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 → e.g., **K-means**

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- It iteratively repeats **2 steps**:
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    - **Update step** → recompute centroids
- The final output depends on key choices (**local optimum**)

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- **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
- 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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- 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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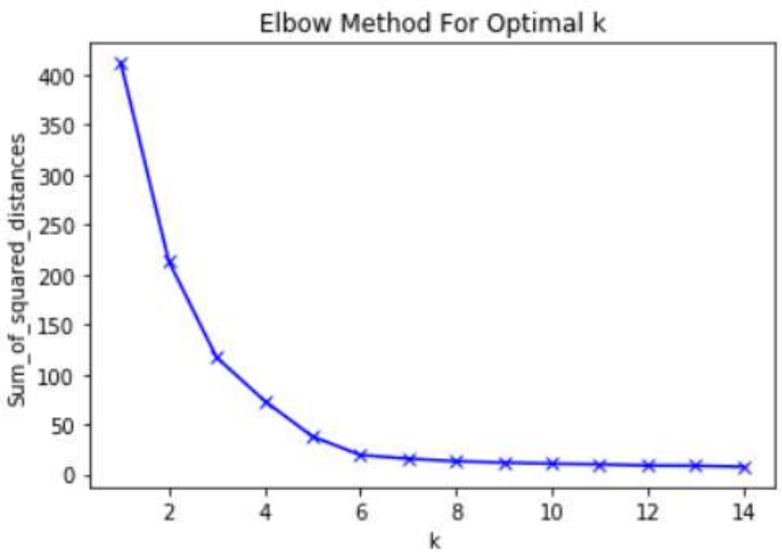

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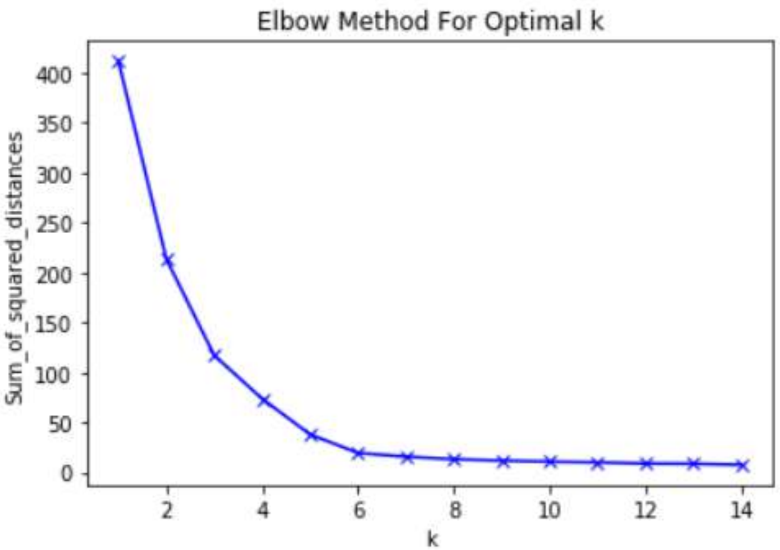

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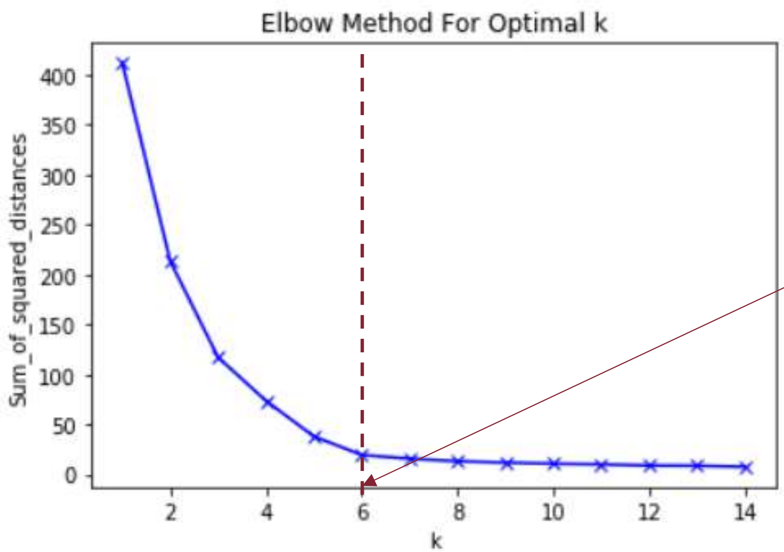

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- The same hard clustering framework can be used with other δ
- Some of them just resemble Euclidean distance, and centroids (i.e., means) still minimize those
  - δ = **Cosine distance** = Euclidean distance on normalized input points
  - δ = **Correlation** = 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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Alternative Formulations: K-medoids

- 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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Measures of Clustering Quality

Clustering Quality

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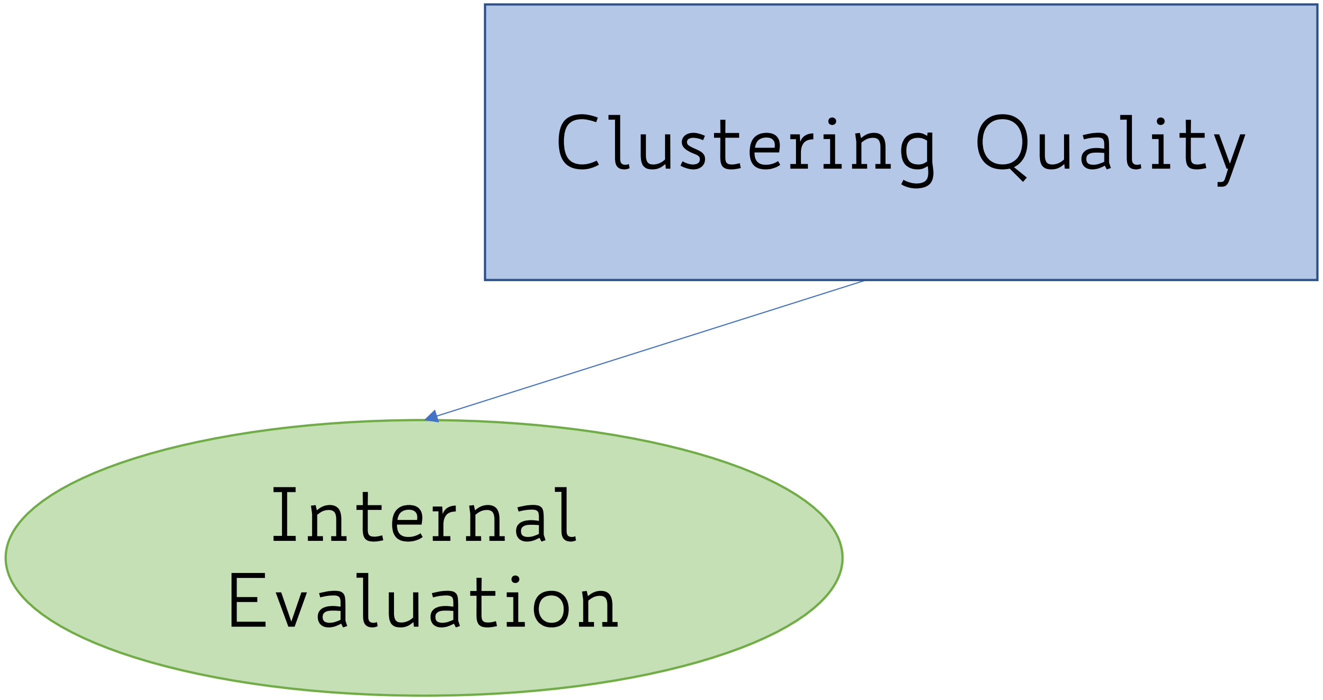

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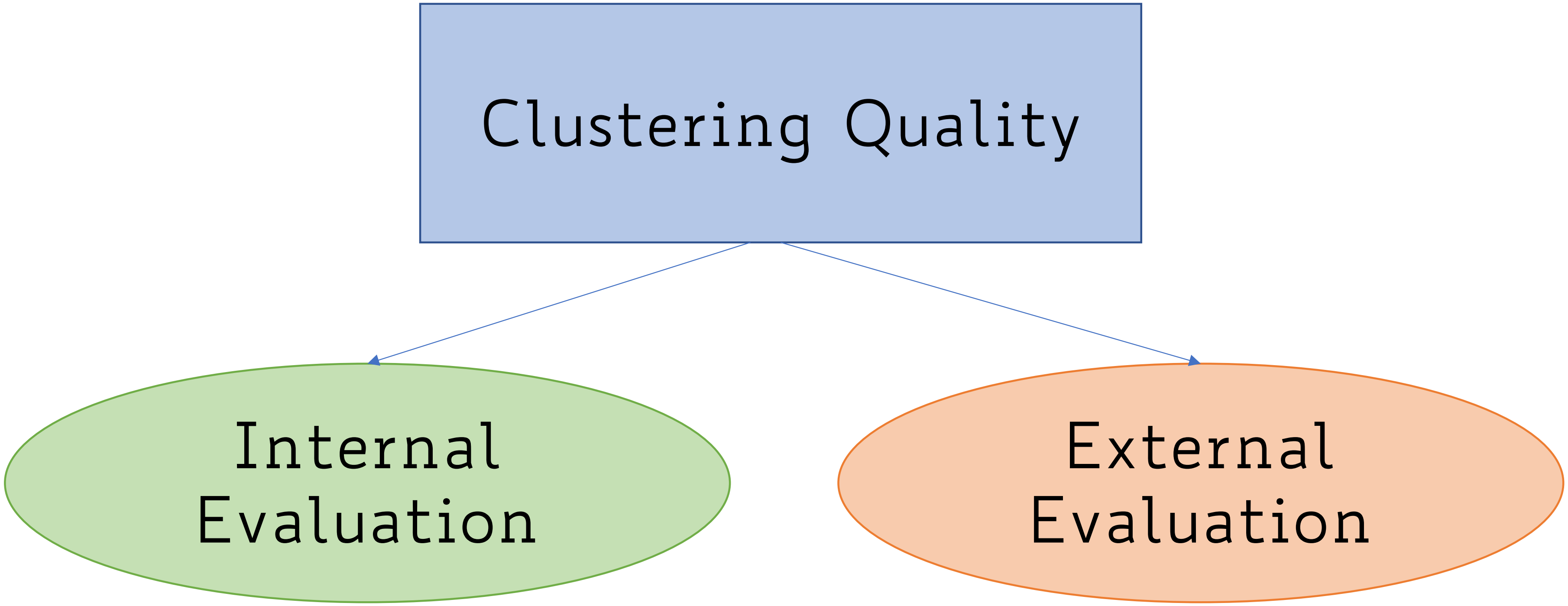

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- A good clustering will produce high quality clusters with:
  - high intra-cluster similarity
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- The measured quality of a clustering depends on
  - data representation
  - similarity measure

Internal Evaluation: Davies-Bouldin Index

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

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

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The smaller the better

Internal Evaluation: Dunn Index

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

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

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

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

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

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- Clustering is evaluated based on data that was not used for clustering, yet pre-classified (**gold standard** data)
- 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

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

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

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

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

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

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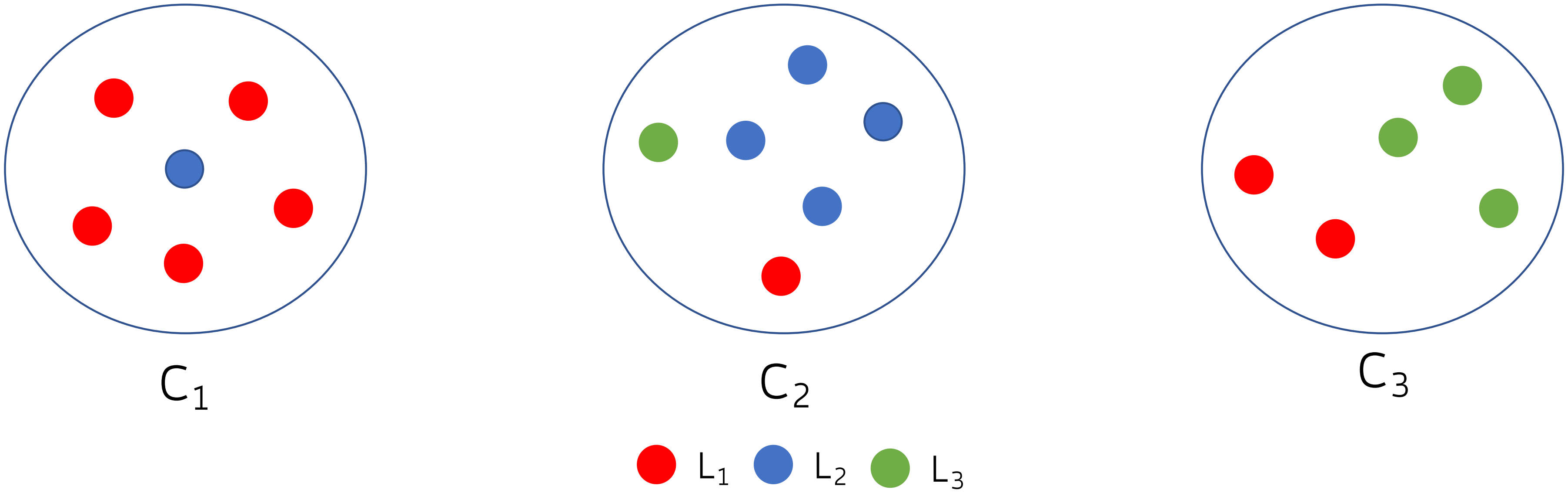
$$\text{purity} = \frac{1}{K} \sum_{i=1}^{K} \text{purity}(C_i)$$

Biased because having as many clusters as items maximizes purity

External Evaluation: Purity Example



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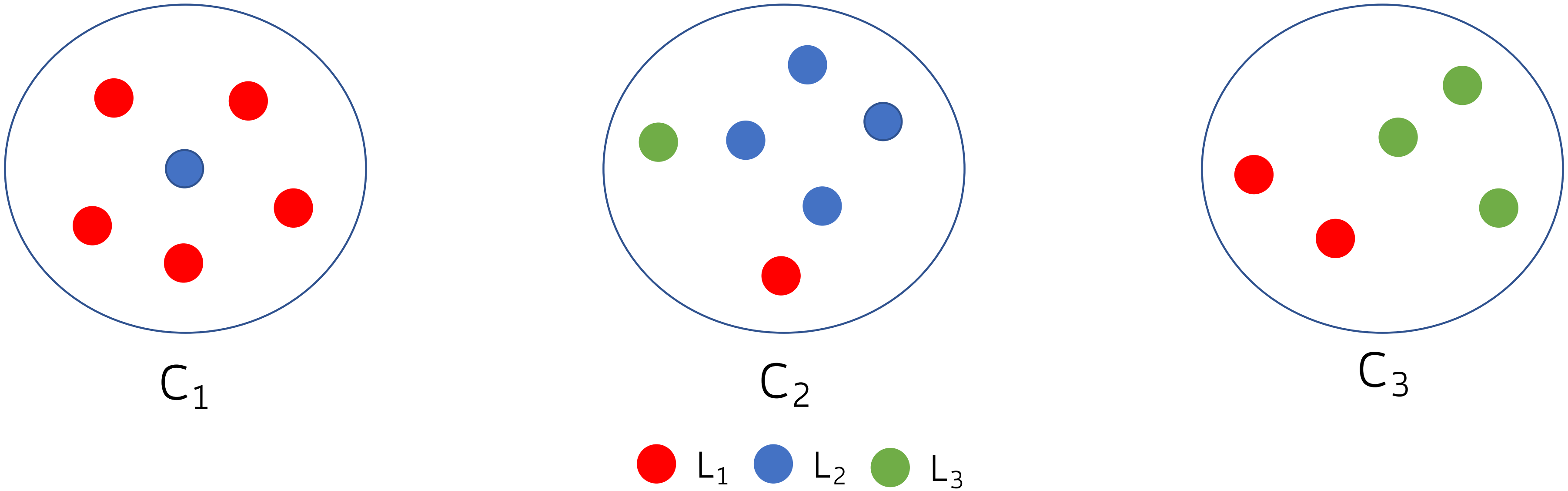

purity(C_1) = 1/6 * max{5, 1, 0} = 5/6

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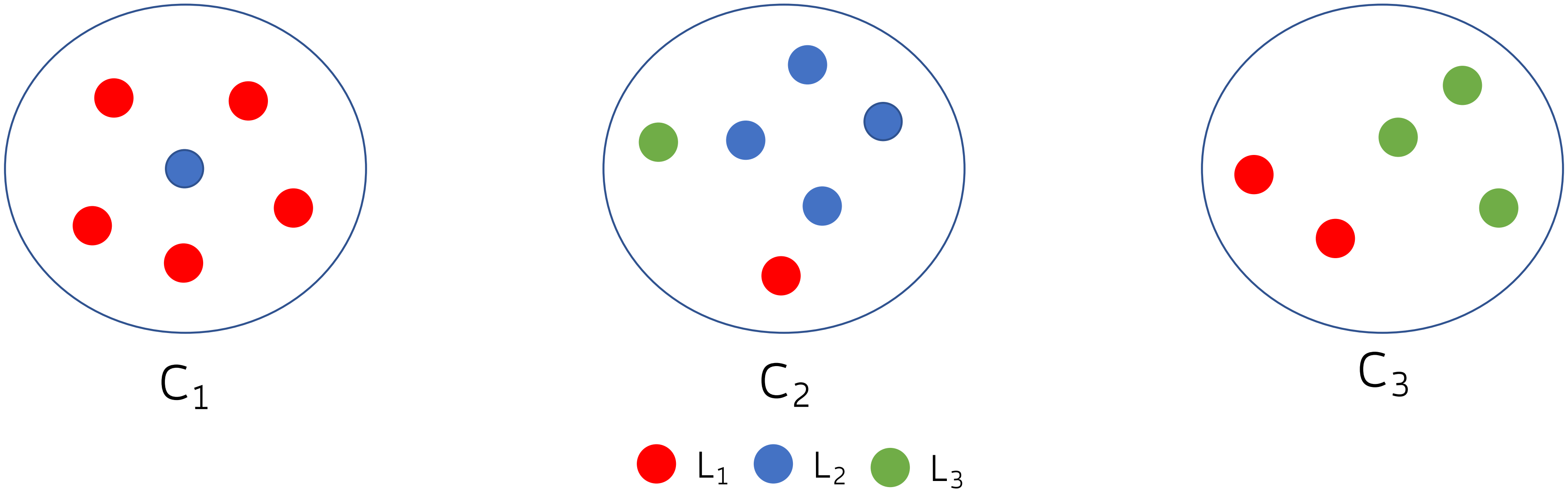

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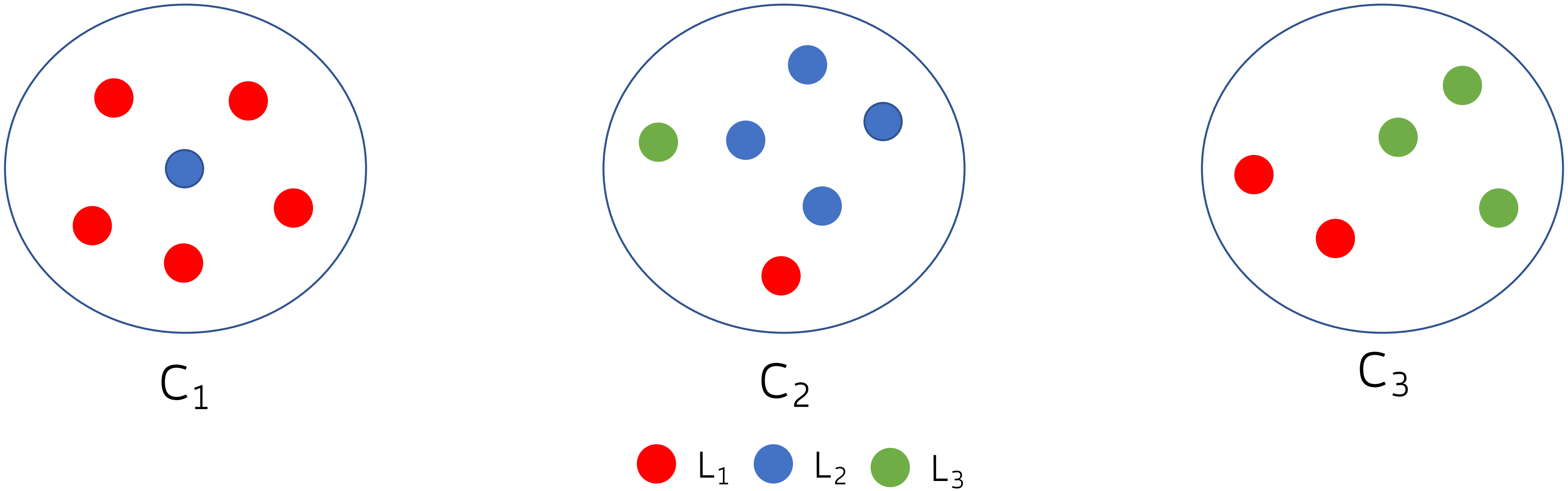

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$\text{purity}(C_3) = 1/5 * \max\{2, 0, 3\} = 3/5$

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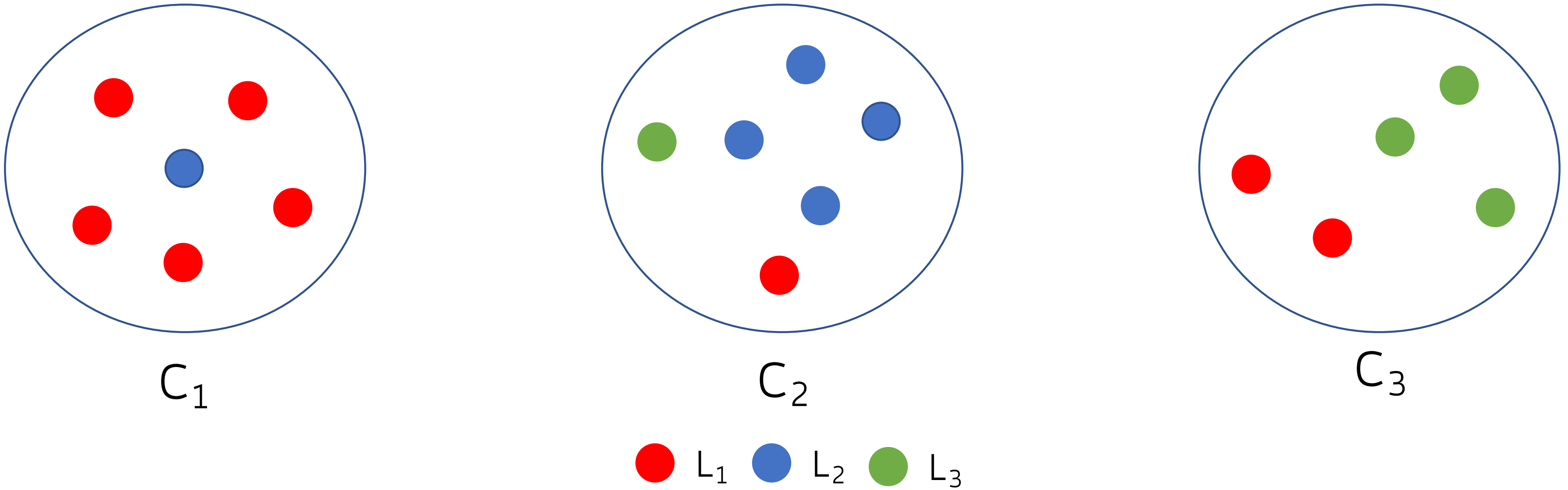

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purity = 1/3 * purity(C_1)+purity(C_2)+purity(C_3) = 7/10

External Evaluation: Rand Index

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

TP = number of *true positives*
TN = number of *true negatives*
FP = number of *false positives*
FN = number of *false negatives*

External Evaluation: Rand Index

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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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Different Clusters in Ground-Truth		TRUE NEGATIVES (TN)

External Evaluation: Rand Index

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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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- Many variants:
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- Internal vs. External measures of **clustering quality**