

Big Data Computing

Master's Degree in Computer Science

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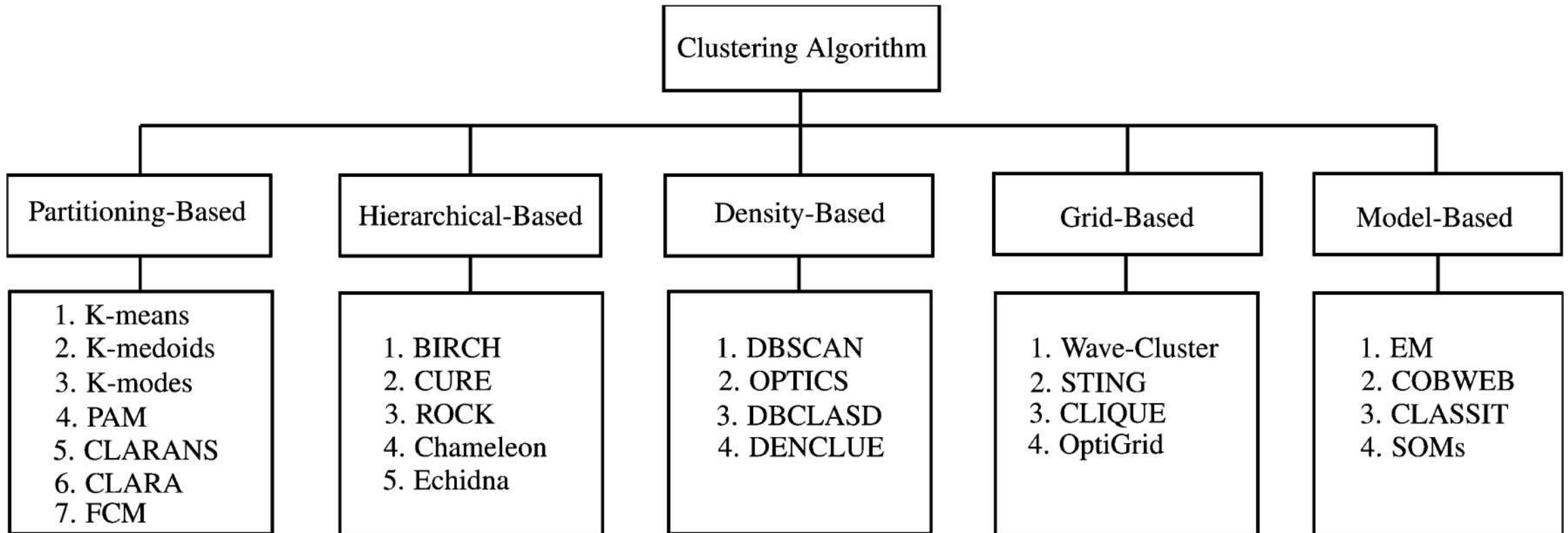
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Recap from Last Lecture(s)

- 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!

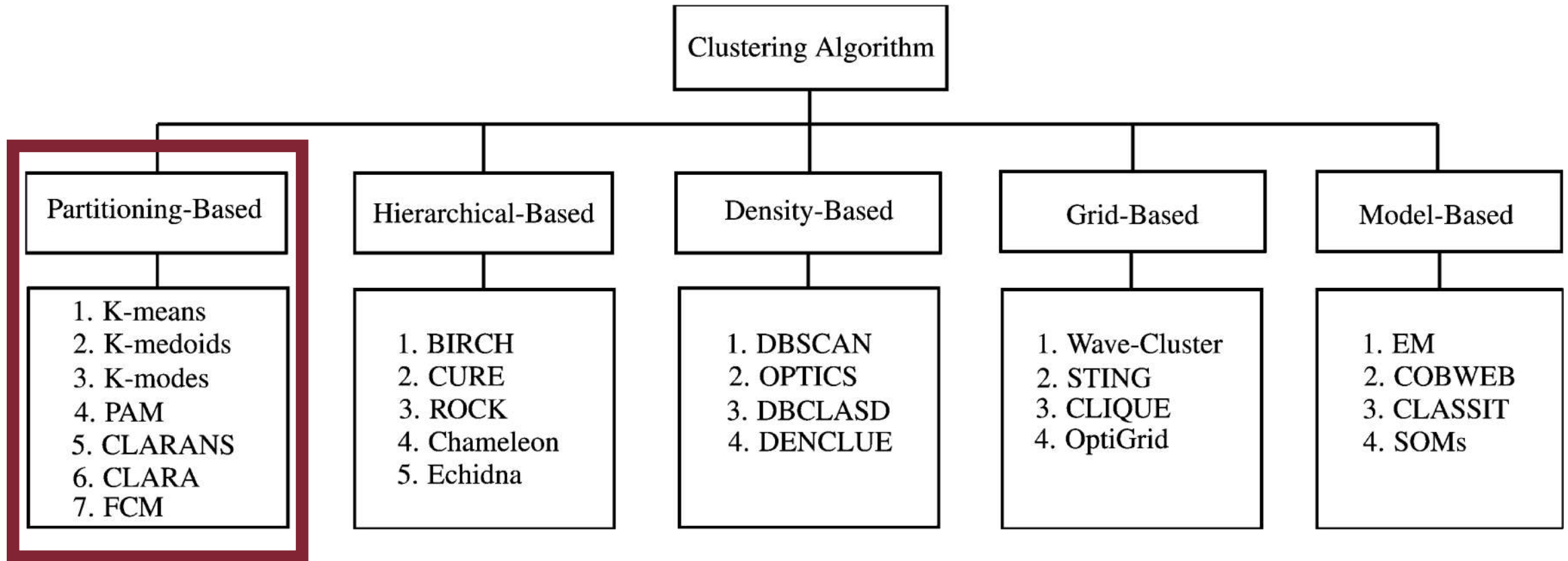
Clustering Algorithms

Clustering Algorithms: Taxonomy



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

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

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Flat Hard Clustering: General Framework

$\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ 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
 $\boldsymbol{\theta}_k$ 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

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

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
- $\Theta = \{\theta_1, \dots, \theta_K\}$ are the cluster representatives
- $\delta(\mathbf{x}_n, \theta_k)$ is a function measuring the distance between \mathbf{x}_n and θ_k

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hard clustering

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

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



NP-hard

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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

Iterative Solution: Lloyd-Forgy Algorithm

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- **Lloyd-Forgy Algorithm**: 2-step **iterative** approximated solution
 - Assignment 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 Θ

$L(\Theta; A)$ fixed Θ 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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Minimize L w.r.t. Θ by fixing A

$L(A; \Theta)$ fixed A parametrized by Θ

We can minimize L by taking the **gradient** of L w.r.t Θ (i.e., the vector of partial derivatives), set it to 0 and solve it for Θ

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$$\nabla L(A; \Theta) = \left(\frac{\partial L(A; \Theta)}{\partial \theta_1}, \dots, \frac{\partial L(A; \Theta)}{\partial \theta_K} \right)$$

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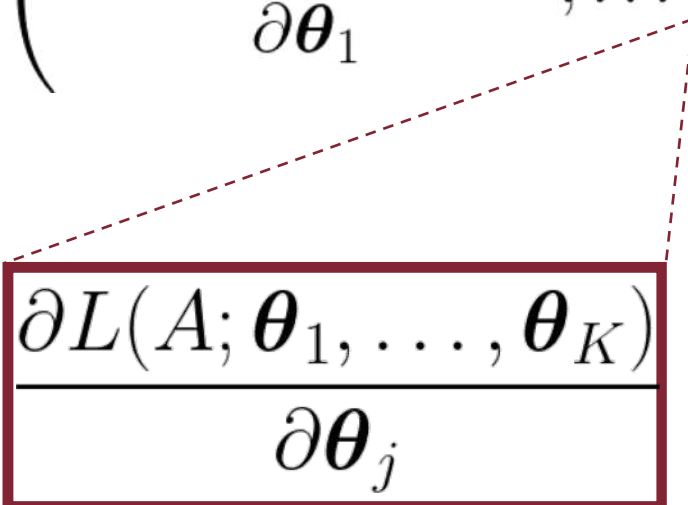
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$$\frac{\partial L(A; \theta_1, \dots, \theta_K)}{\partial \theta_j}$$

The general j -th partial derivative

2-Step Optimization: Update Step

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

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$$\downarrow$$
$$\frac{\partial L}{\partial \theta_j}$$

To make the notation easier!

2-Step Optimization: Update Step

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

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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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- 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

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

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

K-means: Objective Function

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

Euclidean space

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$$\begin{aligned} \delta(\mathbf{x}_n, \boldsymbol{\theta}_k) &= (\|\mathbf{x}_n - \boldsymbol{\theta}_k\|_2)^2 = \\ &= \left[\sqrt{(\mathbf{x}_n - \boldsymbol{\theta}_k)^2} \right]^2 = (\mathbf{x}_n - \boldsymbol{\theta}_k)^2 \end{aligned}$$

Sum of Square Distances
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Minimize L w.r.t. A by fixing Θ

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

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

Compute the gradient w.r.t. Θ , set it to 0 and solve it for Θ

K-means: Update Step

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

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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

$$\begin{aligned} \sum_{n=1}^N -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k^*) &= 0 \Leftrightarrow \\ 2 \sum_{n=1}^N \alpha_{n,k} \boldsymbol{\theta}_k^* &= 2 \sum_{n=1}^N \alpha_{n,k} \mathbf{x}_n \\ \boldsymbol{\theta}_k^* \sum_{n=1}^N \alpha_{n,k} &= \sum_{n=1}^N \alpha_{n,k} \mathbf{x}_n \end{aligned}$$

K-means: Update Step

$\boldsymbol{\theta}_k^*$ does not depend on N,
therefore it can be factored out

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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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- 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

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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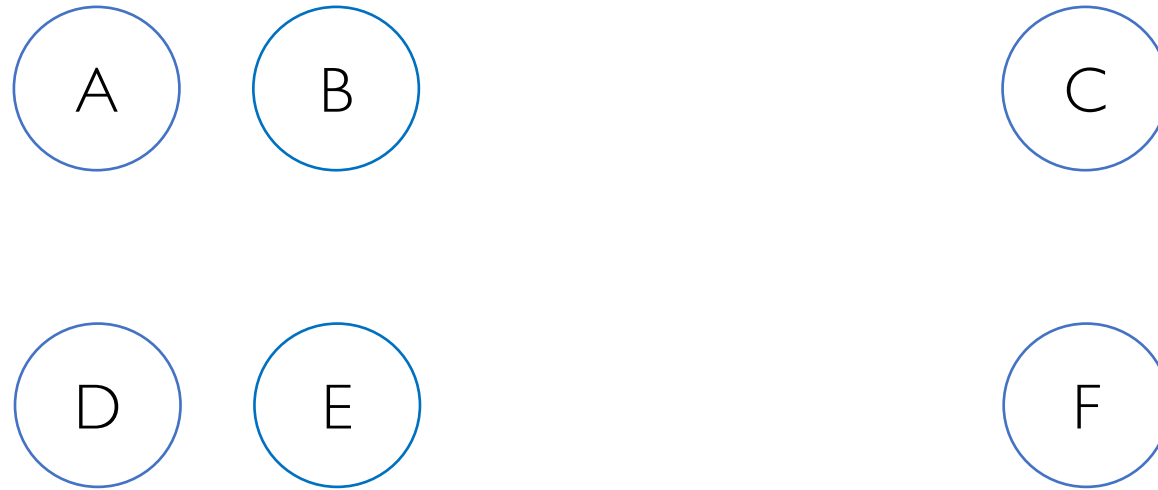
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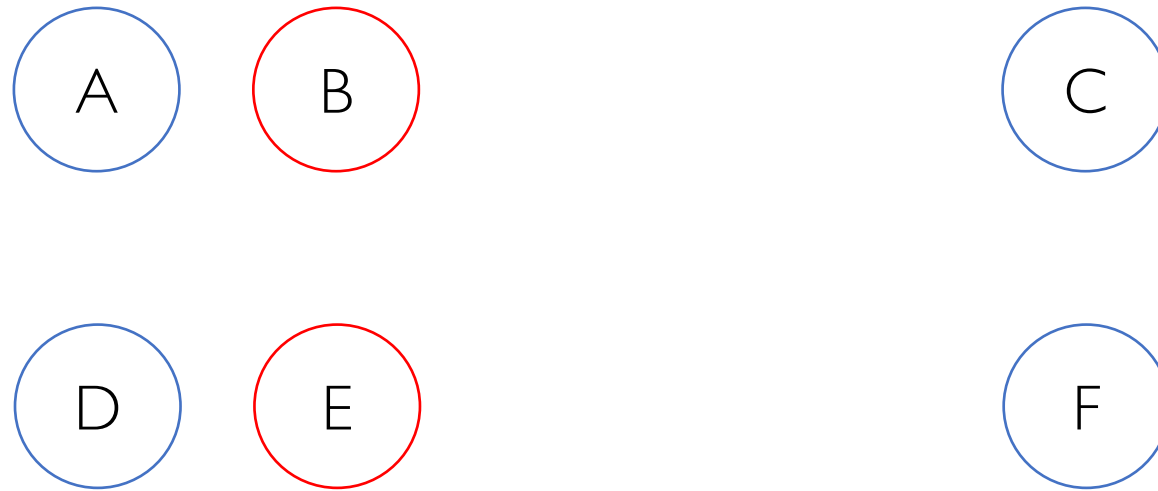
Problem Mitigation:

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

K-means: Seed Choice

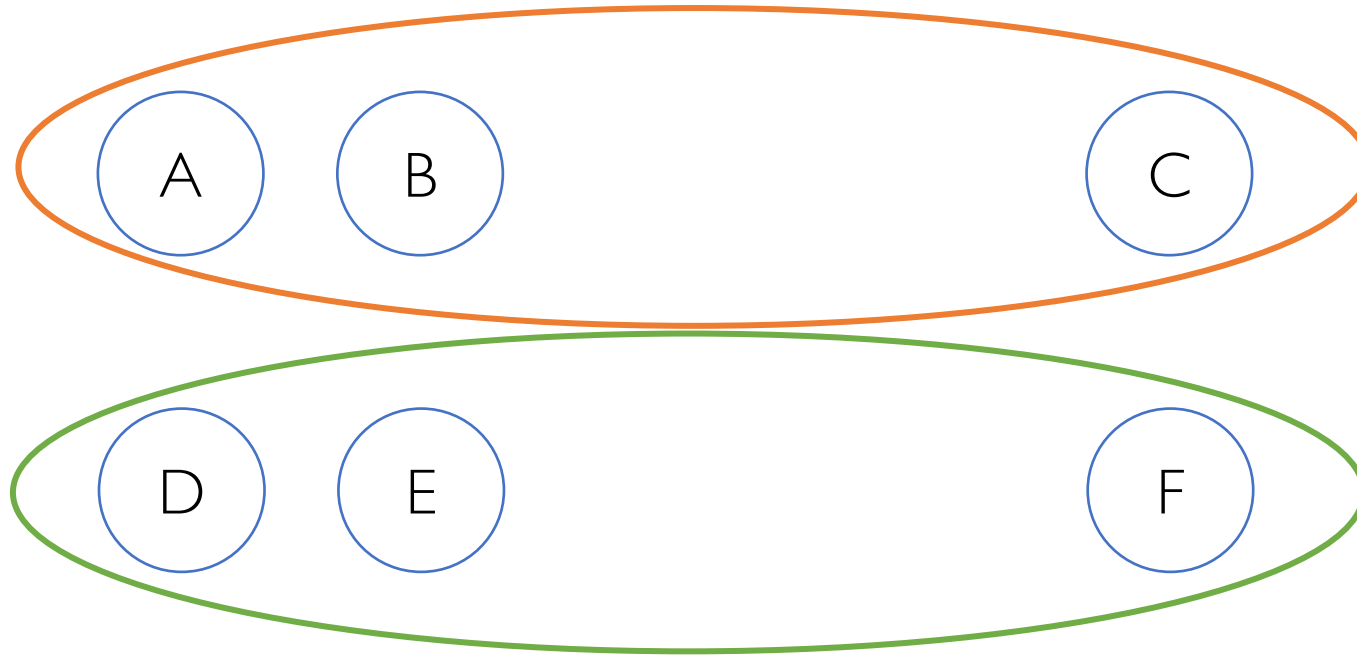


K-means: Bad (Unlucky) Seed Choice



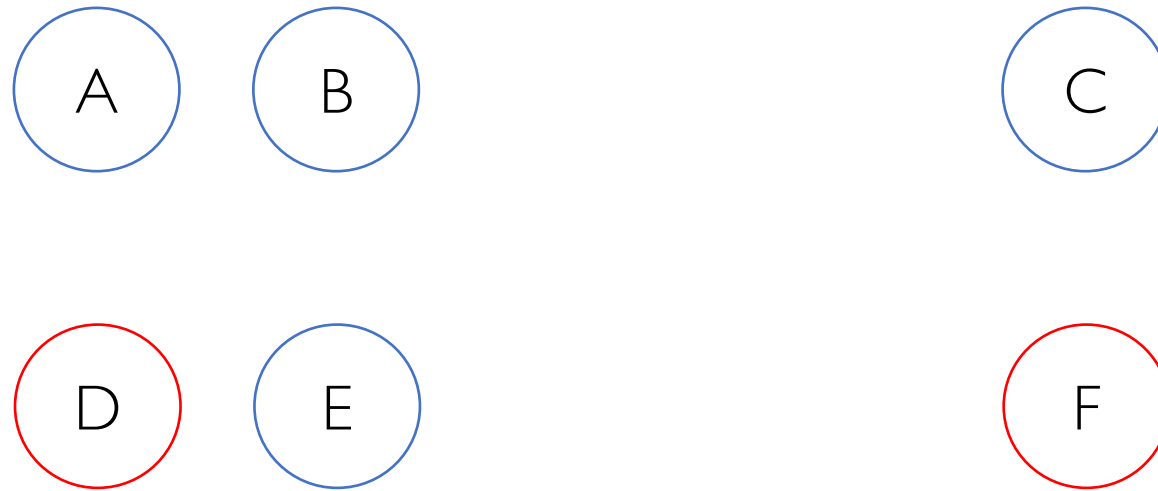
If B and E are randomly chosen as initial centroids...

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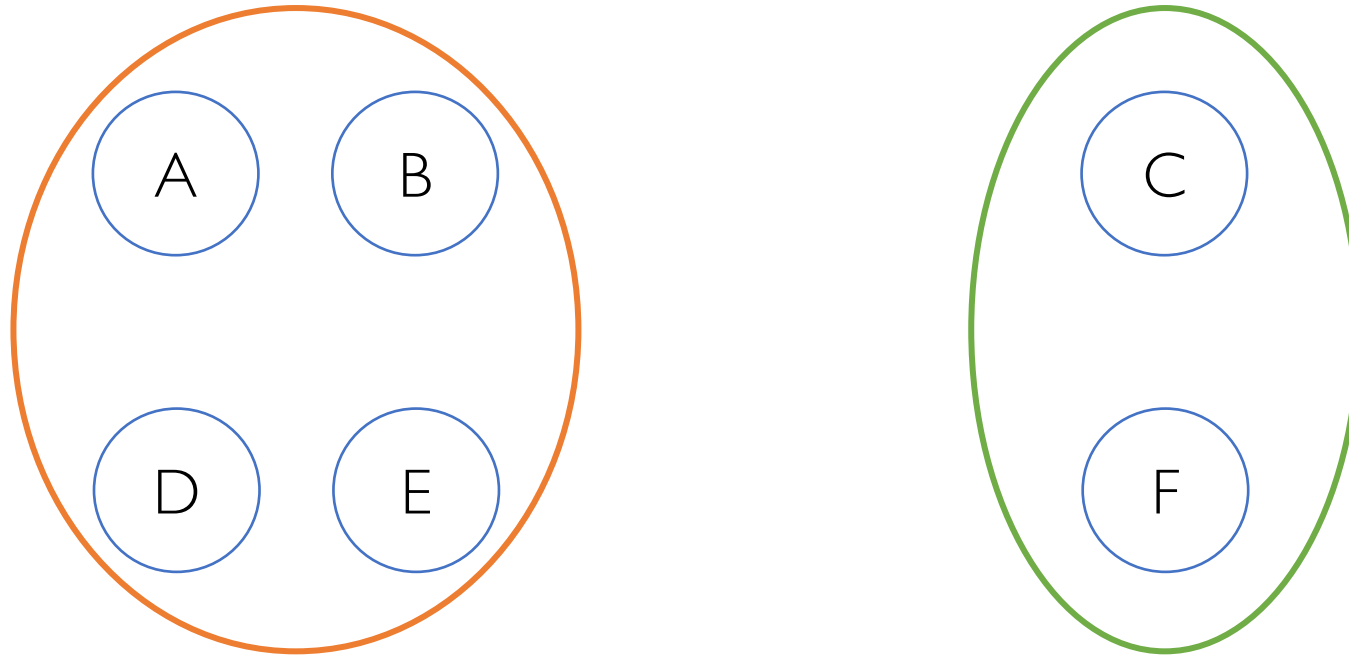
The algorithm converges to the sub-optimal clustering above

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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- 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

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- 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

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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

K-means: "Elbow" Method

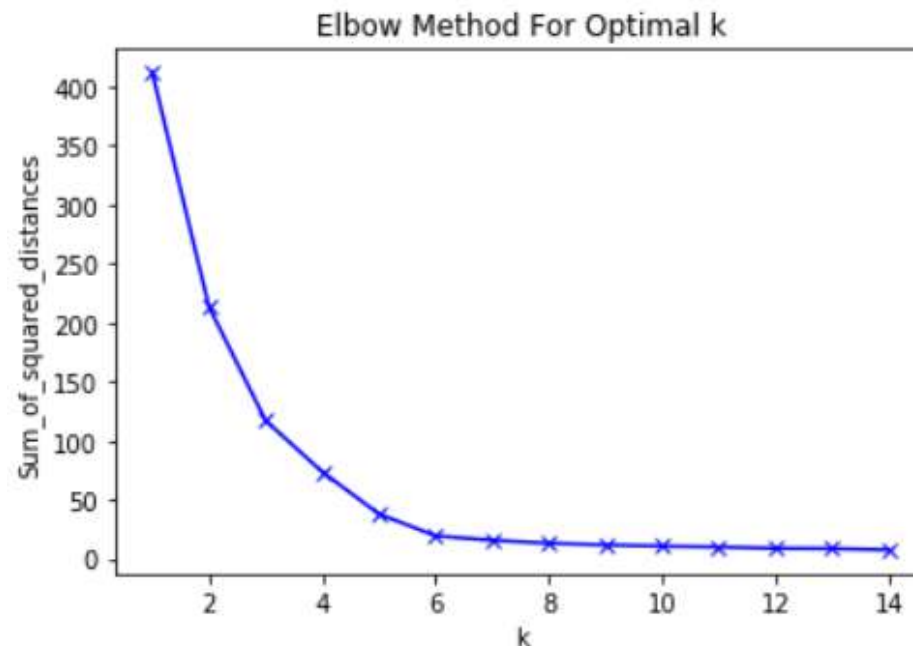
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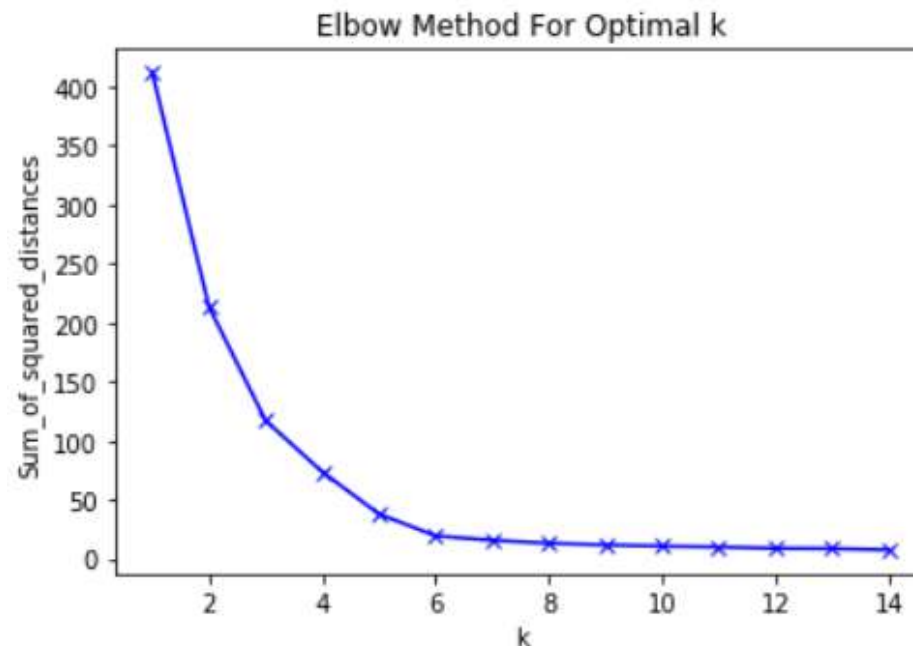
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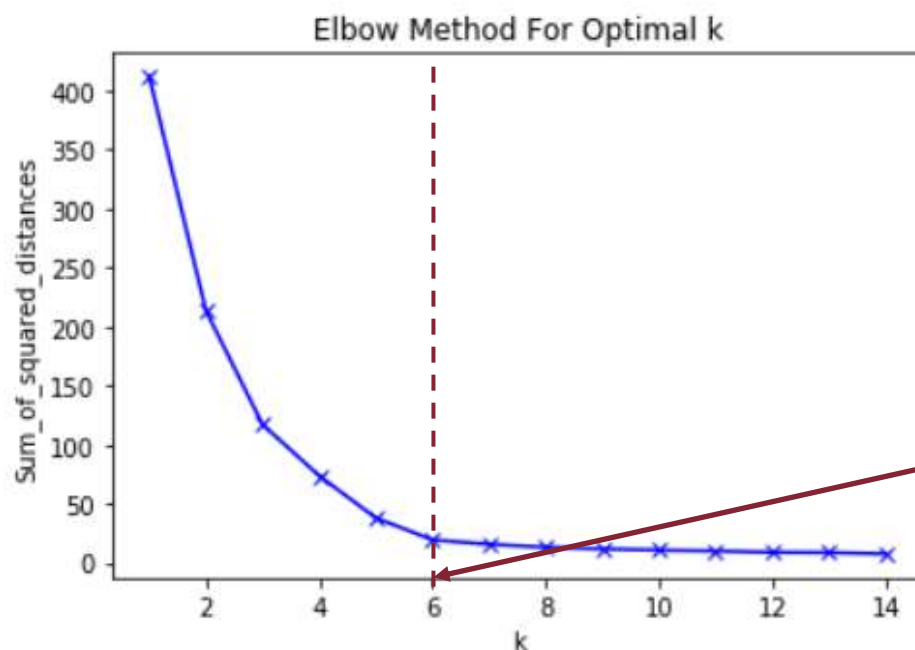
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up to a certain value

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- Others, require specific minimizers
 - $\delta = \text{Manhattan distance}$ (L^1 -Norm) \rightarrow 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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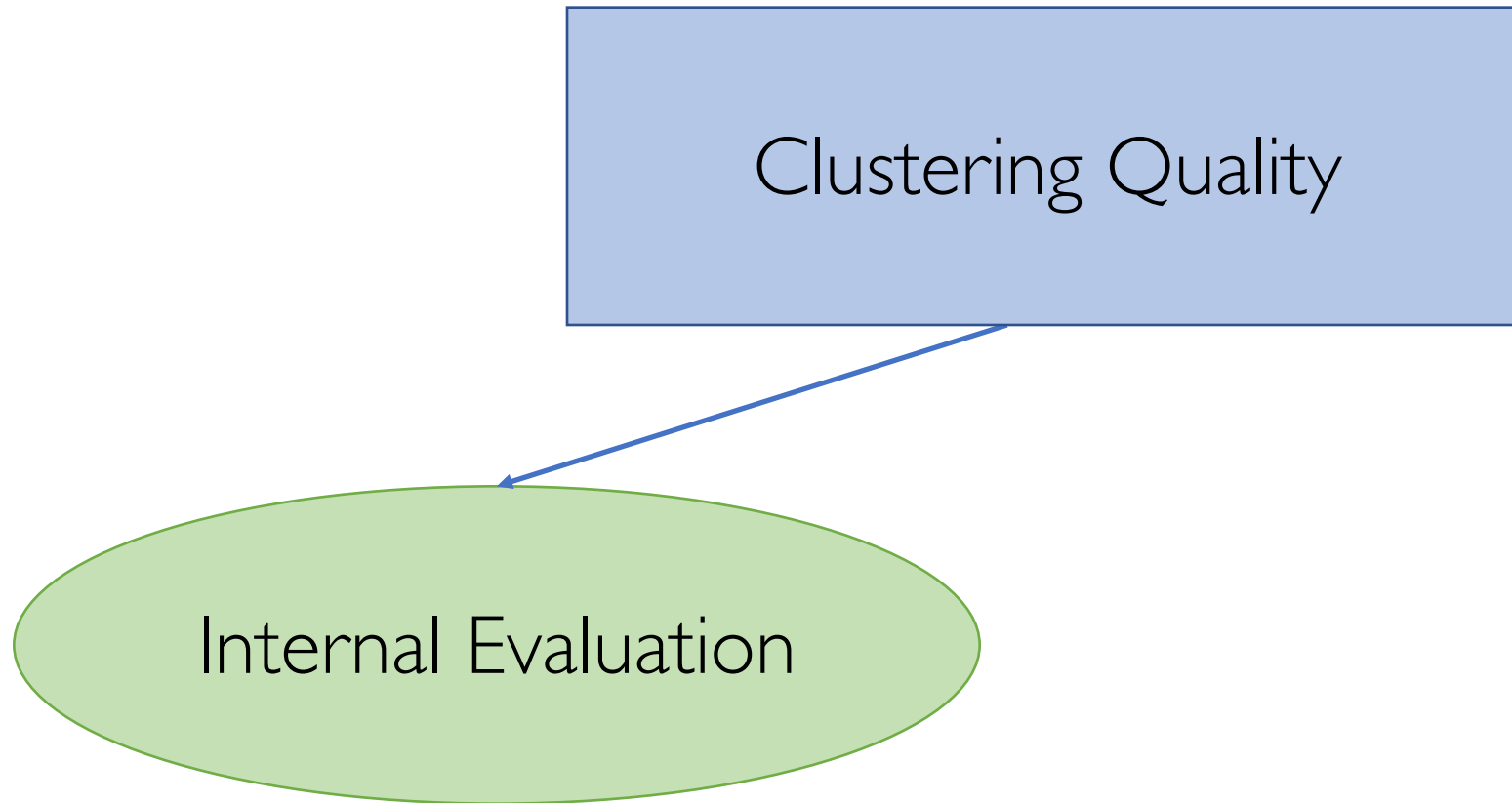
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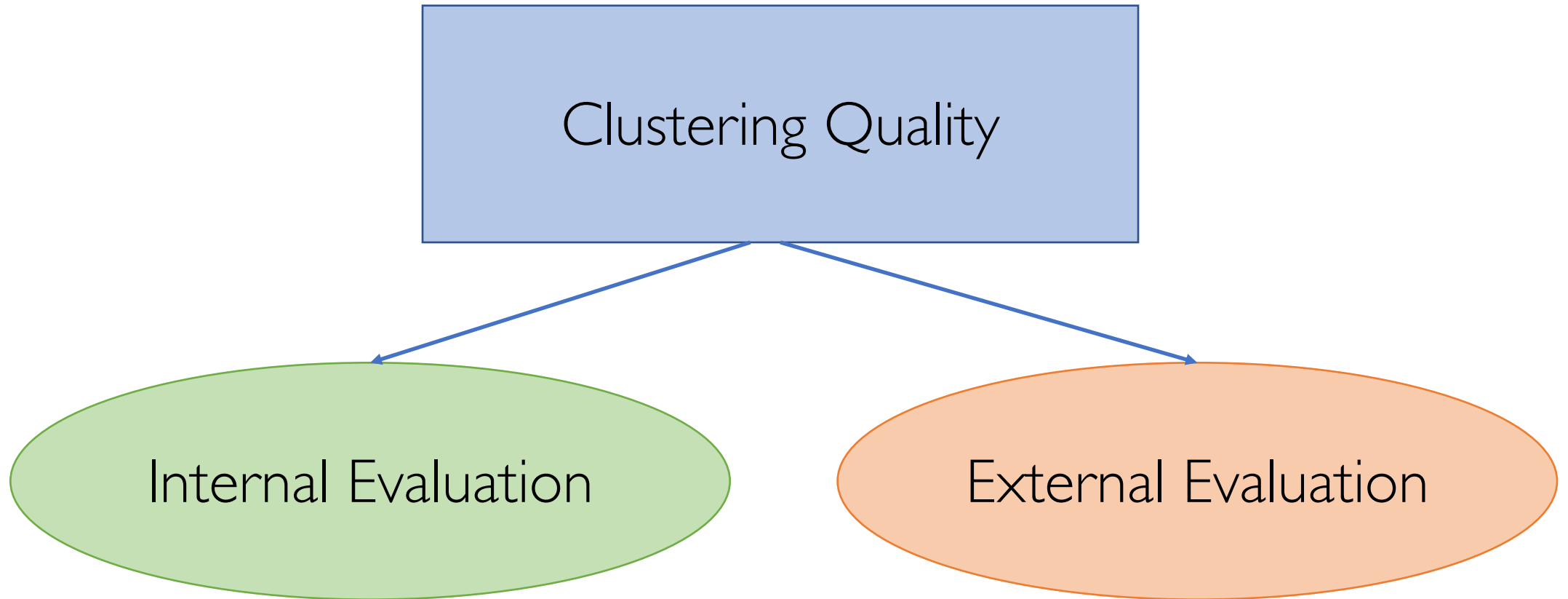
Measures of Clustering Quality

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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

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

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 = 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

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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- 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

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

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

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

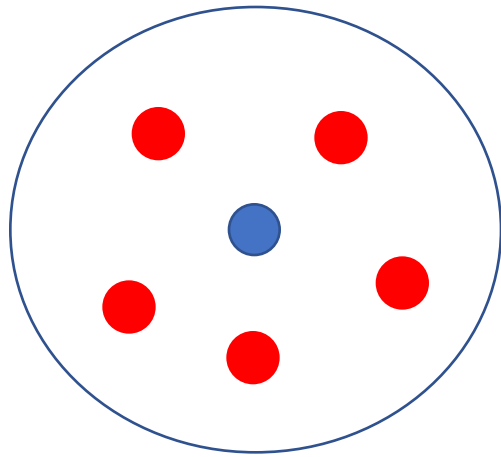
$n_i = \sum_{j=1}^J n_{i,j}$ number of items clustered in C_i

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

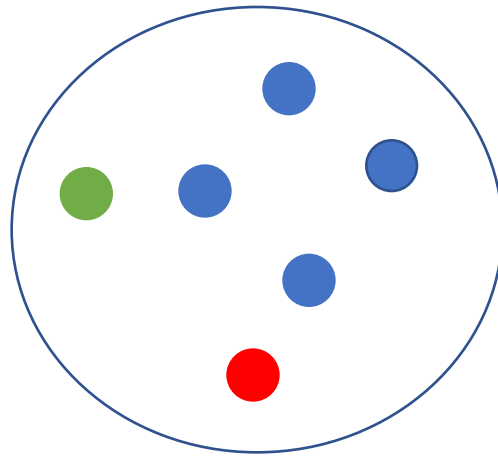
$$\text{purity} = \frac{1}{K} \sum_{i=1}^K \text{purity}(C_i)$$

Biased because having as many clusters as items maximizes purity

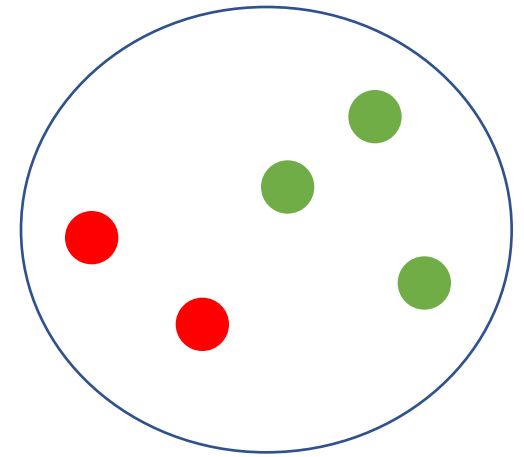
External Evaluation: Purity Example



C_1



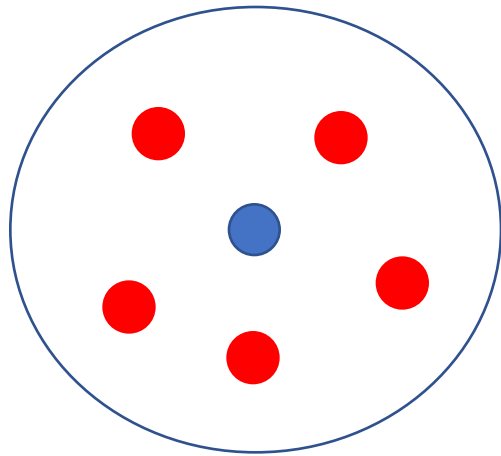
C_2



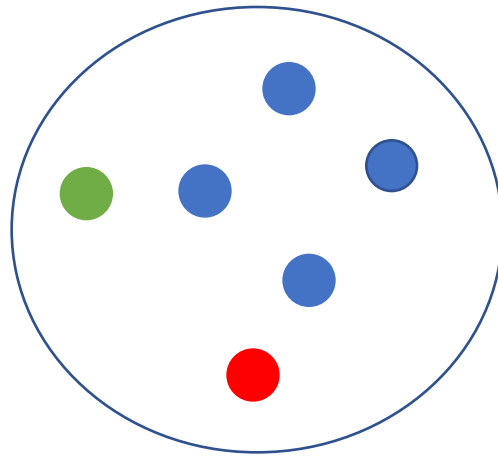
C_3

● L_1 ● L_2 ● L_3

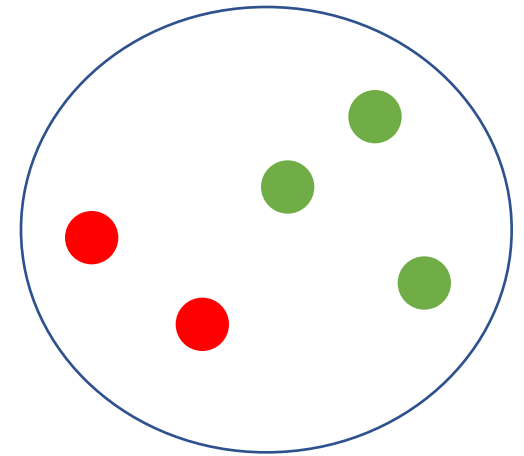
External Evaluation: Purity Example



C_1



C_2

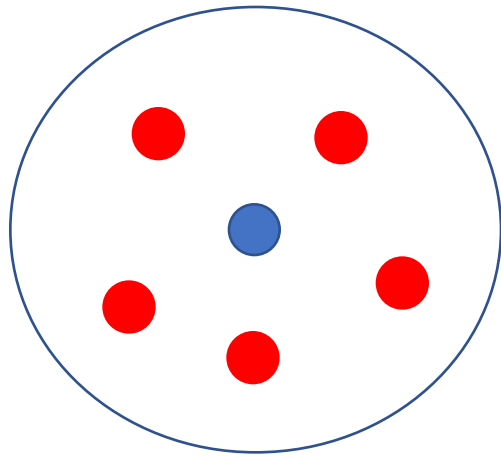


C_3

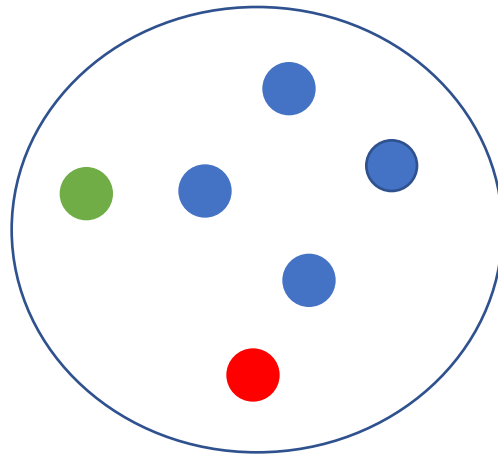
● L_1 ● L_2 ● L_3

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

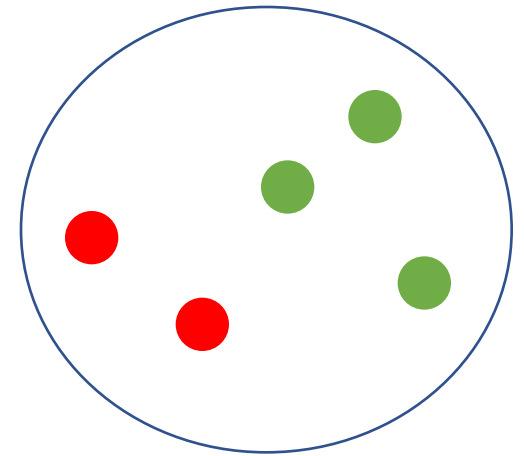
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C_1



C_2



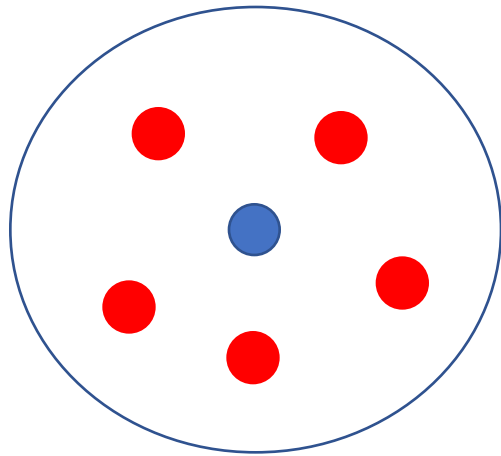
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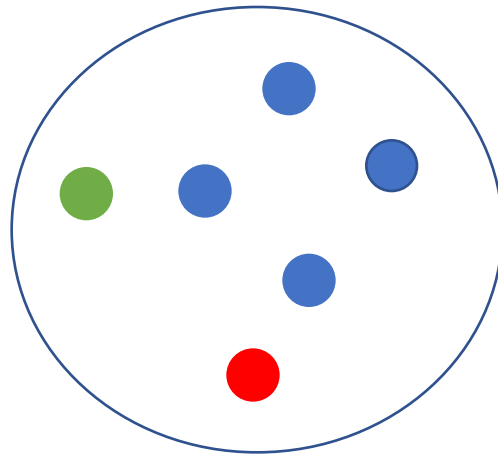
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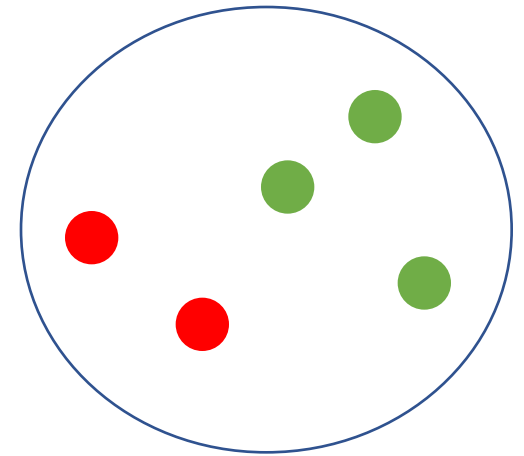
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C_1



C_2



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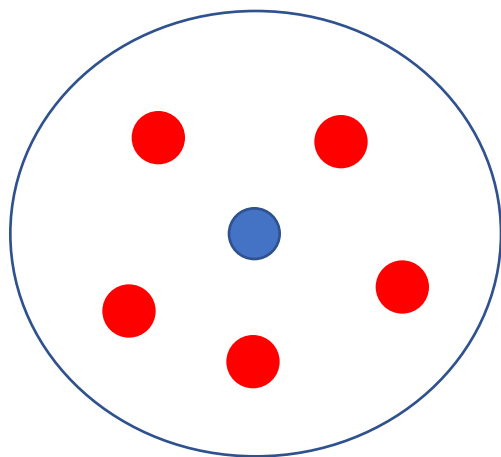
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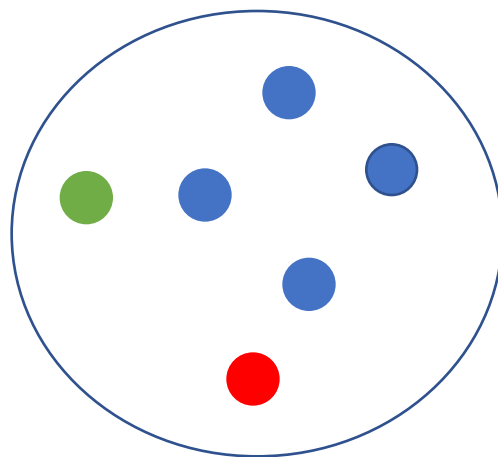
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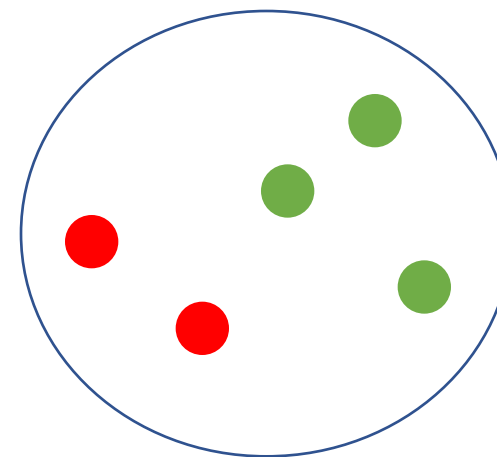
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C_2



C_3

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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 = number of *true positives*

TN = number of *true negatives*

FP = number of *false positives*

FN = number of *false negatives*

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 β

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**