Teoria degli Algoritmi

Corso di Laurea Magistrale in Matematica Applicata

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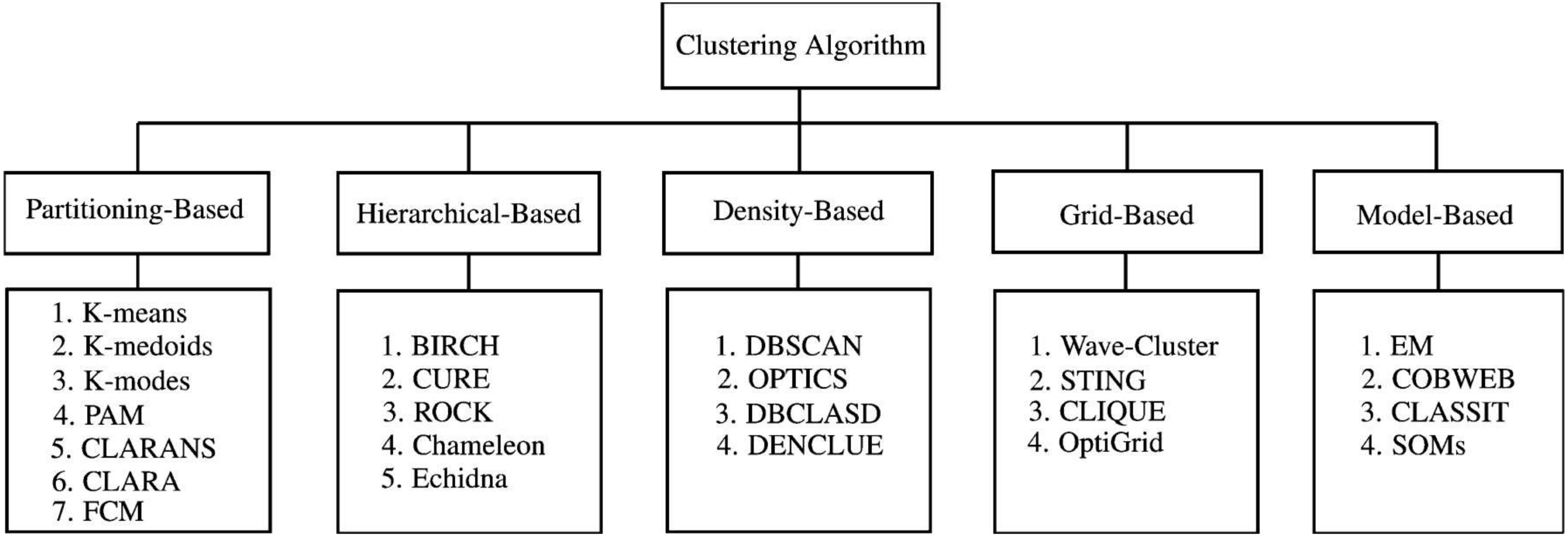
SAPIENZA UNIVERSITÀ DI ROMA

Clustering Algorithms

Clustering Algorithms: Taxonomy



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

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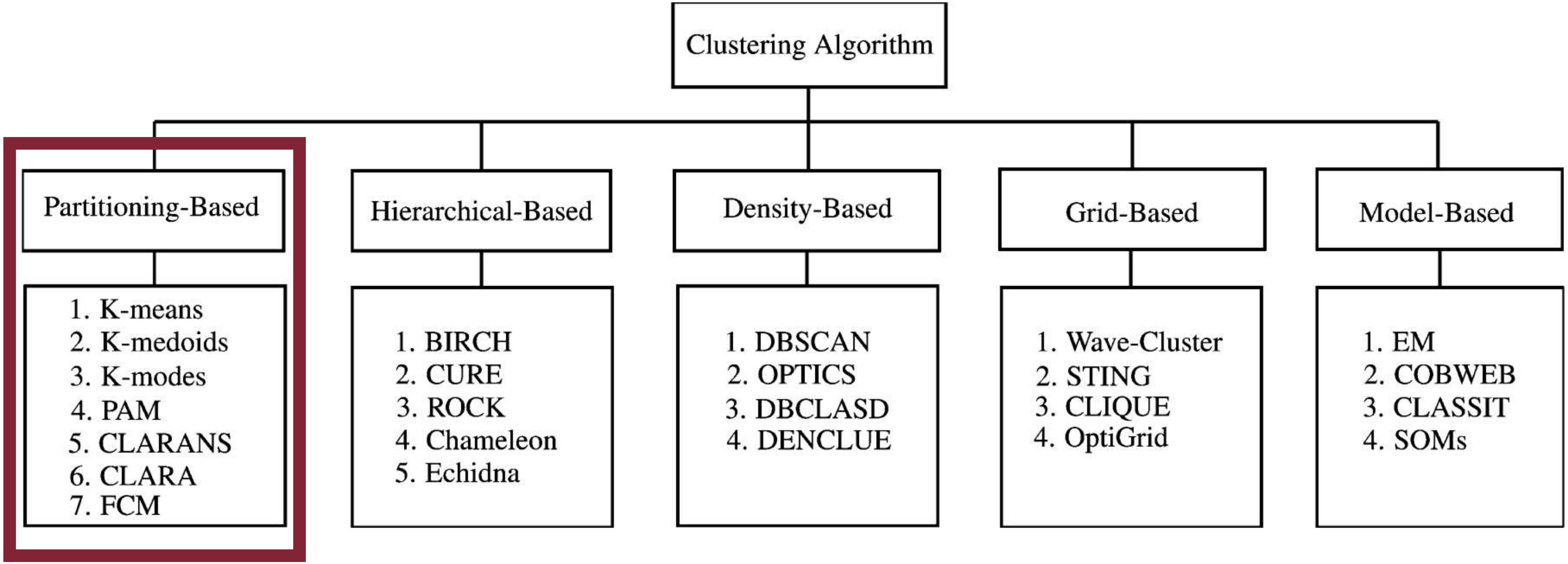

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  - $S(K, N) \sim O(K^N)$ → K-way non-empty partitions of N elements **Stirling partition number**
  - Effective heuristics → K-means, K-medoids, K-means++, etc.

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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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$\boldsymbol{\theta}_k$ 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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$\forall n \; \exists! k$ such that $\alpha_{n,k} = 1 \; \wedge \; \alpha_{n,k'} = 0 \; \forall k' \neq k$

$\boxed{\text{hard clustering}}$

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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) ~ 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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  - Assignment step
  - Update step

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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

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

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

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

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2-Step Optimization: Update Step

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

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

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

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

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

The general *j*-th partial derivative

2-Step Optimization: Update Step

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

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

To make the notation easier!

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

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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!

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

Depends on the distance function δ

A Special Case: K-means

- 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

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

Euclidean space

K-means: Objective Function

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

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

Sum of Square Distances (SSD)

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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 $\boldsymbol{\Theta}$

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)

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

K-means: Update Step

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

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

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

K-means: Update Step

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

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

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

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

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

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

K-means: Lloyd-Forgy Algorithm

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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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- 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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  - Monotonically decreases SSD
- 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 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

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- 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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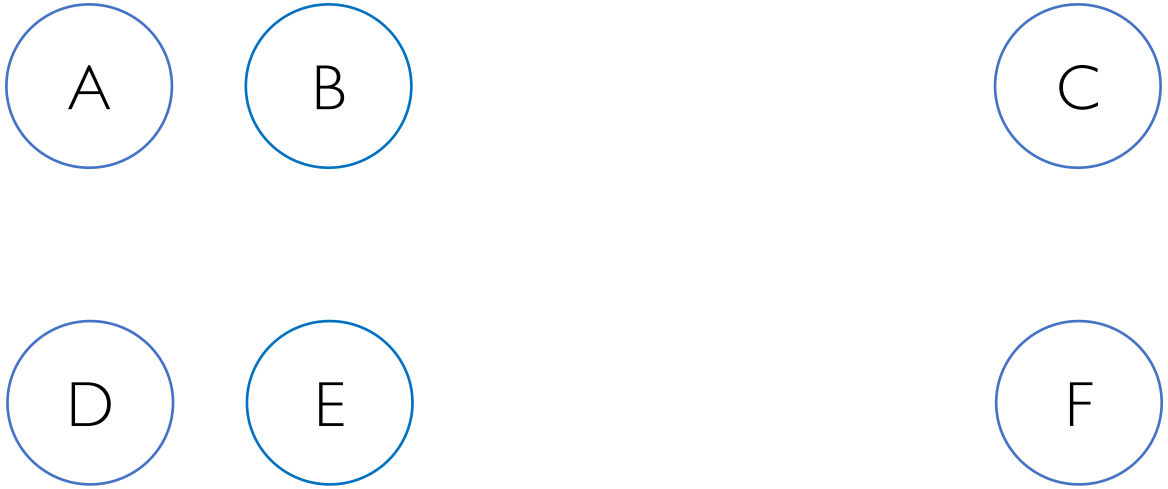
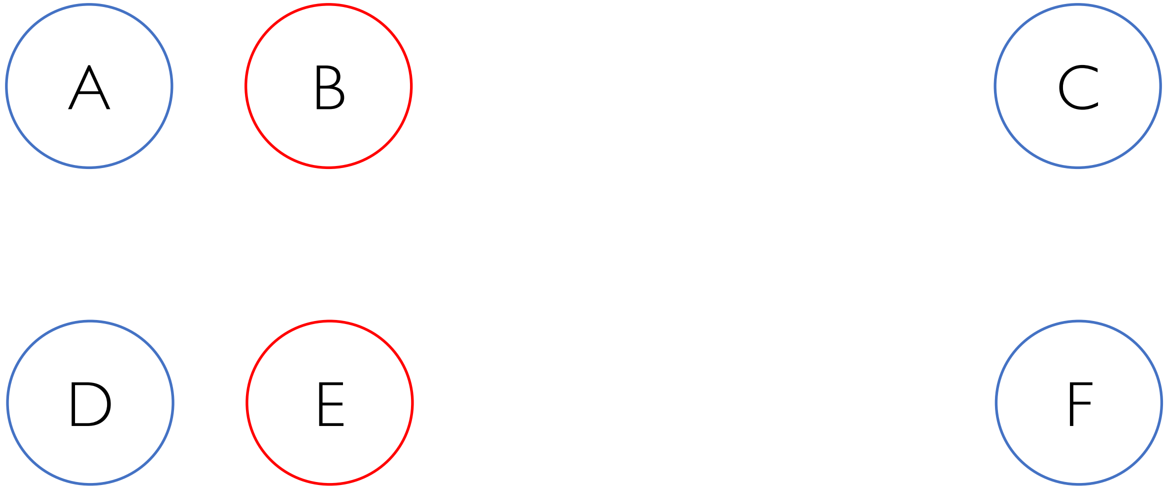
Problem Mitigation:

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

K-means: Seed Choice



K-means: Bad (Unlucky) Seed Choice



If B and E are randomly chosen as initial centroids…

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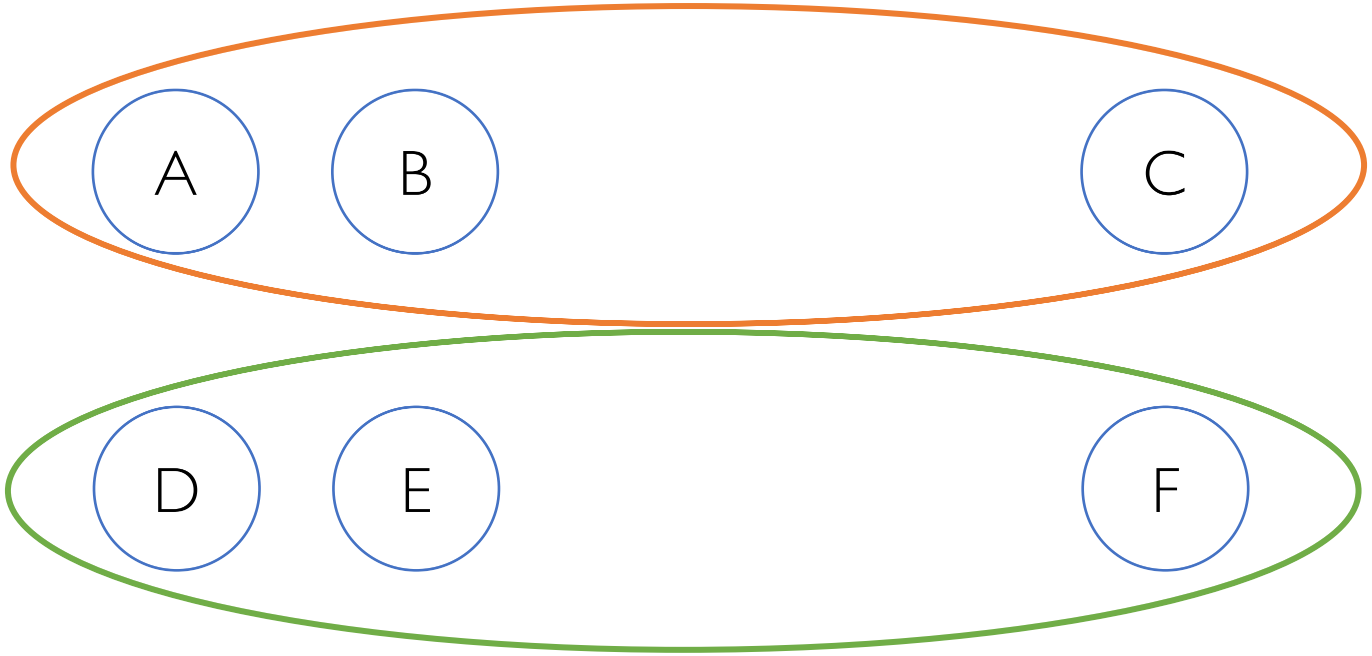
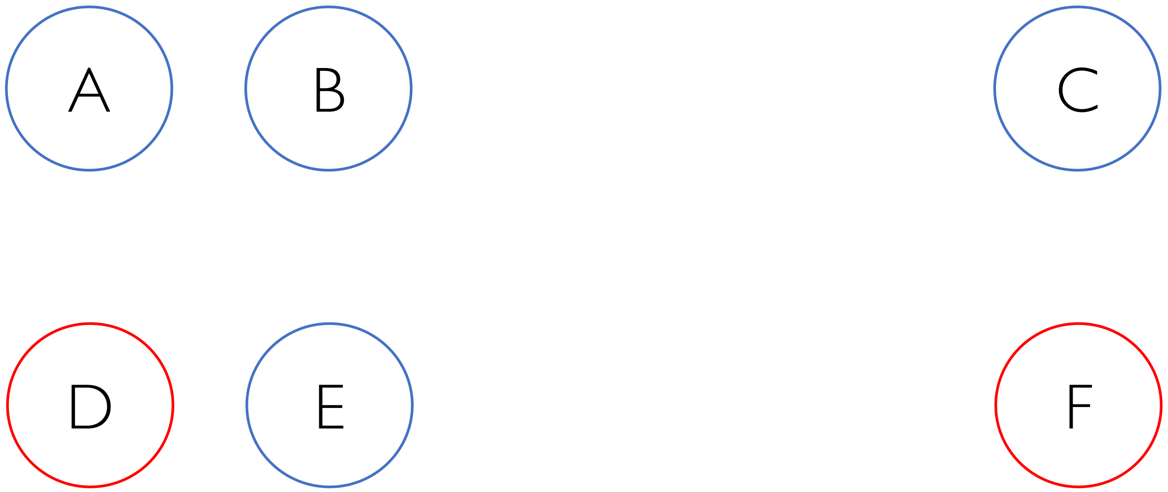


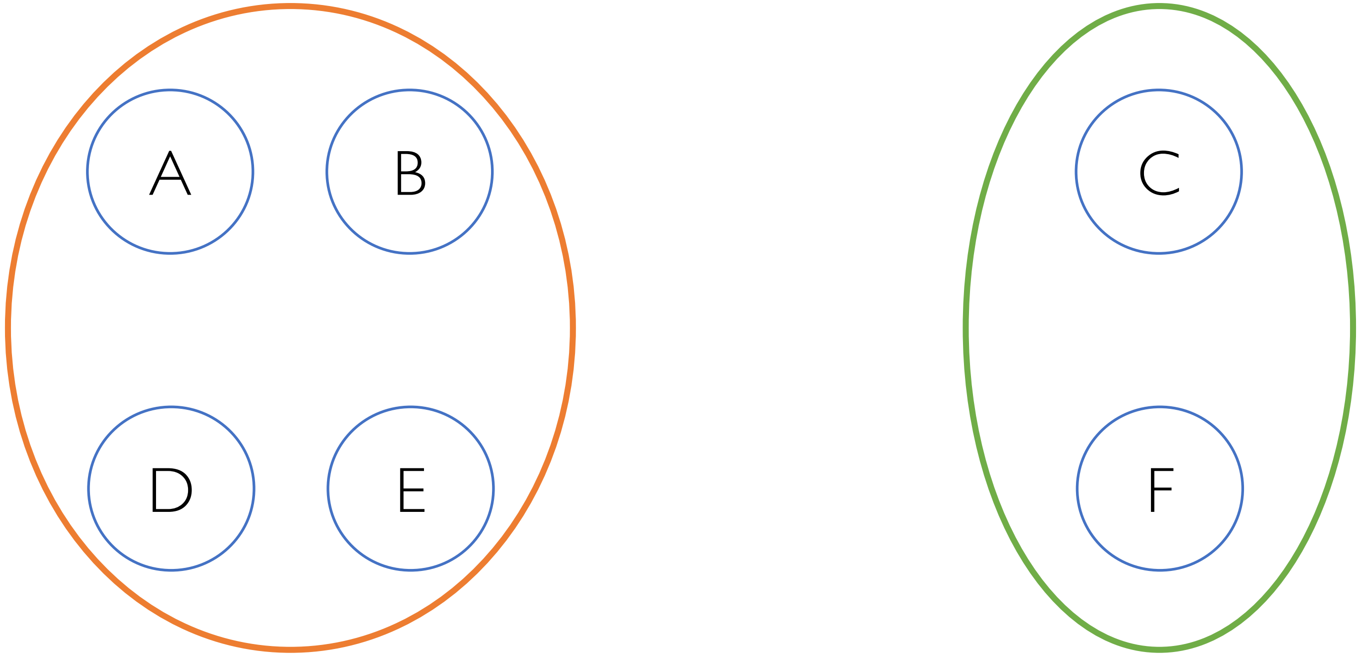
The algorithm converges to the sub-optimal clustering above

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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    4. Repeat steps 2. and 3. until K centers are chosen, then run Lloyd-Forgy

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- 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

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  - Great! Partition N data points into a predetermined number K of 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
- 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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NOTE
There is always a clustering whose total benefit B=N
(where N is the number of data points)

Why?

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

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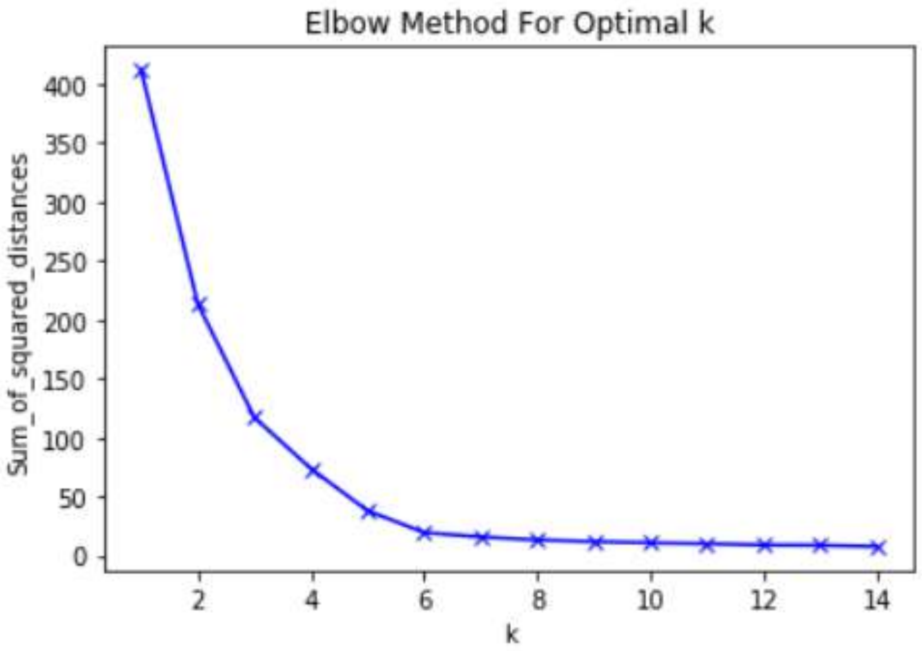

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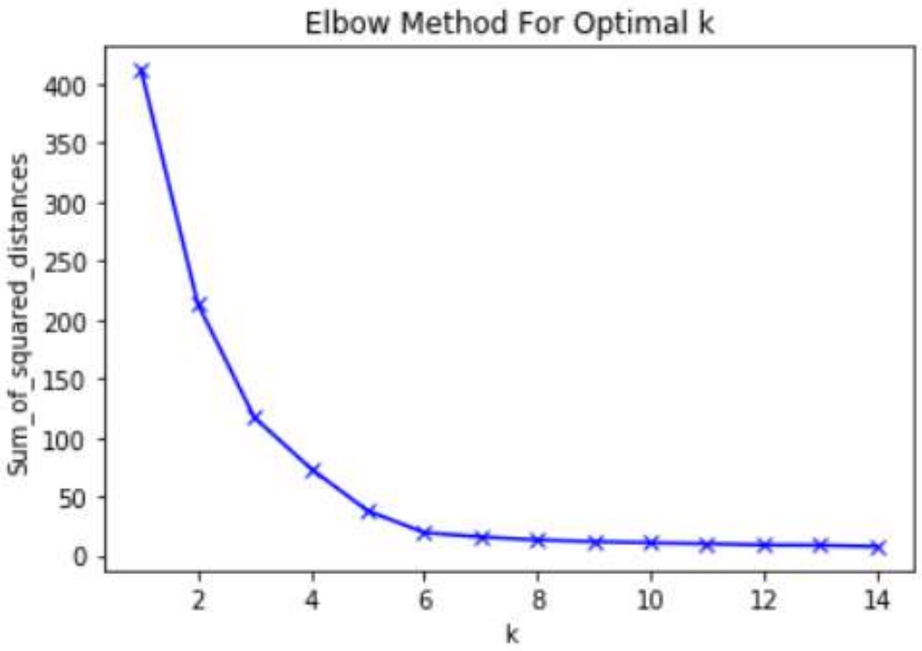

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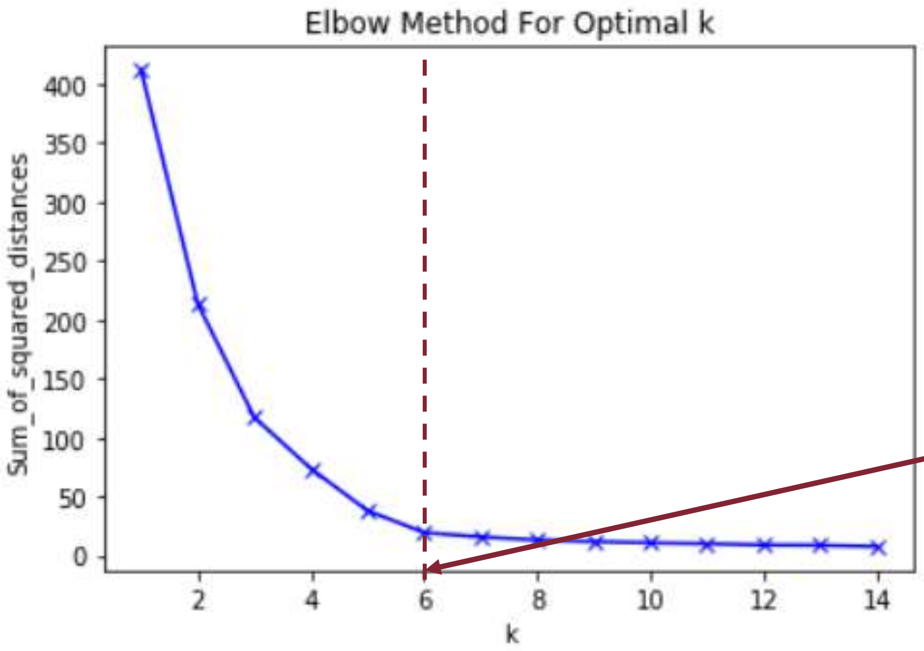

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  - δ = Cosine distance = Euclidean distance on normalized input points
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- Others, require specific minimizers
  - δ = Manhattan distance (L^1-Norm) → median is the minimizer (K-medians)

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Measures of Clustering Quality

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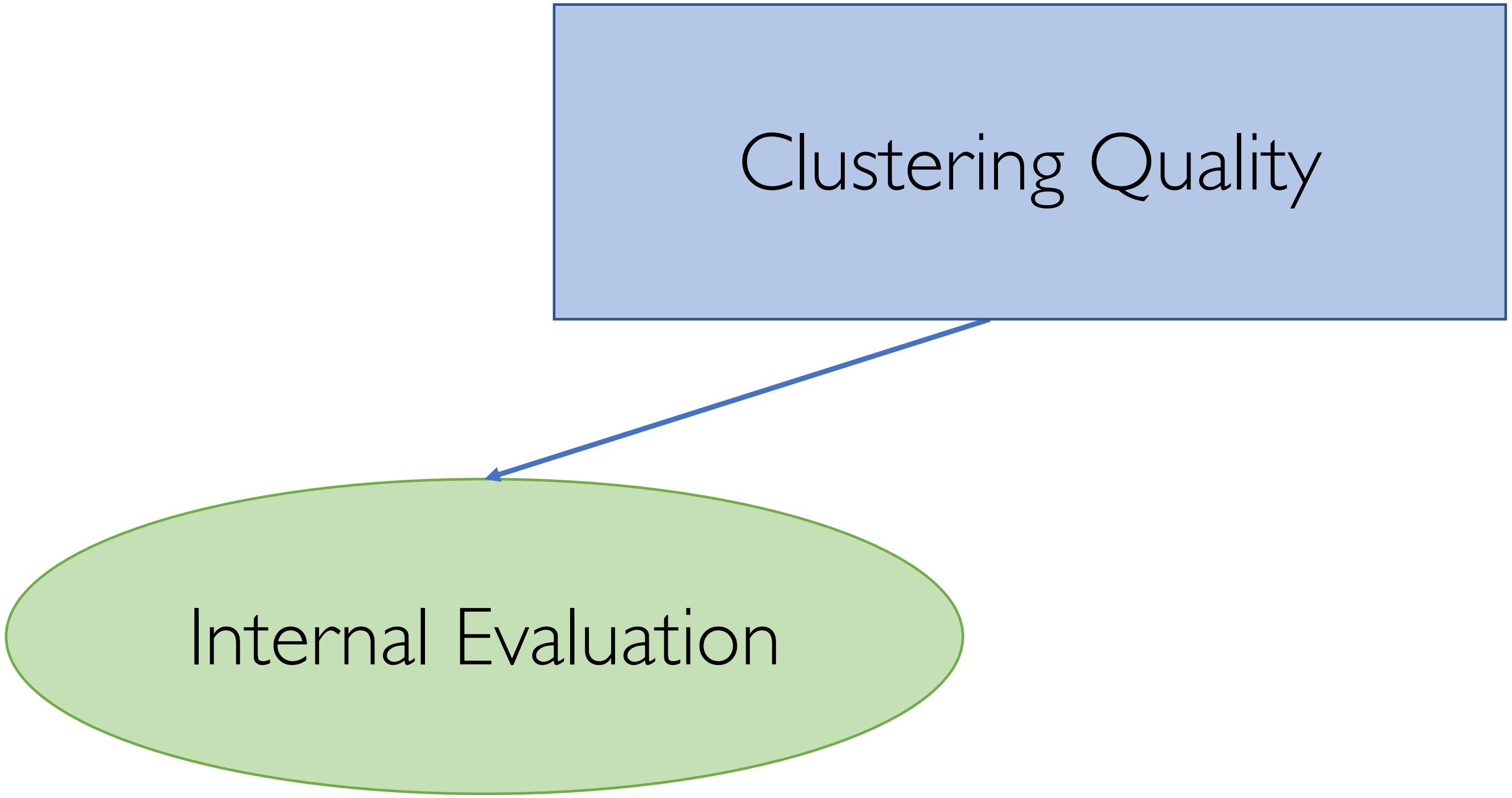

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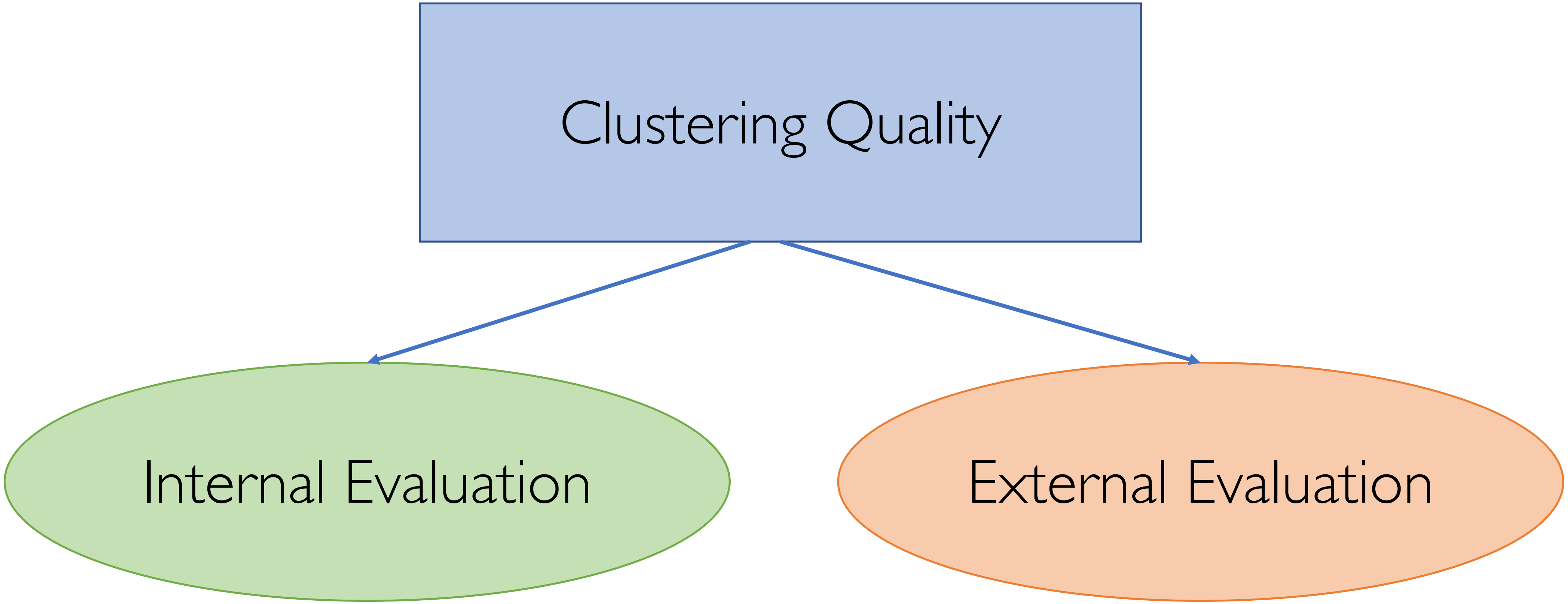

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- The measured quality of a clustering depends on
  - data representation
  - similarity measure

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 = number of clusters

$\boldsymbol{\mu}_k$ = centroid of cluster C_k

σ_k = avg. distance of all elements of cluster C_k from its centroid $\boldsymbol{\mu}_k$

$\delta(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)$ = distance between centroids of C_i 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 != 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

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

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

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

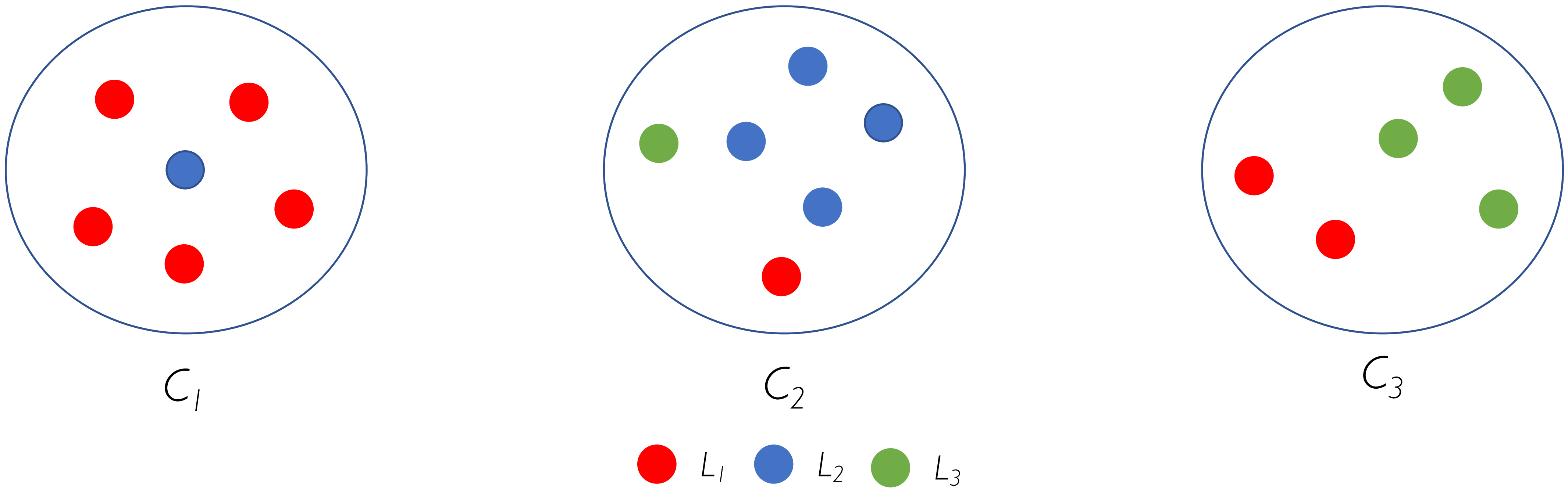
$$n_i = \sum_{j=1}^{J} n_{i,j} \text{ number of items clustered in } C_i$$

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

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

Biased because having as many clusters as items maximizes purity

External Evaluation: Purity Example



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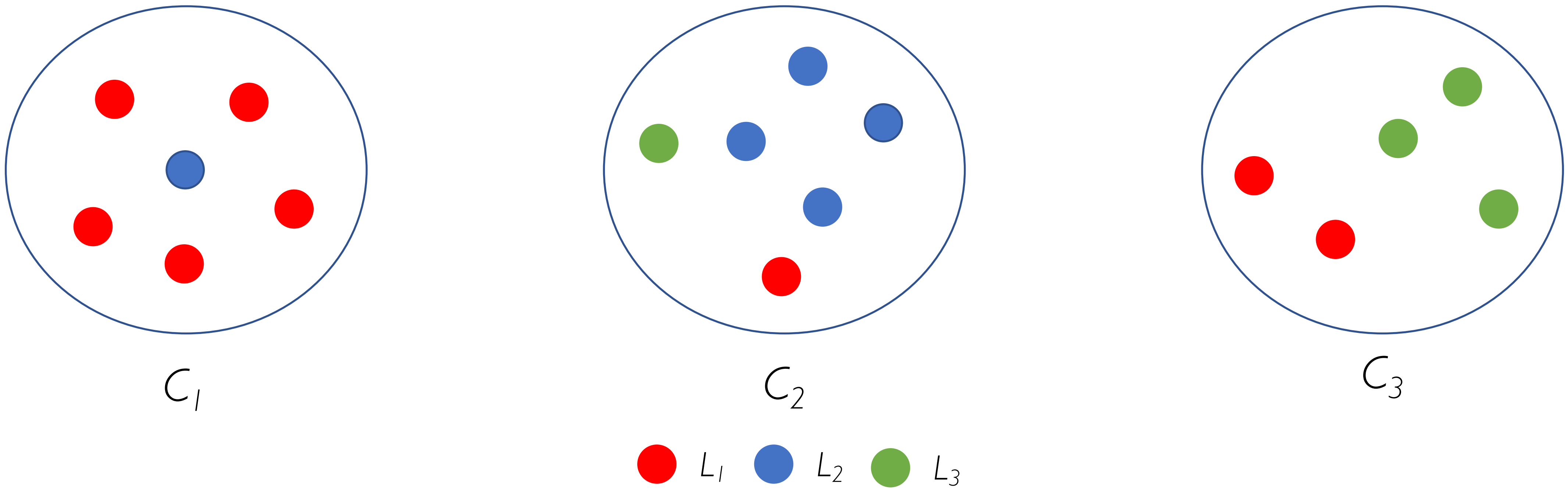

$purity(C_1) = 1/6 * max\{5, 1, 0\} = 5/6$

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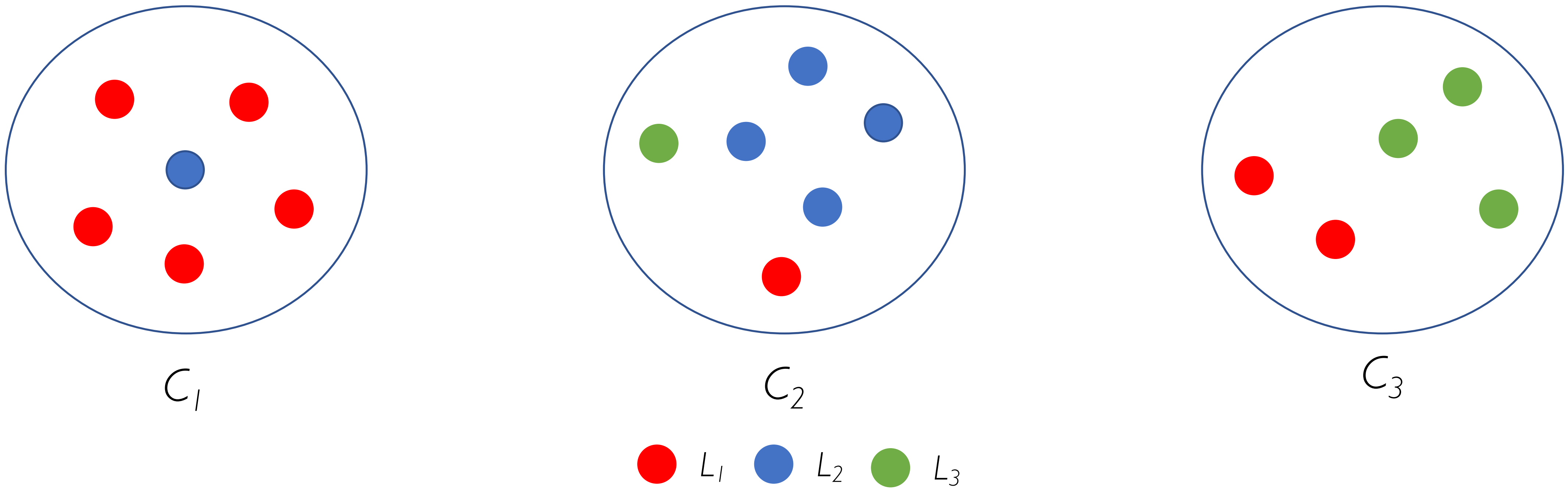

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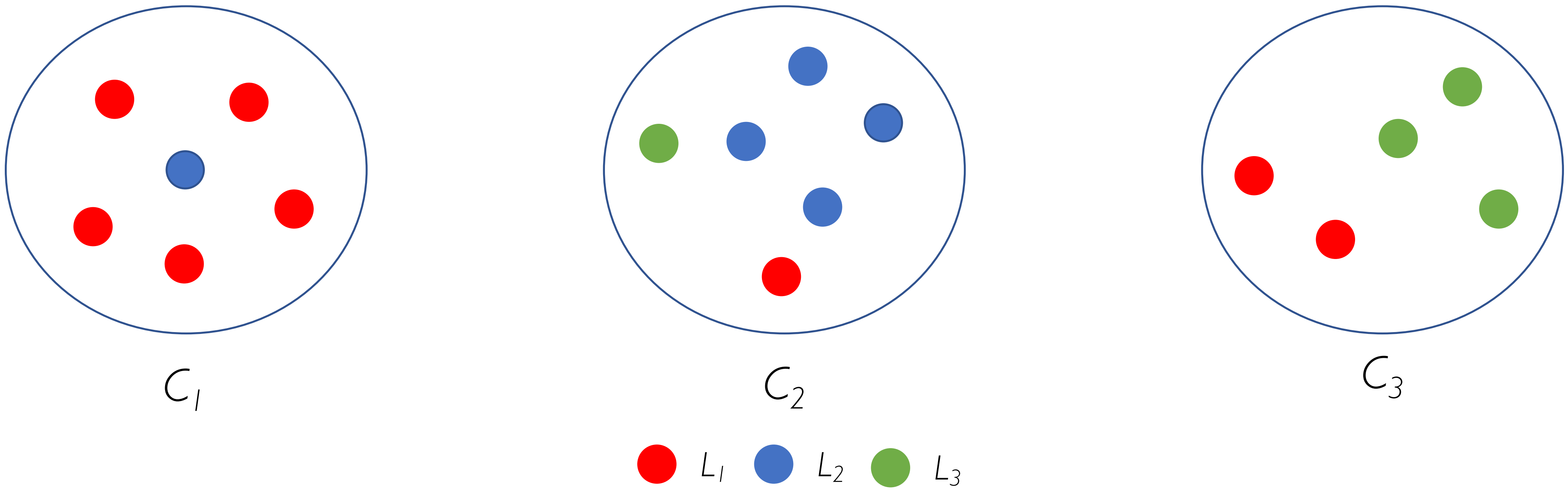

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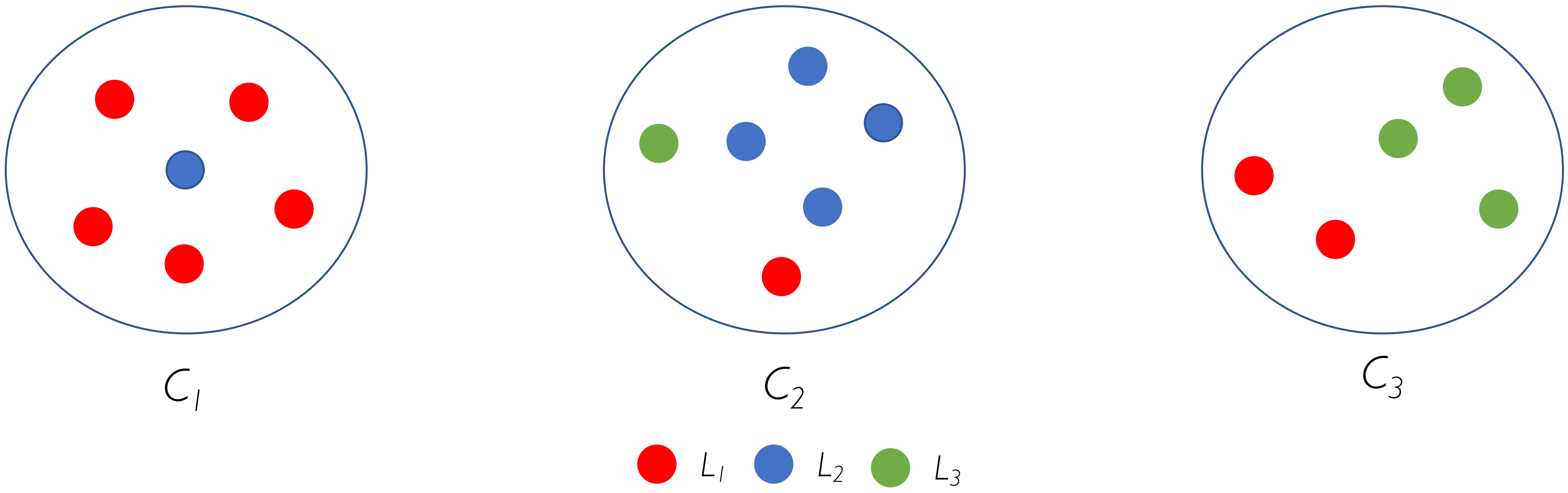

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$$\boxed{\text{purity} = 1/3 * purity(C_1)+purity(C_2)+purity(C_3) = 7/10}$$

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

Suggested Readings

- Kaufman, L., and Rousseeuw, P. J. "*Clustering by Means of Medoids*" (1987)
- Bradley, P. S., Fayyad, U., and Reina, C. "*Scaling Clustering Algorithms to Large Databases*" (KDD 1998)
- Kleinberg, J., "*An Impossibility Theorem for Clustering*" (NIPS 2002)
- Arthur, D., and Vassilvitskii, S. "*k-means++: The Advantages of Careful Seeding*" (SODA 2007)
- Mahajana, M., Nimbhorkara, P., and Varadarajan, K. "*The planar k-means problem is NP-hard*" (Theoretical Computer Science, vol. 442, 2012)