Clustering

- Clustering: Definition, Consideration and Applications
- Point Assignment Methods: k-Means, k-Medoid, k-Mode, PAM
- Agglomerative Clustering
- Validation: Homogeneity and Completeness
- Evaluation: Compactness, Separation, Clustering co-belonging matrix
- External Measures: Purity, Conditional Entropy, Rand Index
- Internal Measures: WSS, BSS, Silhouette coefficient
  - Statistical Significance of Internal Measures

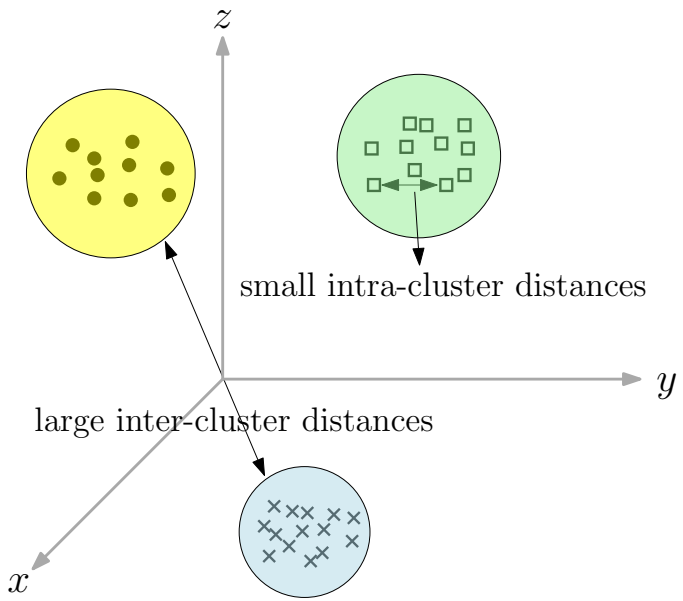
Imdad ullah Khan

Clustering: Definition

Clustering/cluster analysis/data segmentation

Grouping of objects into clusters such that objects in the same cluster are more similar and objects in different clusters are less similar

- Intra-cluster distances (between pairs of points in the same cluster)
- Inter-cluster distances (between pairs of points in different clusters)



Clustering: Definition

- The clustering hypothesis: Points in the same cluster behave similarly with respect to information needs
- Clustering is an unsupervised task, there is no right answer
- There is not even the right number of clusters

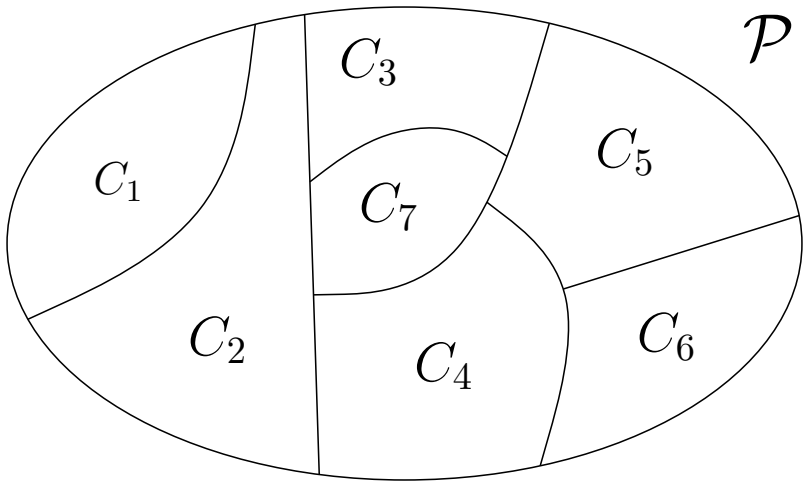
Clustering: Consideration

- Partitioning Level
  - Single level or multi-level (hierarchical partitioning)
  - Some times multiple levels of partitioning are required
    - Students partitioned by schools, by major/minor, even further by CGPA
    - Books in a library clustered into subject areas, topics, sub-topics
- Exclusive or Non-Exclusive Clustering
  - Can points belong to more than one clusters (are clusters intersecting)
  - In social networks typically we get overlapping communities
- Similarity Measure
  - What is type of data, what similarity measure to be used
  - Similarity measure should reflect the inherent grouping in data
- Clustering Space
  - Are all attributes of data points are to be considered (full space)
  - Clustering based on a subspace, e.g. for clustering students based on performance, gender and address info can be ignored

Clustering: Definition

Generally, clustering produces a partition $[C_1, C_2, \ldots, C_k]$ of the dataset $\mathcal{P}$

- Each $C_i \subseteq \mathcal{P}$
- For $i \neq j$, $C_i \cap C_j = \emptyset$
- $\bigcup_{i=1}^{k} C_i = \mathcal{P}$



Clustering: Definition

Generally, clustering produces a partition $[C_1, C_2, \ldots, C_k]$ of the dataset $\mathcal{P}$

Broadly two different ways of clustering depending on input

Input: Given a dataset (feature vectors) and a proximity measure

Output: Clusters of the dataset into k clusters

Alternatively,

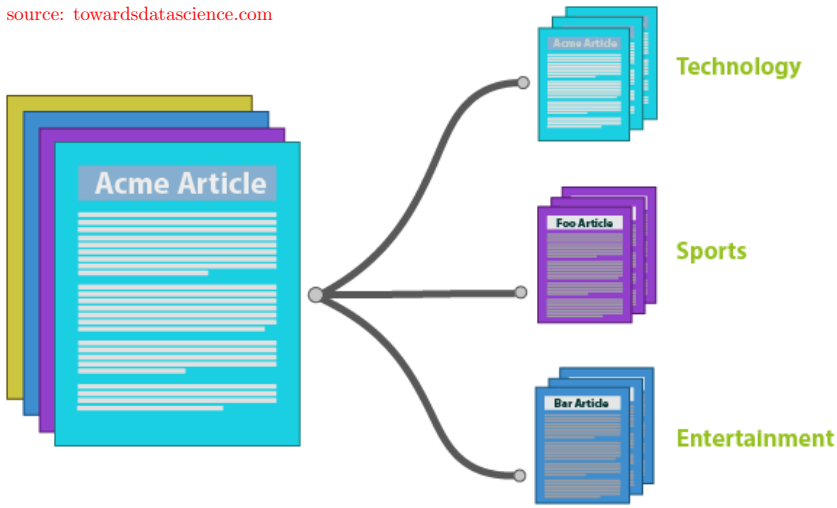
Input: Given pairwise proximity values for a (abstractly described) dataset (e.g. distance or similarity matrix)

Output: Clusters of the dataset into k clusters

The number of clusters k may or may not be part of the input (fixed)

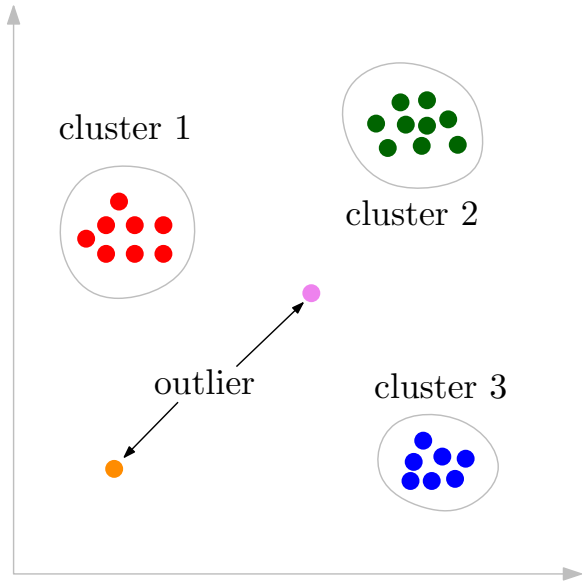
Documents Clustering

- Group documents based on their similarity with other documents
  - document similarity computed from theirTF-IDF vectors
- Documents about same topic or written by same author ideally would form a cluster
  - e.g. sports, politics, entertainment, news
- Benefits: reduces search space, improves search and retrieval cost



Outlier Detection

- Outliers are substantially different from other objects in a dataset
- Identify objects that do not belong to a cluster (or the object itself is a cluster)
- Benefits: fraud detection in financial transactions, data cleaning



Clustering: Applications

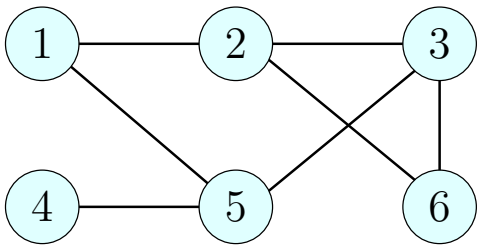
Market Segmentation/ Business Intelligence

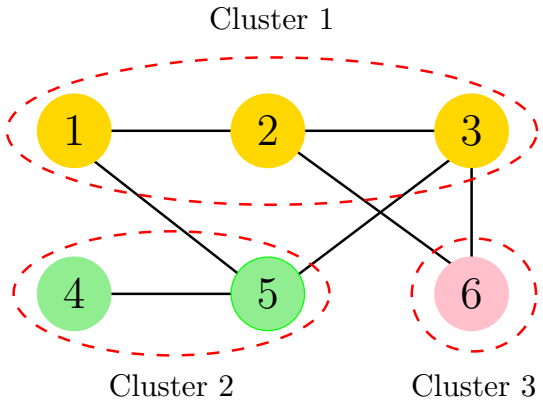
- Subdivide customers into distinct subsets
  - Customers in same subset share common characteristics
- Each subset can be target of different marketing campaigns
- Based on the target, use appropriate proximity measures
  - purchasing history, age, salary, nature of job etc.

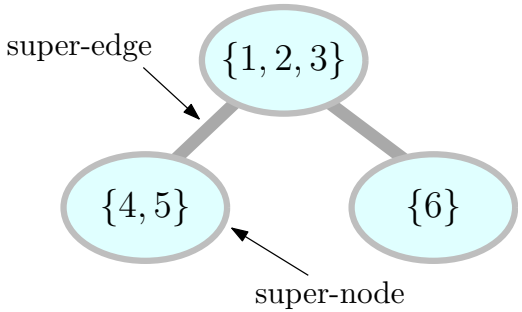
source: medium.com

Data Compression and Graph Summarization

- Make clusters of nodes in a graph
  - Each cluster corresponds to a super node in the graph
- Efficient storage, transmission, processing and analysis of graphs







Basic Clustering Methods

- Clustering methods can be categorized into
  - Distance Based
  - Density and grid-based
  - Generative Model based
  - Other methods used for specific data types
    - e.g. for graph data we used connectivity based clustering

Different methods may generate different clusterings of the same data set

Distance based Clustering

Assumes a meaningful proximity measure is defined over the dataset $\mathcal{P}$

Distance based clustering algorithms can be categorized into

1. Point assignment based methods
   - Require points as feature vectors and the distance measure
   - Assume that number of required clusters k is provided
   - Produces a single level partition of $\mathcal{P}$ into k parts
2. Hierarchical methods
   - Can work with the pairwise distance matrix without explicit points representation or the definition of distance measure
   - Produces multi-level partitions of $\mathcal{P}$
   - Does not require number of clusters k as input
   - Can be further categorized into
     - Agglomerative methods (Bottom-Up Approach)
     - Divisive methods (Top-Down Approach)

Point Assignment Based Clustering

k-Partition Problem

- Given a set of n points, $\mathcal{P} \subset \mathbb{R}^m$ and $k \in \mathbb{Z}$, number of clusters
- Assume Euclidean distance measure over $\mathcal{P}$ ▷ ℓ_p, cosine can be used
- For a subset $C_i \subseteq \mathcal{P}$, denote by $\mathbf{c}_i$ the **centroid** of C_i

$$\mathbf{c}_i := \frac{1}{|C_i|} \sum_{x \in C_i} x$$

- Centroid is the arithmetic mean of m-dim vectors (coordinate-wise mean)
- Goodness of a k-partition $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ is measured by

$$\text{sum of squared error,} \quad SSE(\mathcal{C}) = \sum_{i=1}^{k} \sum_{x \in C_i} \|x - \mathbf{c}_i\|^2$$

also called Within SSE

- **Problem:** Find a k-partition $\mathcal{C}^*$ of $\mathcal{P}$ with minimum SSE
- Brute force approach (try all partitions) is not feasible

k-means Algorithm

- A basic greedy algorithm for the k-Partition problem

Algorithm : k-means algorithm $(\mathcal{P}, k)$

Select k random points as initial centroids

▷ Alternatives of centroids can be used

while Stopping criterion is not met **do** ▷ Many choices

Assign each point $x \in \mathcal{P}$ to the centroid closest to x

▷ closeness w.r.t the similarity measure

▷ Assignment Step

Compute the centroids of (modified) clusters

▷ Refitting Step

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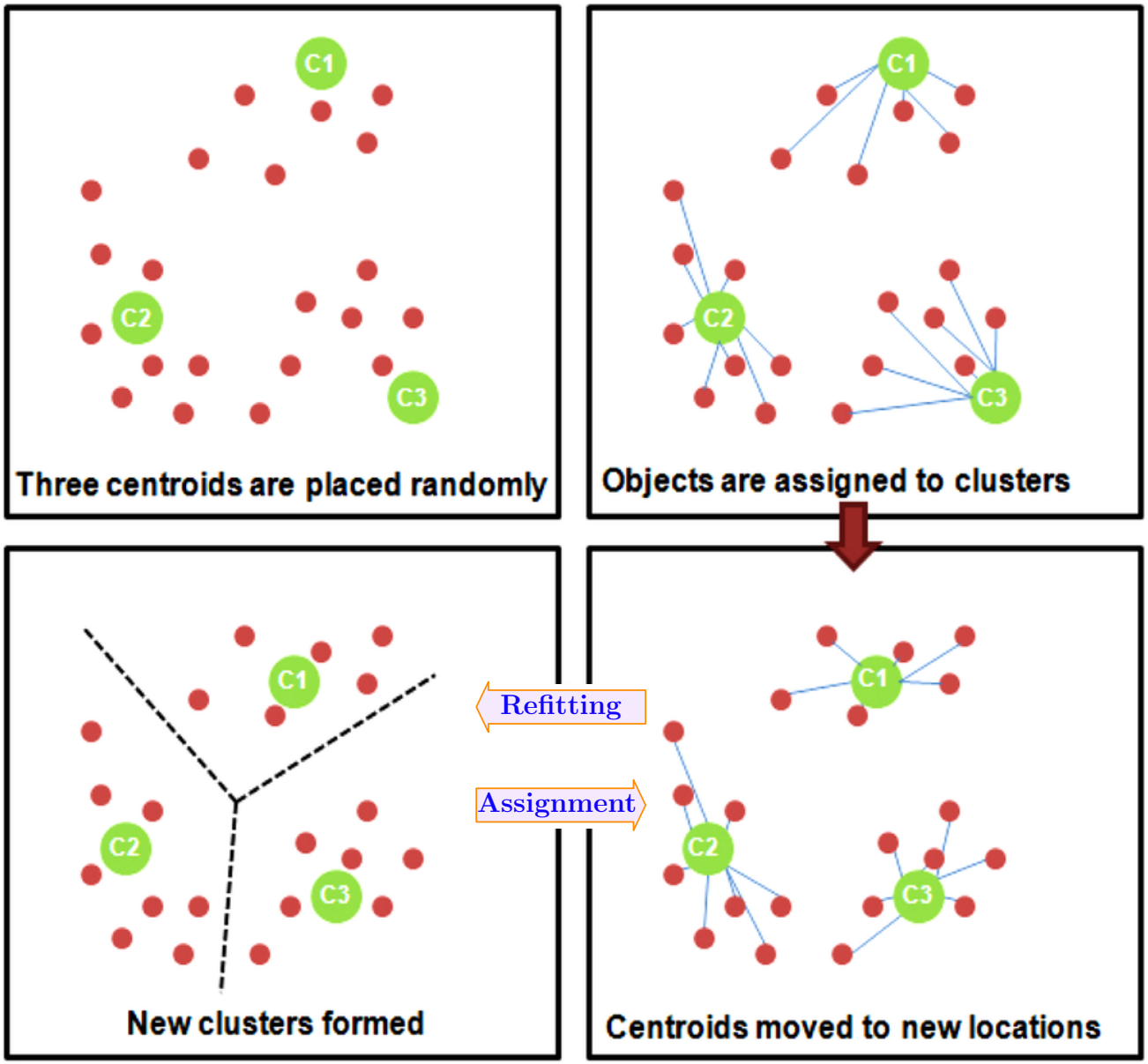
k-means Algorithm: Illustration



k-means Algorithm: Runtime

Algorithm : k-means algorithm $(\mathcal{P}, k)$

Select k random points as initial centroids ▷ Alternatives of centroids can be used
while Stopping criterion is not met **do** ▷ Many choices
  Assign each point $x \in \mathcal{P}$ to the centroid closest to x
  ▷ closeness w.r.t the similarity measure
  Compute the centroids of (modified) clusters

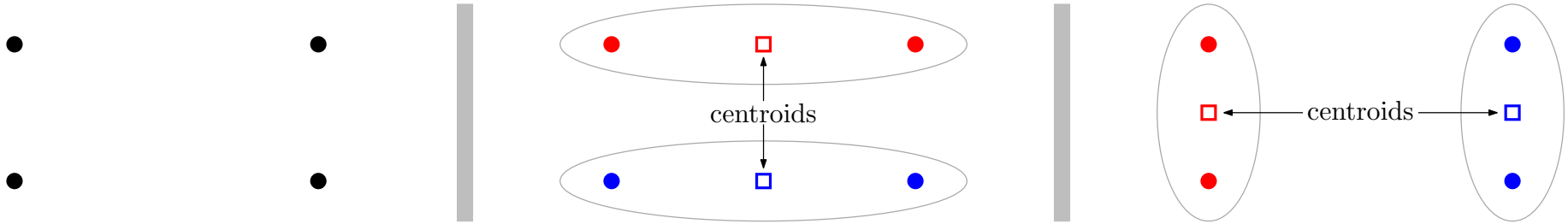
- Each iteration: $O(nk)$ distance computations
  - For each $x \in \mathcal{P}$ compute distances to centroids and find closest
- Recompute centroids: in total takes $O(n)$ time
- number of iterations is $t \implies$ total runtime is $O(tkn)$
- t depends on the stopping rule, generally, $t, k \ll n$
- Total time: $O(n)$ distance computations ▷ very efficient

k-means Algorithm: Stopping Criteria

- A clustering with smaller SSE than another is not necessarily better
- SSE depends on the value of k
  - $k = n \implies SSE = 0$
  - In general large $k \implies$ small SSE
- Stopping criterion could be
  - Stop when there is minimal (less than a threshold) change to SSE
  - Stop when no change in centroids
  - Stop when few points (less than a threshold) change their centroids

k-means Algorithm: Initial k centers

Quality of final clustering critically depends on initial centroids



Different initial centers lead to different clustering, maybe very suboptimal

k-means Algorithm: Initial k centers

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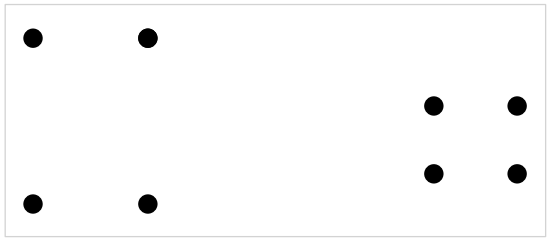
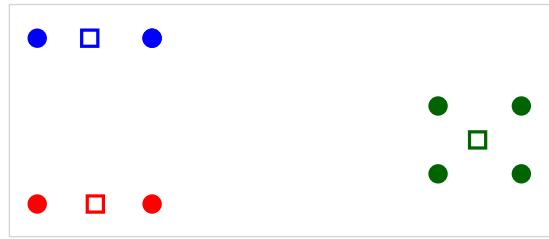




Different initial centers lead to different clustering, maybe very suboptimal

k-means Algorithm: Initial k centers

Quality of final clustering critically depends on initial centroids

k-means Algorithm: Initial k centers

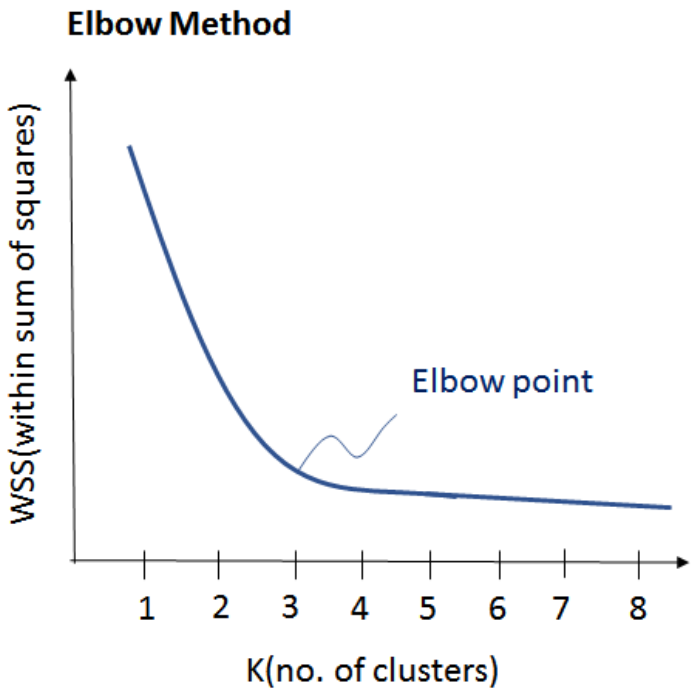
Quality of final clustering critically depends on initial centroids

Some methods used in the literature to choose initial centroids are

- Randomly chose k points in space of $\mathcal{P}$ (e.g. $\mathbb{R}^m$)
- k-means++: Choose first point at random, choose the next point farthest from the first chosen point, repeatedly choose the next point that is farthest from the already chosen points
- Sample a subset of points. Run hierarchical clustering to get k clusters, choose the centroids of each cluster as initial centroids

k-means Algorithm: The right value of k

- Suppose SSE is the right clustering quality parameter
- Suppose k is the right number of clusters
- If we cluster into $k' < k$ clusters, then SSE will go up
- If we cluster into $k' > k$ clusters, then SSE will go sharply down
- Using this *'concavity'*, the right value of k can be found with a binary search



k-means Algorithm: Sensitivity to outliers

k-means algorithm is very sensitive to outliers because mean is an unstable statistic

- Let $\mathcal{P} = \{1, 2, 3, 8, 9, 10, 25\} \subset \mathbb{R}$
- The correct clustering looks like $\{1, 2, 3\}$, $\{8, 9, 10\}$ and 25 is an outlier
  - $SSE(\{1, 2, 3\}, \{8, 9, 10, 25\}) = 196$
  - $SSE(\{1, 2, 3, 8\}, \{9, 10, 25\}) = 189.67$
- k-means will select the latter partition
  - Clearly it is not good, as it separates 8 from 9 and 10

k-means Algorithm: Dealing with instability

- One way to deal with the instability of centroids is to choose some other representative of each cluster
- Representative of a cluster is called **clusteroid**
- Since clusteroid, generally is somewhat central element of the cluster, it is also called **medoid**
- The goal here is to choose k clusteroids and minimize the sum of distances from each point to its clusteroid

k-Medians algorithm

- Median is less sensitive to outliers than mean
- We use *'median of clusters'* instead of centroids as clusteroids
- Let med_i be the *'median'* of a cluster C_i.
- Goodness of a k-partition $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ is measured by

$$S_{med}(\mathcal{C}) := \sum_{i=1}^{k} \sum_{x \in C_i} \|x_i - med_i\|^2$$

Problem: Find a k-partition $\mathcal{C}^*$ of $\mathcal{P}$ with minimum $S_{med}(\cdot)$

- Various definitions of median for points in higher dimensions
- Oja Median, Simplicial Median, 1-Median, Coordinate-wise median

k-Medians algorithm

- We give a generic version of k-medians algorithms

Algorithm : k-medians algorithm $(\mathcal{P}, k)$

Select k points as initial medians ▷ randomly or arbitrarily

while Stopping criterion is not met **do** ▷ many choices

Assign each point $x \in \mathcal{P}$ to the median closest to x ▷ closeness w.r.t the similarity measure

Compute the medians of (modified) clusters

▷ using the adopated definition of median

Partition Around Medoids

A pseudocode of Partition Around Medoids (PAM) is as follows:

Algorithm : Partition Around Medoids $(\mathcal{P}, k)$

Select k points as initial clustroids (medoids) arbitrarily

while Stopping criterion is not met **do** ▷ many choices

Choose a non-medoid point p

Compute change in SSE with replacing a medoid m with p

If the change in SSE is negative, then swap m with p

Runtime is $O(k(n-k)^2)$ in each iteration

k-modes algorithm: Categorical Data

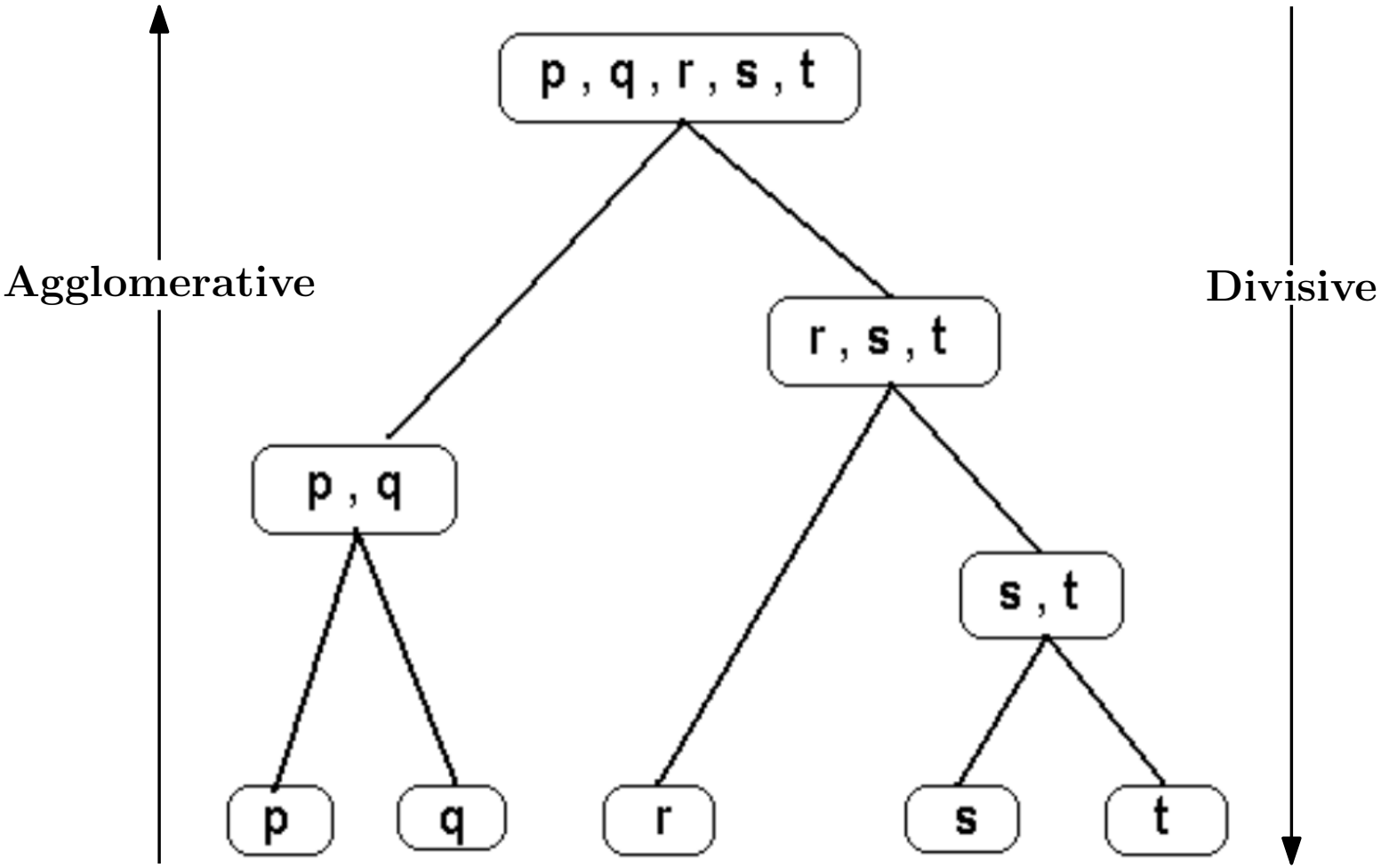
- k-Means or k-Medians cannot handle nominal data
- k-Modes algorithm is an extension for nominal data
- It just replaces mean with mode of the cluster
- Mode of multidimensional data is vector of coordinate wise modes
- Some distance to the clusteroid also needs to be defined
- In the above definition of modes, distance to clusteroid (mode) can be for instance the Hamming distance
- We can use any of the distance measures discussed for nominal data

Agglomerative Clustering

Hierarchical Clustering

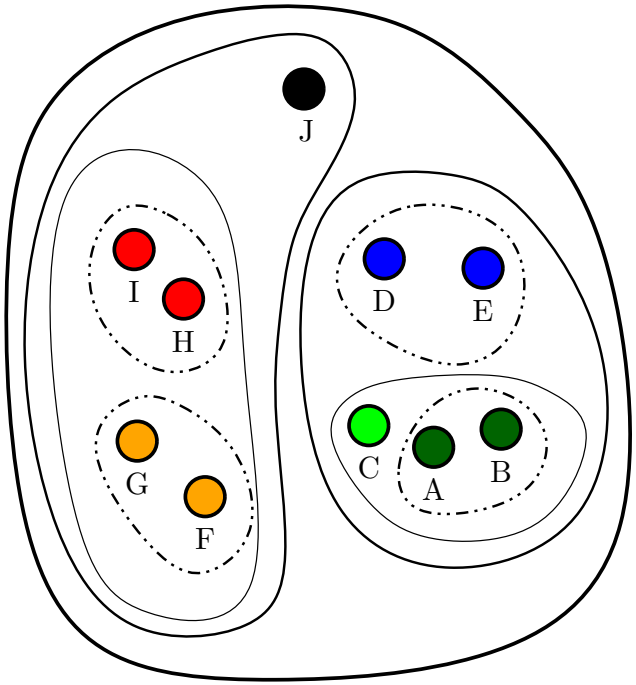
- Creates a hierarchy of clusters (multi-level partitions)
  - returns a set of nested clusters
- Generally no requirement of a fixed number of k clusters
- Hierarchical method can be
- Divisive Approach (Top-Down)
  - Initially all points are in one huge cluster
  - In every step one current cluster is split into two
  - Generates a top-down hierarchy of clusters
- Agglomerative Approach (Bottom-Up)
  - Initially each point is a cluster itself
  - In every step two clusters are merged into one
  - Generates a bottom-up hierarchy of clusters

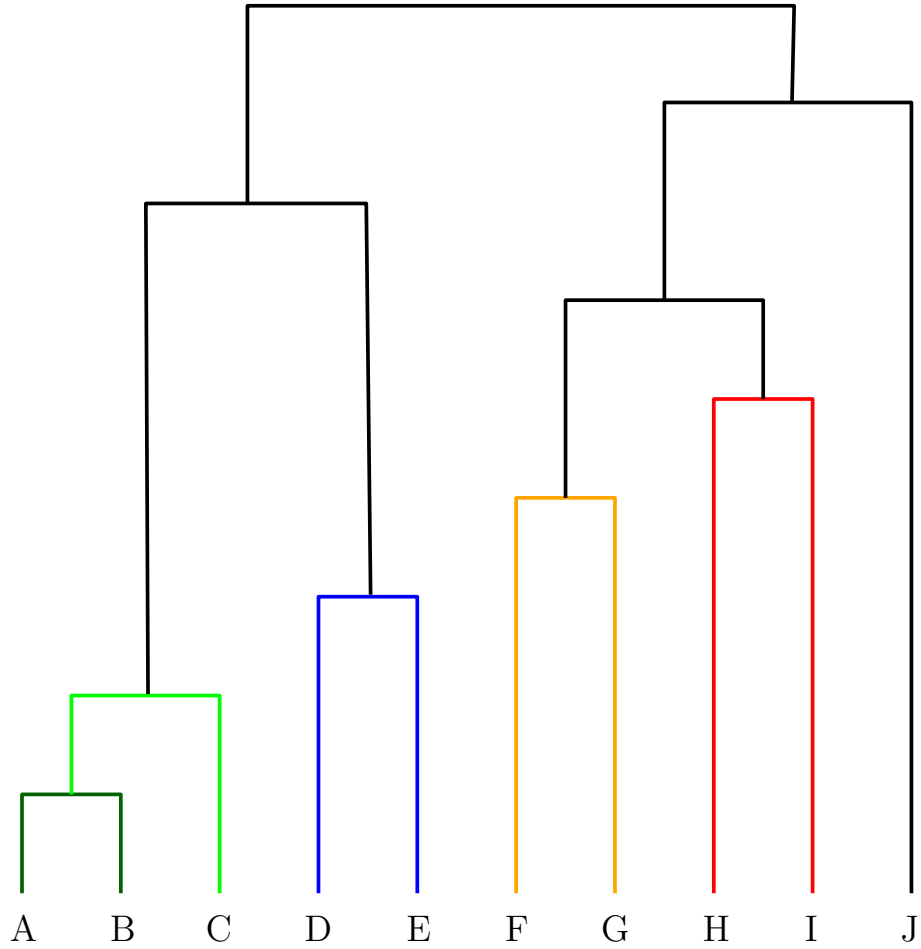
Hierarchical Clustering: Agglomerative and Divisive Approach



Hierarchical Clustering

Output of hierarchical clustering is represented by a **dendrogram** (a tree recording the sequence of merges or splits)





Hierarchical Clustering: Divisive Approach

We will discuss spectral clustering a divisive clustering approach

Hierarchical Clustering: Agglomerative Approach

Agglomerative Clustering

- Initially each point is a cluster itself
- In every step two *'close by'* clusters are merged into one
- Generates a bottom-up hierarchy of clusters

Key considerations:

- Representation of clusters
- Distance between clusters
- The choice of pairs of clusters to be merged
- A stopping criterion

Agglomerative Clustering

Algorithm : Generic Agglomerative Clustering ($\mathcal{P}$)

Initialize with each point as a cluster in $\mathcal{C}$

while stopping criterion is not met **do**

Choose the best pair of clusters $(C_i, C_j) \in \binom{\mathcal{C}}{2}$

$C_m \leftarrow \text{MERGE}(C_i, C_i)$

$\mathcal{C} \leftarrow \mathcal{C} \setminus \{C_i, C_j\} \cup \{C_m\}$

Agglomerative Clustering

Generic Agglomerative Clustering

$\mathcal{P} = \{A, B, C, D, E, F, G, H, I\}$

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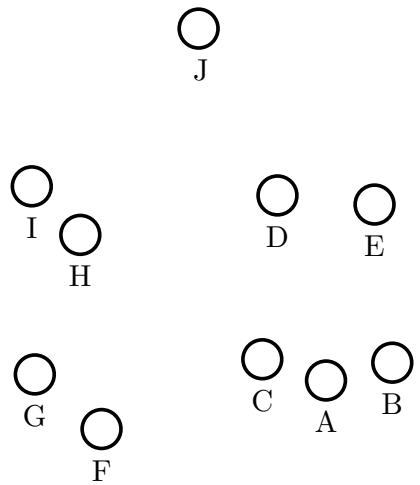

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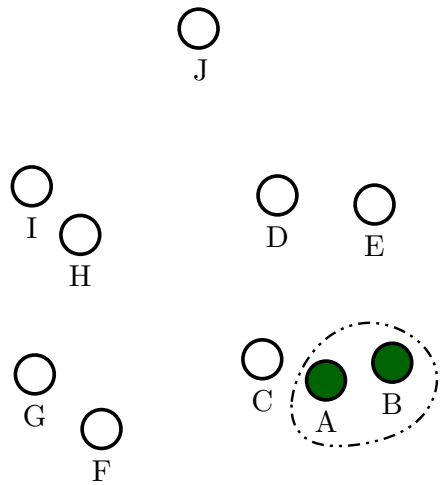

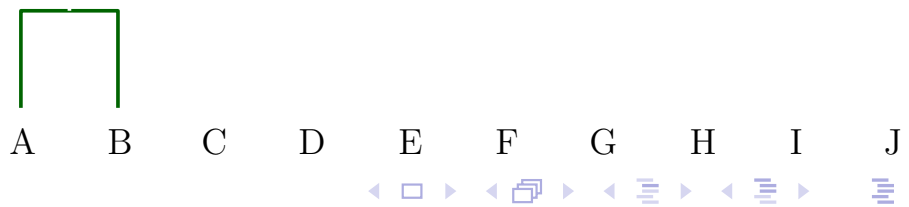

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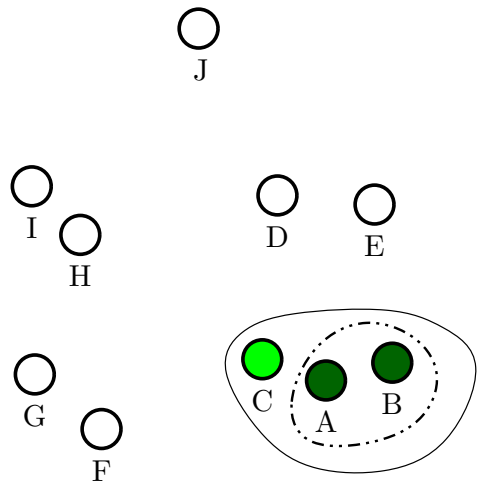

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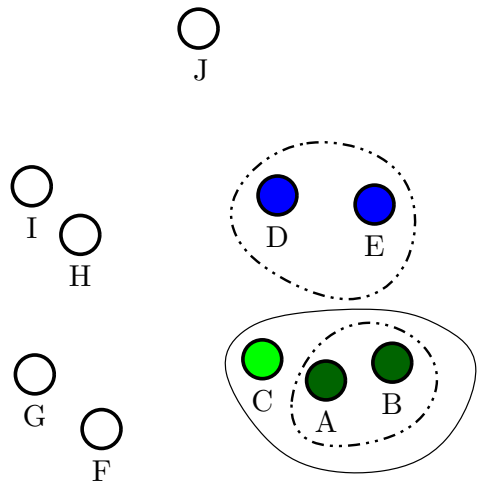

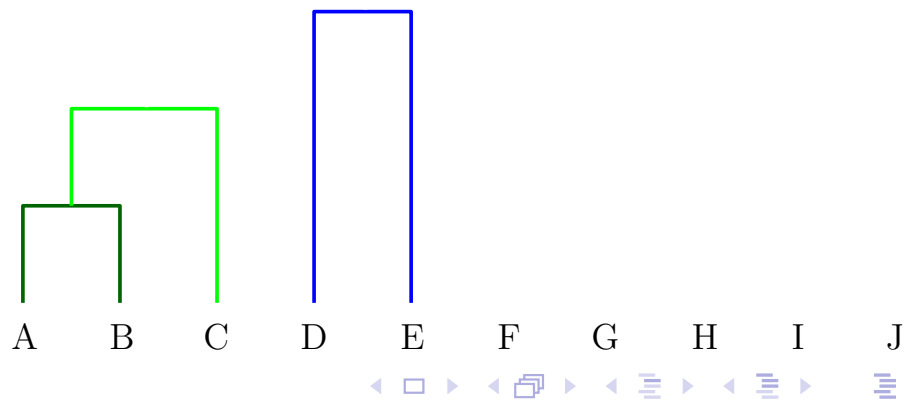

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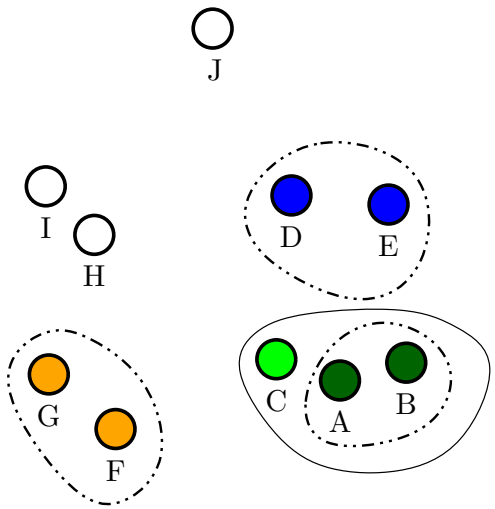

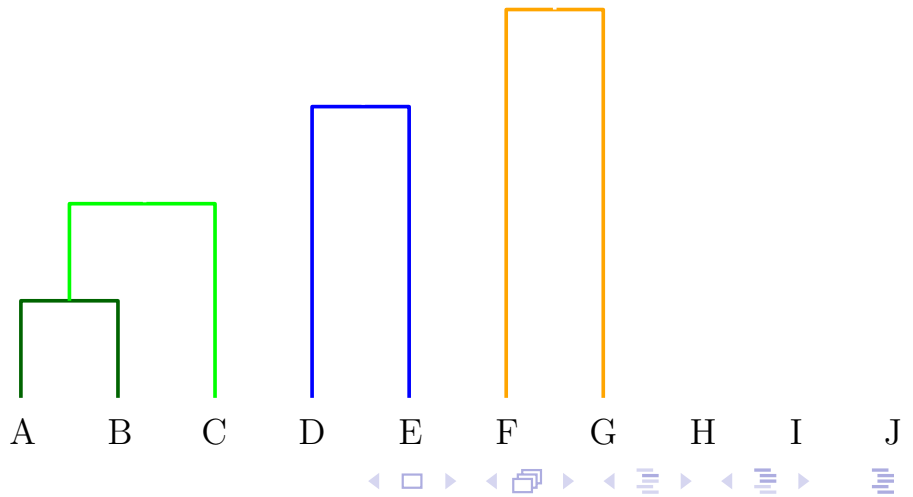

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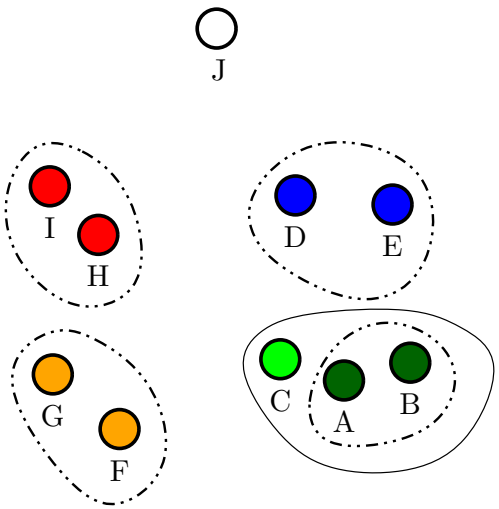

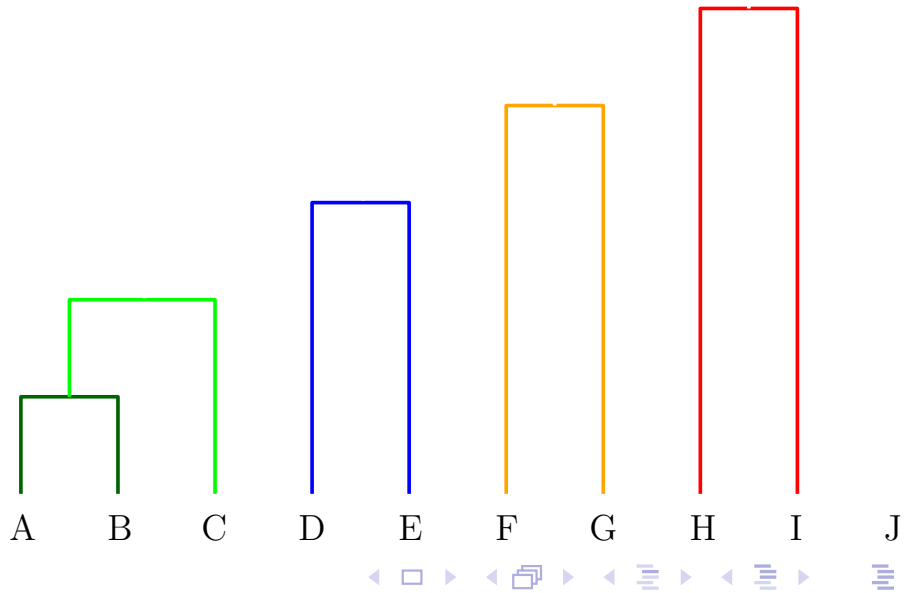

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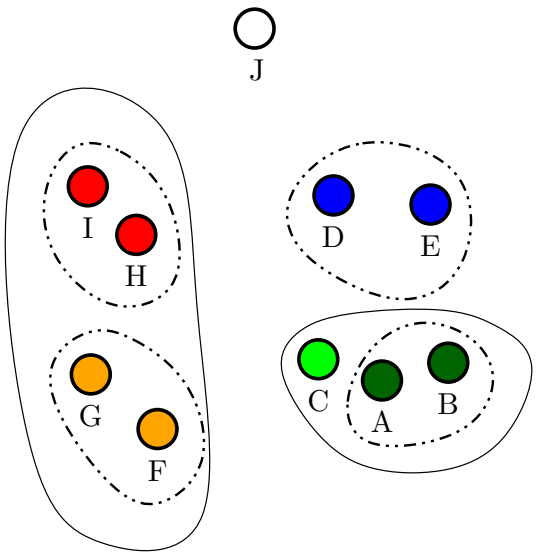

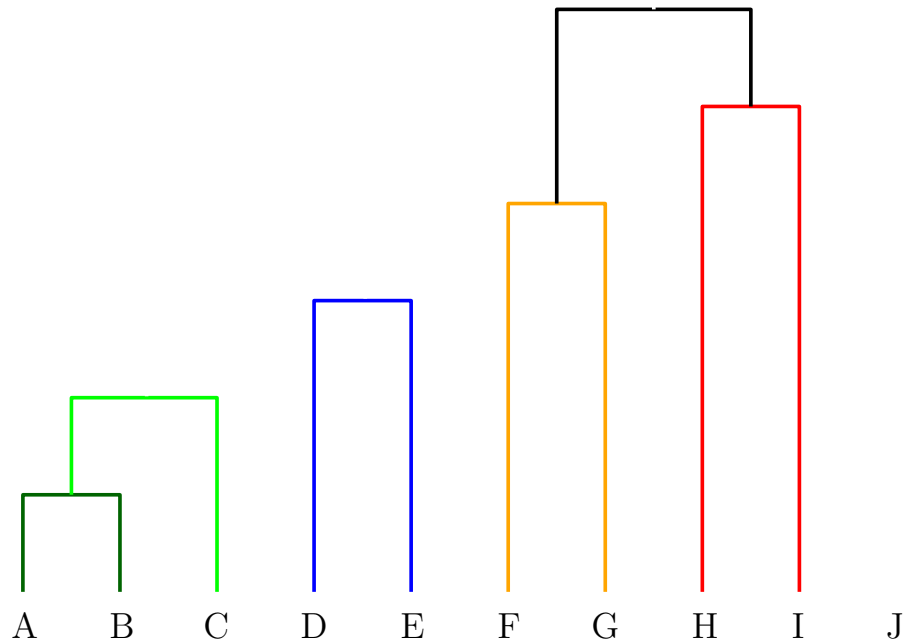

Agglomerative Clustering

Generic Agglomerative Clustering

$$\mathcal{P} = \{A, B, C, D, E, F, G, H, I\}$$

Initialize with each point as a cluster in $\mathcal{C}$
while stopping criterion is not met **do**
  Choose the best pair of clusters $(C_i, C_j) \in \binom{\mathcal{C}}{2}$
  $\mathcal{C} \leftarrow \text{MERGE}(C_i, C_i)$
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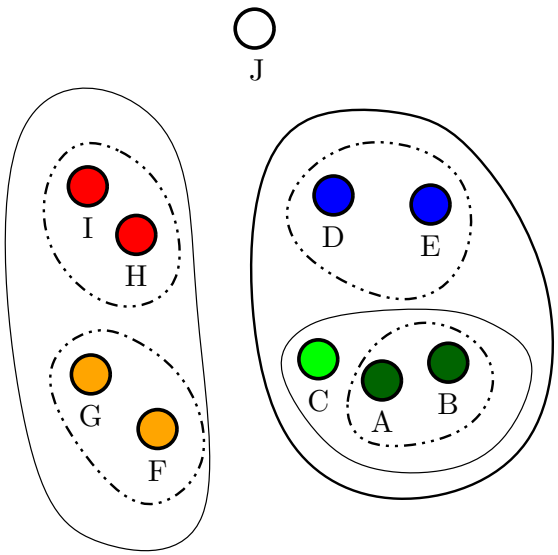

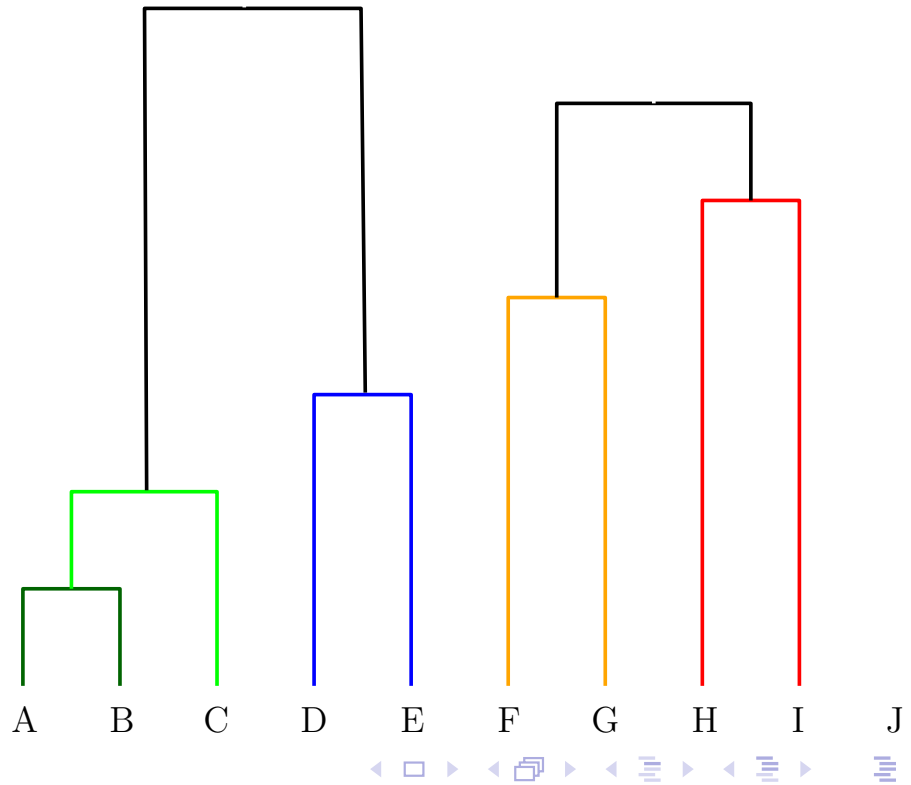

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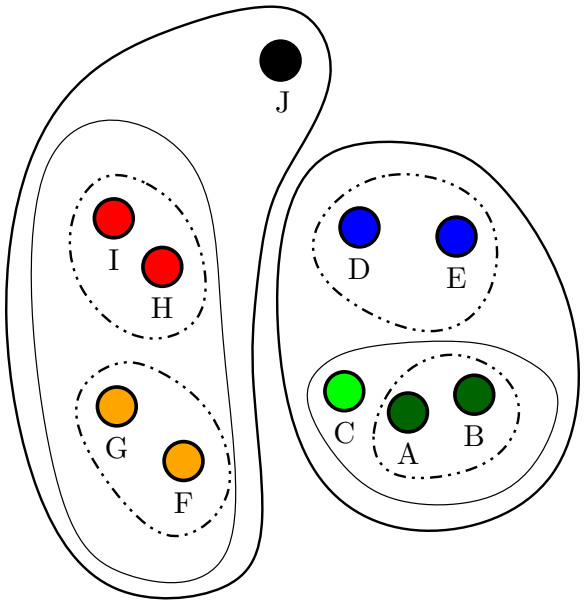

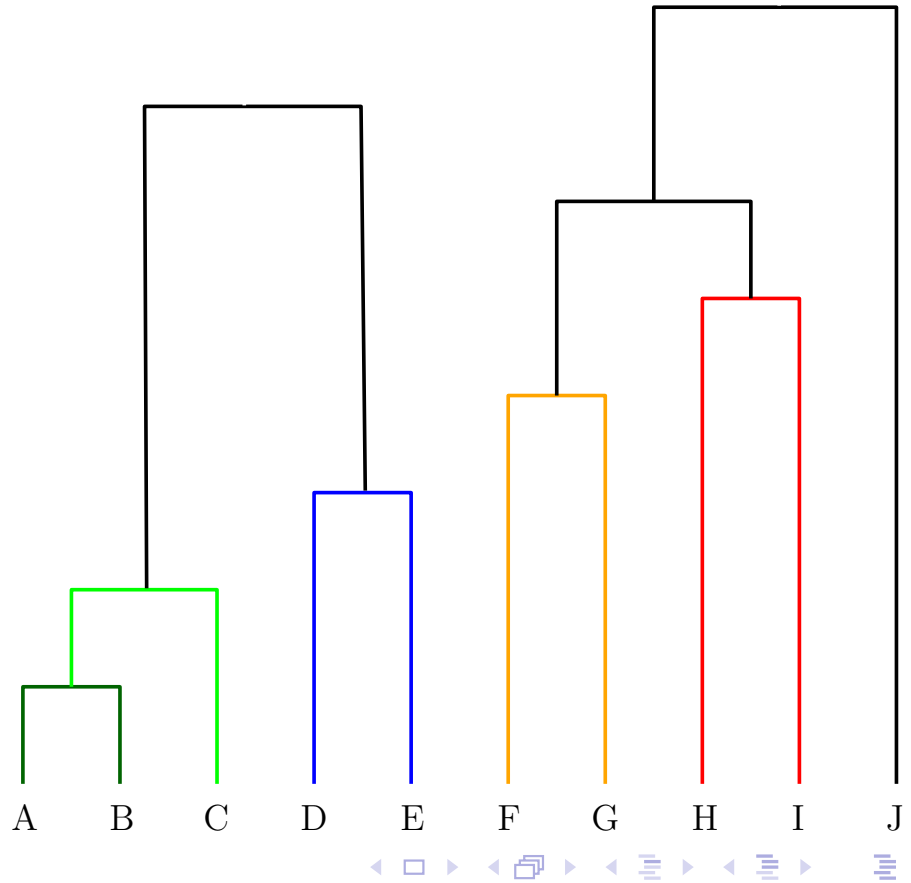

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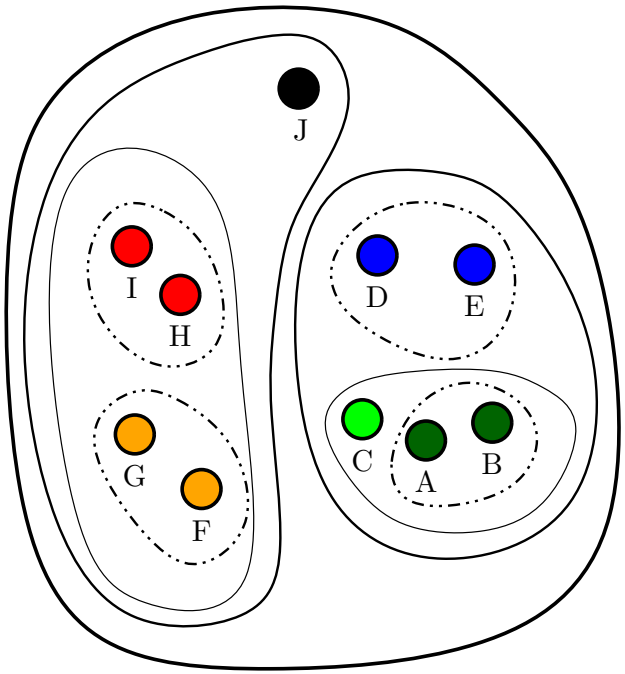
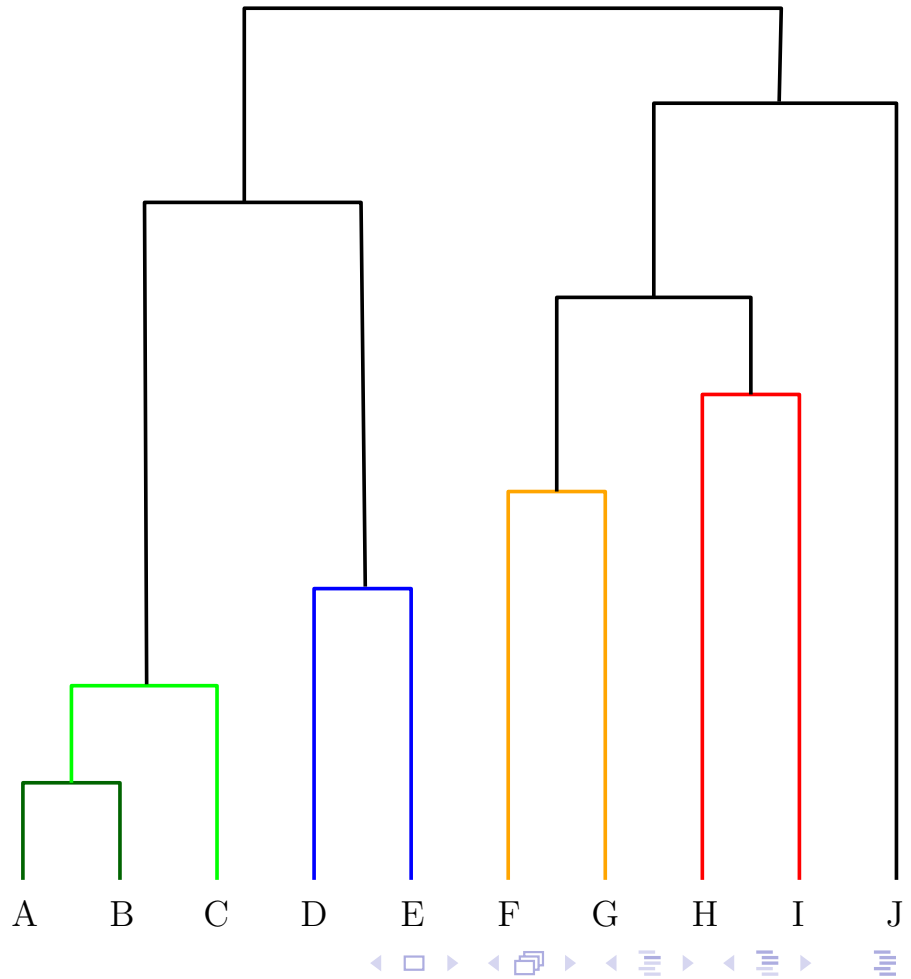




Hierarchical Clustering

Hierarchical Clustering (both divisive and agglomerative)

- is rigid in nature
  - once a cluster is made, it cannot be undone
  - less chances of improvement
- generally less computational cost
- does not require specific number of clusters
- Can stop when clustering is good enough (stopping criterion)

Agglomerative Clustering

Agglomerative Clustering

- Initially each point is a cluster itself
- In every step two *'close by'* clusters are merged into one
- Generates a bottom-up hierarchy of clusters

Key considerations:

- Representation of clusters
- Distance between clusters
- The choice of pairs of clusters to be merged
- A stopping criterion

Agglomerative Clustering: Euclidean Space

Let $\mathcal{P} = \{x_1, \ldots, x_N\}$, each $x_i \in \mathbb{R}^n$

- **Represent** each cluster by its centroid
- **Distance** between two clusters is the distance between their centroids
- **Select** a pair of clusters with minimum (inter-centroid) distance
- **Stop** when the number of clusters is equal to k

Note that this representation requires explicit feature vectors for points

Cluster: Diameter, Radius and Density

- **Diameter** of a cluster C, $dia(C)$ is the max inter-point distance in C

$$dia(C) = \max_{x,y \in C} \{d(x,y)\}$$

- **Radius** of a cluster C with centroid $\mathbf{c}$, $rad(C)$ is the maximum distance of a point in C from the centroid $\mathbf{c}$

$$rad(C) = \max_{x \in C} \{d(x,\mathbf{c})\}$$

- **Density** of a cluster C: is mass (number of points) over volume
  - What is volume (shape) of the cluster? Use an estimate

$$den(C) = \frac{|C|}{dia(C)^2} \quad \text{or} \quad den(C) = \frac{|C|}{rad(C)^2} \quad \text{or} \quad den(C) = \frac{|C|}{rad(C)^n}$$

The exponent in denominator is usually $1, 2$, or n (dimensionality of points)

Agglomerative Clustering: Stopping Criteria

Stop based on *'quality'* of recently merged cluster, e.g. when the

- average inter-point distance of the merged cluster is above a threshold
- diameter of the merged cluster is above a threshold
- radius of the merged cluster is above a threshold
- the average distance from the centroid is above a threshold
- sum of squared distances from the centroid is above a threshold

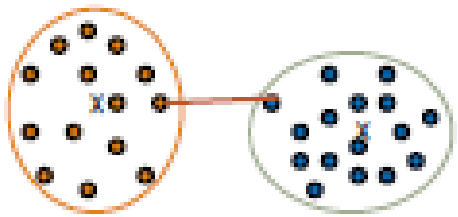
Stop based on a global *'quality'* measure. e.g. when

- the average diameter of all clusters increases above a threshold
  - the idea is as long as we merge cluster that truly should be merged, the average diameter will not significantly increase
  - when we merge a pair that should not be merged, there would be a sudden jump in the average diameter

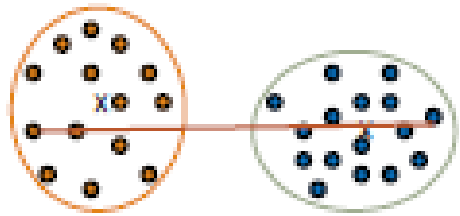
Agglomerative Clustering: Distance between Clusters

Distance Between two cluster C_i and C_j can be defined as

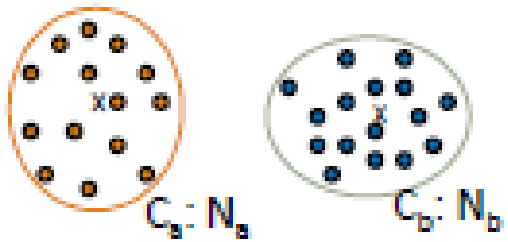
- Centroid Link: distance between centroids of C_i and C_j
  - Requires points as numeric vectors
- Single Link: Minimum inter-point distance between C_i and C_j
- Average Link: Average inter-point distance between C_i and C_j
- Complete Link: Maximum Inter-point distance between C_i and C_j



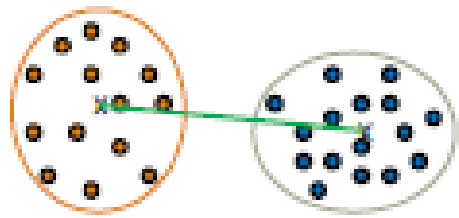
Single Link



Complete Link



Average Link



Centroid Link

Agglomerative Clustering: Pair Selection Criteria

Pair selection can be based on any distance measures between two clusters

e.g. select a pair of clusters with minimum

- Centroid link
- Single Link
- Average Link
- Complete Link

Can also select pair based on *'quality'* of the resulting (merged) cluster

e.g. choose a pair

- resulting in the lowest radius of a merged cluster
- resulting in the lowest diameter of a merged cluster

Agglomerative Clustering: Cluster Representation

We cannot compute centroids if

- points are not real vectors (non-Euclidean space)
- points are only abstractly described (no explicit vectors) and only distance matrix is provided

We can represent clusters by a central element. Any definition of clusteroid of a cluster C can b used , e.g. a point in C

- with minimum sum (average) of distances to other points in C
- with minimum largest distance to a point in C
- with minimum sum of squared distances to other points in C

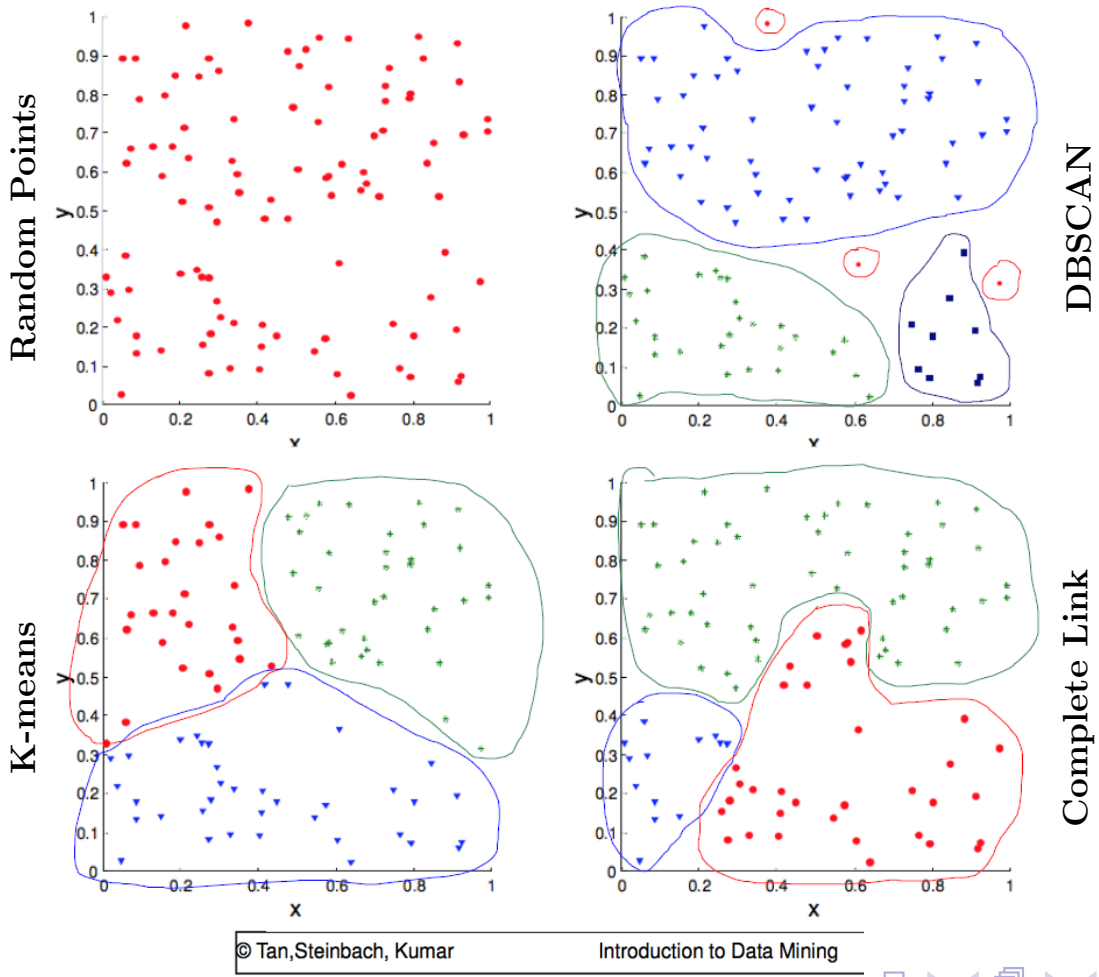
Notions of inter-cluster distances, pair selection and stopping rules can be adapted to this version of problem (replace clustroid for centroid if needed)

Clustering Quality Assessment

Validation and Evaluation

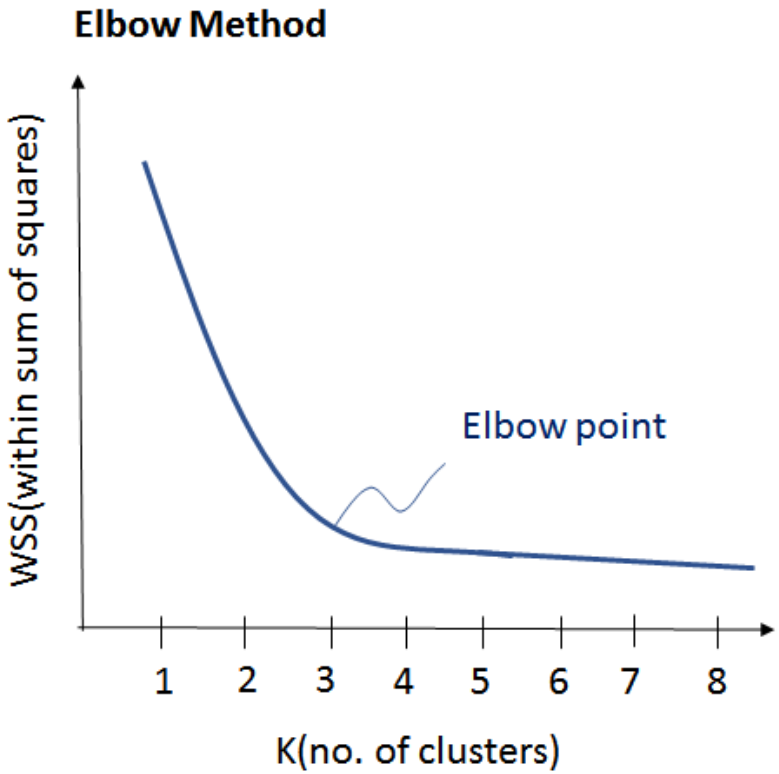
Goals and Aspects of Clustering Quality Assessment

1. Determine cluster tendency of dataset
   - Are there meaningful groups (non-random structure) in the data
   - or clusters represent some patterns in noise



Goals and Aspects of Clustering Quality Assessment

1. Determine cluster tendency of dataset
2. Find the correct number of clusters
   - Recall the elbow method



Goals and Aspects of Clustering Quality Assessment

1. Determine cluster tendency of dataset
2. Find the correct number of clusters
3. Evaluate Clustering Quality
   - Validate the output clustering by comparing with known results (class labels or manual clustering by experts)
   - Evaluate how well the output clustering fit the data without reference to external results
4. Compare two clustering algorithms
   - Observe the kind of patterns each try to mine and determine which algorithm is suitable for the task at hand
5. Compare two clusters in a clustering

Clustering: Evaluation and Validation

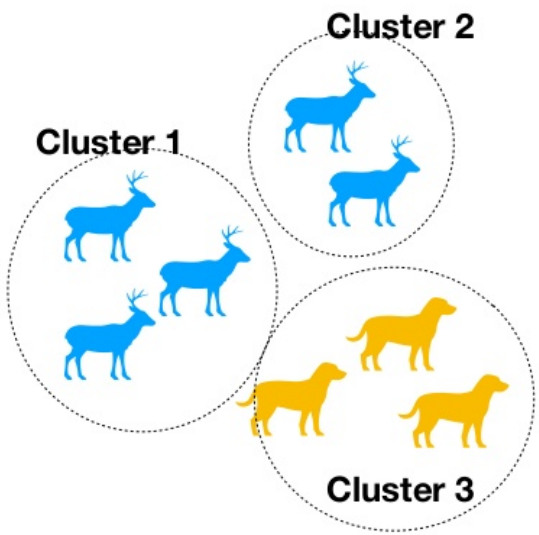
Clustering is an unsupervised task (cannot use ground truth in the clustering algorithm)

- Cluster Validation against Class Labels: If true class labels are available, we can see how well clusters match with class labels
- Cluster Evaluation with No Class Labels: Assess cluster quality w.r.t proximity measure

Validation of Clustering

Two basic criteria for validating clusterings are:

1. Cluster homogeneity
   - Clusters should contain objects of a single class only
   - Such clusters are called pure, the purer the clusters the better
   - Singleton clusters are the most homogeneous



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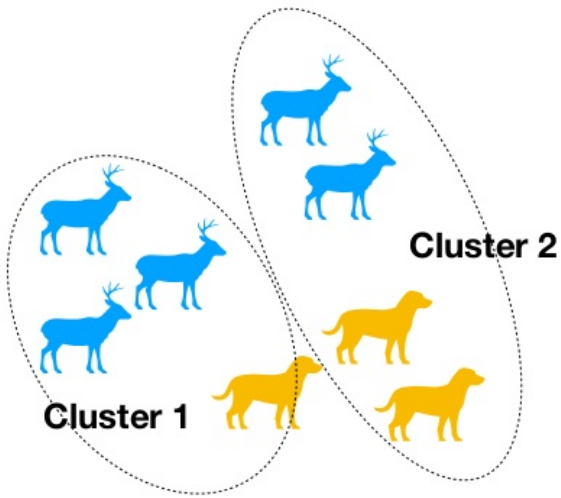

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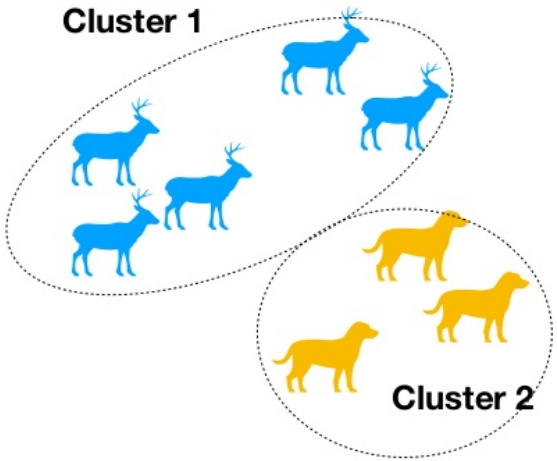
Validation of Clustering

Two basic criteria for validating clusterings are:

1. Cluster homogeneity
2. Cluster Completeness
   - Objects in the same class should be contained in a single cluster
   - Classes should not be split into multiple clusters
   - Singleton clusters may not be complete



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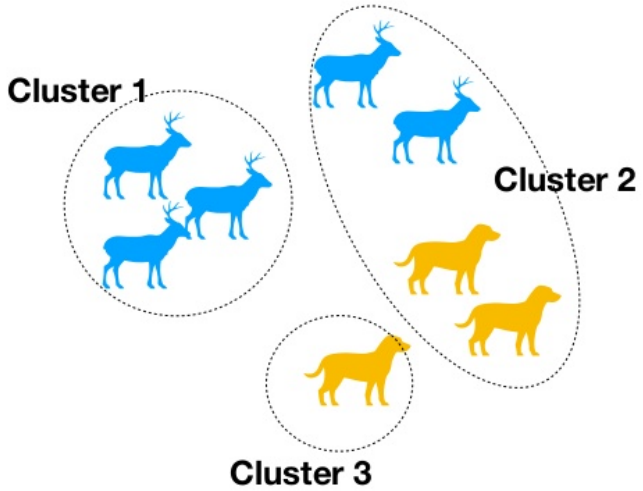

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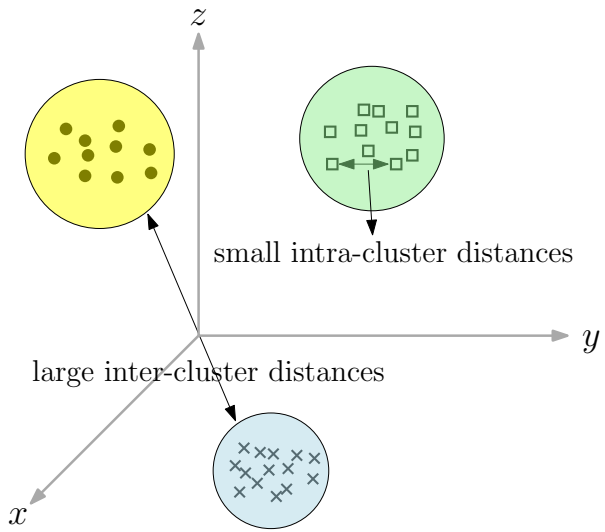
Evaluation of Clustering

Three basic criteria for evaluating clusterings are:

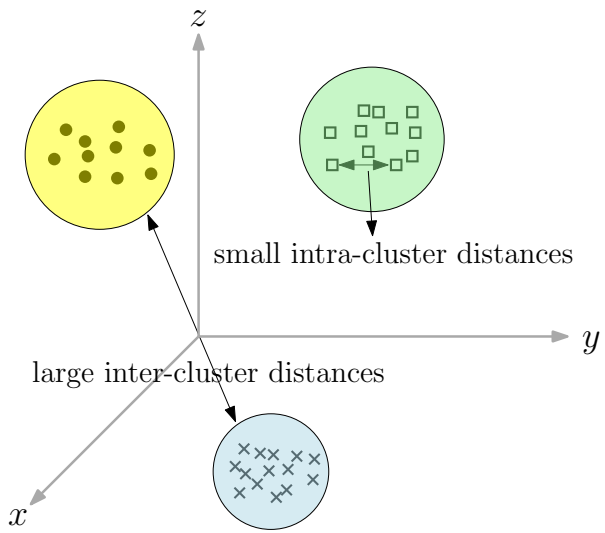
1. Cluster Compactness
   - Objects in a cluster should be highly similar, Intra-Cluster-Low distances
   - generally desired in classification type tasks such as image recognition
   - Proximity measure should be meaningful (similarity $\sim$ homogeneity)
   - Also called cluster cohesion



Evaluation of Clustering

Three basic criteria for evaluating clusterings are:

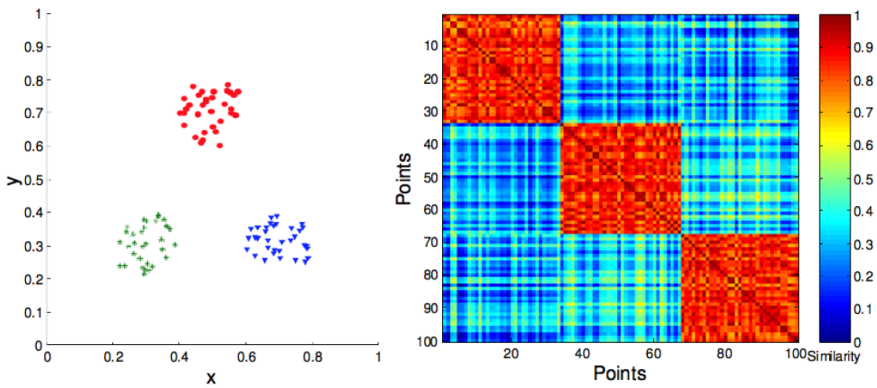
1. Cluster Compactness
2. Cluster Separation
   - Clusters should be well-separated (far apart)
   - Objects in two different clusters should be highly dissimilar
   - Inter-cluster high distances
   - Again proximity measure should be meaningful

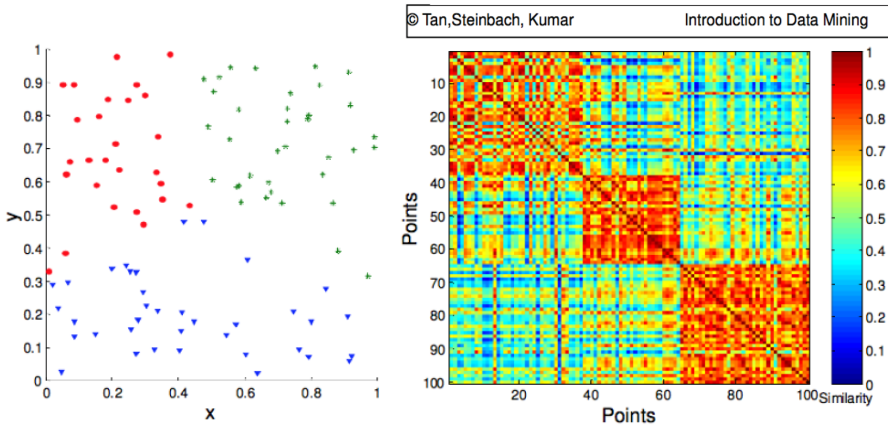


Evaluation of Clustering

Three basic criteria for evaluating clusterings are:

1. Cluster Compactness
2. Cluster Separation
3. Agreement of pairwise proximity with clustering-induced metric
   - Clustering should respect the pairwise proximity measure
   - Similar/distant pairs should be in the same/different clusters
   - Somewhat encompasses both compactness and separation





Arrange rows and columns of similarity matrix by cluster ids and inspect it

External and Internal Measures of Clustering Quality

External and Internal Measures of Clustering Quality

Numerical measures for clustering validation and evaluation

- **External or Extrinsic Measures** ▷ used for validation
  - They use class labels
  - Some are indexes to measure for a specific criterion
  - Different Indexes on a common scale can be combined to measure for combination of criteria
- **Internal or Intrinsic Measures** ▷ used for evaluation
  - They do not use class labels
  - Some are indexes to measure for a specific criterion
  - Different Indexes on a common scale can be combined to measure for combination of criteria
  - Generally a statistical significance of index values needs to be ascertained

External Measures

Any measures for assessment of quality of classification can be used

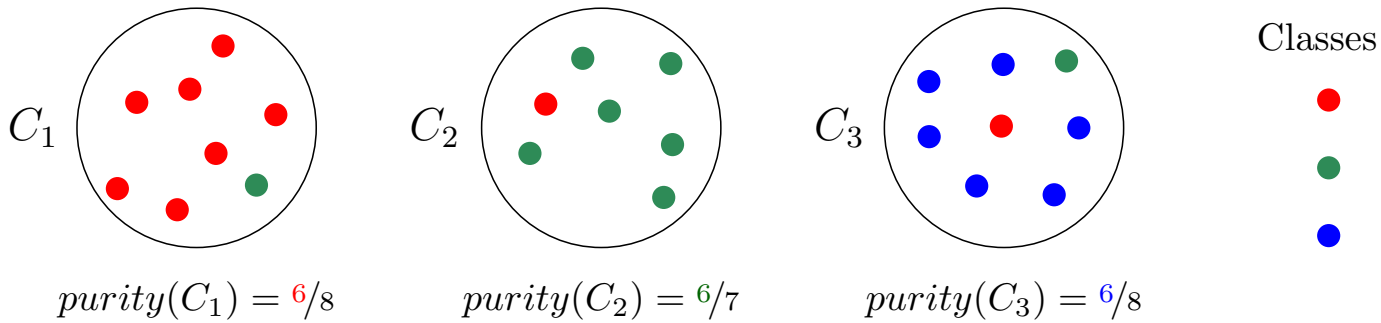
- Accuracy
- Error
- Precision, Recall, F1 measure
- Purity
- Entropy
- Conditional Entropy
- Normalized Mutual Information (NMI)
- Maximum Matching: Match clusters to class and see goodness of matching

External Measures: Purity

- Let $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$, L classes
- Let n_{ij} be objects of class i in cluster C_j

Purity of C_j: ratio of dominant class in C_j to $|C_j|$

$$purity(C_j) = \frac{\max\limits_{1 \le i \le L} n_{ij}}{|C_j|}$$



Purity of clustering $\mathcal{C}$:

$$purity(\mathcal{C}) = \sum_{j=1}^{k} \frac{|C_j|}{N} purity(C_j)$$

- $purity(\mathcal{C}) = 8/23 \times 7/8 + 7/23 \times 6/7 + 8/23 \times 6/8 = 19/23$

External Measures: Purity

- Let $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$, L classes
- Let n_{ij} be objects of class i in cluster C_j

Purity of C_j: ratio of dominant class in C_j to $|C_j|$

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Purity of clustering $\mathcal{C}$:

$$purity(\mathcal{C}) = \sum_{j=1}^{k} \frac{|C_j|}{N} purity(C_j)$$

- Highest purity is 1 when clusters are the purest
- Singleton clusters maximize purity
- Purity favors homogeneity only
- Ignores cluster completeness

External Measure: Conditional Entropy

- Let $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ ▷ Clustering into k clusters
- $\mathcal{T} = \{T_1, T_2, \ldots, T_L\}$ ▷ True partition into L classes
- n_{ij} : objects of class T_i in cluster C_j
- $p_{ij} = {}^{n_{ij}}/_{|C_j|}$ ▷ class (probability) distribution in C_j

Conditional entropy of $\mathcal{T}$ w.r.t cluster C_j: entropy of class distrib. in C_j

$$H(\mathcal{T}|C_j) = -\sum_{i=1}^{L} p_{ij} \log p_{ij}$$

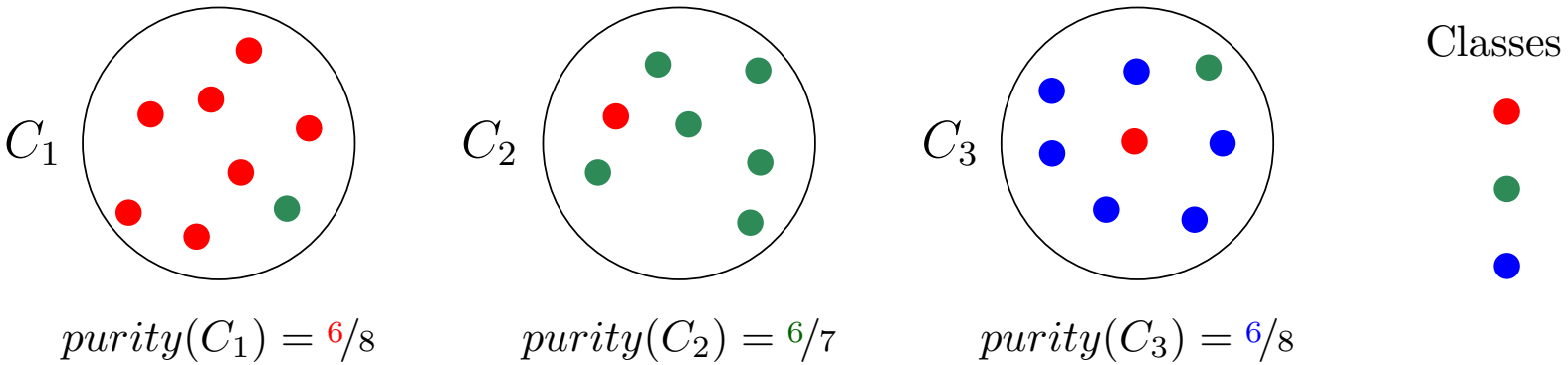
Conditional entropy of $\mathcal{T}$ w.r.t clustering $\mathcal{C}$:

$$H(\mathcal{T}|\mathcal{C}) = -\sum_{j=1}^{k} \frac{|C_j|}{N} H(\mathcal{T}|C_j) = -\sum_{j=1}^{k} \frac{|C_j|}{N} \sum_{i=1}^{L} p_{ij} \log p_{ij}$$

External Measure: Conditional Entropy

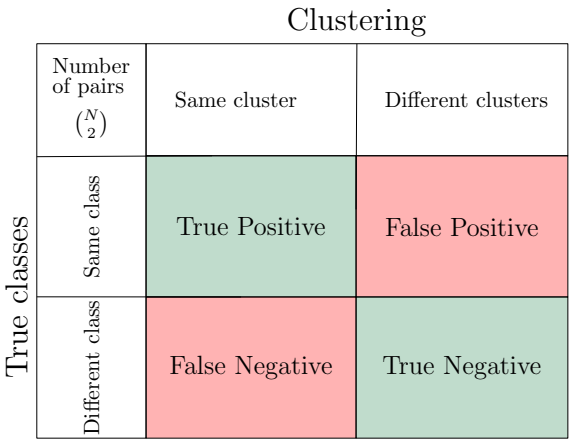
- Highest possible value is log L
- Split classes results in higher entropy
- For perfectly complete clusters conditional entropy is 0
- Conditional entropy favors completeness

Compute values of conditional entropies in this example



External Measure: Rand and Jaccard Index of clustering

- Let $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ ▷ Clustering into k clusters
- $\mathcal{T} = \{T_1, T_2, \ldots, T_L\}$ ▷ True partition into L classes
- Measures of pairwise agreement of class labels and clustering parts



Rand Index of $\mathcal{C}$: $$RI(\mathcal{C}) := \frac{TP + TN}{\binom{N}{2}}$$

▷ Compare with standard precision and recall

Jaccard Index of $\mathcal{C}$: $$J(\mathcal{C}) := \frac{TP}{TP + FN + FP}$$

Internal Measure: Within sum of squared error (WSSE)

A measure of compactness of a cluster or clustering is SSE or average SSE

For a k-partition $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ sum of squared error (SSE) is:

Let $\mathbf{c}_i = centroid(C_i)$, then

$$\text{SSE}(\mathcal{C}) = \sum_{i=1}^{k} \sum_{x \in C_i} ||x - \mathbf{c}_i||^2$$

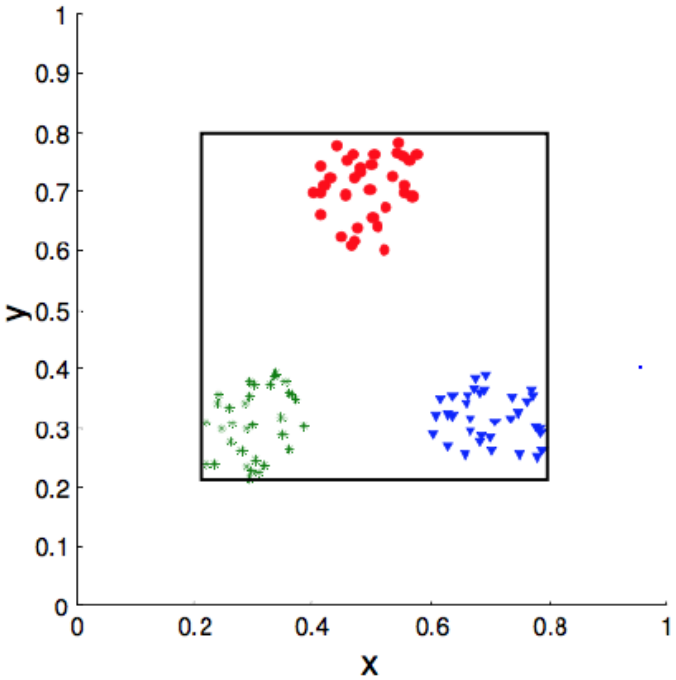
also called **within sum of squared error** (WSSE or WSS)

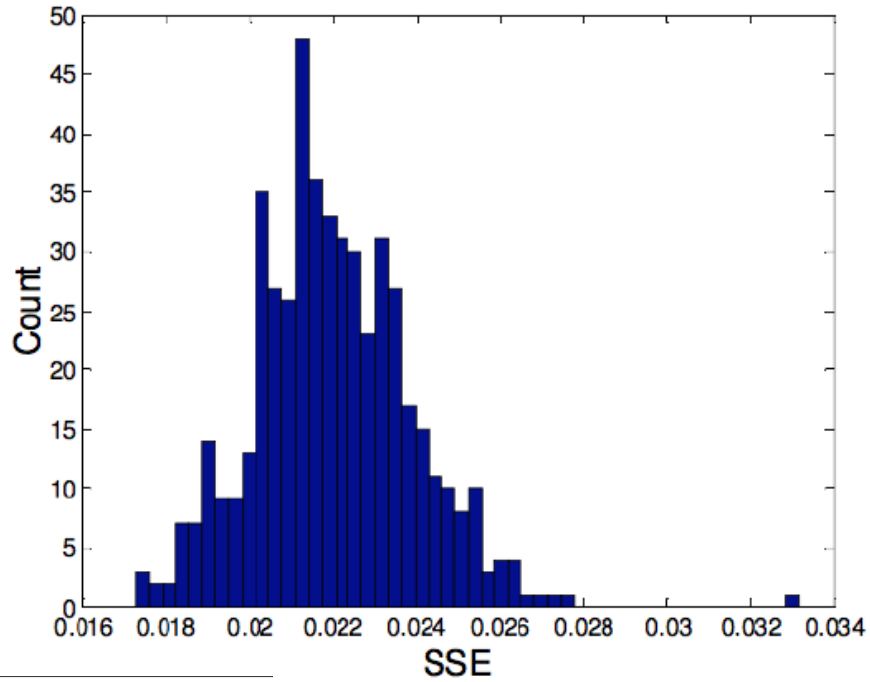
Internal Measure: Statistical Significance

- For SSE and other internal measures need to see whether the values are meaningful or statistically significant (deep statistical theories)
- A rough idea (rule of thumb is) to see if e.g. the obtained SSE for a clustering of N points in a certain space into k clusters is good
- Generate random datasets of N points in the same space (same ranges and dimensions) and then cluster them into k clusters using the same algorithm
- Observe the distribution of the SSE of these trials (say get the mean and st-dev)
- If the mean SSE of these random points is significantly higher than our SSE, then SSE is significant (and clustering is good)

Internal Measure: Statistical Significance

- Compare SSE of 0.005 against three clusters in random data
- Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values





Internal Measure

- Some other internal measures for cluster (or clustering) compactness
  - (weighted) average of intra-cluster pairwise distances
  - Correlation between proximity matrix and cluster co-belonging matrix (see below)
- Smaller values of an index means clusters are compact

Internal Measure: BSS

- Clustering Separation can be measured by
  - (weighted) average of inter-cluster pairwise distances
  - The Between Sum of Squares (BSS) is given by

    Let $\mathbf{c}_i = centroid(C_i)$ and let $\mathbf{c} = centroid(\mathcal{P})$ (centroid of the whole dataset), then

$$\text{BSS}(\mathcal{C}) = \sum_{i=1}^{k} |C_i|(\mathbf{c} - \mathbf{c}_i)^2$$

- Larger values of an index means clusters are well-separated

Internal Measure: Silhouette Coefficient

Silhouette Coefficient incorporates both cohesion and separation

Let $\mathcal{C} = \{C_1, \ldots, C_k\}$. For a point x in C_i

- $a(x) = \frac{1}{|C_i|} \sum_{x \neq y \in C_i} d(x, y)$ ▷ mean distance from x in its cluster
- $b(x) = \min_{j \neq i} \frac{1}{|C_j|} \sum_{y \in C_j} d(x, y)$ ▷ mean distance from x in closest cluster

Silhouette Coefficient of $x \in \mathcal{P}$: $s(x) := \frac{b(x) - a(x)}{\max\{a(x), b(x)\}}$

Silhouette Coefficient of $\mathcal{C}$ is the mean value of $s(x)$ over points in $\mathcal{P}$

$$SC(\mathcal{C}) := \frac{1}{N} \sum_{x \in \mathcal{P}} s(x)$$

- $SC(\mathcal{C}) \in [-1, 1]$ ▷ the closer to 1 the better clustering

Internal Measure: Clustering co-belonging matrix

Correlation between proximity and clustering induced co-belonging matrices

- Let D be the pairwise proximity matrix
- Let C be the co-belonging matrix induced by clustering
  - A row and column for each point, and $C(i, j) = 1$ or 0 depending on whether $x_i \neq x_j \in \mathcal{P}$ belong to the same cluster
- High correlation between these two symmetric matrices means good clustering and vice-versa (if proximity is similarity)
- For distance matrix low correlation indicates good clustering
- Incorporates both compactness and separation, also measures agreement of clustering-induced metric and pairwise proximity measure