Big Data Computing

Master's Degree in Computer Science

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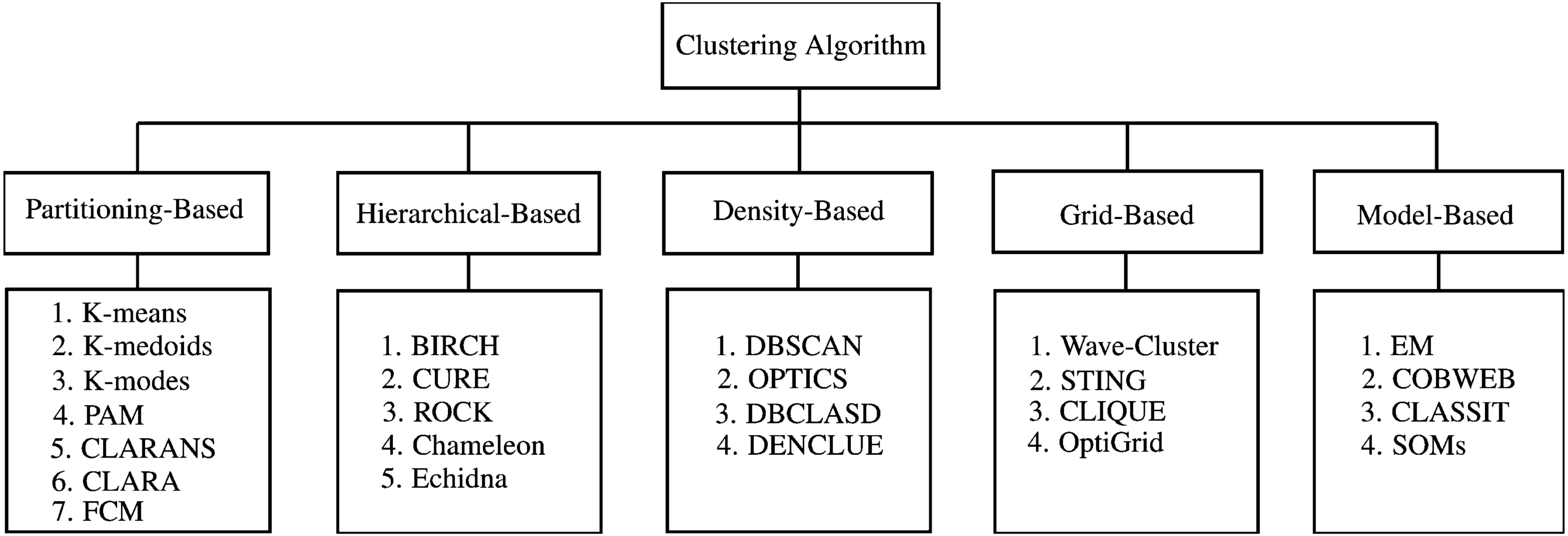
Recap from Last Lecture(s)

- 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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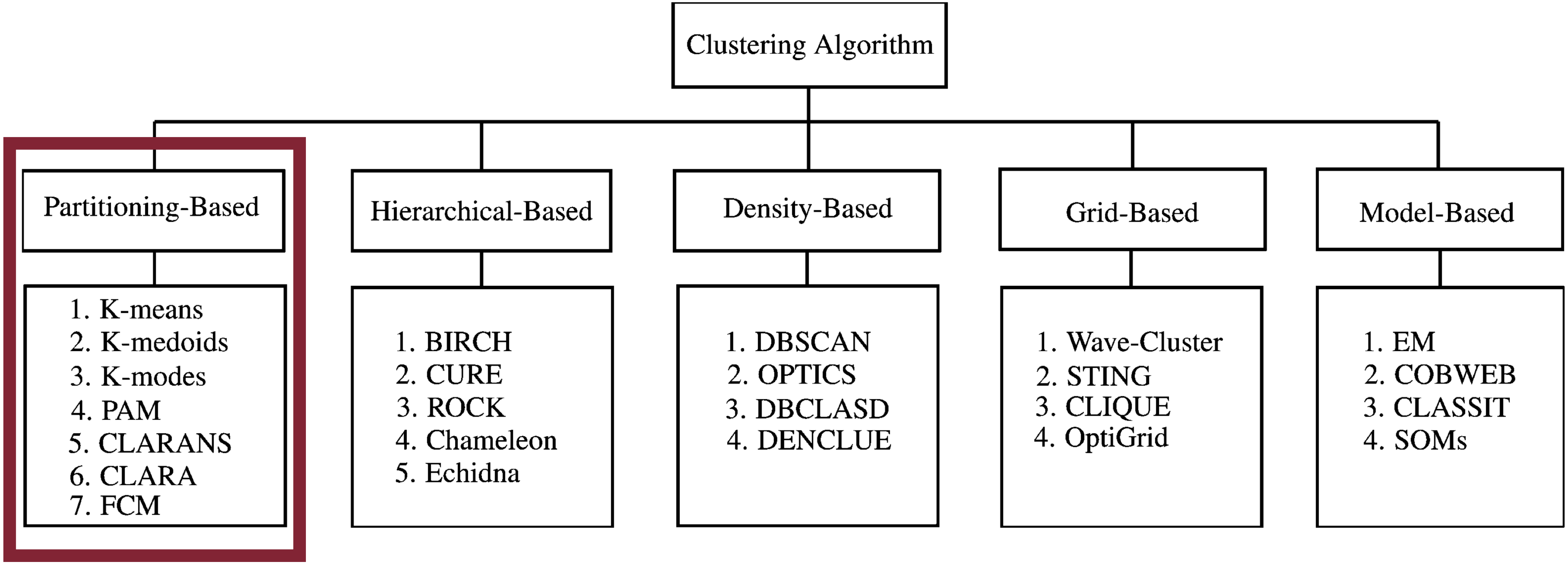

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Partitioning: Hard Clustering

- **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
  - Global optimum → Intractable for many objective function (might require to enumerate all the possible partitions)*
  - $S(K, N) \sim O(K^N)$ → K-way non-empty partitions of N elements **Stirling partition number**
  - Effective heuristics → K-means, K-medoids, K-means++, etc.

*Kleinberg, J., "An Impossibility Theorem for Clustering" (NIPS 2002)

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

Note:

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

Objective Function

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

$$\sum_{k=1}^{K} \alpha_{n,k} = 1$$

hard clustering

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 $\boldsymbol{\theta}_k$

Objective Function

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

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

⇒

NP-hard

Objective Function

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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
- Non-convexity doesn't allow us to rely on nice property of convex optimization with numerical methods (unique global minimum)
- **Lloyd-Forgy Algorithm:** 2-step **iterative** approximated solution
  - **Assignment step**
  - **Update step**

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

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

$$L(\boldsymbol{\Theta}; A) \text{ fixed } \boldsymbol{\Theta} \text{ parametrized by } A$$

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

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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 centroid according to δ

(L is just the summation of all the distances from each data point to its assigned 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

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

$$L(A; \boldsymbol{\Theta}) \text{ fixed } A \text{ parametrized by } \boldsymbol{\Theta}$$

2-Step Optimization: Update Step

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$$L(A; \mathbf{\Theta}) \text{ fixed } A \text{ parametrized by } \mathbf{\Theta}$$

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

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

$$\nabla L(A; \boldsymbol{\Theta}) = 0 \Leftrightarrow \frac{\partial L}{\partial \boldsymbol{\theta}_k} = 0 \ \forall k \in \{1, \ldots, K\}$$

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

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

Depends on the distance function δ

A Special Case: K-means

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- 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

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

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

C_k the generic k-th cluster

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

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

K-means: Objective Function

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

Euclidean space

K-means: Objective Function

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

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

Sum of Square Distances (SSD)

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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

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

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

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

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

K-means: Update Step

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

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

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

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

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

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

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

K-means: Lloyd-Forgy Algorithm

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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

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  - A state in which clusters do not change

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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

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

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

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- (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) assuming the 2 steps above are repeated R times

K-means: Seed Choice

- Convergence (rate) and clustering quality depends on the selection of **initial centroids**
  - Forgy method **randomly** chooses K data points as the initial means
  - Random Partition method **randomly** assigns a cluster to each observation

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Problem Mitigation:

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

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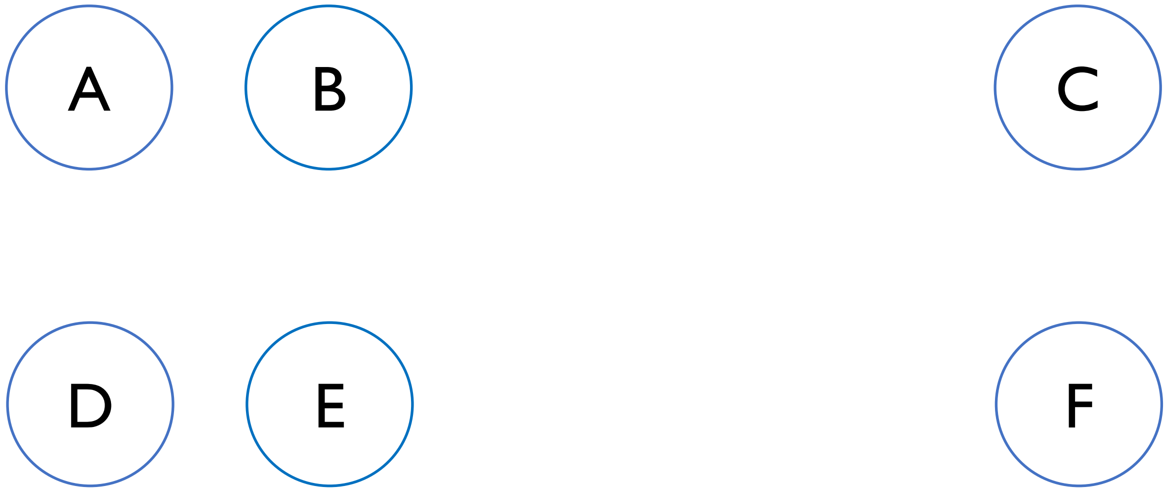

K-means: Bad (Unlucky) Seed Choice

If B and E are randomly chosen as initial centroids…

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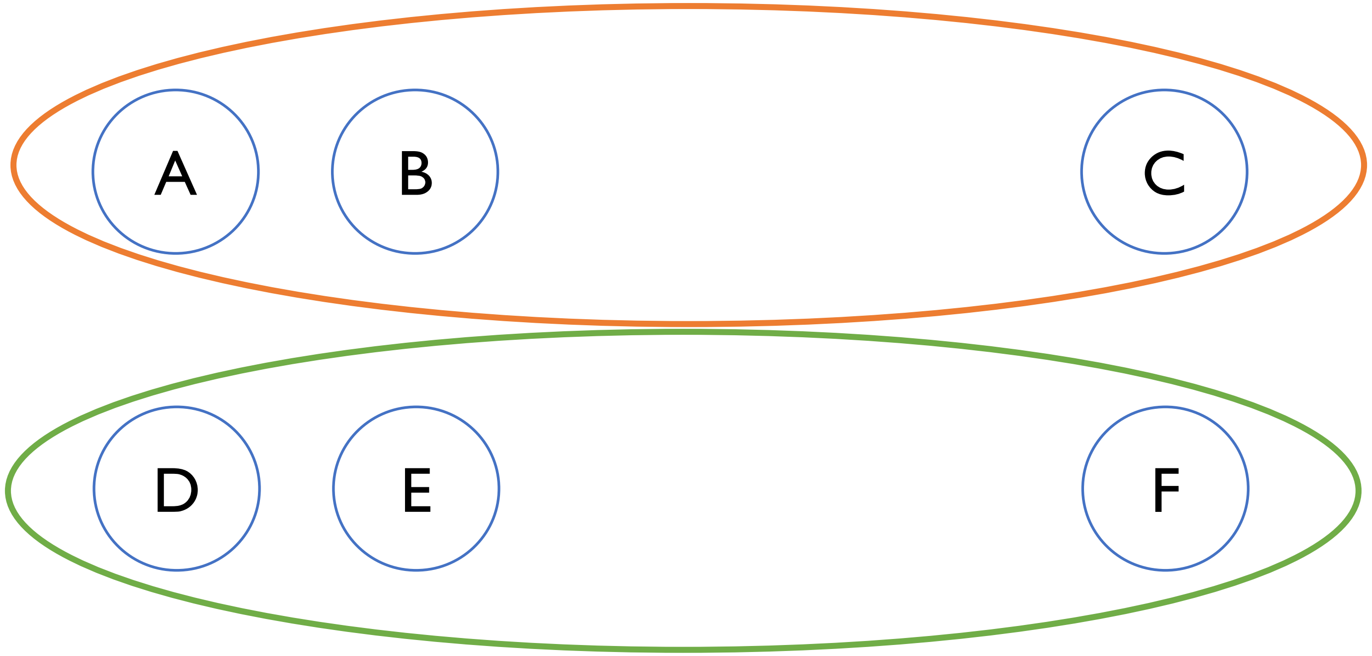
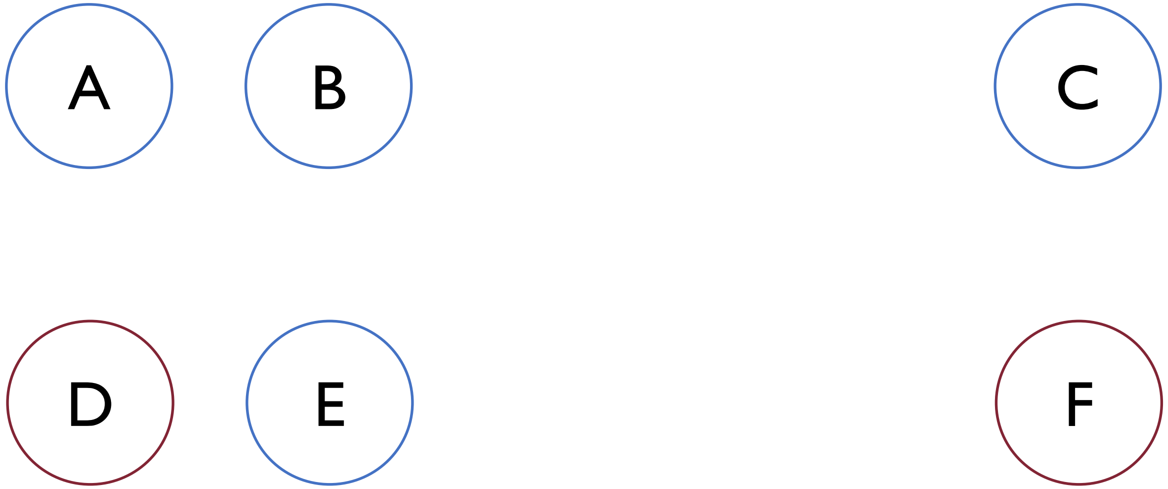


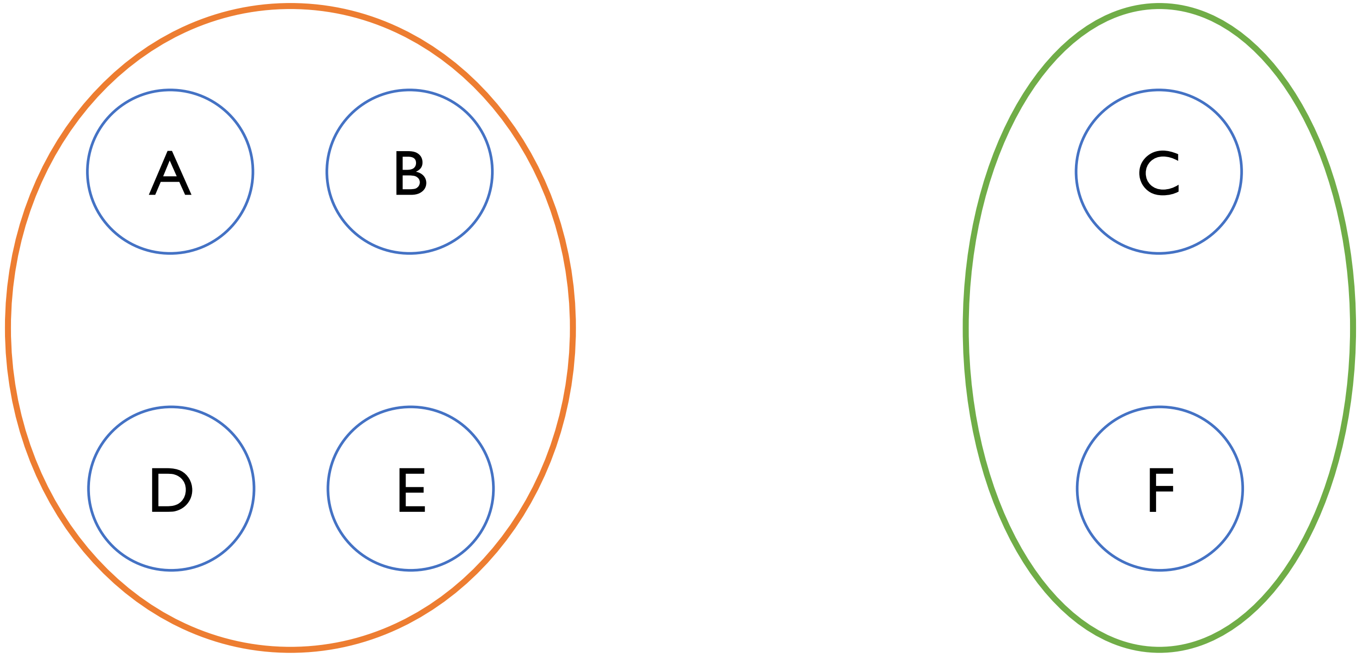
The algorithm converges to the sub-optimal clustering above

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

Alternative Seed Choice: K-means++

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    1. Choose one center uniformly at random from among initial data points

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  1. Choose one center uniformly at random from among initial data points
  2. For each data point **x**, compute D(**x**) as the distance between **x** and the nearest center that has already been chosen

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  1. Choose one center uniformly at random from among initial data points
  2. For each data point $\mathbf{x}$, compute $D(\mathbf{x})$ as the distance between $\mathbf{x}$ and the nearest center that has already been chosen
  3. Choose one new data point at random as a new center with probability proportional to $D(\mathbf{x})^2$
  4. Repeat steps 2. and 3. until K centers are chosen, then run Lloyd-Forgy

"Vanilla" K-means vs. K-means++

- Random initialization used with "vanilla" K-means may produce clusters that are **arbitrarily worse** than optimum

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"Vanilla" K-means vs. K-means++

- Random initialization used with "vanilla" K-means may produce clusters that are **arbitrarily worse** than optimum
- K-means++ provides an upper-bound to the approximation obtained w.r.t. the optimal solution
- At most, clusters obtained with K-means++ initialization are O(log K) worse than the optimal partitioning

K-means: How Many Clusters?

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  - Great! Partition N data points into a predetermined number K of clusters
  - Unfortunately, it is very uncommon to know K in advance

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- Number of clusters K is given
  - Great! Partition N data points into a predetermined number K of clusters
  - Unfortunately, it is very uncommon to know K in advance
- Finding the "right" number K of clusters is part of the problem!
  - Trade-off between having too few and too many clusters
  - Total benefit vs. Total cost

K-means: Total Benefit

- Given a clustering, define the benefit b_i for a data point $\mathbf{x}_i$ to be the similarity to its assigned centroid

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- Define the total benefit B to be the sum of the individual benefits

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- Define the total benefit B to be the sum of the individual benefits

NOTE

There is always a clustering whose total benefit B=N
(where N is the number of data points)

Why?

K-means: Total Cost

- Assign a cost p to each cluster, thereby a clustering with K clusters has a total cost $P = Kp$

K-means: Total Cost

- Assign a cost p to each cluster, thereby a clustering with K clusters has a total cost $P = Kp$
- Define the value V of a clustering to be total benefit-total cost

$$\boxed{V = B - P}$$

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B increases with larger values of K, but P allows to stop that

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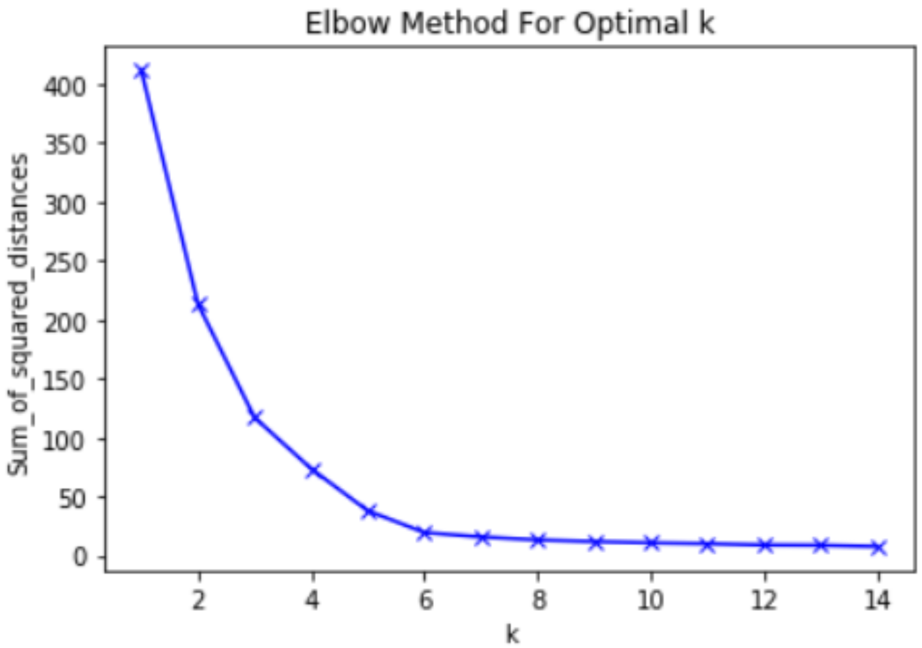

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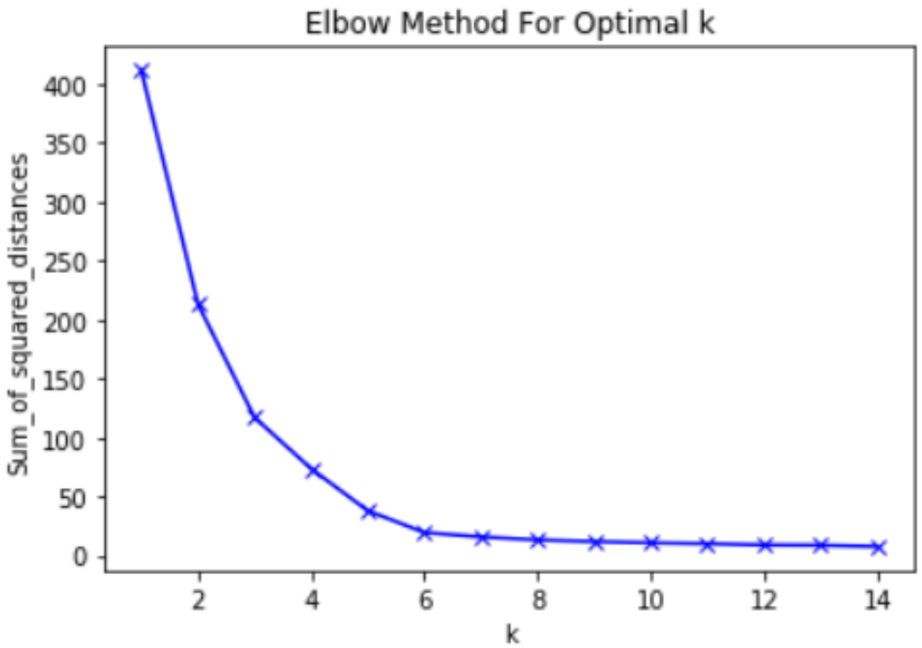

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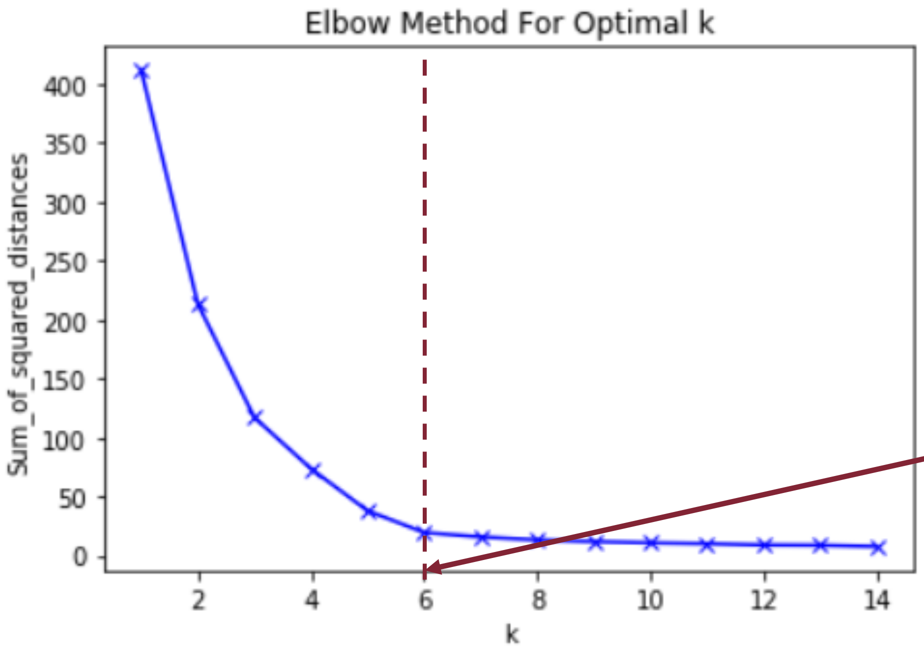

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  - δ = **Cosine distance** = Euclidean distance on normalized input points
  - δ = **Correlation** = Euclidean distance on standardized input points
- Others, require specific minimizers
  - δ = **Manhattan distance** (L^1-Norm) → median is the minimizer (K-medians)

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- Robust to outliers yet computationally expensive $O(K(N-K)^2)$

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Measures of Clustering Quality

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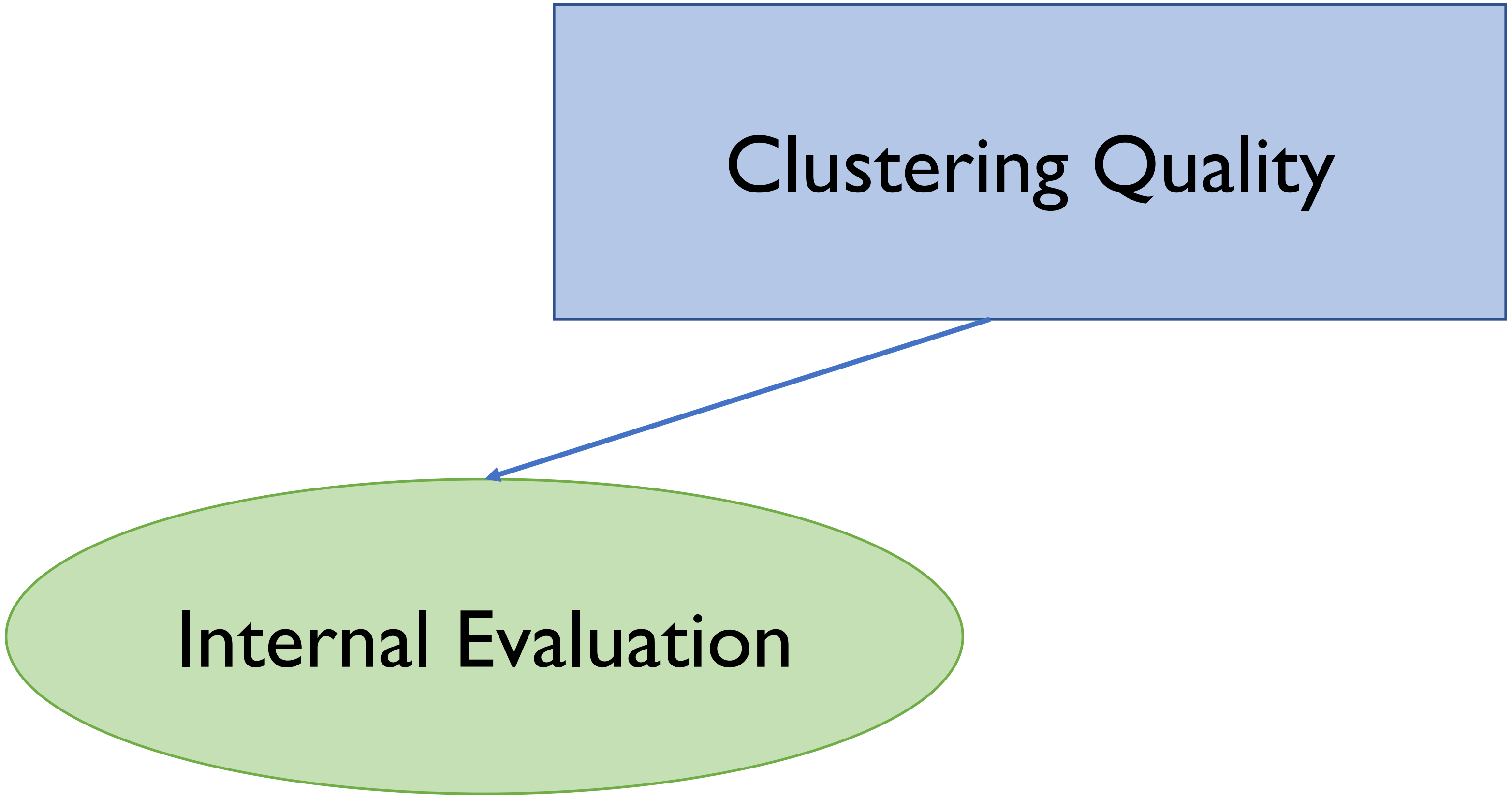

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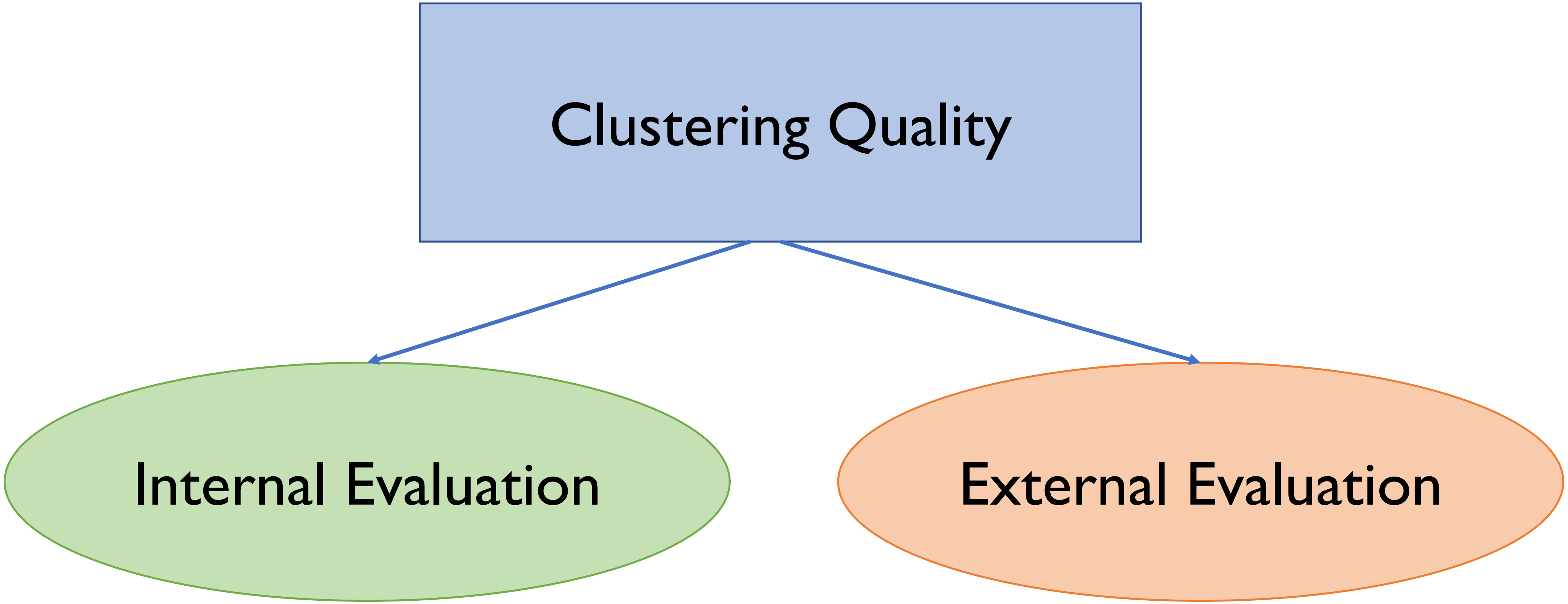

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- The measured quality of a clustering depends on
  - **data representation**
  - **similarity measure**

Internal Evaluation: Davies-Bouldin Index

$$DB = \frac{1}{K}\sum_{i=1}^{K} \max_{j \neq i}\left(\frac{\sigma_i + \sigma_j}{\delta(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)}\right)$$

$$K = \text{number of clusters}$$
$$\boldsymbol{\mu}_k = \text{centroid of cluster } C_k$$
$$\sigma_k = \text{avg. distance of all elements of cluster } C_k \text{ from its centroid } \boldsymbol{\mu}_k$$
$$\delta(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j) = \text{distance between centroids of } C_i \text{ and } C_j$$

The smaller the better

Internal Evaluation: Dunn Index

$$D = \frac{\min_{1 \leq i < j \leq K} \delta(C_i, C_j)}{\max_{1 \leq k \leq K} \delta'(C_k)}$$

$$K = \text{number of clusters}$$
$$\delta(C_i, C_j) = \text{distance between cluster } C_i \text{ and } C_j$$
$$\delta'(C_k) = \text{intra-cluster distance of cluster } C_k$$

Distance between centroids

Max distance between any pair of objects

The higher the better

Internal Evaluation: Silhouette Coefficient

mean distance between *i* and all other data points in the same cluster C_i

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i, j \neq i} \delta(i, j)$$

smallest mean distance of *i* to all points in any other cluster $C_k \neq C_i$

$$b(i) = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} \delta(i, j)$$

$$s(i) = \begin{cases} 1 - a(i)/b(i) & \text{if } a(i) < b(i) \\ 0 & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1 & \text{if } a(i) > b(i) \end{cases}$$

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- Hard as it requires labeled data typically provided by human experts

External Evaluation: Purity

$$C_1 \ldots, C_K = \text{set of } K \text{ clusters}$$

$$L_1 \ldots, L_J = \text{set of } J \text{ labels}$$

$$n_{i,j} = \text{number of items with label } L_j \text{ clustered in } C_i$$

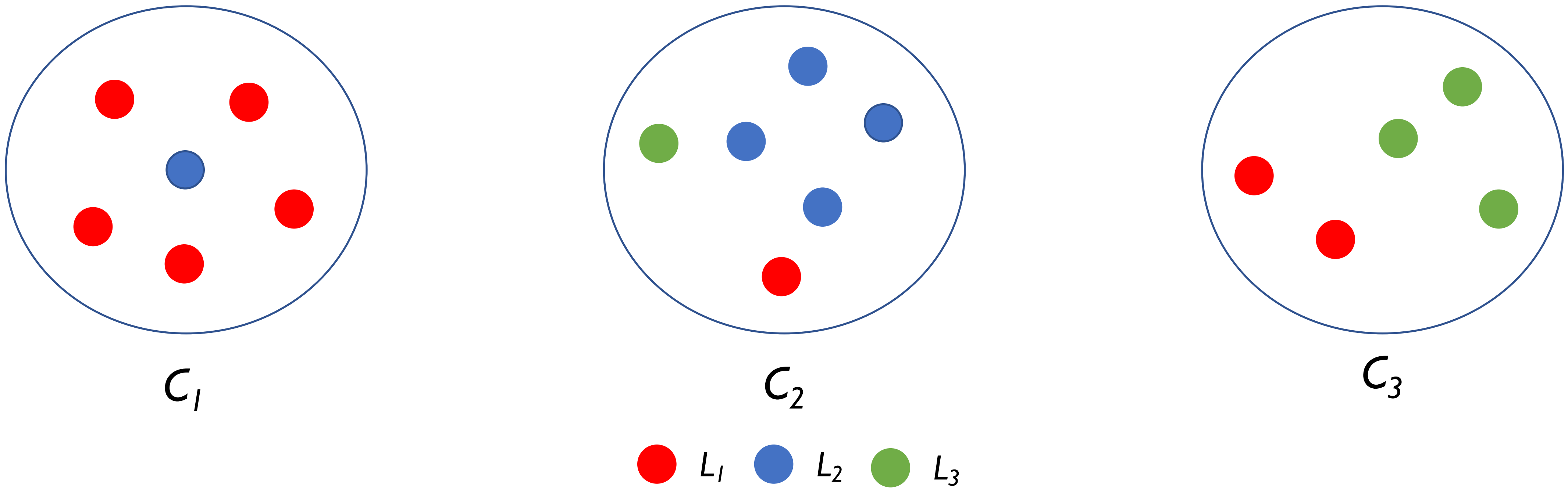
$$n_i = \sum_{j=1}^{J} n_{i,j} \text{ number of items clustered in } C_i$$

$$\text{purity}(C_i) = \frac{1}{n_i} \max_{j \in \{1,\ldots,J\}} n_{i,j}$$

$$\text{purity} = \frac{1}{K} \sum_{i=1}^{K} \text{purity}(C_i)$$

Biased because having as many clusters as items maximizes purity

External Evaluation: Purity Example



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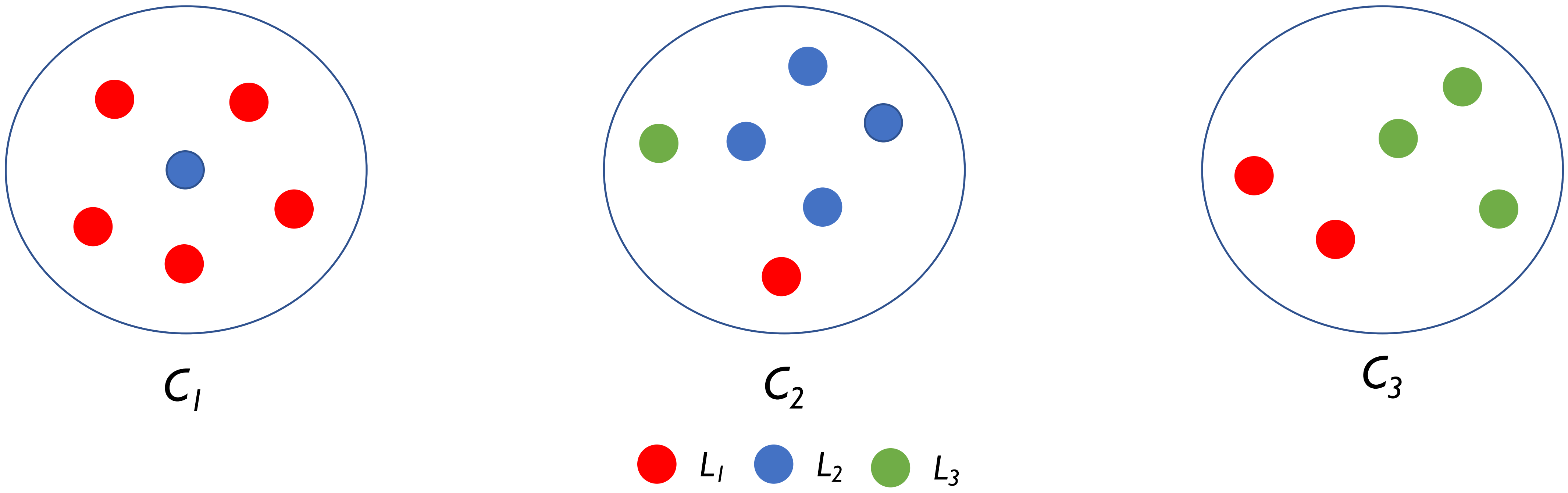

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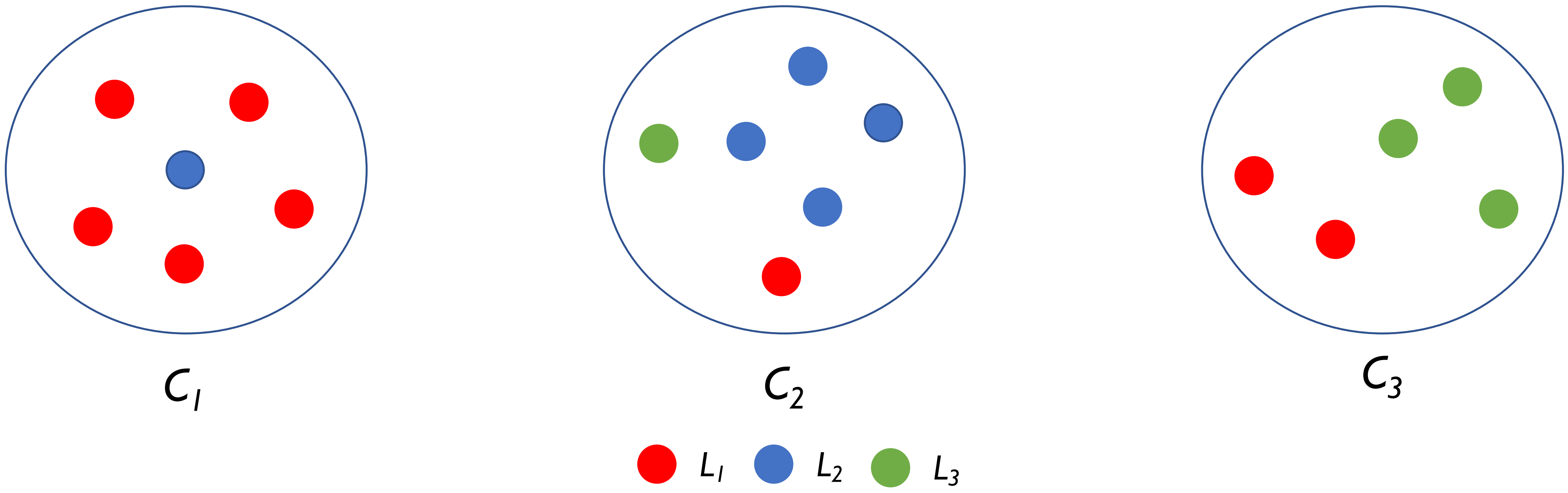

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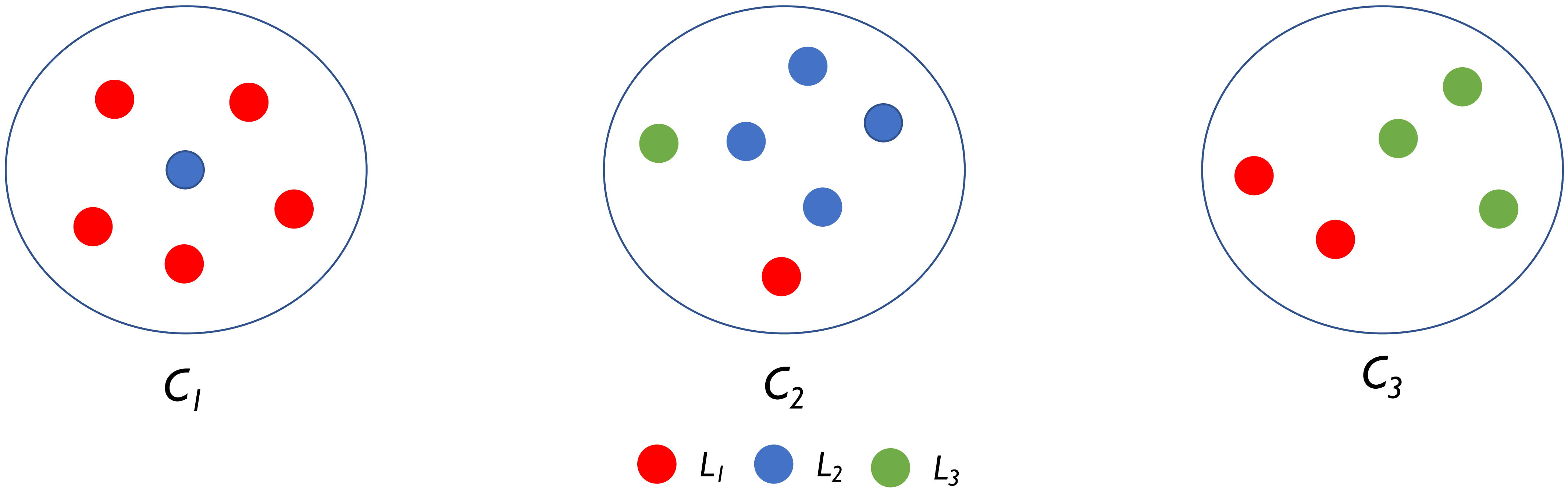

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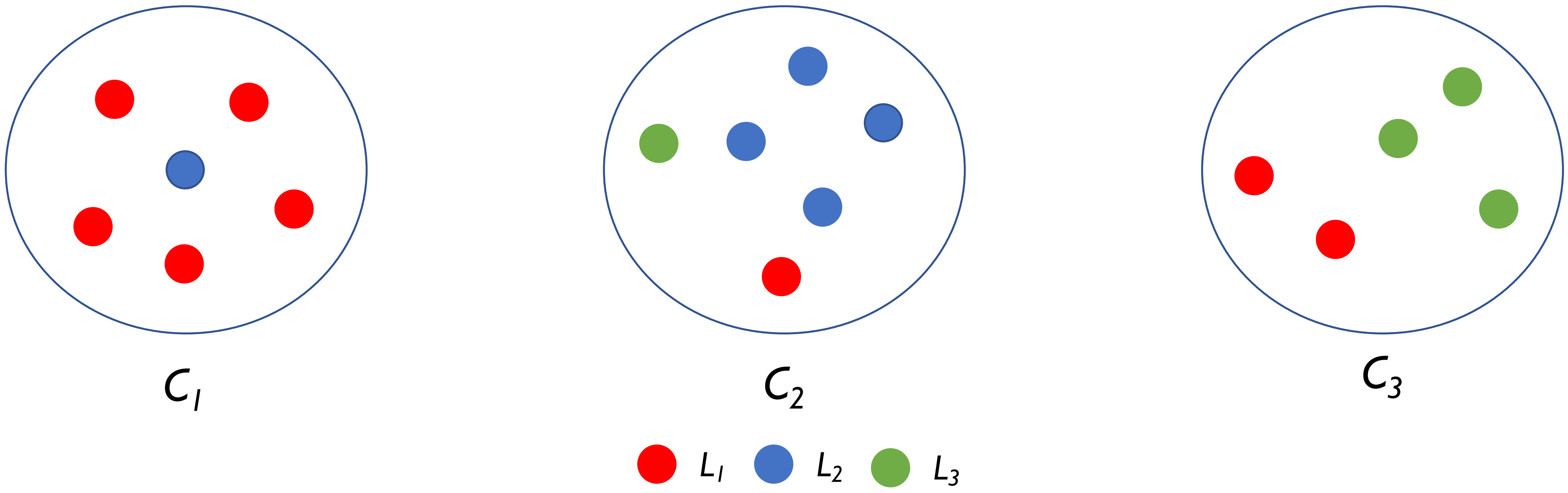

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purity = 1/3 * purity(C_1)+purity(C_2)+purity(C_3) = **7/10**

External Evaluation: Rand Index

$$\text{Rand} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$\left.\begin{aligned} TP &= \text{number of } \textit{true positives} \\ TN &= \text{number of } \textit{true negatives} \\ FP &= \text{number of } \textit{false positives} \\ FN &= \text{number of } \textit{false negatives} \end{aligned}\right\}$$

All computed from **pairs** of elements

Measures the level of agreement between clustering and ground truth

External Evaluation: Rand Index

n. of pairs	Same Cluster in Clustering	Different Clusters in Clustering
Same Cluster in Ground-Truth	TRUE POSITIVES (**TP**)	FALSE NEGATIVES (**FN**)
Different Clusters in Ground-Truth	FALSE POSITIVES (**FP**)	TRUE NEGATIVES (**TN**)

Confusion Matrix

External Evaluation: Precision, Recall, F-measure

$$P = \frac{TP}{TP + FP} \quad R = \frac{TP}{TP + FN}$$

$$F_\beta = \frac{(\beta^2 + 1) \cdot P \cdot R}{\beta^2 \cdot P + R}$$

$$F_1 = \frac{2 \cdot P \cdot R}{P + R}$$

Balances the contribution of false negatives by weighting recall through a parameter $\boldsymbol{\beta}$

External Evaluation: Many Other Measures

- Jaccard index
- Dice index
- Fowlkes-Mallows index
- Mutual information
- etc.

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- Internal vs. External measures of **clustering quality**