Big Data Computing

Master's Degree in Computer Science

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SAPIENZA
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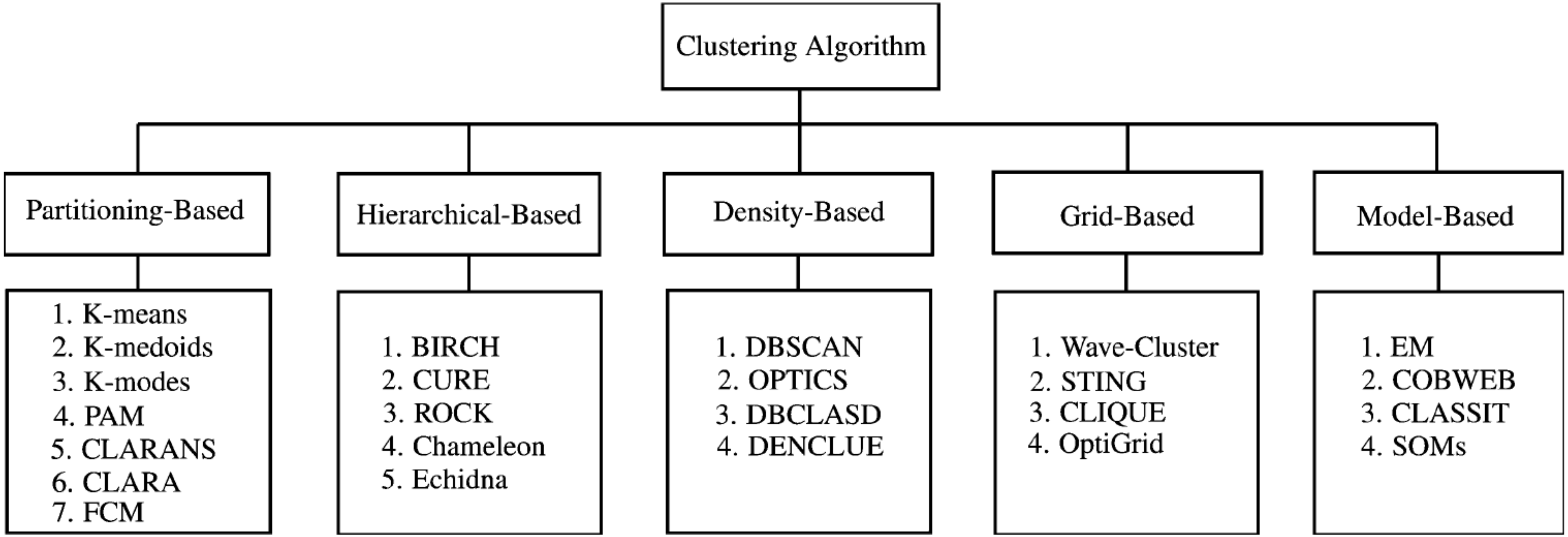
Recap from Last Lecture(s)

- 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



source: https://www.computer.org/csdl/journal/ec/2014/03/06832486/13rRUEgs2xB

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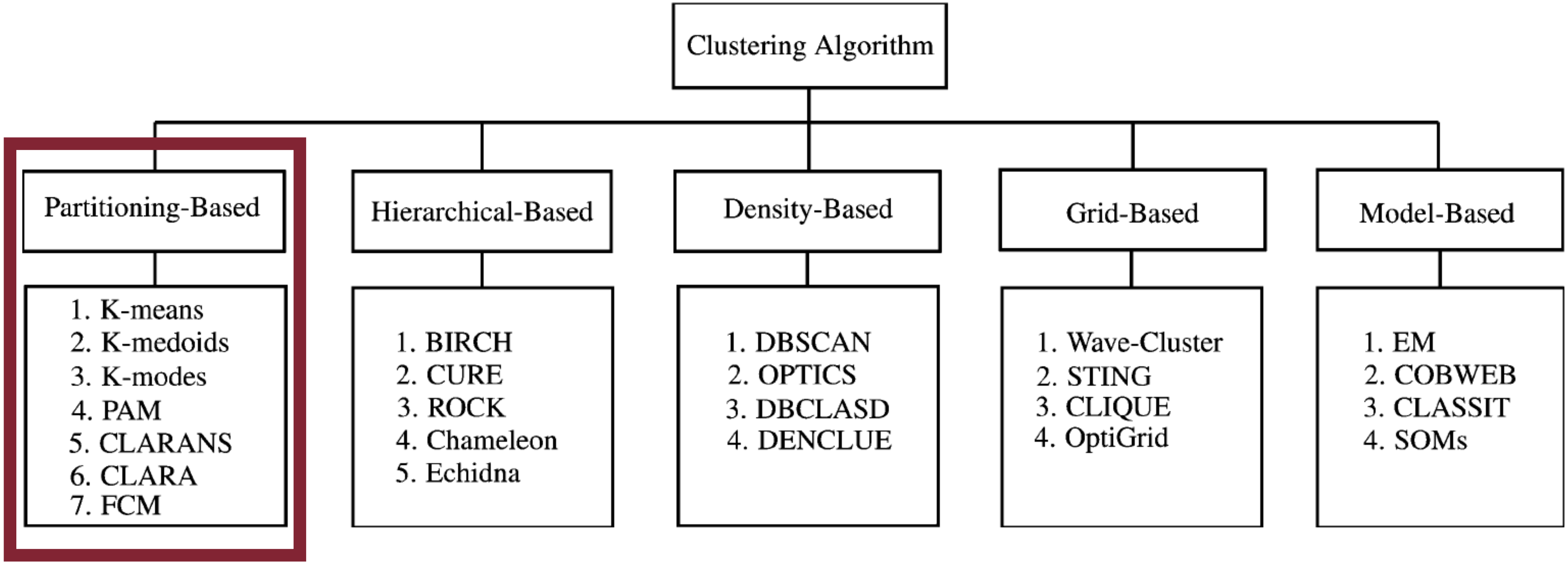

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Partitioning: Hard Clustering

- **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

$\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ 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

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

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

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

$\Rightarrow$ 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

- **NP-hardness** doesn't allow us to compute the exact solution (i.e., global optimum)

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Iterative Solution: Lloyd-Forgy Algorithm

- **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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- 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

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

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

2-Step Optimization: Update Step

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

2-Step Optimization: Update Step

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

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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

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

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

To make the notation easier!

2-Step Optimization: Update Step

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2-Step Optimization: Update Step

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

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!

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

Depends on the distance function δ

Take-Home Message of Today

- Focus on hard partitioning clustering

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  - Minimizing "some" aggregated internal cluster distance

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- 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