Big Data Computing

Master's Degree in Computer Science

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Recap from Last Lecture

- 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

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- 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

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

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

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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

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

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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K-means: Update Step

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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

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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

- 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

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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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- (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

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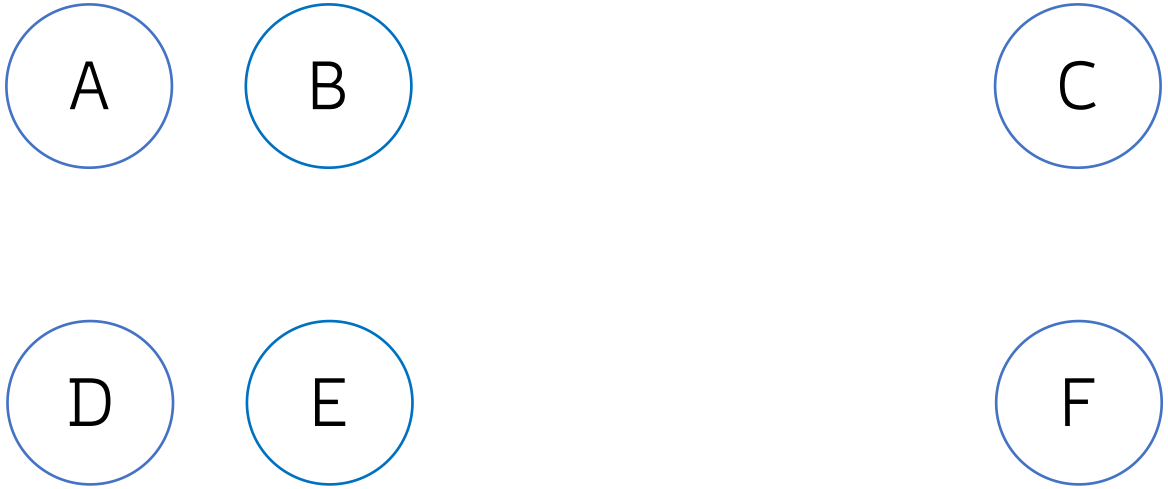
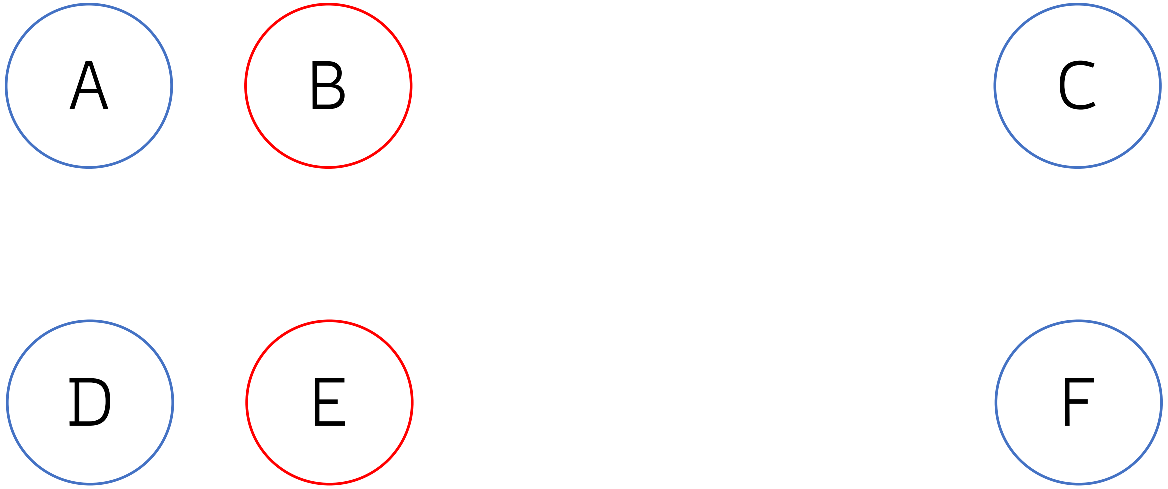
Problem Mitigation:

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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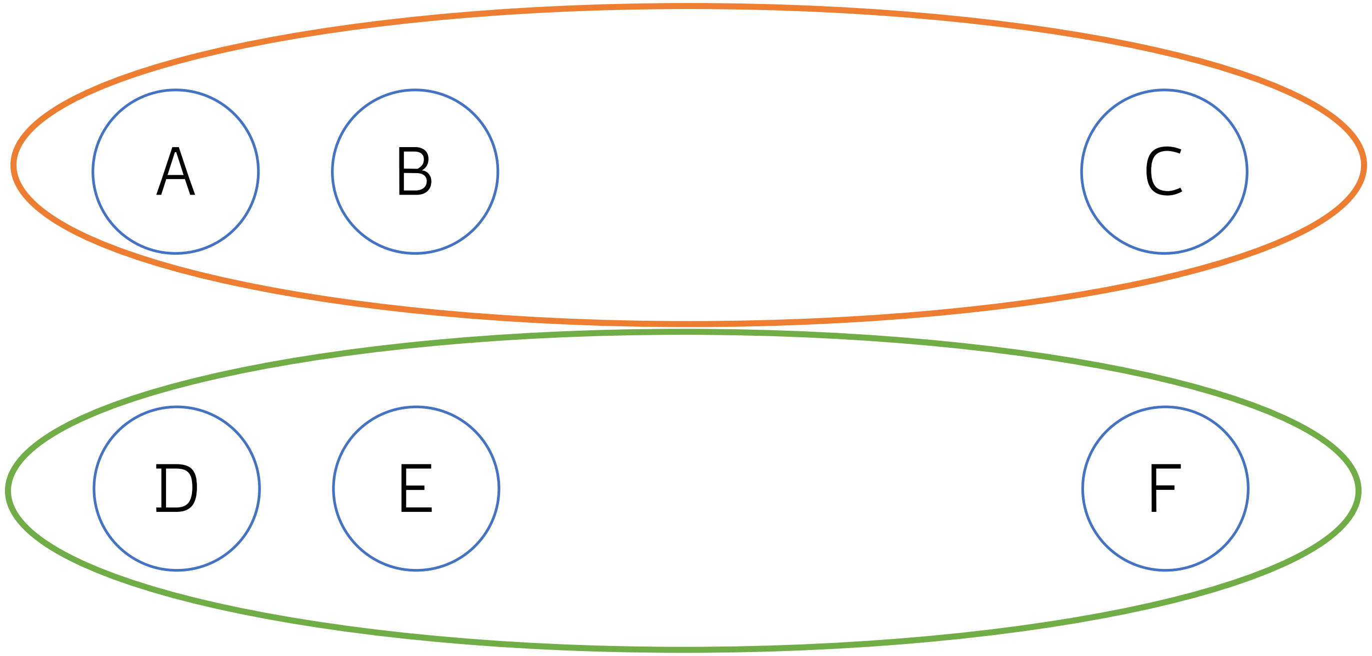
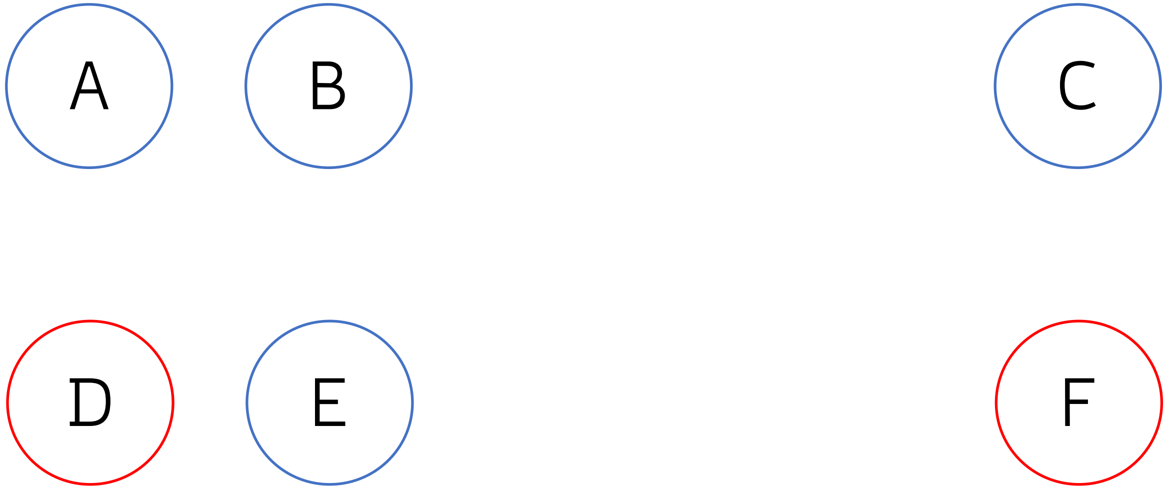


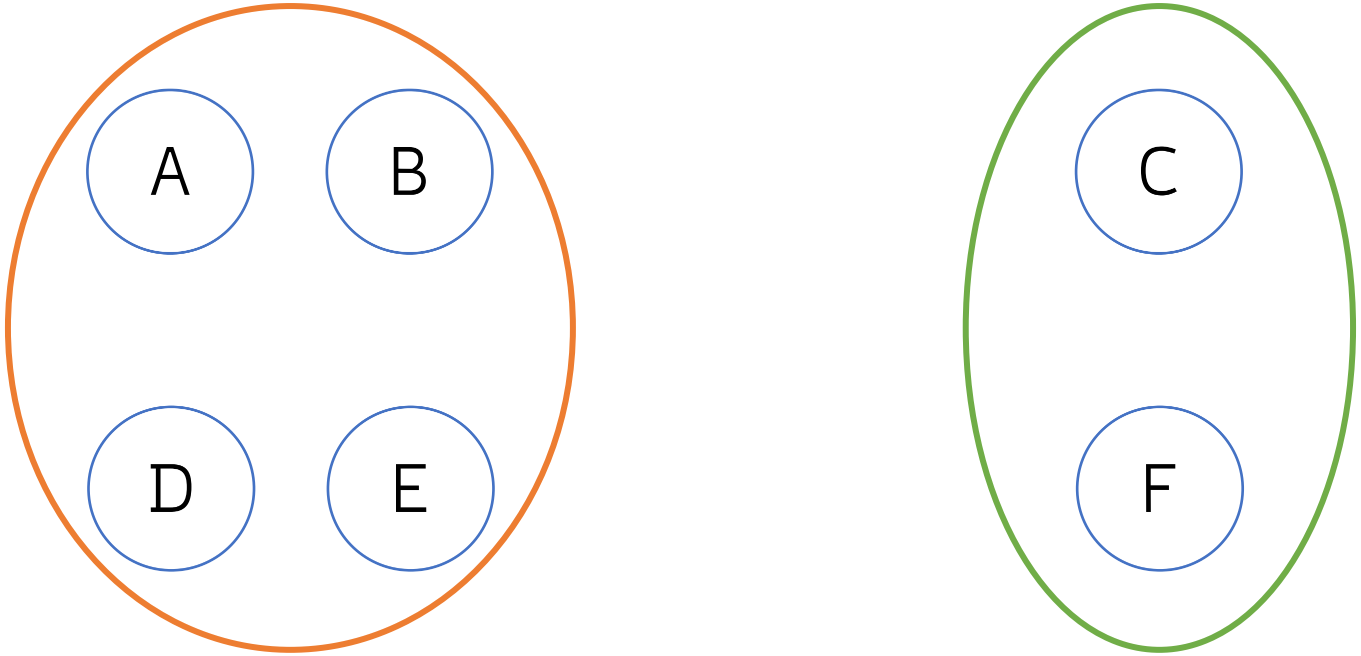
The algorithm converges to the sub-optimal clustering above

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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Alternative Seed Choice: K-means++

- A method to carefully select initial centroids
- Proposed in 2007 by Arthur and Vassilvitskii [paper]
- **Intuition:** Spreading out the K initial cluster centers is a good thing
- Select the i-th centroid as the farthest data point to any other already selected centroids

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

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- Random initialization of "vanilla" K-means may give clusters that are **arbitrarily worse** than optimum

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- Random initialization of "vanilla" K-means may give 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

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  - Great! Partition N data points into a predetermined number K of clusters
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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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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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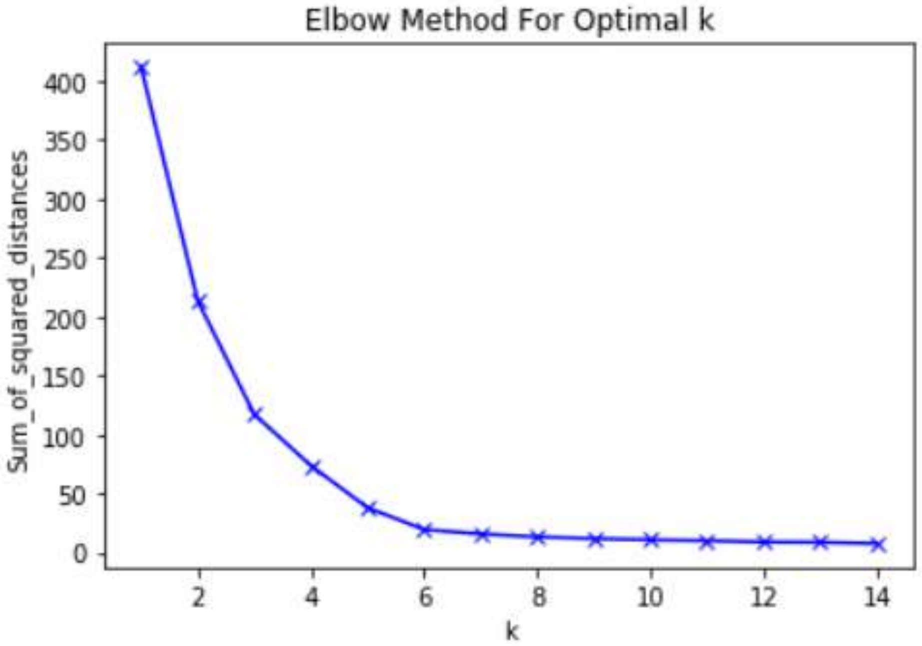

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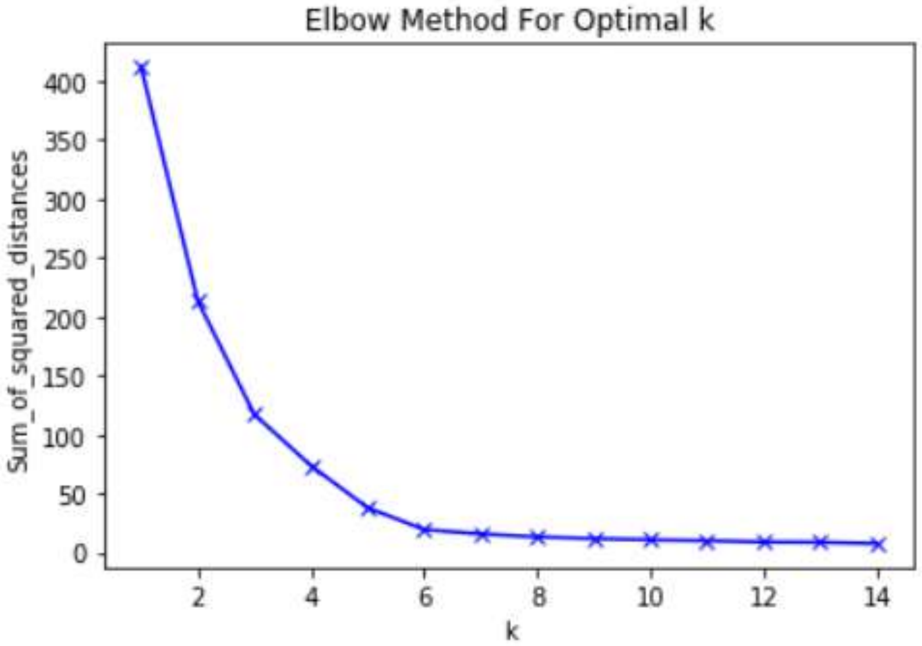

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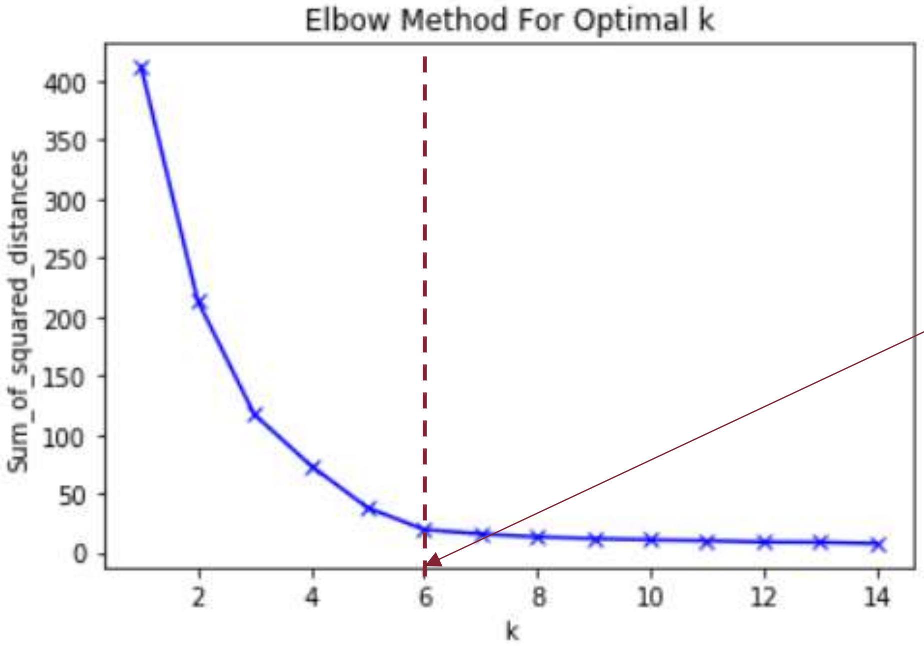

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up to a certain value

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- Some of them just resemble Euclidean distance, and centroids (i.e., means) still minimize those
  - 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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- Similar to K-means yet chooses input data points as centers (**medoids**)
- A medoid is the closest object to any other point in the cluster
- Works with **any arbitrary distance** δ
- PAM (Partitioning Around Medoids) greedy Algorithm, introduced by Kaufman and Rousseeuw in 1987 [paper] vs. Lloyd-Forgy
- Robust to outliers yet computationally expensive $O(K(N-K)^2)$

Bradley-Fayyad-Reina (BFR) K-means

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Clustering Quality

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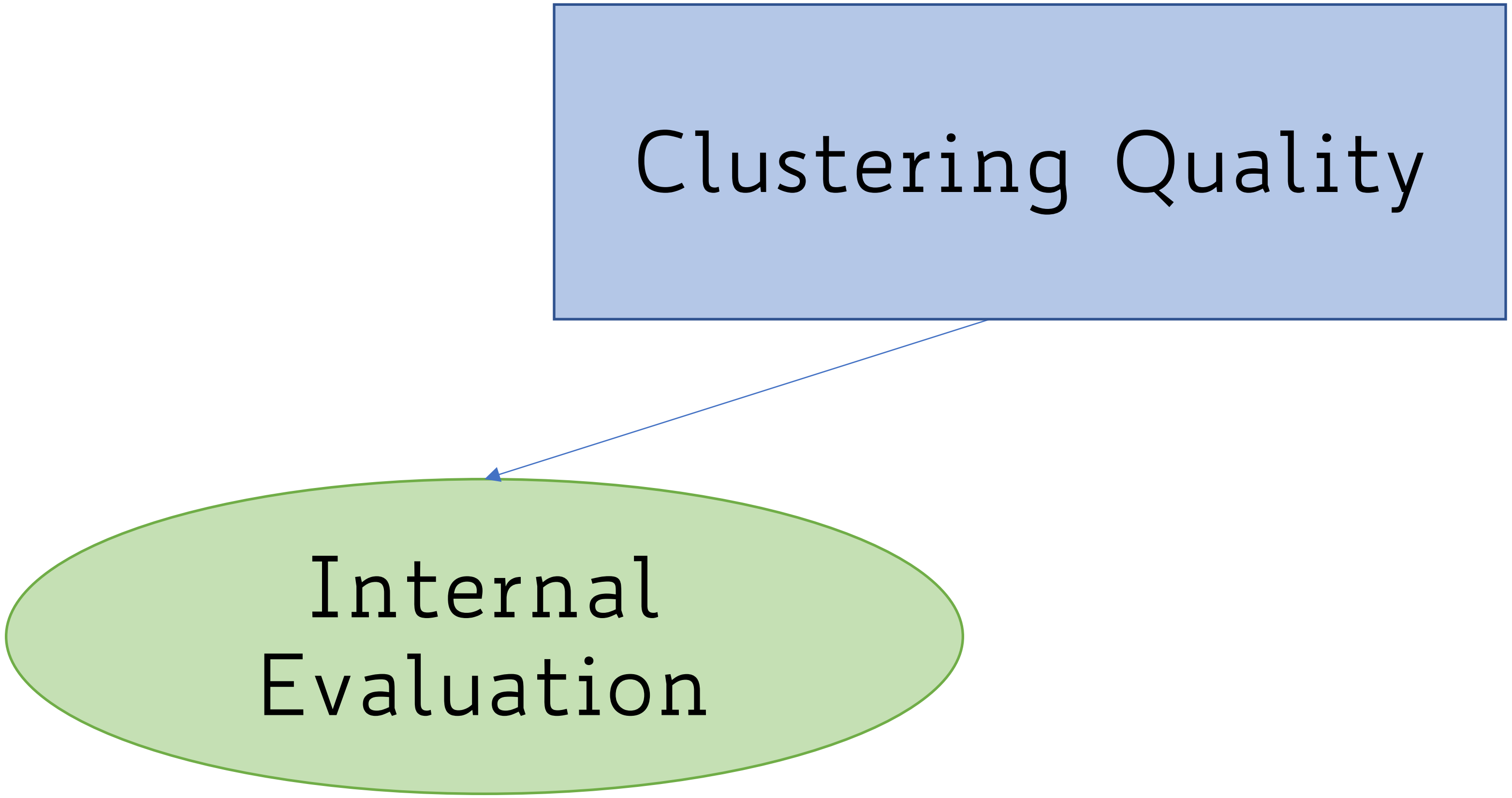

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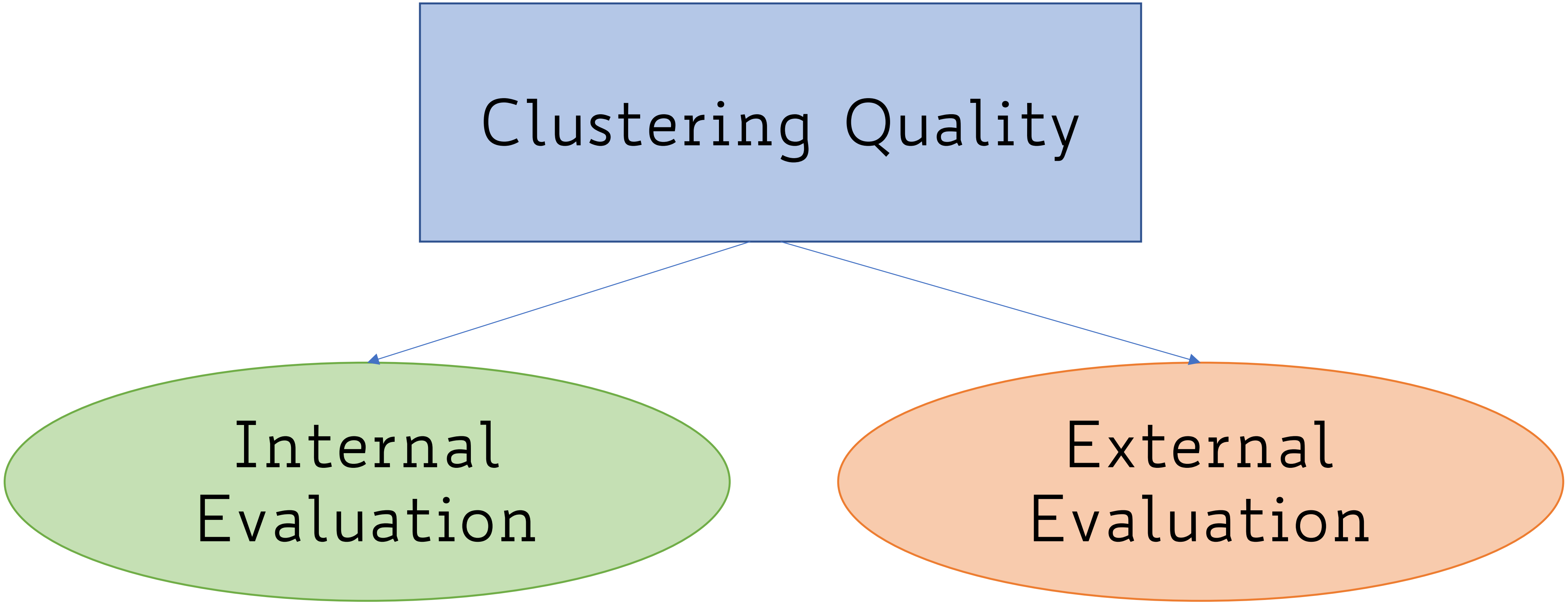

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- A good clustering will produce high quality clusters with:
  - high intra-cluster similarity
  - low inter-cluster similarity
- The measured quality of a clustering depends on
  - data representation
  - similarity measure

Internal Evaluation: Davies-Bouldin Index

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

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

Internal Evaluation: Davies-Bouldin Index

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

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

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

Distance between centroids

Max distance between any pair of objects

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

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smallest mean distance of i to all points in any other cluster C_k != C_i

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

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- Quality measured by the ability to discover some or all of the hidden patterns in gold standard data
- Hard as it requires labeled data typically provided by human experts

External Evaluation: Purity

$C_1 \ldots, C_K$ = set of K clusters

$L_1 \ldots, L_J$ = set of J labels

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

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

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

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

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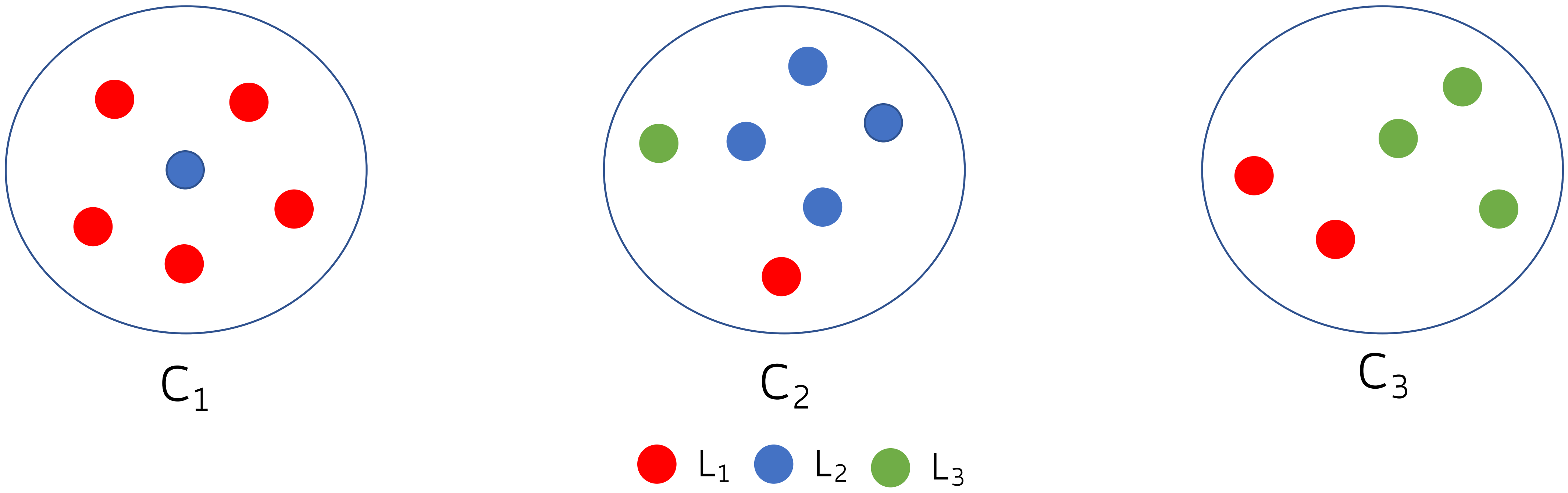
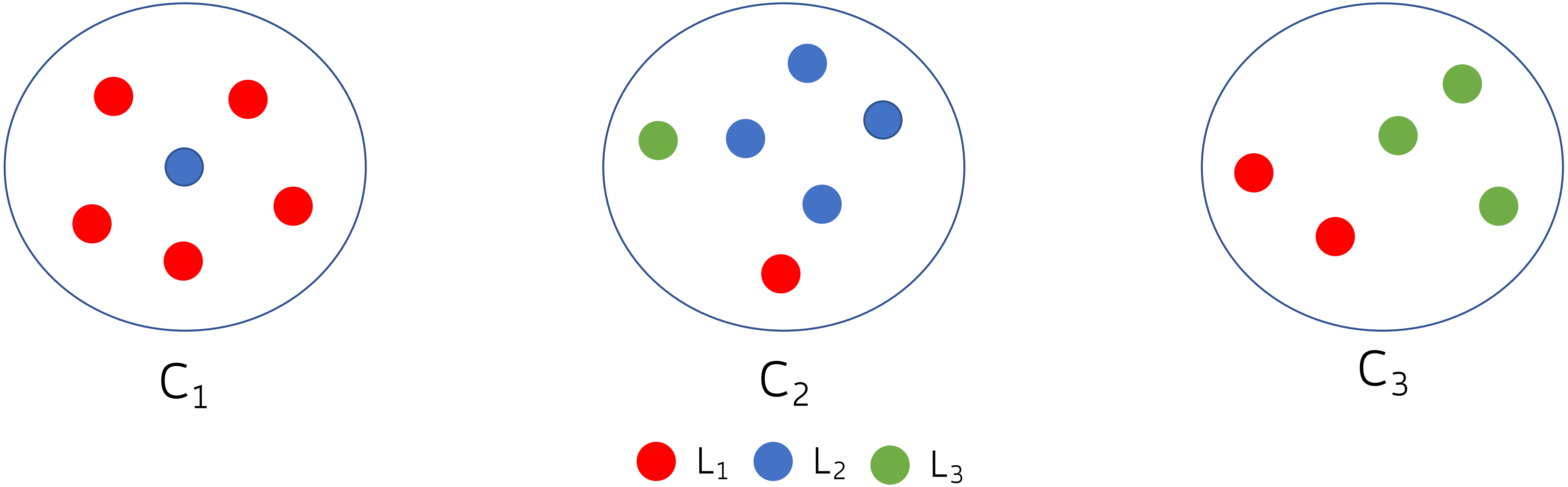
Biased because having as many clusters as items maximizes purity

External Evaluation: Purity Example

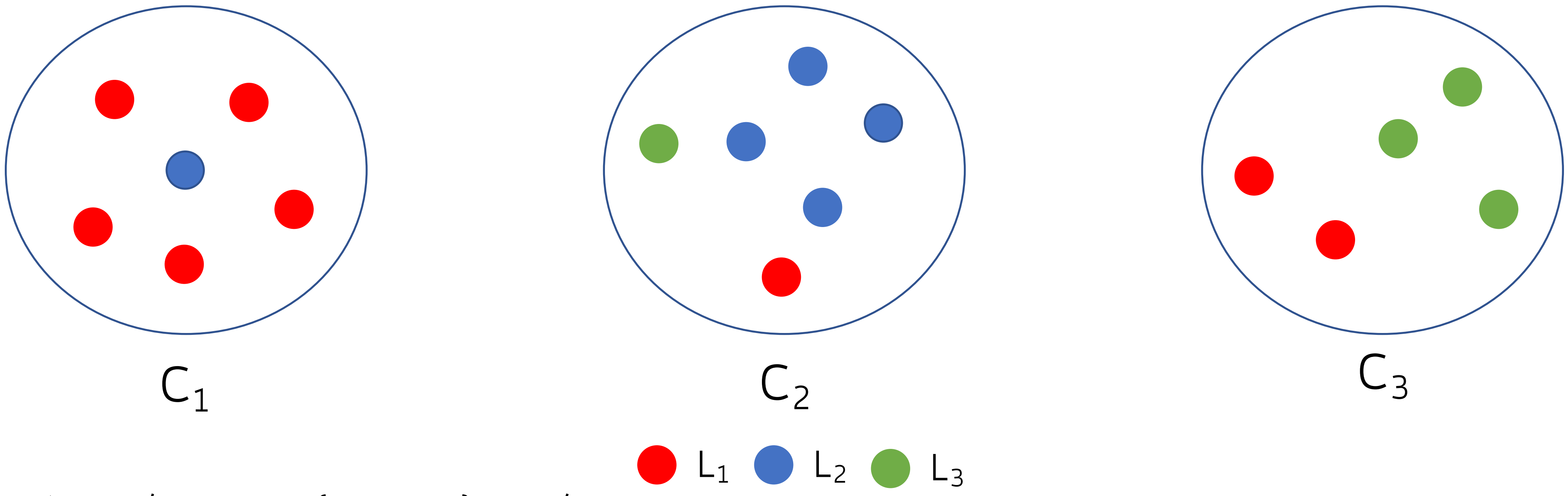


External Evaluation: Purity Example



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

External Evaluation: Purity Example



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

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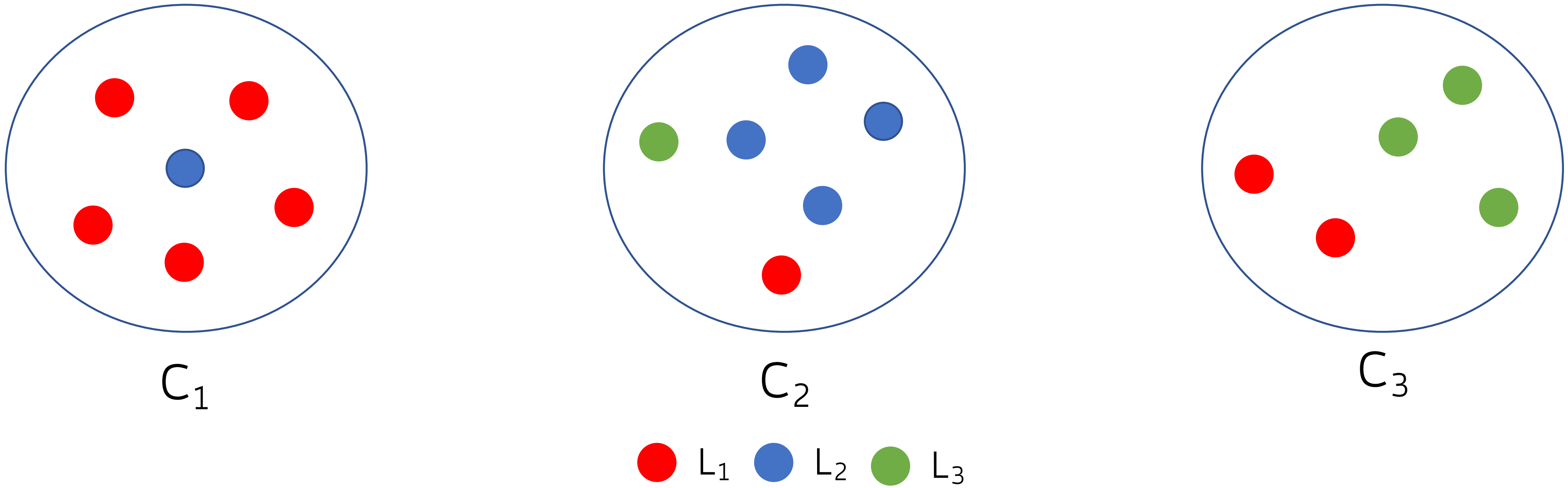
External Evaluation: Purity Example



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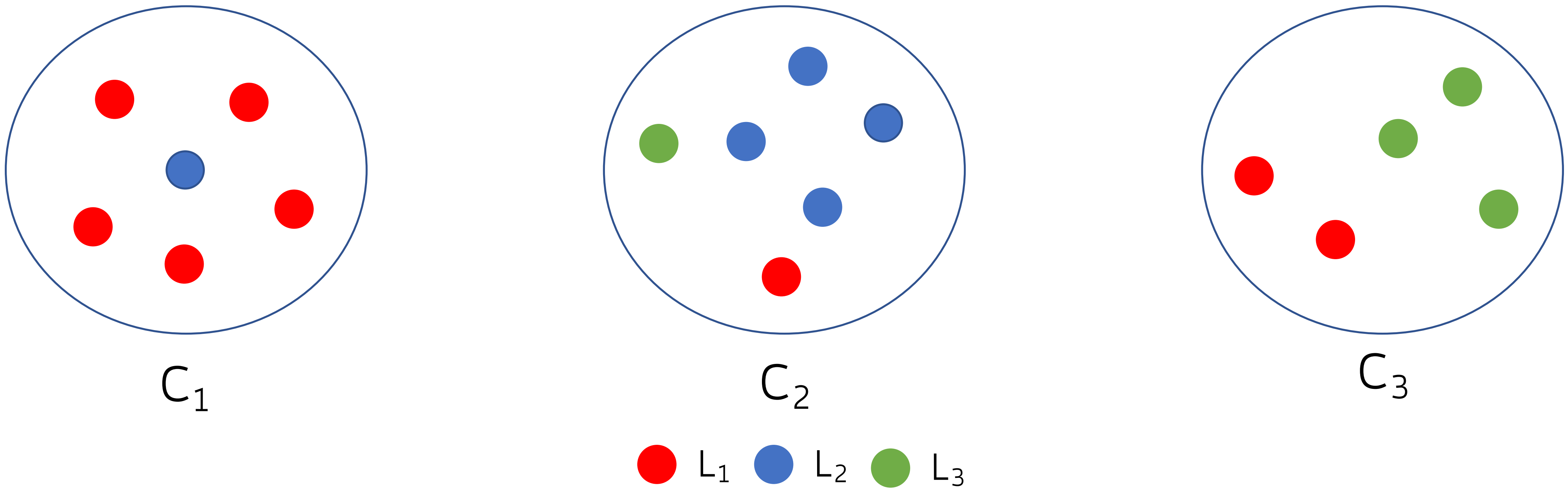

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$\text{purity} = 1/3 * \text{purity}(C_1)+\text{purity}(C_2)+\text{purity}(C_3) = 7/10$

External Evaluation: Rand Index

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

$$TP = \text{number of } \textit{true positives}$$
$$TN = \text{number of } \textit{true negatives}$$
$$FP = \text{number of } \textit{false positives}$$
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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		
Different Clusters in Ground-Truth		

External Evaluation: Rand Index

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External Evaluation: Rand Index

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Same Cluster in Ground-Truth		
Different Clusters in Ground-Truth		TRUE NEGATIVES (TN)

External Evaluation: Rand Index

n. of pairs	Same Cluster in Clustering	Different Clusters in Clustering
Same Cluster in Ground-Truth		
Different Clusters in Ground-Truth	FALSE POSITIVES (FP)	

External Evaluation: Rand Index

n. of pairs	Same Cluster in Clustering	Different Clusters in Clustering
Same Cluster in Ground-Truth		FALSE NEGATIVES (FN)
Different Clusters in Ground-Truth		

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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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- Tries to minimize the internal sum of squared Euclidean distances (Lloyd-Forgy Algorithm)
- Many variants:
  - **K-means++**, **K-medoids** (PAM Algorithm), **BFR K-means**, etc.
- Internal vs. External measures of **clustering quality**