0..K-1}	{0..K-1}	...	{0..K-1}	{0..K-1}	{0..K-1}	...	{0..K-1}	{0..K-1}

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In the previous example (K=2), the following is **not** allowed

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- Effective heuristics → K-means, K-medoids, K-means++, etc.

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Flat Hard Clustering: General Framework

$$\{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \text{ the set of } N \text{ input data points}$$
$$\{C_1, \ldots, C_K\} \text{ the set of } K \text{ output clusters}$$
$$C_k \text{ the generic } k\text{-th cluster}$$
$$\boldsymbol{\theta}_k \text{ is the } \textit{representative} \text{ of cluster } C_k$$

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C_k the generic k-th cluster

$\boldsymbol{\theta}_k$ is the *representative* of cluster C_k

Note:

At this stage we haven't yet specified what a cluster representative actually is

Objective Function

$$L(A, \boldsymbol{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \delta(\mathbf{x}_n, \boldsymbol{\theta}_k)$$

where:

- A is an $N \times K$ matrix s.t. $\alpha_{n,k} = 1$ iff $\mathbf{x}_n$ is assigned to cluster C_k, 0 otherwise
- $\boldsymbol{\Theta} = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_K\}$ are the cluster representatives
- $\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)$ is a function measuring the distance between $\mathbf{x}_n$ and $\boldsymbol{\theta}_k$

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$$\boxed{A^*, \boldsymbol{\Theta}^* = \text{argmin}_{A,\boldsymbol{\Theta}} \underbrace{\sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \delta(\mathbf{x}_n, \boldsymbol{\theta}_k)}_{L(A,\boldsymbol{\Theta})}}$$

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exact solution must explore exponential search space
S(K, N) ~ O(K^N)

⇒ NP-hard

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exact solution must explore exponential search space $S(K, N) \sim O(K^N)$ ⇨ NP-hard

non-convex due to the discrete assignment matrix A ⇨ multiple local minima

Iterative Solution: Lloyd-Forgy Algorithm

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- NP-hardness doesn't allow us to compute the exact solution (i.e., global optimum)
- Non-convexity doesn't allow us to rely on nice property of convex optimization (unique global optimum)
- A convex objective can be (approximately) solved with numerical methods to find the global optimum

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- **Lloyd-Forgy Algorithm:** 2-step **iterative** approximated solution

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- Assignment step
- Update step

Iterative Solution: Lloyd-Forgy Algorithm

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Does not guarantee to find the global optimum as it may stuck to a local optimum or a saddle point

2-Step Optimization: Assignment Step

$\boxed{\text{Minimize L w.r.t. A by fixing } \boldsymbol{\Theta}}$

$L(A|\boldsymbol{\Theta}) = L(A;\boldsymbol{\Theta}) = L$ is a function of A parametrized by $\boldsymbol{\Theta}$

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Note:
Can't take the gradient of L w.r.t. A since A is discrete!

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Intuitively, given a set of fixed representatives, L is minimized if each data point is assigned to the closest cluster representative according to δ

(L is the sum of all the distances from each data point to its representative)

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$$\alpha_{n,k} = \begin{cases} 1 & \text{if } \delta(\mathbf{x}_n, \boldsymbol{\theta}_k) = \min_{1 \leq j \leq K}\{\delta(\mathbf{x}_n, \boldsymbol{\theta}_j)\} \\ 0 & \text{otherwise} \end{cases}$$

2-Step Optimization: Update Step

$\boxed{\text{Minimize L w.r.t. } \boldsymbol{\Theta} \text{ by fixing A}}$

$L(\boldsymbol{\Theta}|A) = L(\boldsymbol{\Theta}; A) = L$ is a function of $\boldsymbol{\Theta}$ parametrized by A

2-Step Optimization: Update Step

Minimize L w.r.t. $\mathbf{\Theta}$ by fixing A

$$L(\mathbf{\Theta}|A) = L(\mathbf{\Theta}; A) = L \text{ is a function of } \mathbf{\Theta} \text{ parametrized by } A$$

We can minimize L by taking the gradient of L w.r.t $\mathbf{\Theta}$ (i.e., the vector of partial derivatives), set it to 0 and solve it for $\mathbf{\Theta}$

2-Step Optimization: Update Step

$$\nabla L(\mathbf{\Theta}; A) = \left(\frac{\partial L(\mathbf{\Theta}; A)}{\partial \boldsymbol{\theta}_1}, \ldots, \frac{\partial L(\mathbf{\Theta}; A)}{\partial \boldsymbol{\theta}_K} \right)$$

2-Step Optimization: Update Step

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$$\boxed{\frac{\partial L(\boldsymbol{\theta}_1 \ldots \boldsymbol{\theta}_K; A)}{\partial \boldsymbol{\theta}_j}}$$

The general j-th partial derivative

2-Step Optimization: Update Step

$$\nabla L(\mathbf{\Theta}; A) = \mathbf{0} \Leftrightarrow \frac{\partial L(\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_K; A)}{\partial \boldsymbol{\theta}_j} = 0 \; \forall j \in \{1, \ldots, K\}$$

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$$\frac{\partial L}{\partial \boldsymbol{\theta}_j}$$

To make the notation easier!

2-Step Optimization: Update Step

$$\frac{\partial L}{\partial \boldsymbol{\theta}_j} = \frac{\partial}{\partial \boldsymbol{\theta}_j}\left[\sum_{n=1}^{N}\sum_{k=1}^{K}\alpha_{n,k}\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)\right] = 0$$

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When computing the partial derivative w.r.t. $\boldsymbol{\theta}_j$ any other term $\boldsymbol{\theta}_k$ of the inner summation is treated as constant!

2-Step Optimization: Update Step

$$\frac{\partial L}{\partial \boldsymbol{\theta}_j} = \frac{\partial}{\partial \boldsymbol{\theta}_j}\left[\sum_{n=1}^{N}\sum_{k=1}^{K}\alpha_{n,k}\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)\right] = 0$$

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$$= \frac{\partial}{\partial \boldsymbol{\theta}_j}\left[\sum_{n=1}^{N}\alpha_{n,j}\delta(\mathbf{x}_n, \boldsymbol{\theta}_j)\right] = 0$$

Solve for each $\boldsymbol{\theta}_j$ independently

Depends on the distance function δ

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- Each cluster representative is its center of mass (i.e., **centroid**)

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A Special Case: K-means

- Each cluster representative is its center of mass (i.e., **centroid**)
- The centroid of a cluster is the **mean** of the instances assigned to that cluster
- (Re)Assignment of instances to clusters is based on distance/similarity to the current cluster centroids
- The basic idea is constructing clusters so that the total within-cluster **Sum of Square Distances** (**SSD**) is minimized

K-means: Setup

$\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ the set of N input data points

$\{C_1, \ldots, C_K\}$ the set of K output clusters

C_k the generic k-th cluster

$$\boldsymbol{\theta}_k = \frac{\sum_{n=1}^{N} \alpha_{n,k} \mathbf{x}_n}{\sum_{n=1}^{N} \alpha_{n,k}} = \boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{n \in C_k} \mathbf{x}_n$$

$$\text{where } |C_k| = \sum_{n=1}^{N} \alpha_{n,k}$$

K-means: Objective Function

$$L(A, \boldsymbol{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \underbrace{\left(||\mathbf{x}_n - \boldsymbol{\theta}_k||_2 \right)^2}_{\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)}$$ Euclidean space

K-means: Objective Function

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$$\delta(\mathbf{x}_n, \boldsymbol{\theta}_k) = (||\mathbf{x}_n - \boldsymbol{\theta}_k||_2)^2 =$$

$$= \left[\sqrt{(\mathbf{x}_n - \boldsymbol{\theta}_k)^2}\right]^2 = (\mathbf{x}_n - \boldsymbol{\theta}_k)^2$$

Sum of Square Distances (SSD)

K-means: Objective Function

$$L(A, \boldsymbol{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \underbrace{(||\mathbf{x}_n - \boldsymbol{\theta}_k||_2)^2}_{\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)}$$

$$\delta(\mathbf{x}_n, \boldsymbol{\theta}_k) = (||\mathbf{x}_n - \boldsymbol{\theta}_k||_2)^2 =$$

$$= \left[\sqrt{(\mathbf{x}_n - \boldsymbol{\theta}_k)^2}\right]^2 = (\mathbf{x}_n - \boldsymbol{\theta}_k)^2$$

Sum of Square Distances (SSD)

$$\boxed{L(A, \boldsymbol{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} (\mathbf{x}_n - \boldsymbol{\theta}_k)^2}$$

K-means: Assignment Step

$\boxed{\text{Minimize L w.r.t. A by fixing } \mathbf{\Theta}}$

Intuitively, given a set of fixed centroids, L is minimized if each data point is assigned to the centroid with the smallest SSD

(L is just the SSD from each data point to its assigned centroid)

$$\alpha_{n,k} = \begin{cases} 1 & \text{if } (\mathbf{x}_n - \boldsymbol{\theta}_k)^2 = \min_{1 \le j \le K}\{(\mathbf{x}_n - \boldsymbol{\theta}_j)^2\} \\ 0 & \text{otherwise} \end{cases}$$

K-means: Update Step

$\boxed{\text{Minimize L w.r.t. } \boldsymbol{\Theta} \text{ by fixing A}}$

$$\boldsymbol{\Theta}^* = \text{argmin}_{\boldsymbol{\Theta}} \left\{ \underbrace{\sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} (\mathbf{x}_n - \boldsymbol{\theta}_k)^2}_{L(\boldsymbol{\Theta};A)} \right\}$$

$\boxed{\text{Compute the gradient w.r.t. } \boldsymbol{\Theta}\text{, set it to 0 and solve it for } \boldsymbol{\Theta}}$

K-means: Update Step

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \frac{\partial}{\partial \boldsymbol{\theta}_k}\left[\sum_{n=1}^{N} \alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k)^2\right] = 0 \quad \forall k \in \{1, \ldots, K\}$$

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$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k)$$

$$\text{Find } \boldsymbol{\theta}_k^* \text{ s.t. } \sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k^*) = 0$$

K-means: Update Step

$$\sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k^*) = 0 \Leftrightarrow$$

$$2\sum_{n=1}^{N} \alpha_{n,k}\boldsymbol{\theta}_k^* = 2\sum_{n=1}^{N} \alpha_{n,k}\mathbf{x}_n$$

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$\boldsymbol{\theta}^*_k$ does not depend on N, therefore it can be factored out

K-means: Update Step

$$\boldsymbol{\theta}_k^* \sum_{n=1}^{N} \alpha_{n,k} = \sum_{n=1}^{N} \alpha_{n,k} \mathbf{x}_n$$

$$\boldsymbol{\theta}_k^* = \frac{\sum_{n=1}^{N} \alpha_{n,k} \mathbf{x}_n}{\sum_{n=1}^{N} \alpha_{n,k}} = \boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{n \in C_k} \mathbf{x}_n$$

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The cluster centroid (i.e., mean) minimizes the objective (for a fixed assignment A)

K-means: Lloyd-Forgy Algorithm

1. Specify the number of output clusters K

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5. Iteratively repeat steps 3-4 until a **stopping criterion** is met

Stopping Criterion

- Several options to choose from:
  - Fixed number of iterations
  - Cluster assignments stop changing (beyond some threshold)
  - Centroid doesn't change (beyond some threshold)

Lloyd-Forgy's Convergence

- How/Why are we guaranteed the K-means algorithm ever reaches a fixed point?
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- How/Why are we guaranteed the K-means algorithm ever reaches a fixed point?
  - A state in which clusters do not change
- Intuitively, in both steps we either improve the objective or not
- It is an instance of more general **Expectation Maximization** (**EM**)
  - EM is known to converge (although not necessarily to a global optimum)

Lloyd-Forgy's Relationship with EM

- E-step = Assignment step
  - Each object is assigned to the closest centroid, i.e., to the most likely cluster
  - Monotonically decreases SSD

Lloyd-Forgy's Relationship with EM

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  - Monotonically decreases SSD
- M-step = Update step
  - The model (i.e., centroids) are updated (i.e., SSD optimization)
  - Monotonically decreases each SSD_k

Lloyd-Forgy's Complexity Analysis

- Computing the distance between two d-dimensional data points takes O(d)

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- Computing the distance between two *d*-dimensional data points takes O(d)
- (Re-)Assigning clusters [E-step]: O(KN) distance computations or O(KNd)
- Computing centroids [M-step]: O(Nd) as there are O(N) average computations since each data point is added to a cluster exactly once *at each iteration*, each one taking O(d)
- Overall: O(RKNd) if the 2 steps above are repeated R times

K-means: Seed Choice

- Convergence (rate) and clustering quality depends on the selection of **initial centroids**

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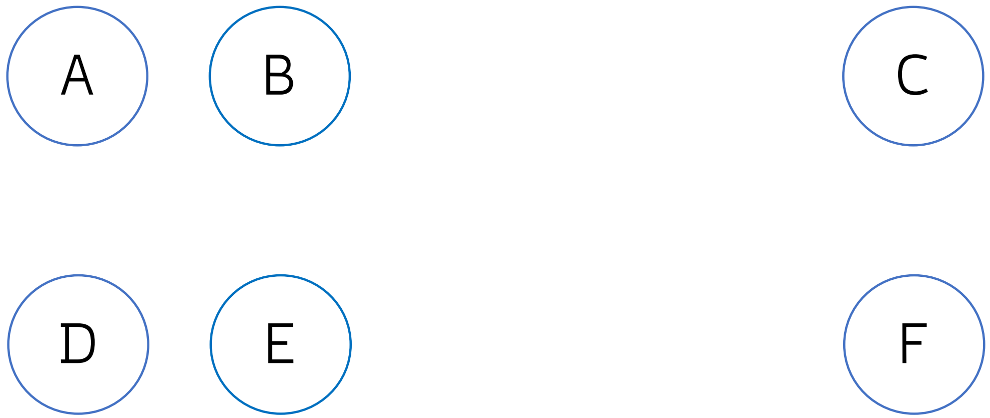
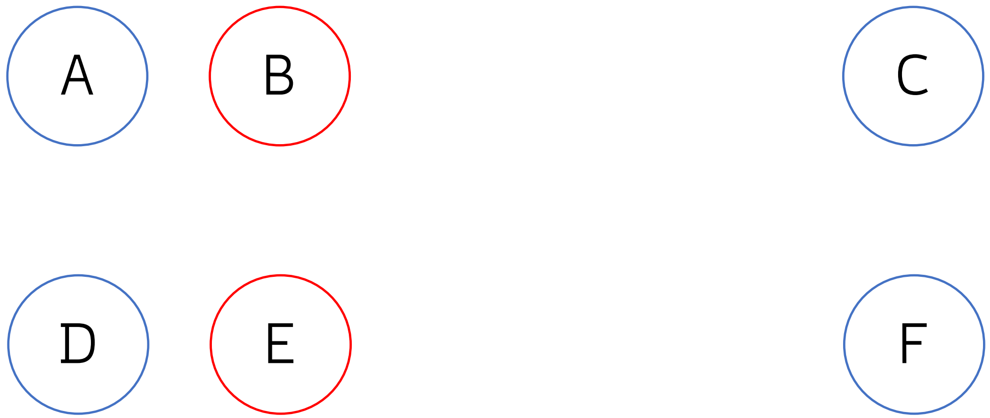
Problem Mitigation:

Execute several runs of the Lloyd-Forgy algorithm with multiple random initialization seeds

K-means: Seed Choice

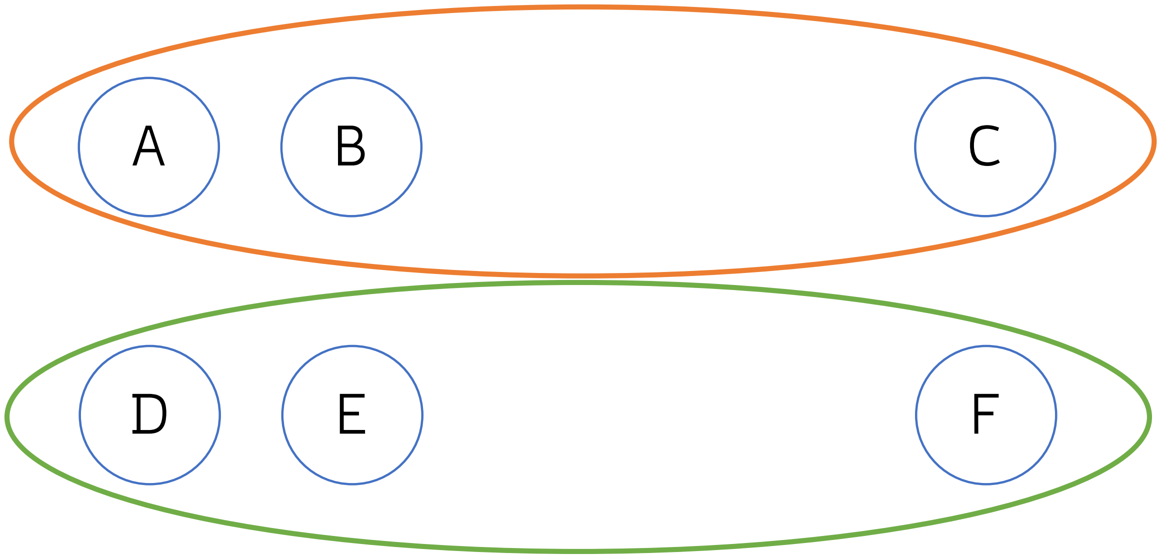


K-means: Bad (Unlucky) Seed Choice



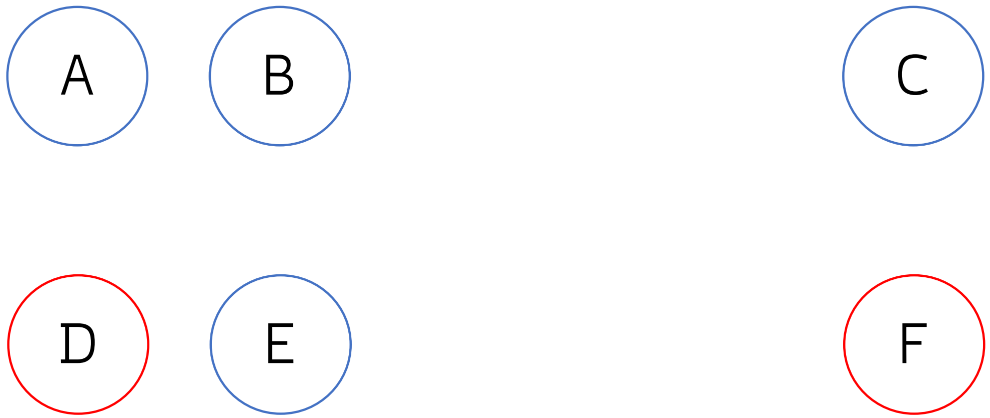
If B and E are randomly chosen as initial centroids…

K-means: Bad (Unlucky) Seed Choice



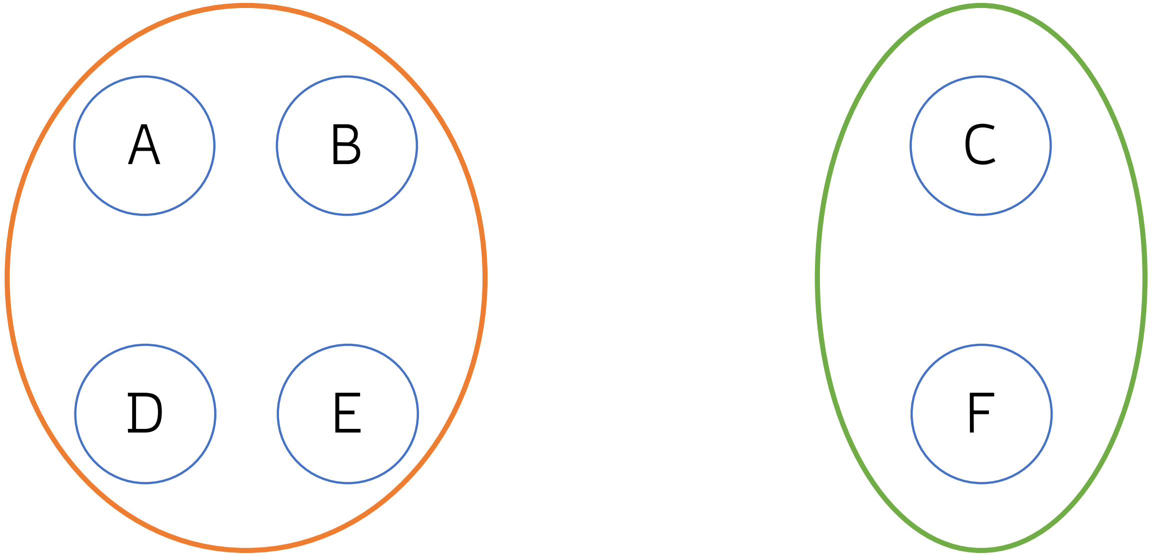
The algorithm converges to the sub-optimal clustering above

K-means: Good (Lucky) Seed Choice



If D and F are randomly chosen as initial centroids instead...

K-means: Good (Lucky) Seed Choice



The algorithm converges to a better clustering

Take-Home Message of Today

- Focus on hard partitioning clustering

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- Formulate hard partitioning clustering as a (**non-convex**) optimization problem
  - Minimizing "some" aggregated internal cluster distance

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Take-Home Message of Today

- Focus on hard partitioning clustering
- Formulate hard partitioning clustering as a (**non-convex**) optimization problem
  - Minimizing "some" aggregated internal cluster distance
- Computing exact solution is **NP-hard** due to exponential search space
- Use an iterative (approximate) solution → e.g., **K-means**