Hierarchical Methods

Group 5

Khanh Le Tran Quoc Khoa Tran Nhat Khoa Huynh Tong Dang

University of Information Technology

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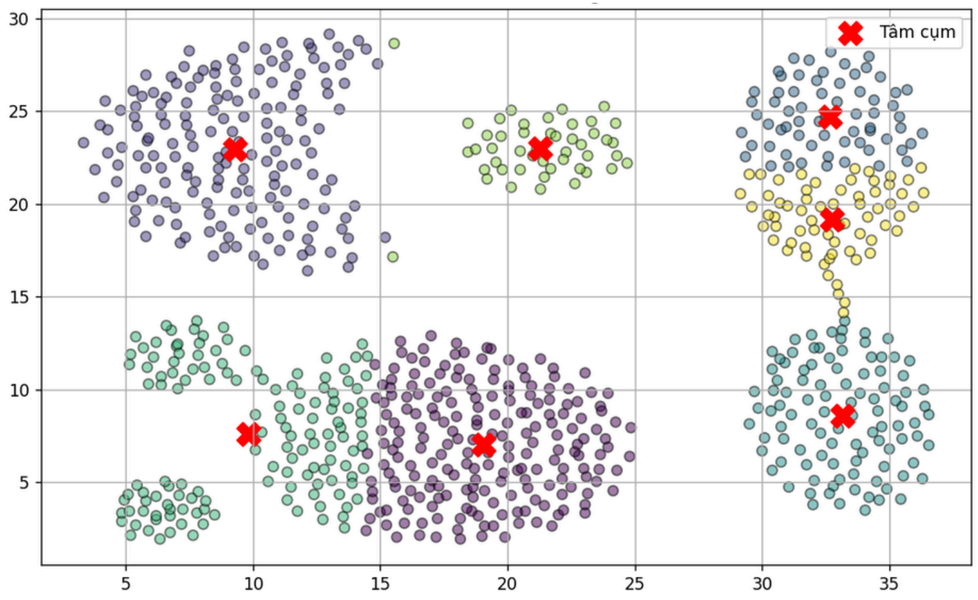
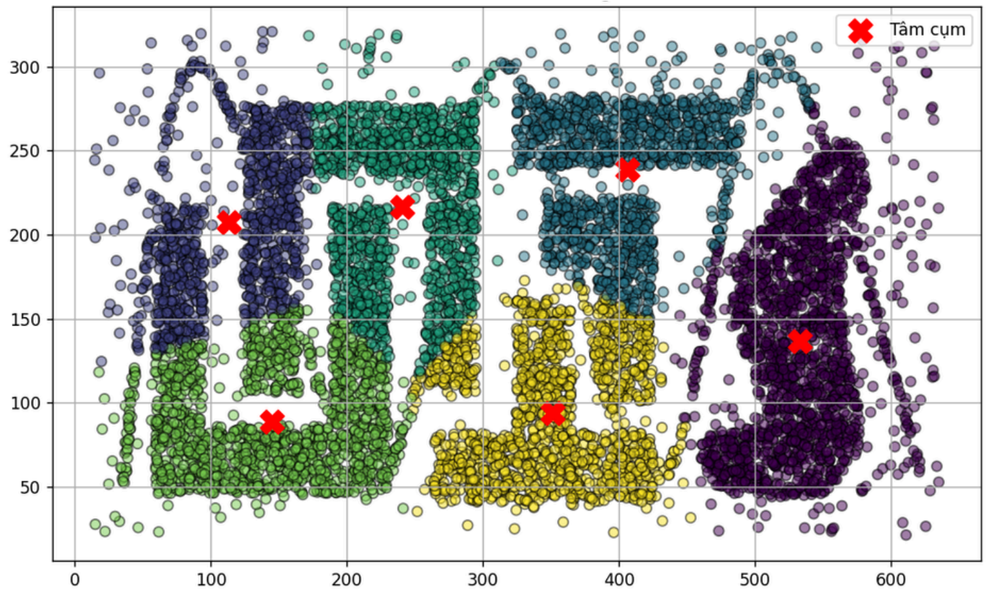
Link Github

Motivation

- Partitioning methods are widely used due to their simplicity, but they come with certain limitations:
  - **Require the number of clusters.**
  - **Struggle with data that has complex struture.**





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- We want to understand why the model decides to form specific clusters.

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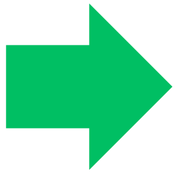
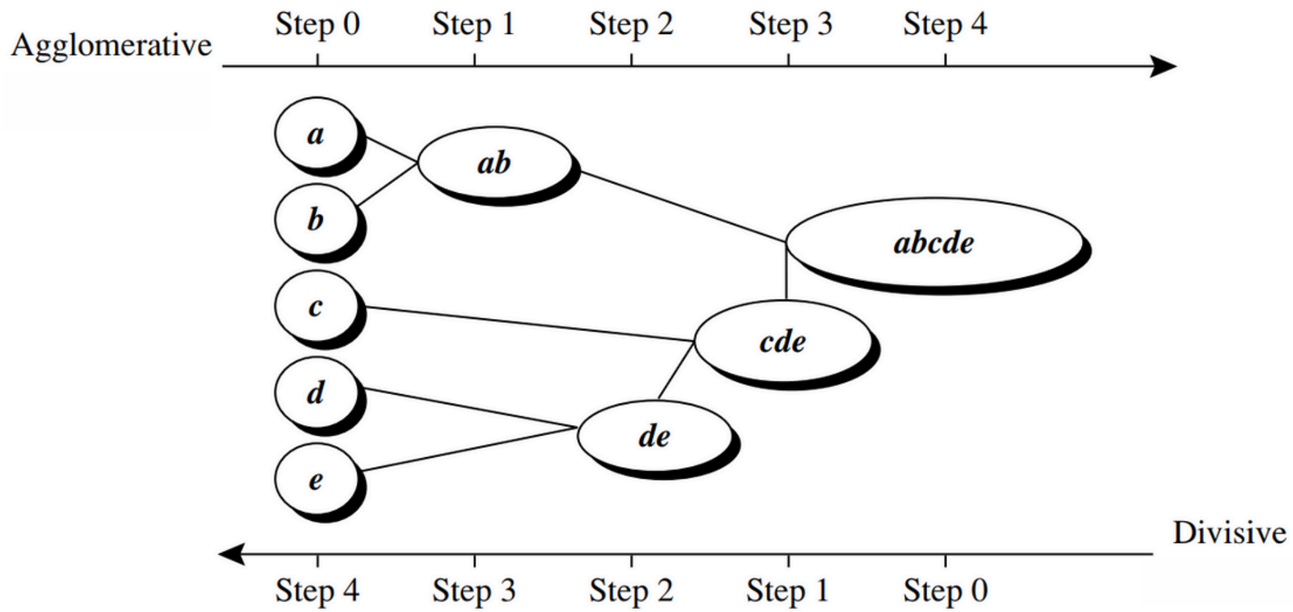


Hierachical Clustering Methods

Hierarchical Clustering Introduction

- **Hierarchical clustering** is a clustering method in which data objects are **arranged into a hierarchical structure**. It can be performed in two main ways:
  - **Agglomerative (bottom-up)**
  - **Divisive (top-down)**



Agglomerative Hierarchical Clustering

- A **bottom-up** approach to clustering
- Begin with each the data point is a cluster and progressively **merge** them into **bigger clusters**.
- This process continues recursively until there is only **a cluster**.
- How we decide to merge two clusters of each iter?

→ How **“close”** or **“similarity”** between two clusters

Agglomerative Hierarchical Clustering

- Ward method: how much the **sum of squares will increase when we merge them.**

$$D(C_i, C_j) = \sum_{x \in C_i \cup C_j} \|x - \mu_{C_i \cup C_j}\|^2 - \sum_{x \in C_i} \|x - \mu_{C_i}\|^2 - \sum_{x \in C_j} \|x - \mu_{C_j}\|^2$$

- Complete method: **maximum distance** beetween points in two clusters.

$$D(C_i, C_j) = \max_{x \in C_i, y \in C_j} d(x, y)$$

- Average method: **Average distance** beetween points in two clusters.

$$D(C_i, C_j) = \frac{1}{|C_i| \cdot |C_j|} \sum_{x \in C_i} \sum_{y \in C_j} d(x, y)$$

- Single method: **minimum distance** beetween points in two clusters.

$$D(C_i, C_j) = \min_{x \in C_i, y \in C_j} d(x, y)$$

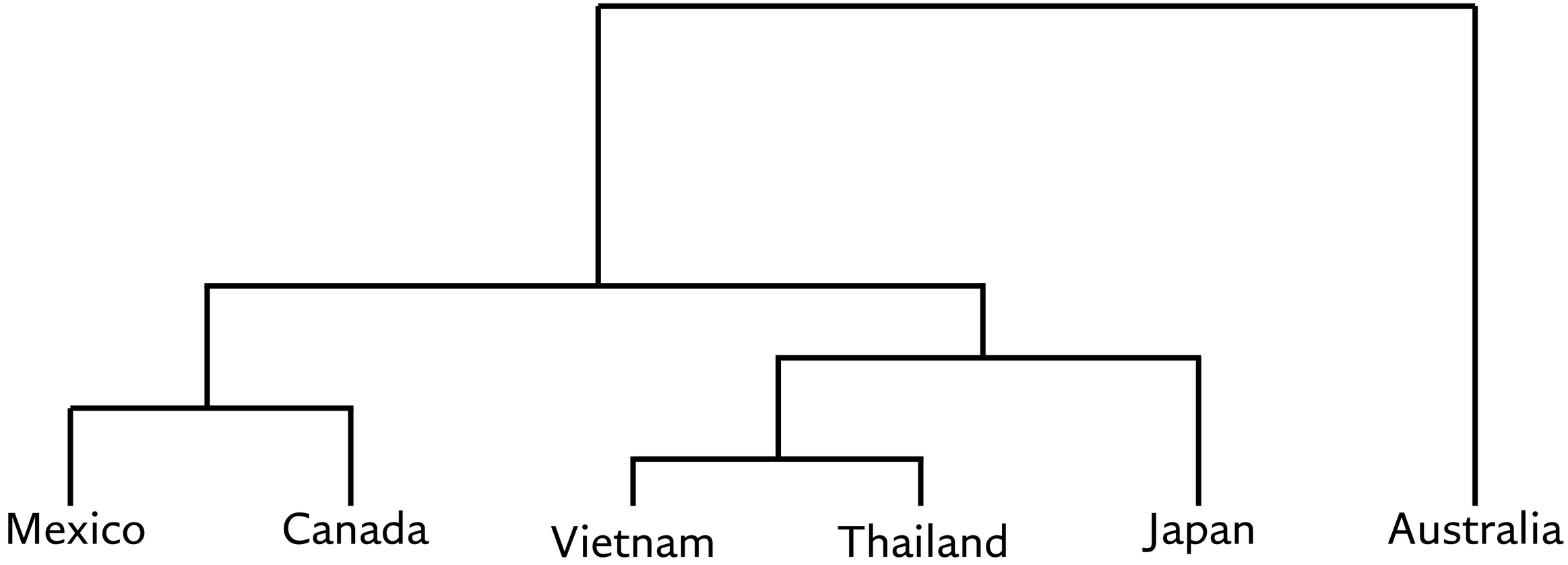
Agglomerative Hierarchical Clustering

Algorithm 1 Agglomerative Clustering

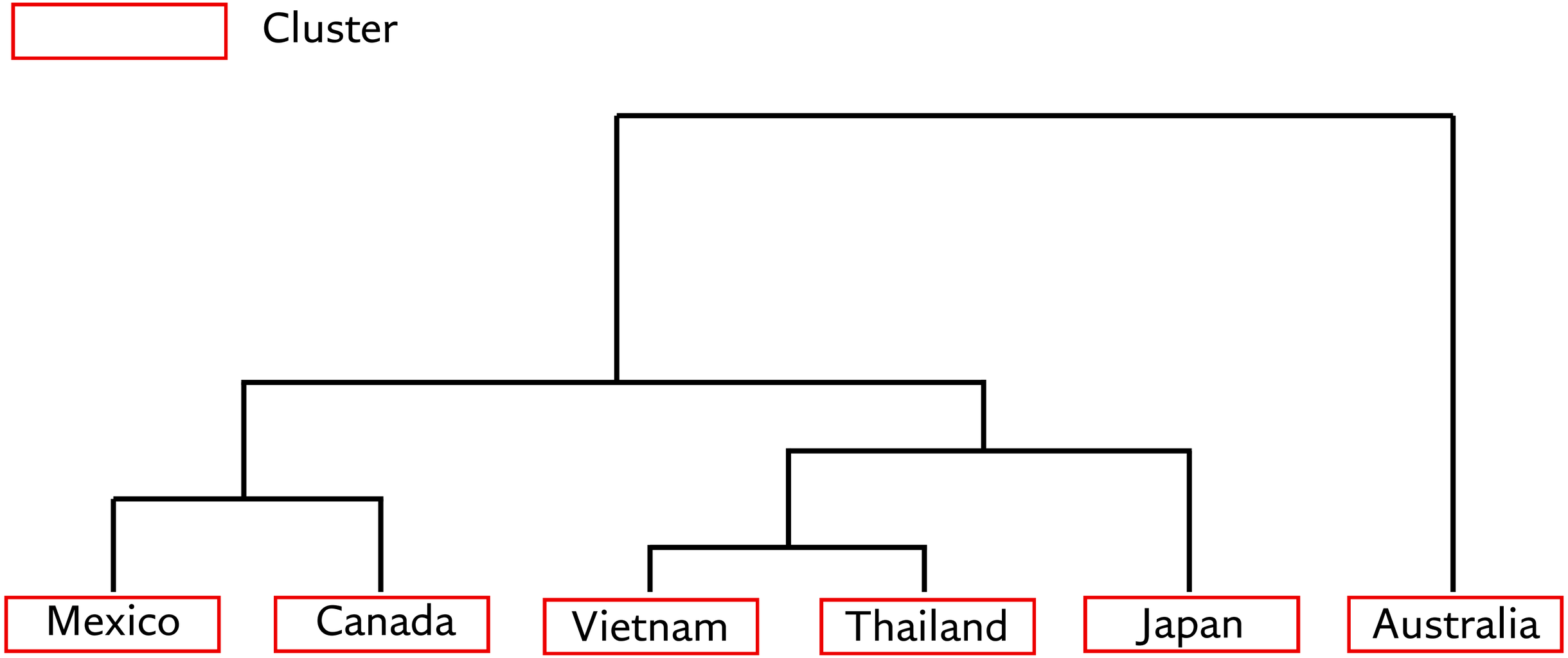
Require: Set of data points $X = \{x_1, x_2, \ldots, x_n\}$, number of clusters k
Ensure: k clusters containing all data points

1: Initialize each data point as its own cluster: $C = \{\{x_1\}, \{x_2\}, \ldots, \{x_n\}\}$
2: **while** $|C| > k$ **do**
3: Calculate **the distance** between each pair of clusters in C
4: Select the pair of clusters (C_i, C_j) with the minimum distance
5: Merge clusters C_i and C_j to form a new cluster C_{ij}
6: Update the set of clusters: $C = (C \setminus \{C_i, C_j\}) \cup \{C_{ij}\}$
7: **end while**
8: **return** C as the final set of clusters

Dendrogram



Dendrogram



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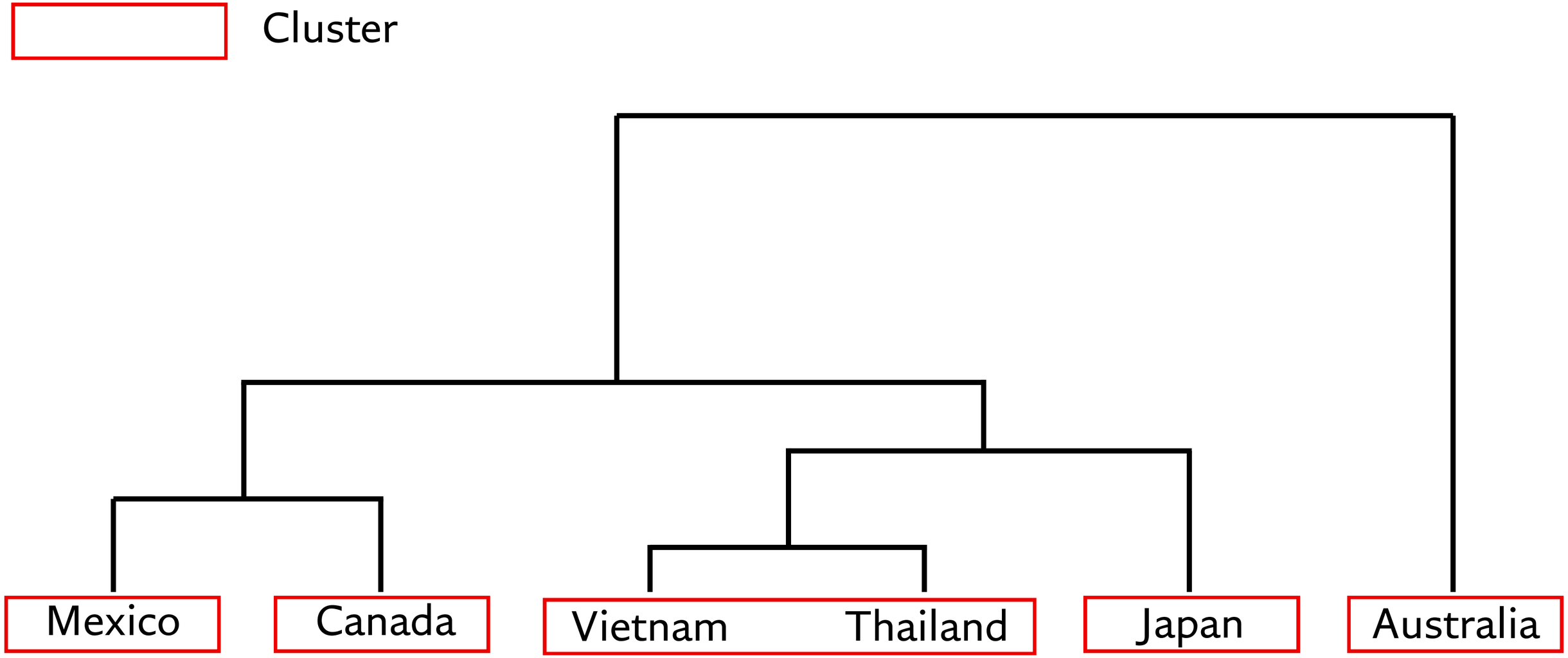

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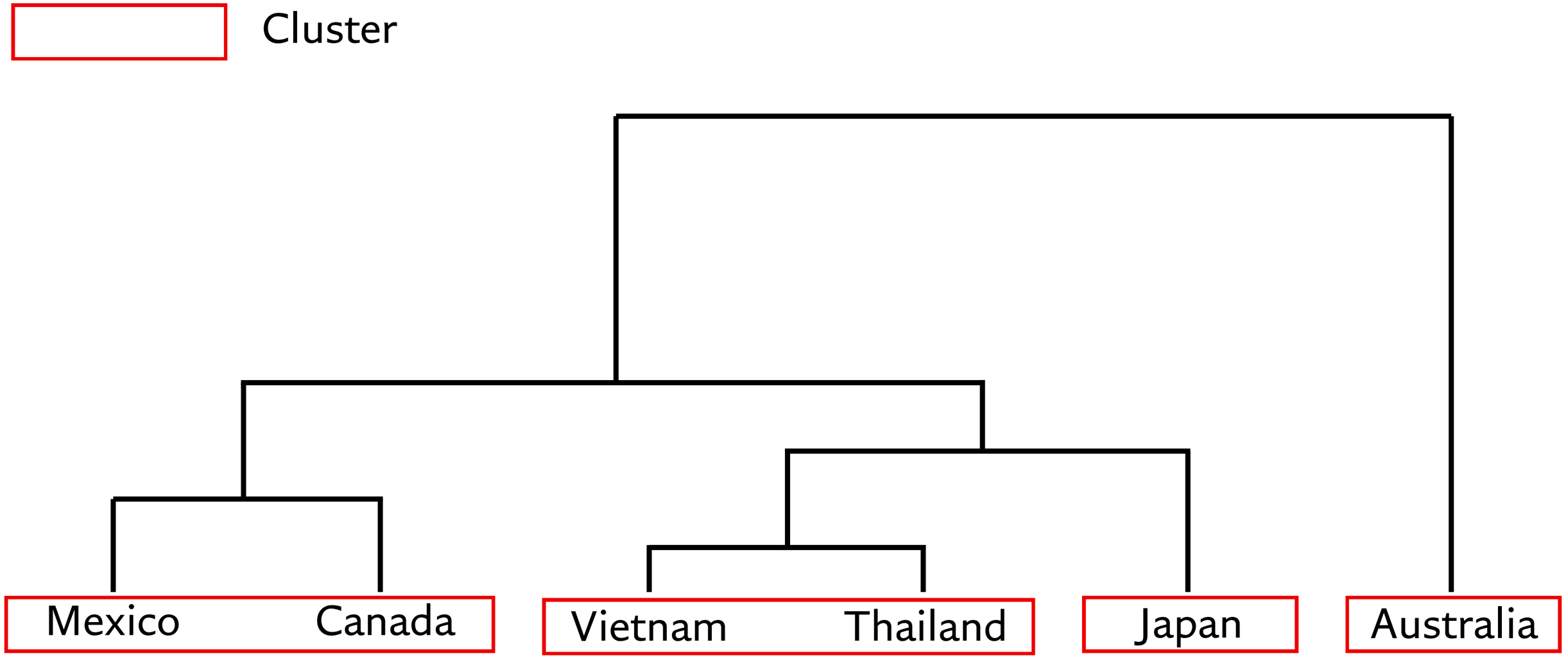
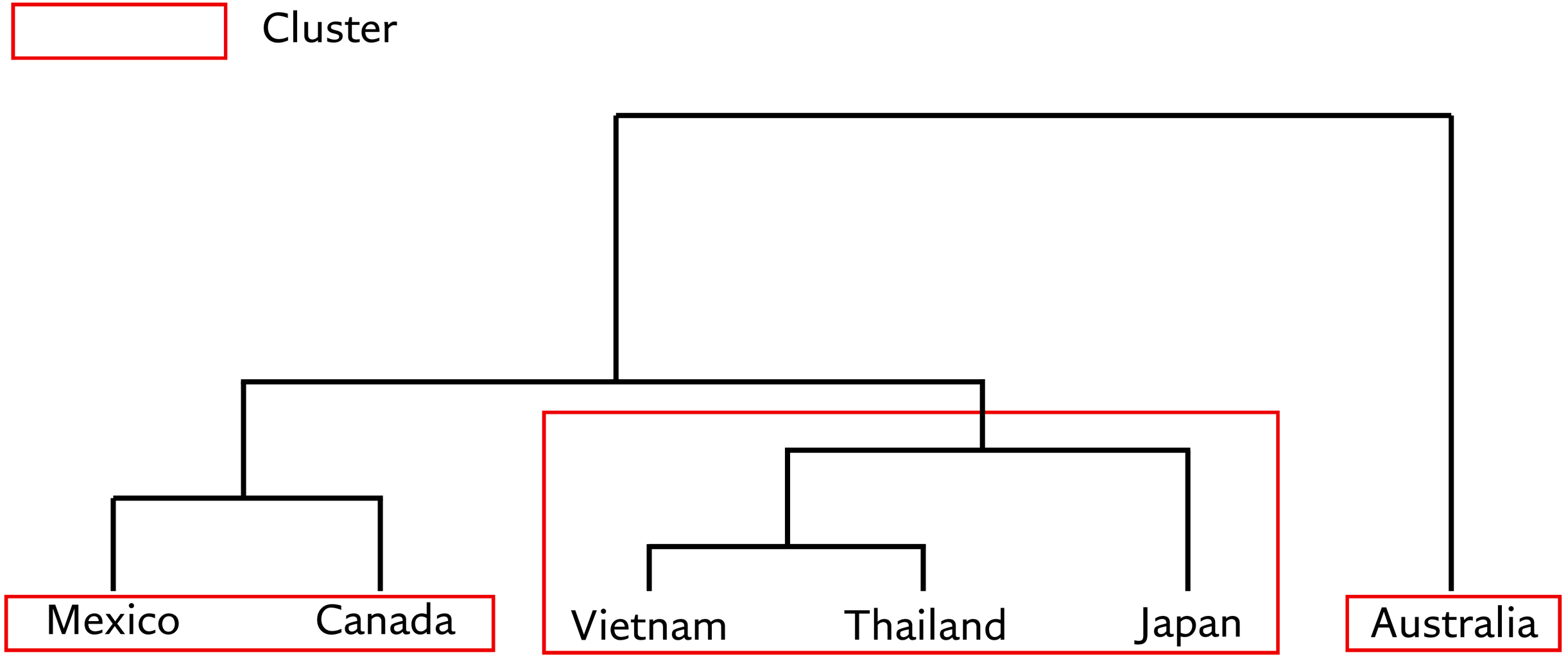


Dendrogram



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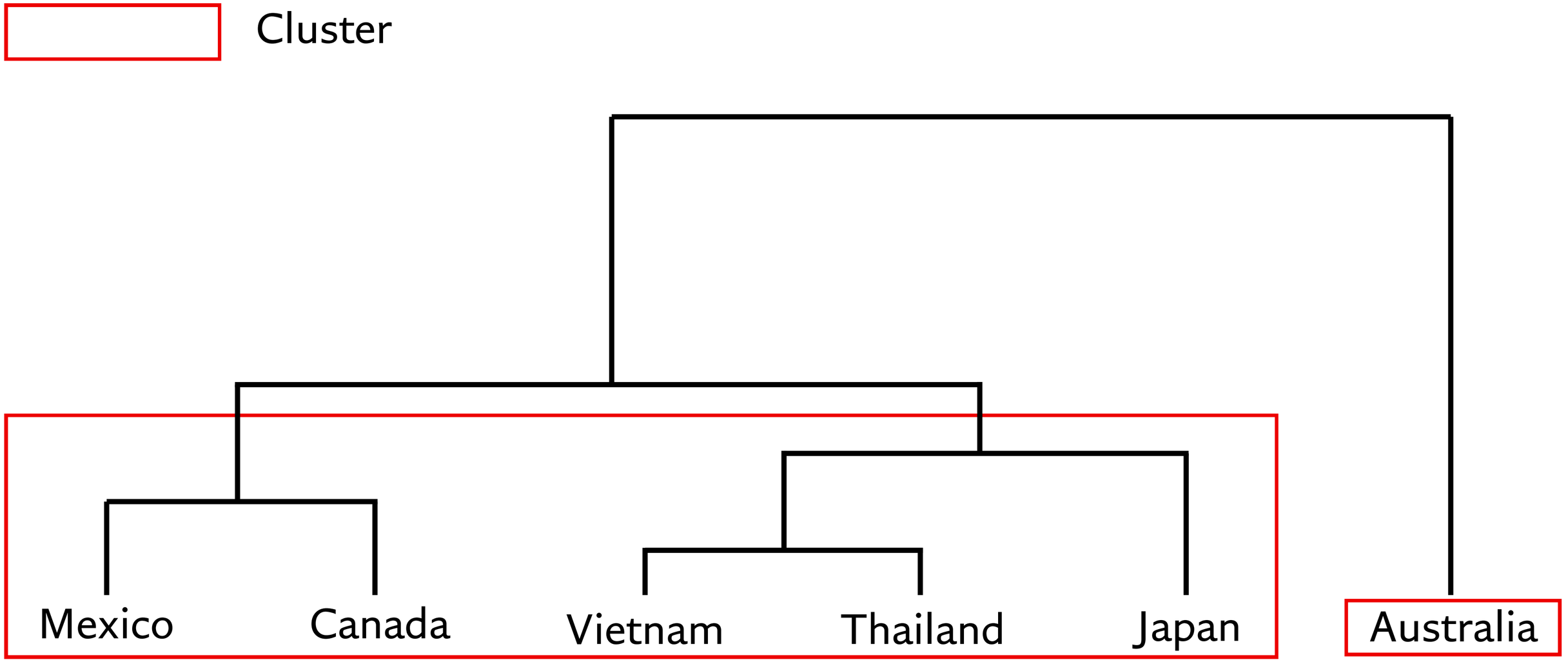
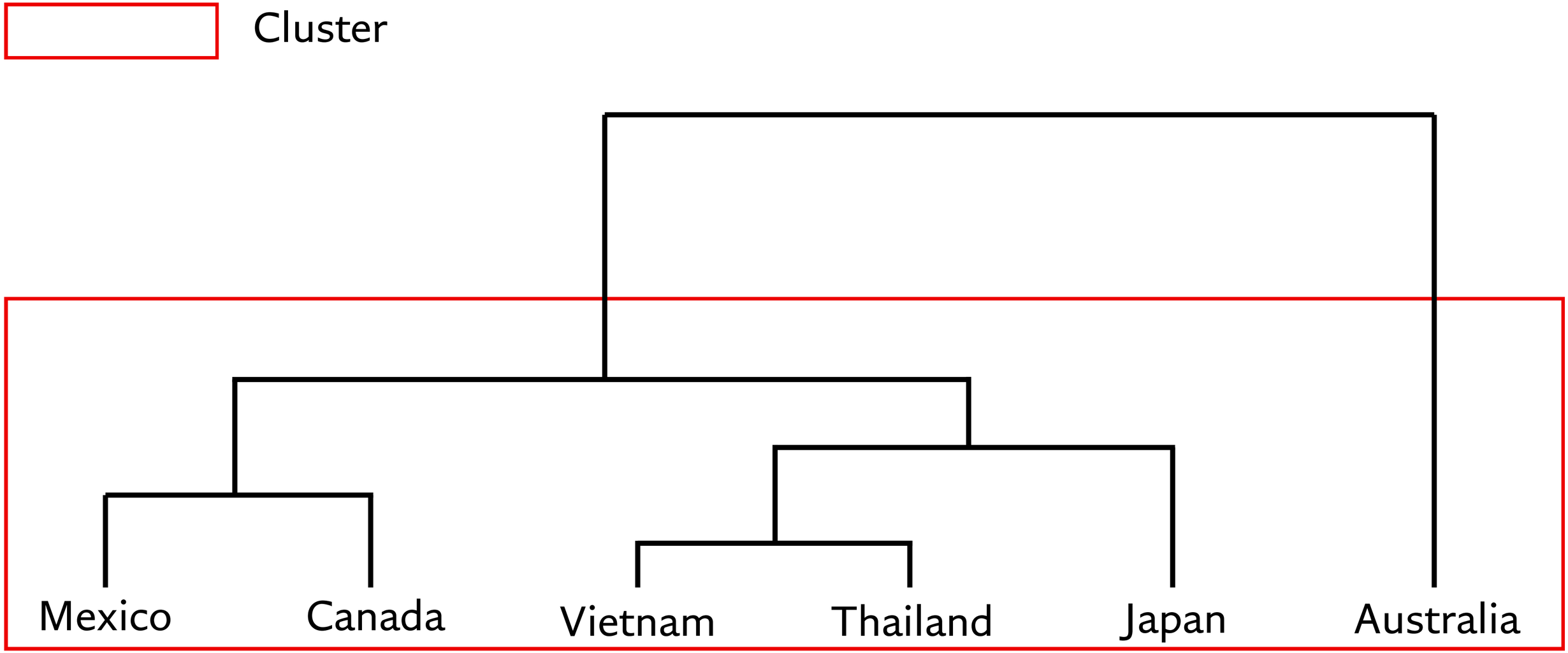
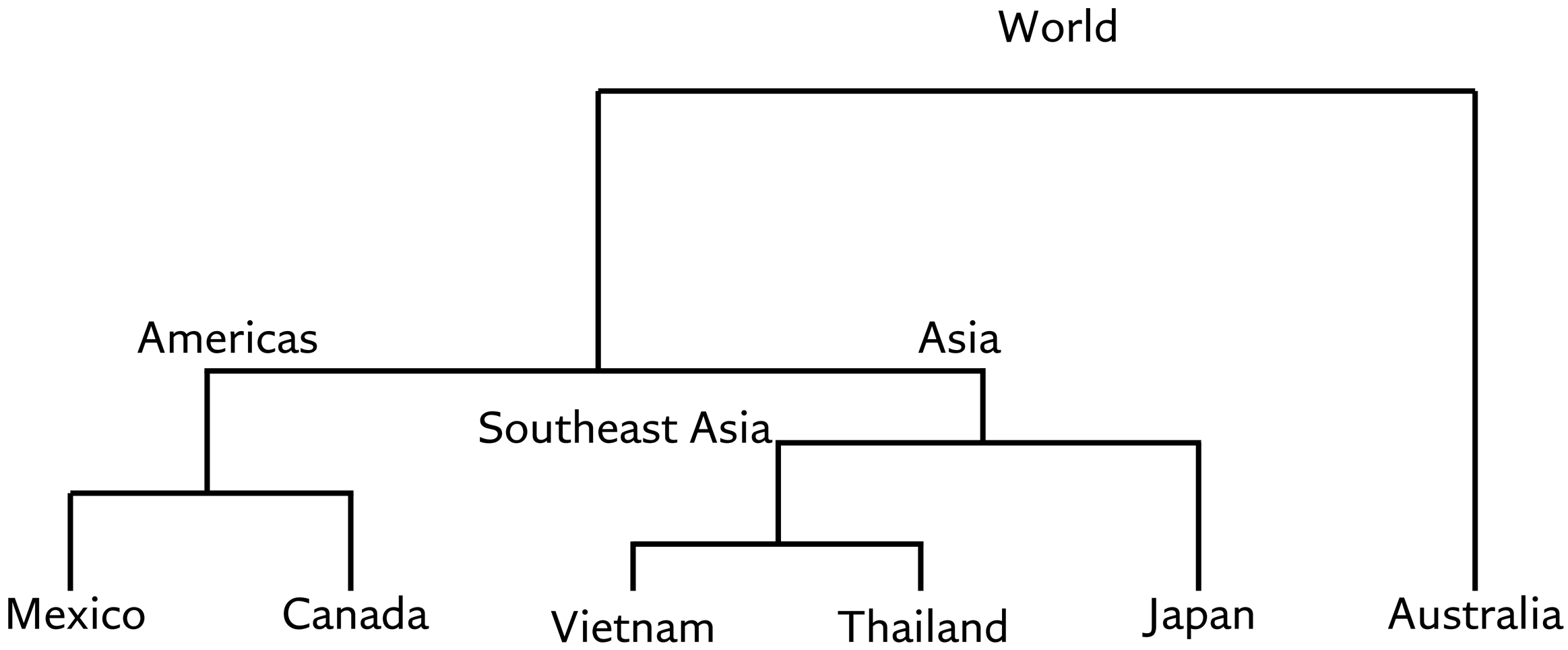


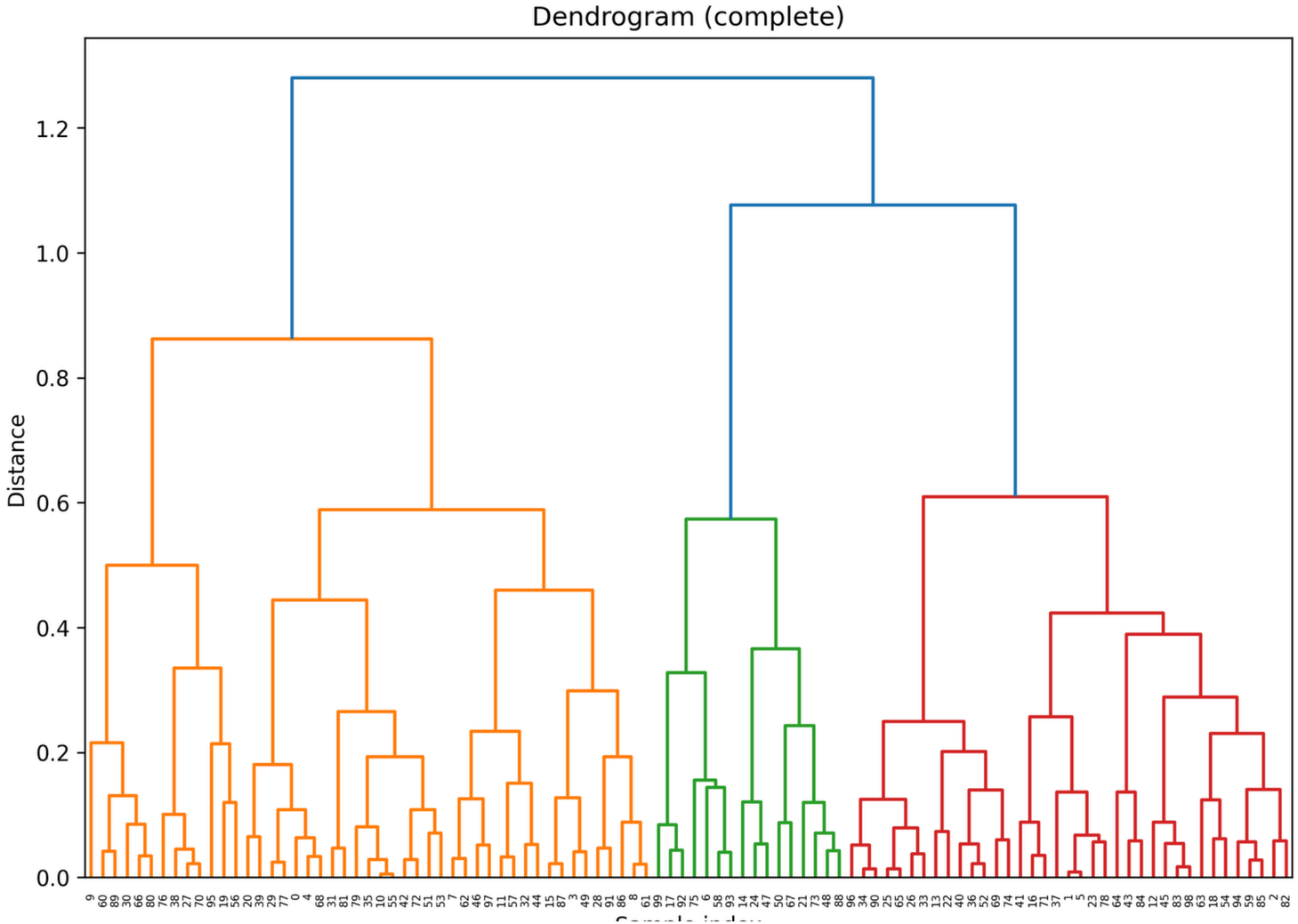
Dendrogram



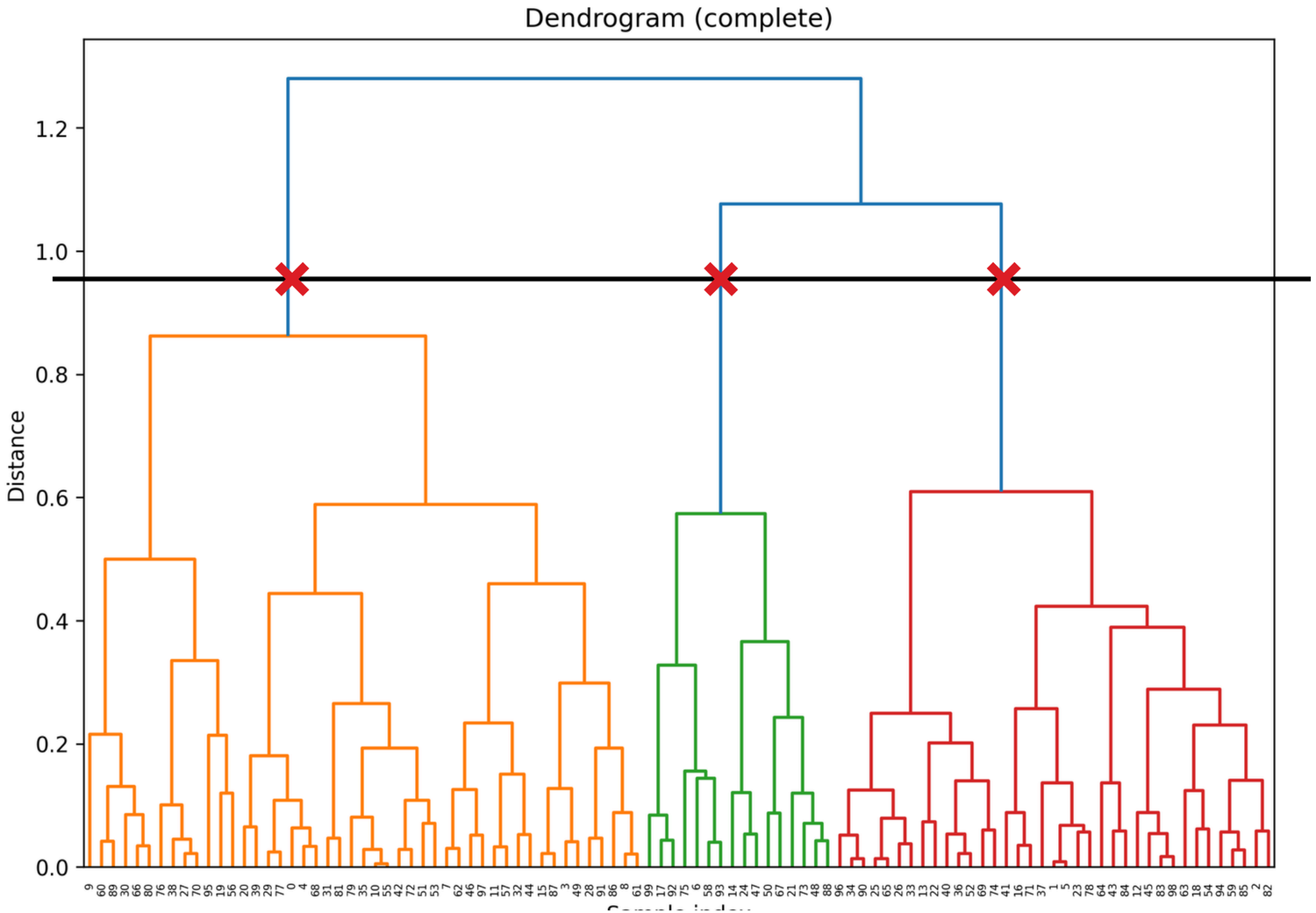
Dendrogram


World
Americas
Asia
Southeast Asia
Mexico
Canada
Vietnam
Thailand
Japan
Australia

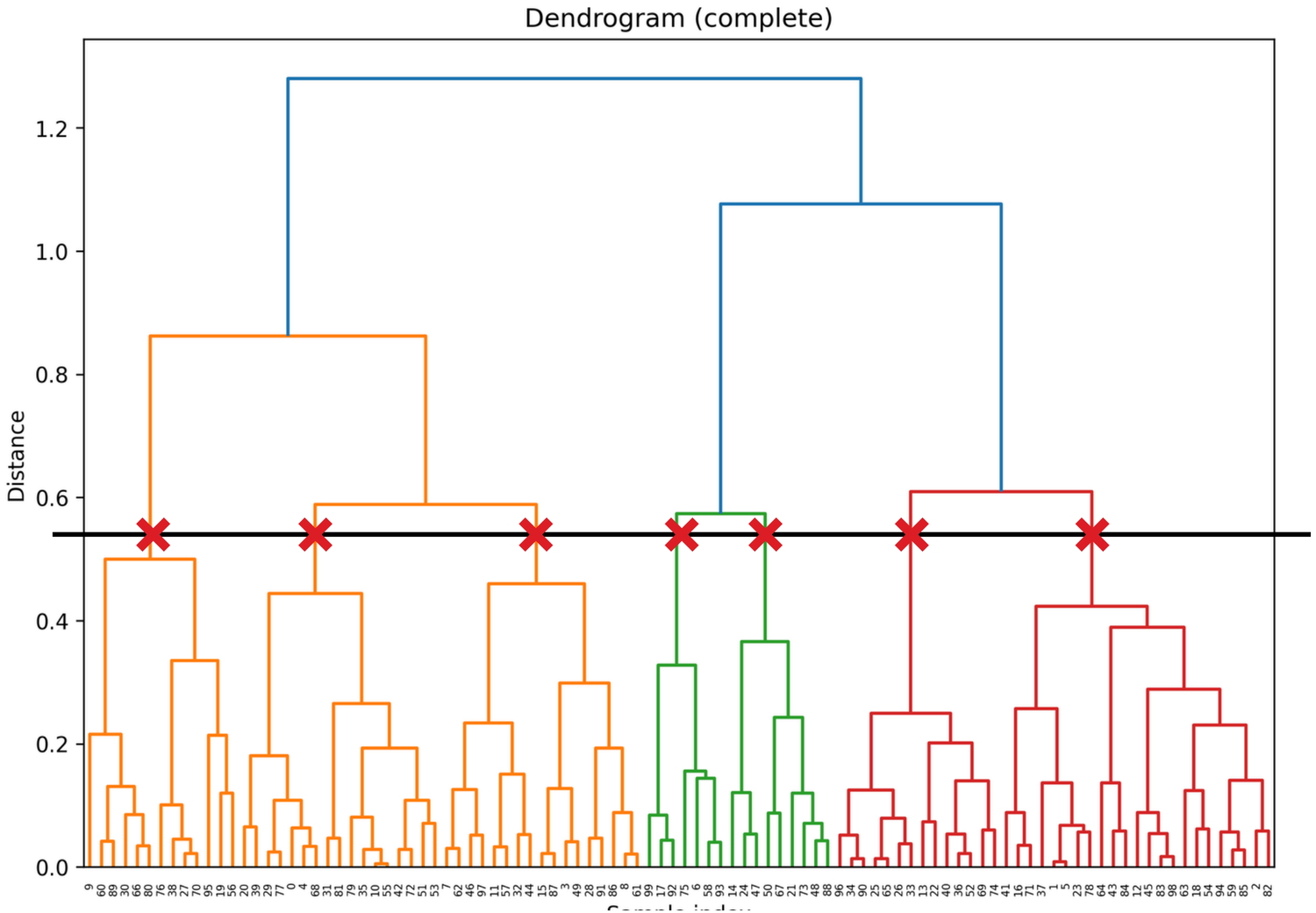
Dendrogram



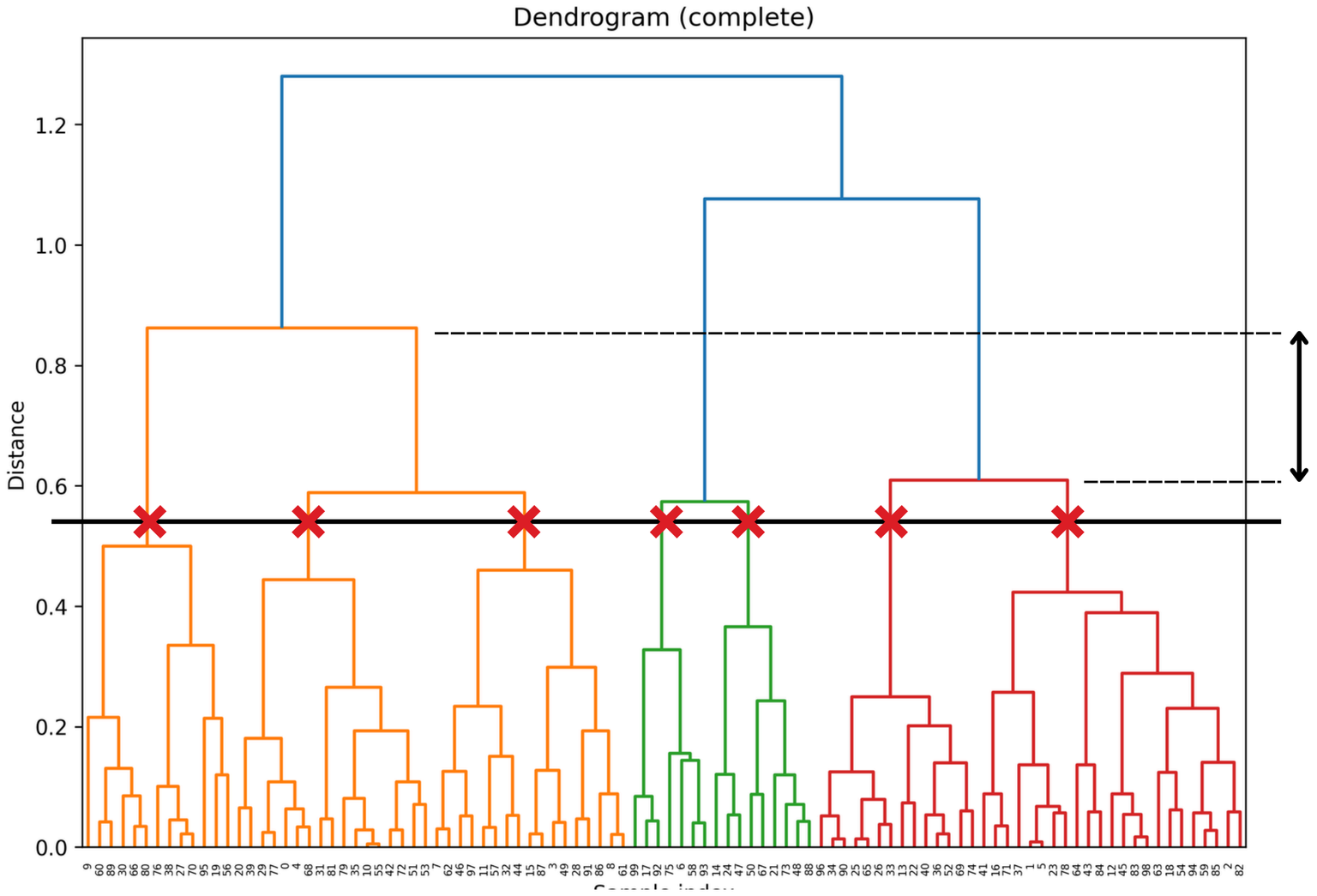
Dendrogram

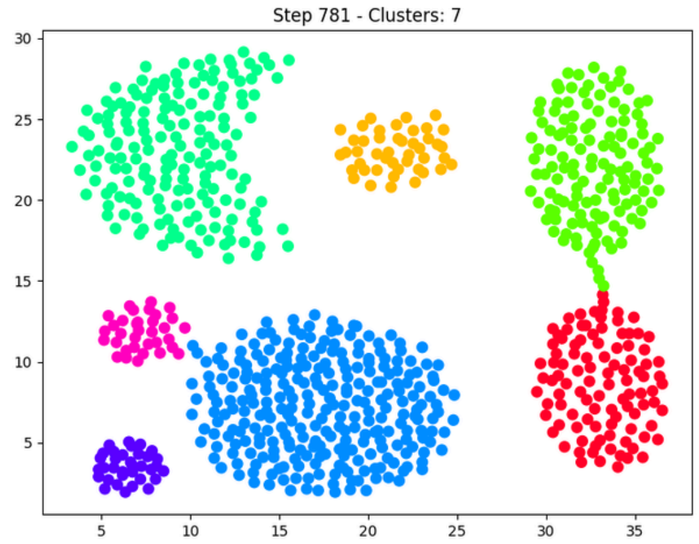


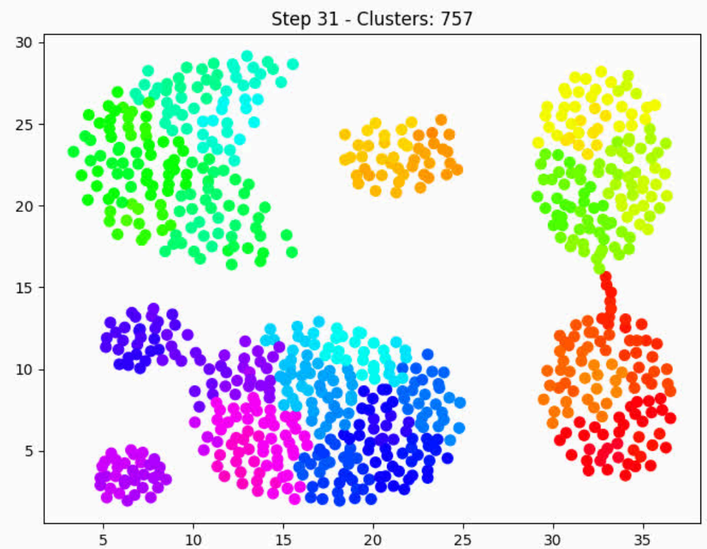
Dendrogram



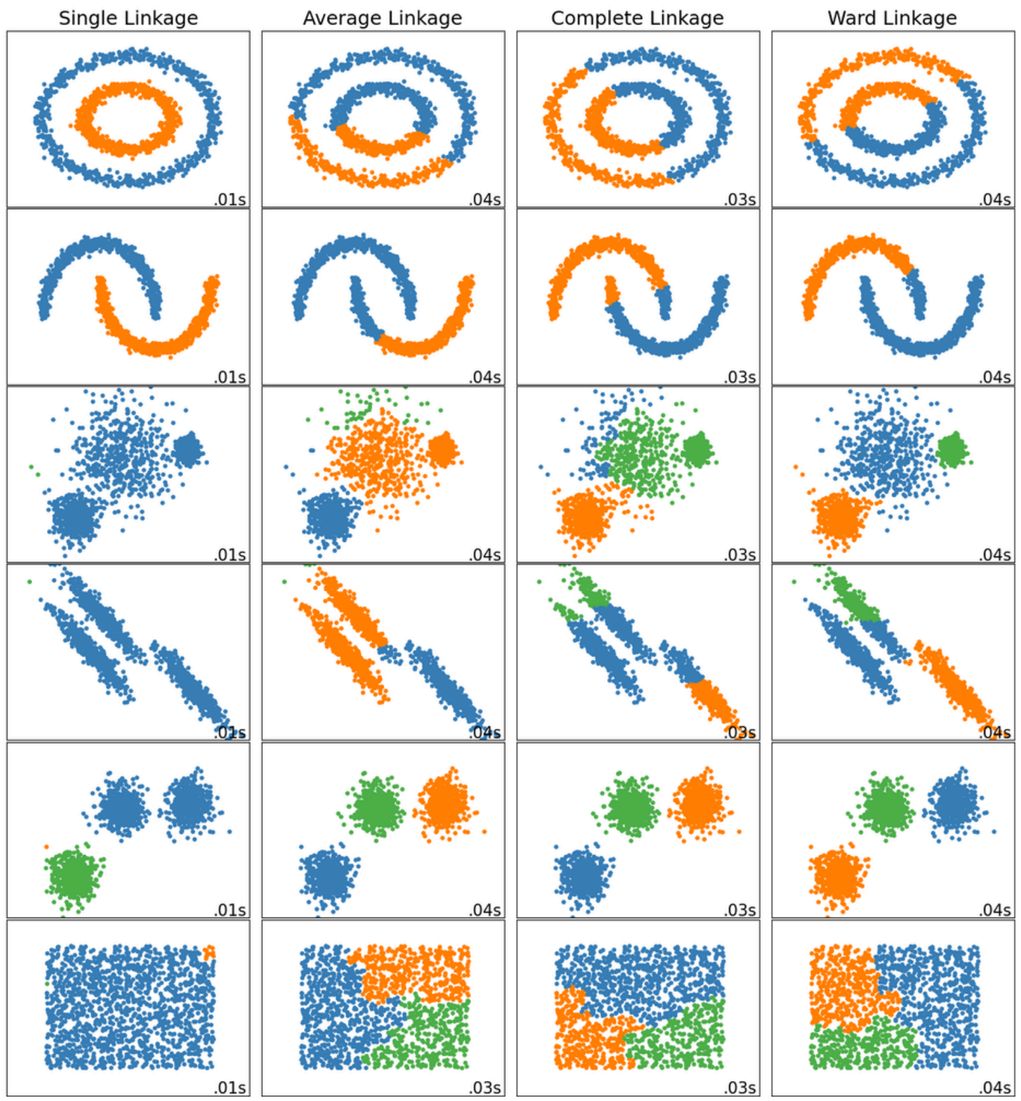
Dendrogram


Dendrogram (complete)
Distance
1.2
1.0
0.8
0.6
0.4
0.2
0.0


Step 781 - Clusters: 7


Step 31 - Clusters: 757

Experiment



- **Single**: fast, and can **perform well on non-globular data**, but it performs **poorly in the presence of noise**.
- **Average**, **Complete**: perform well on cleanly separated globular clusters, but have mixed results otherwise.
- **Ward**: the most effective method for noisy data.

Divisive Hierarchical Clustering

- A **top-down** approach to clustering, which is the opposite of the more common **agglomerative** clustering.
- Begin with all the data points in **one single cluster** and progressively split them into **smaller clusters**.
- This process continues recursively until each data point is its own cluster.
- The challenge in divisive hierarchical clustering is deciding **the best way to split** clusters at each step.

Divisive Hierarchical Clustering

Algorithm 2 Divisive Clustering

Require: Set of data points $X = \{x_1, x_2, \ldots, x_n\}$, number of clusters k
Ensure: k clusters containing all data points

1: Initialize the set of clusters: $C = \{X\}$
2: **while** $|C| < k$ **do**
3: Select the cluster C_i in C with **the lowest connection**
4: Split the cluster C_i into two sub-clusters (C_{i1}, C_{i2})
5: Update the set of clusters: $C = (C \setminus \{C_i\}) \cup \{C_{i1}, C_{i2}\}$
6: **end while**
7: **return** C as the final set of clusters

Divisive Hierarchical Clustering

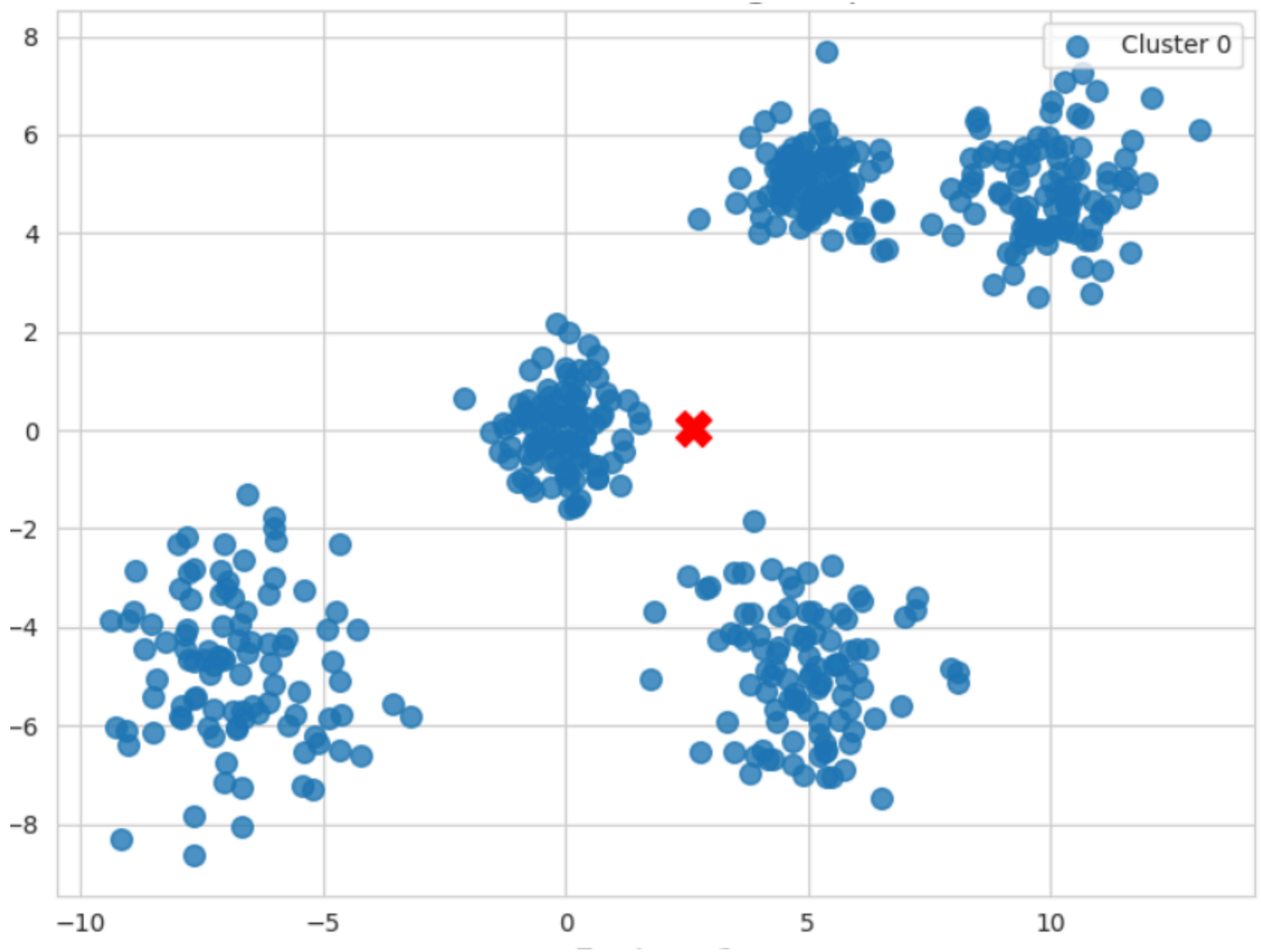
- There are **three key aspects** that must be addressed when designing a divisive hierarchical clustering algorithm:

  Splitting Criterion:
  - A common criterion for evaluating splits is the **Sum of Squared Errors (SSE),** which helps to minimize the within-cluster variance.

  Splitting Method:
  - Evaluate every possible way of dividing the data points **into two clusters**.
  - One practical and popular heuristic is to use the **bisecting k-means** method, where **k = 2.**

  Cluster Selection for Splitting:
  - Which cluster should we split next?
  - A simple yet effective approach is to choose the **loosest cluster**, i.e., the cluster with the **largest average SSE**.

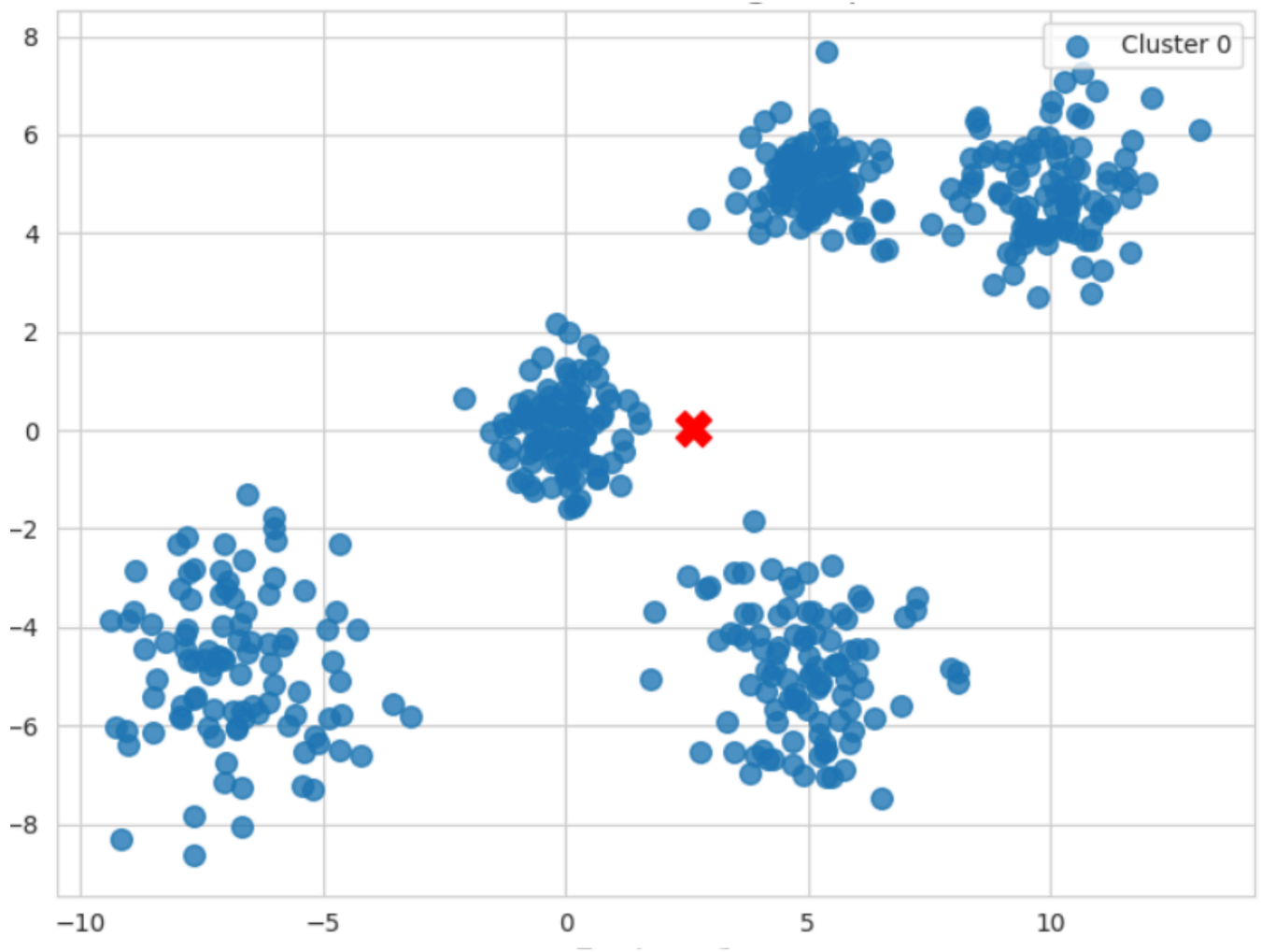
Divisive Hierarchical Clustering



The SSE for a cluster **C** is defined as:

$$SSE = \sum_{\mathbf{x} \in C} \|\mathbf{x} - \mathbf{m}_C\|^2$$

Divisive Hierarchical Clustering

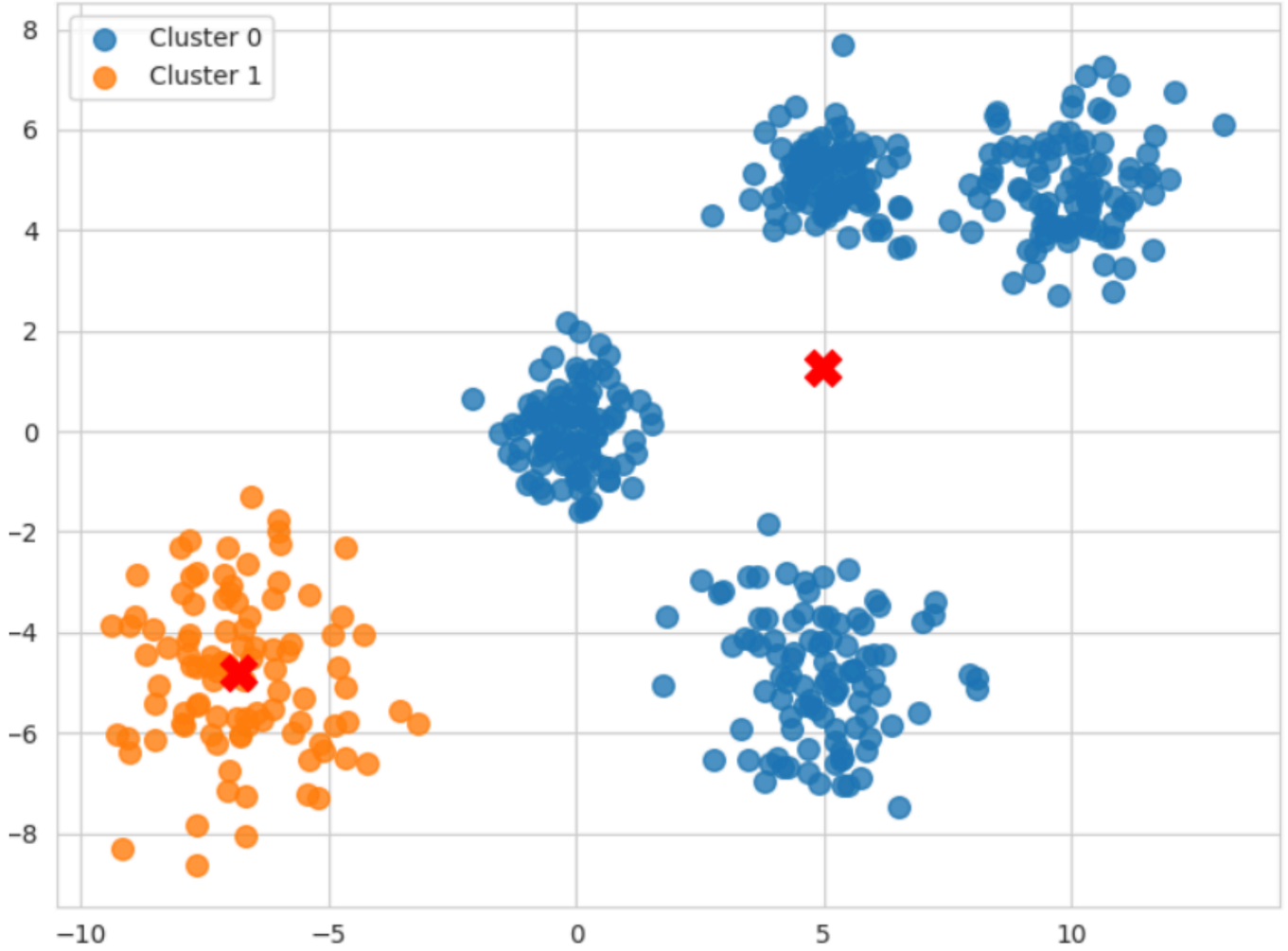


Formally, for each cluster C_i, we compute the average SSE:

$$E_{C_i} = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2$$

Cluster SSE scores: 53.69

Divisive Hierarchical Clustering



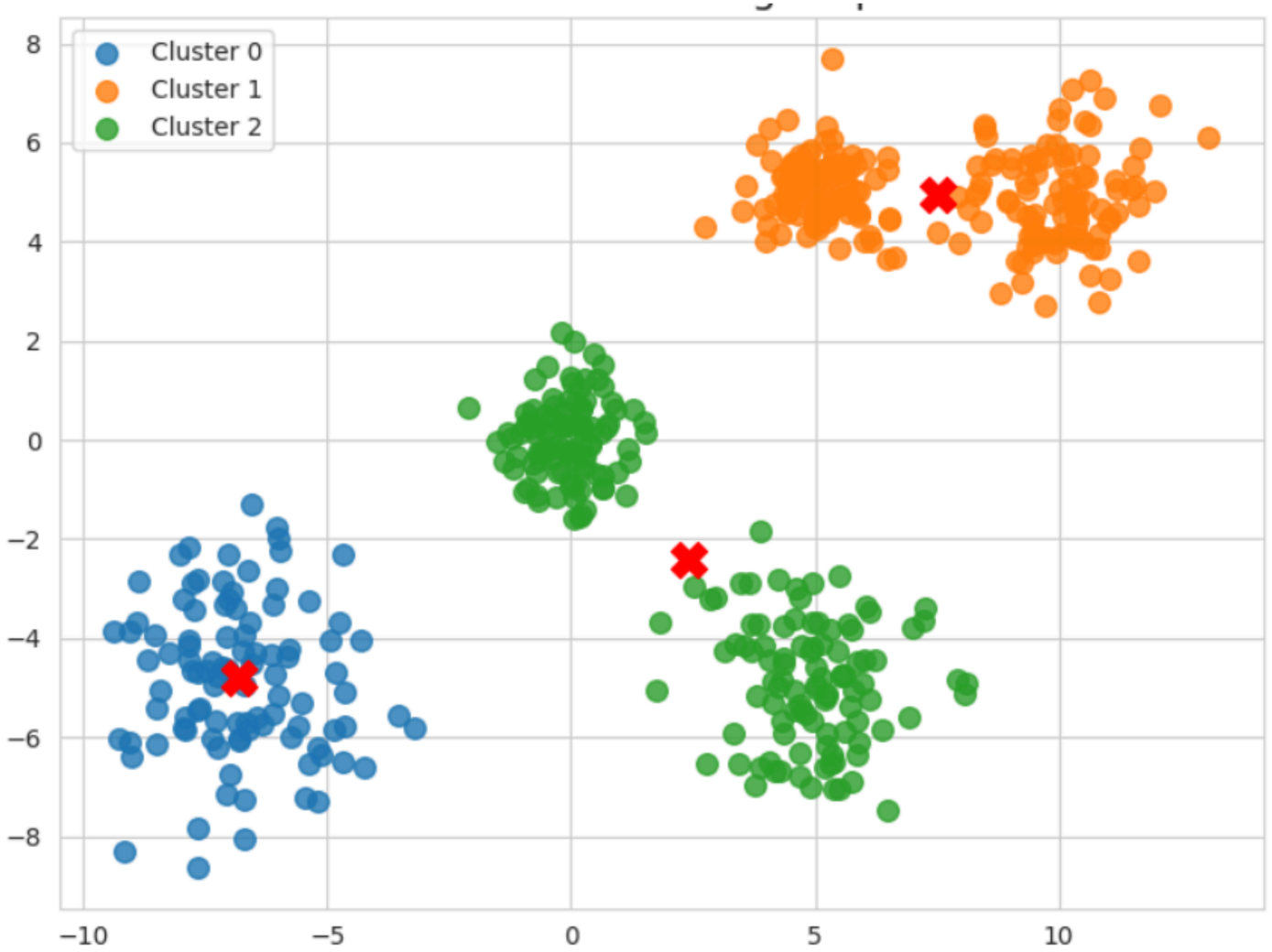
Use the bisecting k-means method, where k = 2.

$$E_{C_i} = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2$$

Cluster SSE scores (0): 31.0

Cluster SSE scores (1): 4.09

Divisive Hierarchical Clustering



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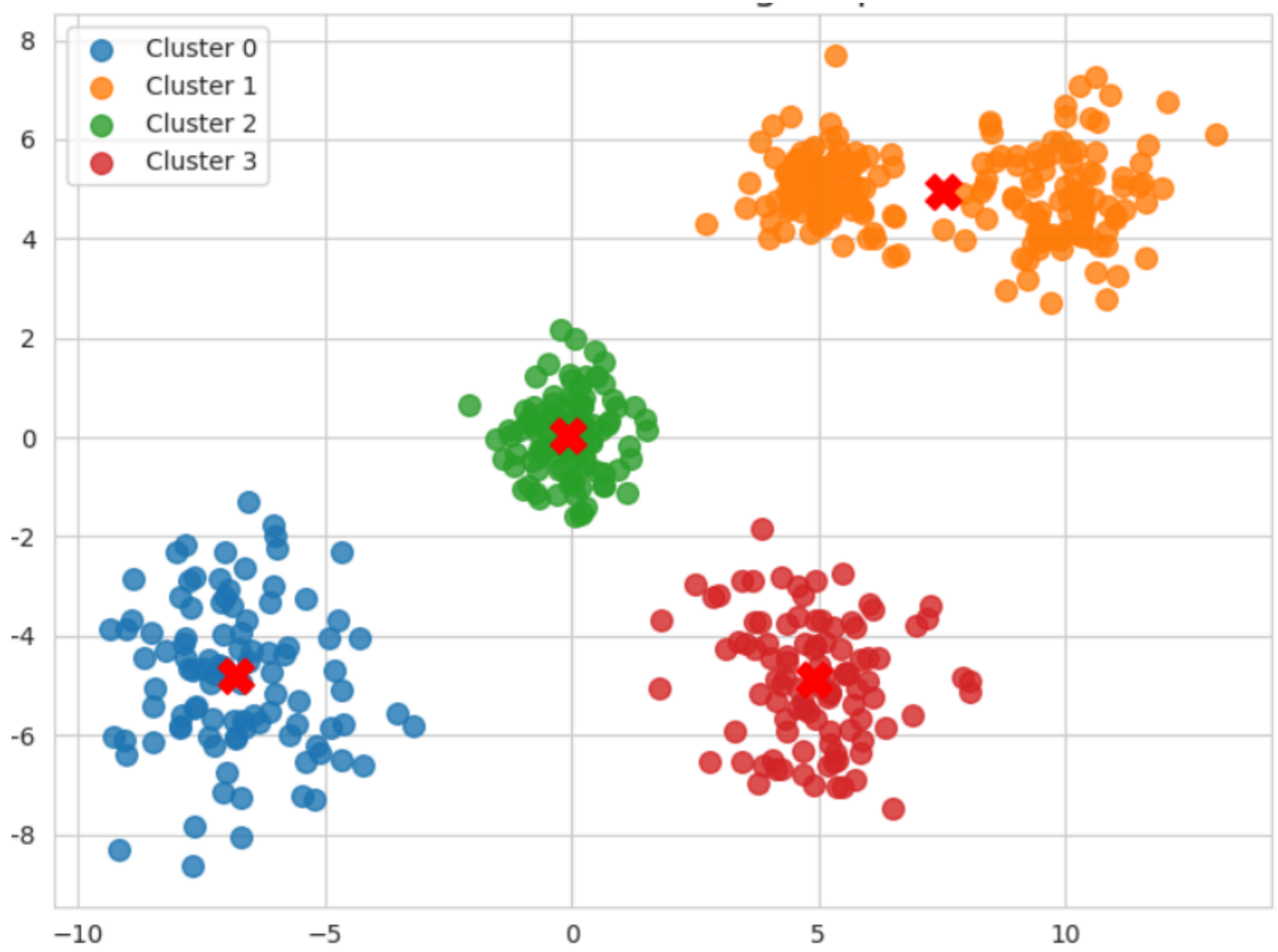
Cluster SSE scores (0): 4.09

Cluster SSE scores (1): 7.38

Cluster SSE scores (2): 14.31

Divisive Hierarchical Clustering



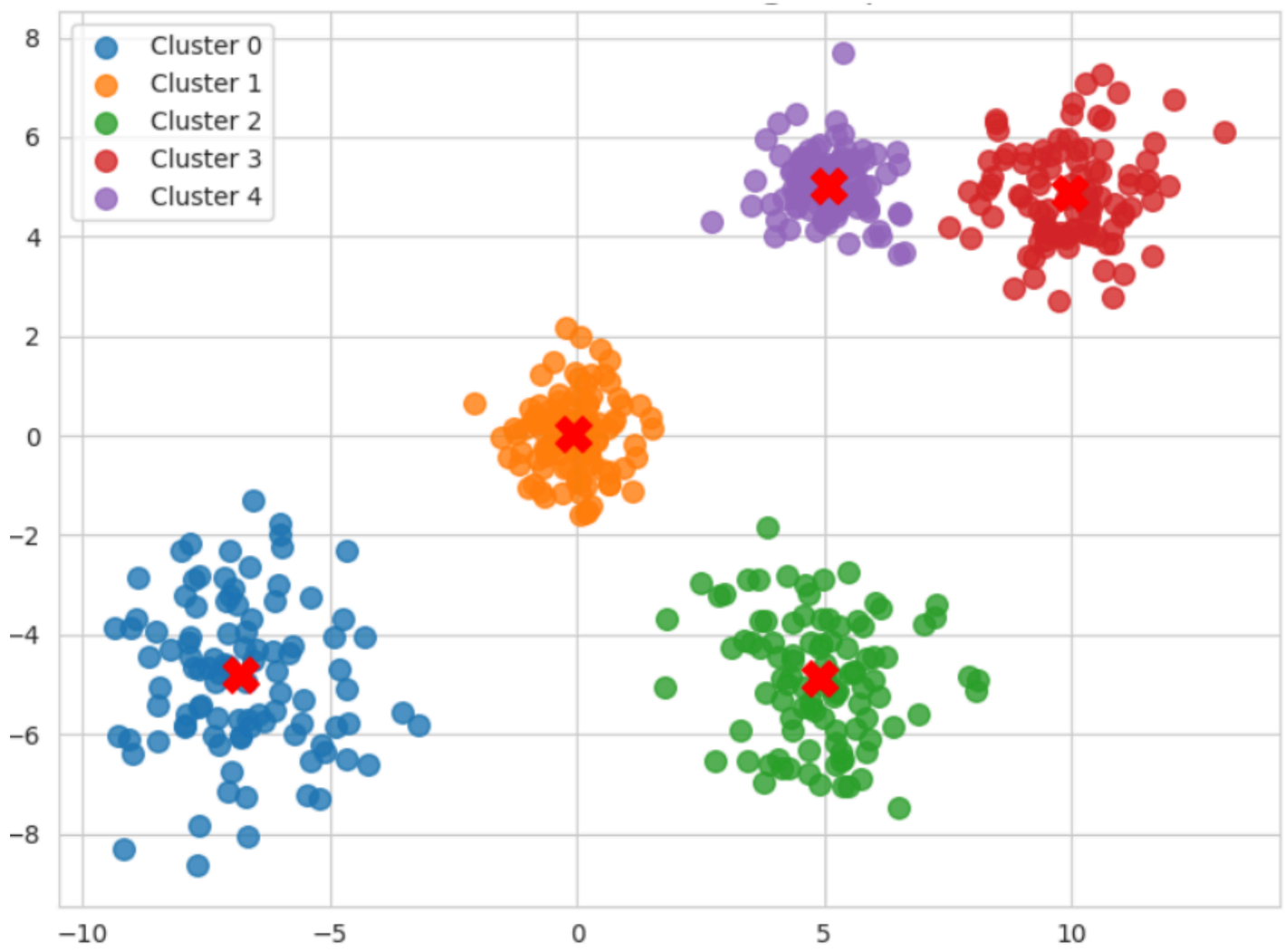
Cluster SSE scores (0): 4.09

Cluster SSE scores (1): 7.38

Cluster SSE scores (2): 1.09

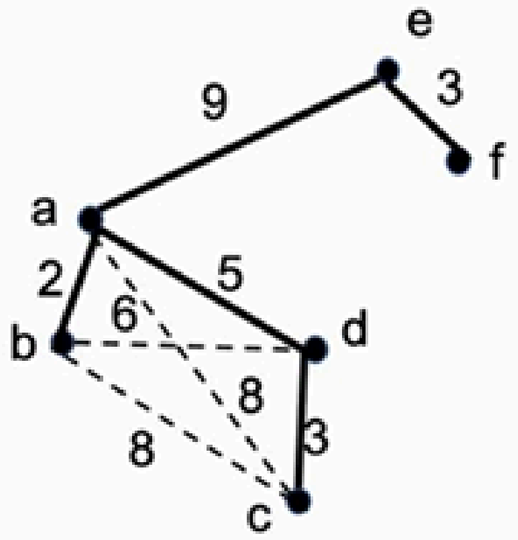
Cluster SSE scores (3): 2.96

Divisive Hierarchical Clustering



Minimum Spanning Tree-based Approach

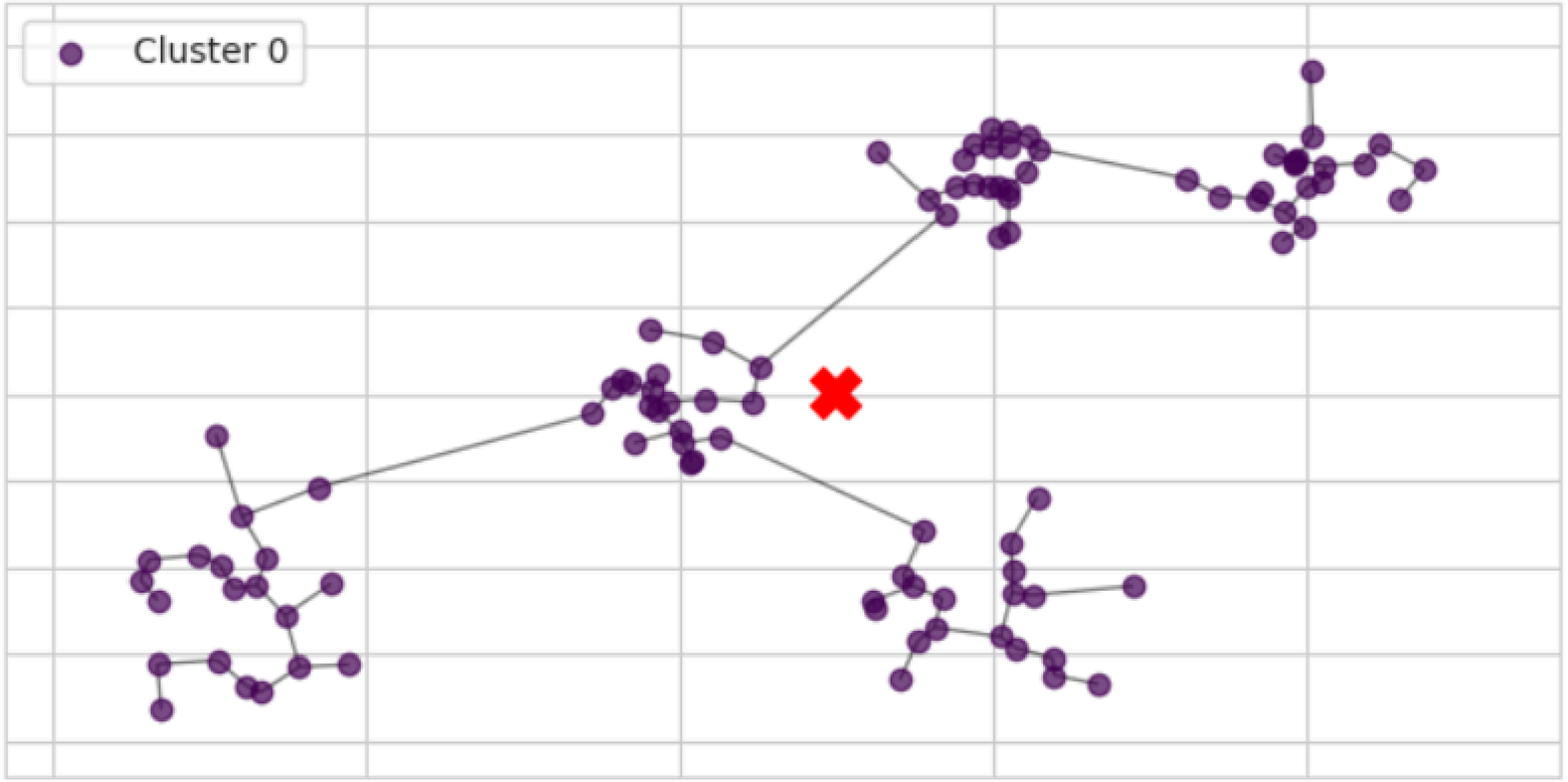
- Based on the concept of the **minimum spanning tree (MST)**
- In a weighted graph G, a minimum spanning tree is an acyclic subgraph of G that contains all nodes in G, and the sum of edge weights of the tree is minimized.



Minimum Spanning Tree-based Approach

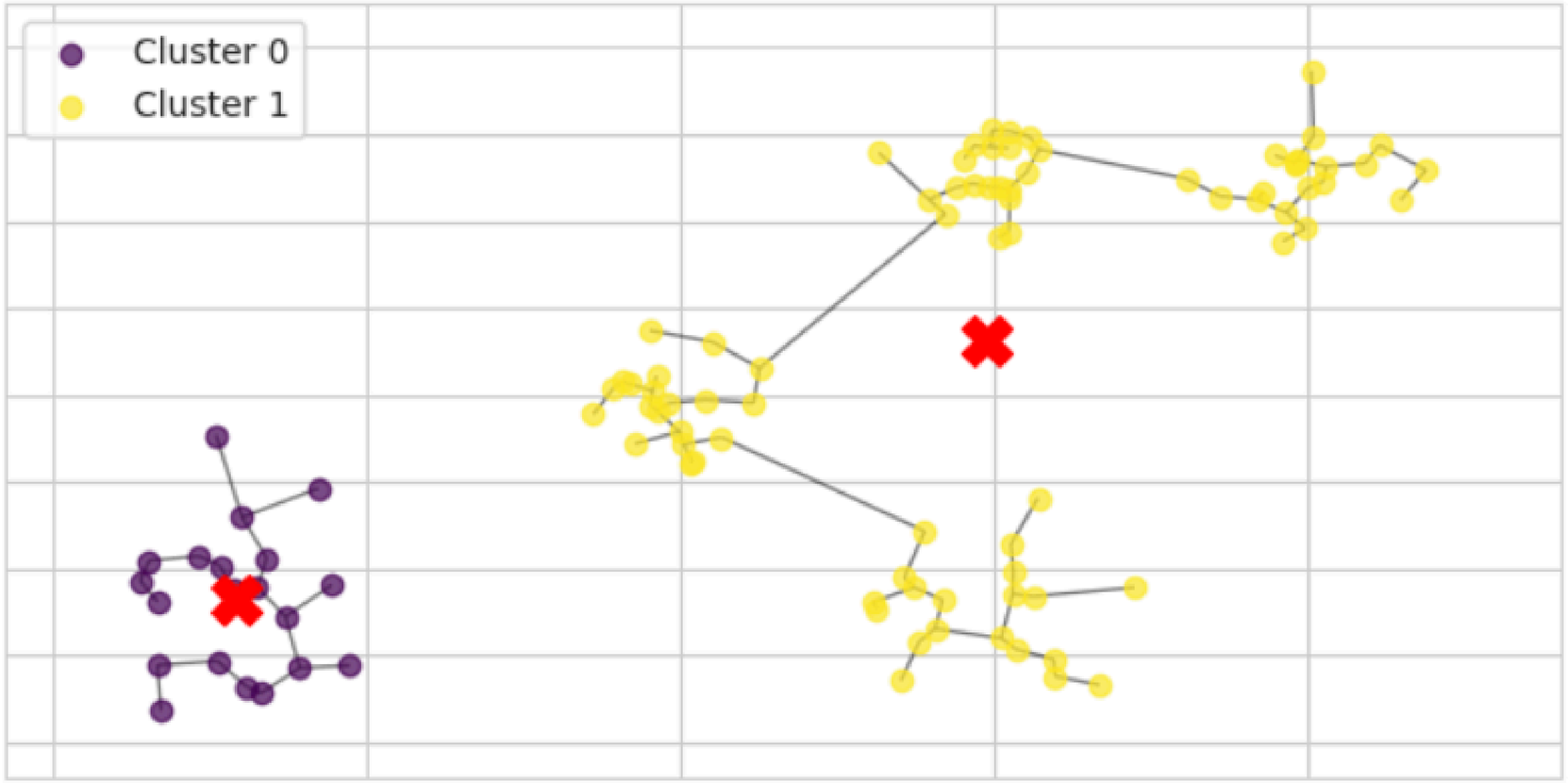
- To perform divisive hierarchical clustering using the MST, we follow these steps:
  - Construct a weighted graph where each node represents a data point, and the edge weights correspond to the distance between points
  - Compute the MST of the graph.
  - At each step, delete the edge with the largest weight in the MST. This will split the cluster into two sub-clusters.
  - Repeat the process of deleting the largest edge until each point is its own cluster or the desired number of clusters is reached.

Minimum Spanning Tree-based Approach



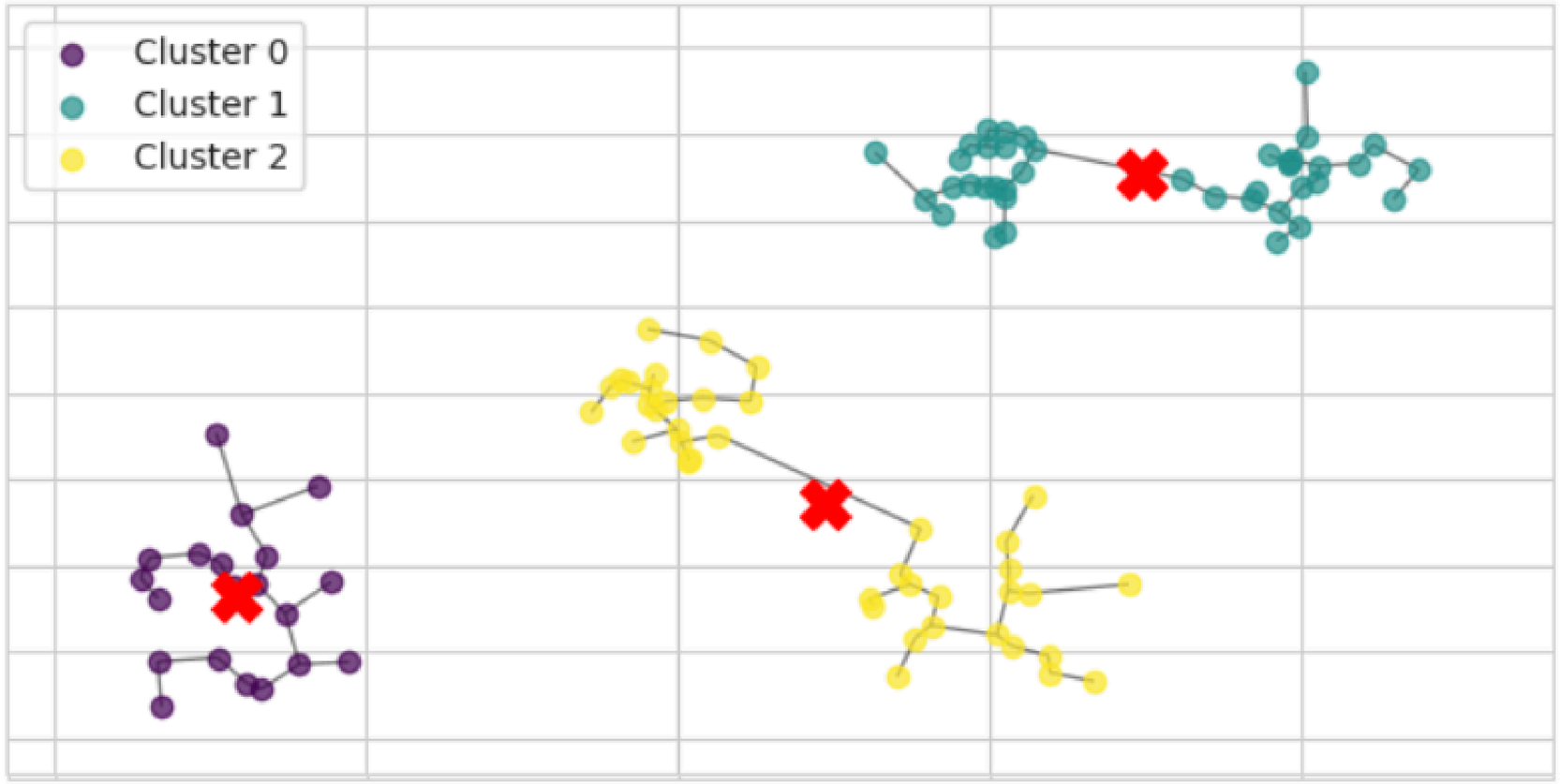
Compute the MST of the graph.

Minimum Spanning Tree-based Approach



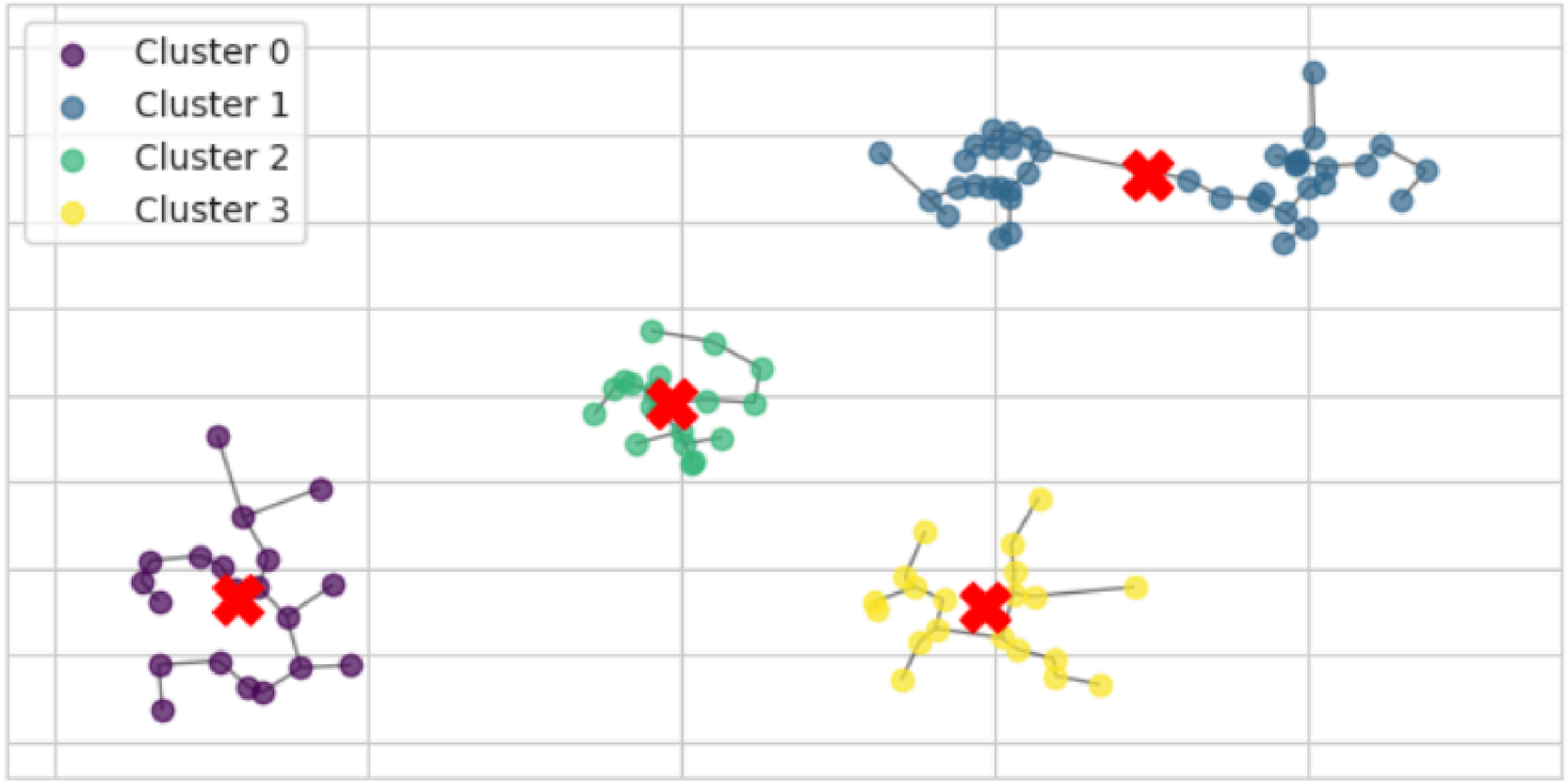
At each step, delete the edge with the largest weight in the MST. This will split the cluster into two sub-clusters.

Minimum Spanning Tree-based Approach



Repeat the process of deleting the largest edge until each point is its own cluster or the desired number of clusters is reached (5).

Minimum Spanning Tree-based Approach



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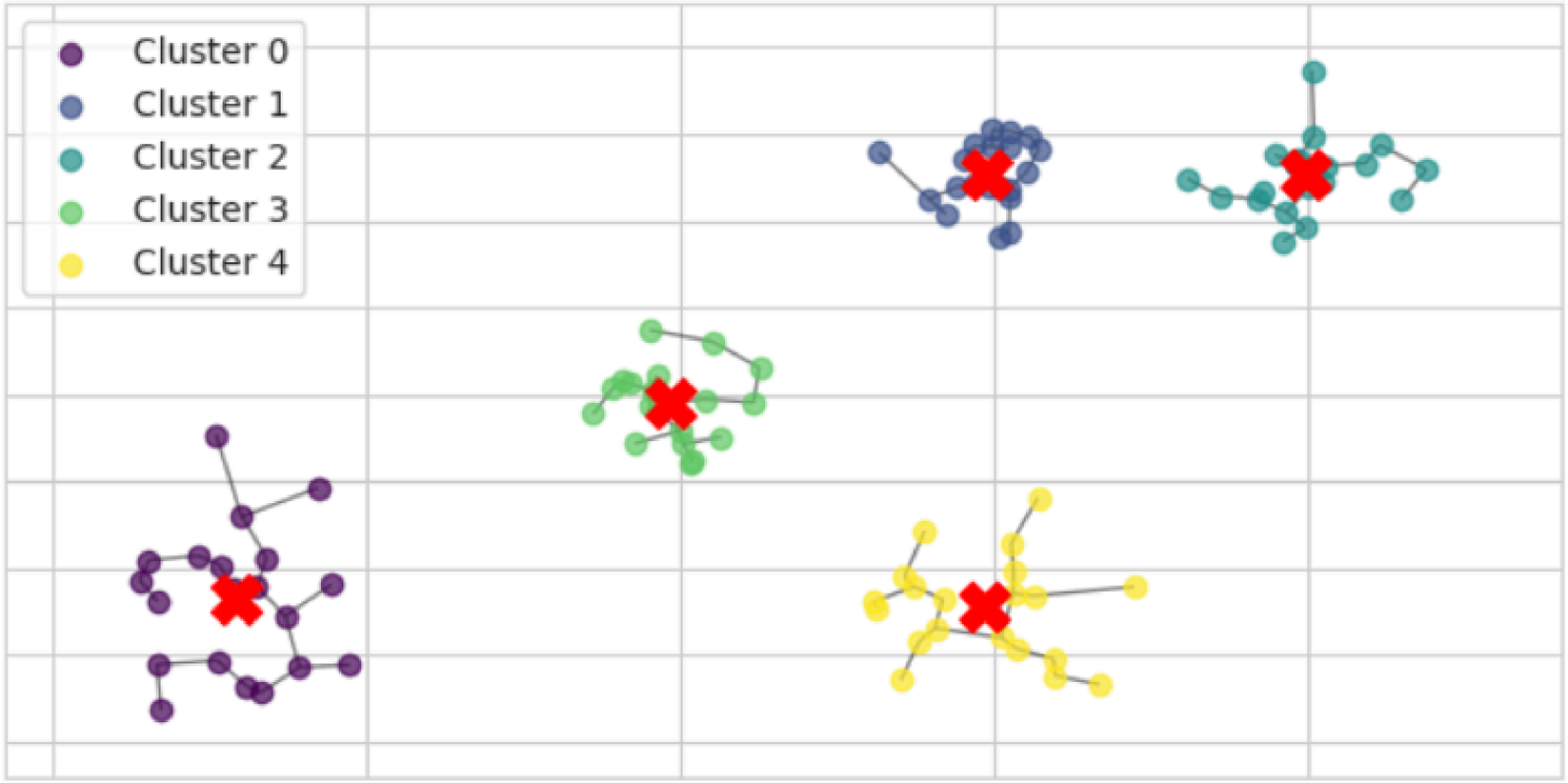

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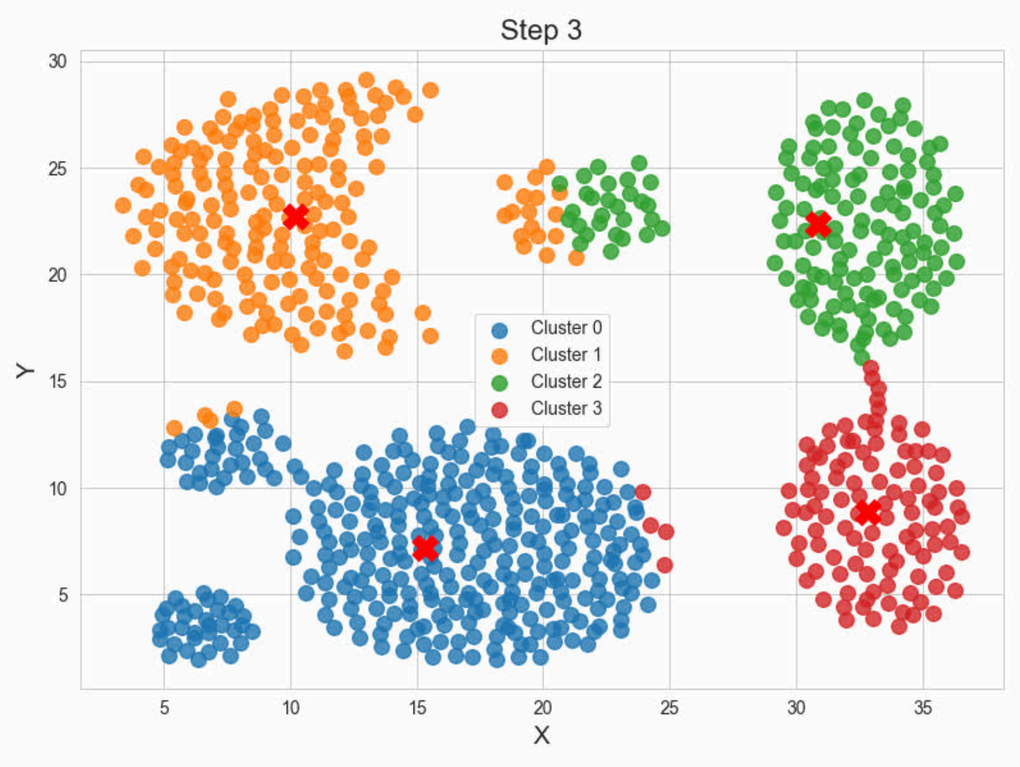
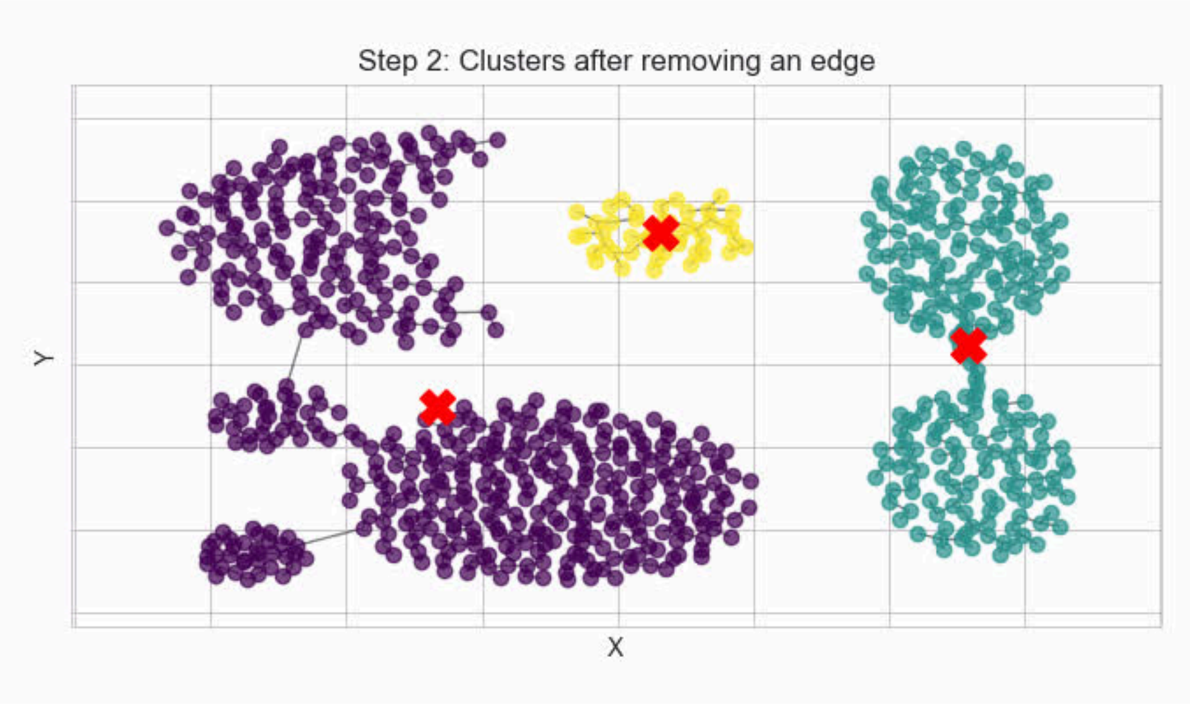
Experiments

BisectingKMeans

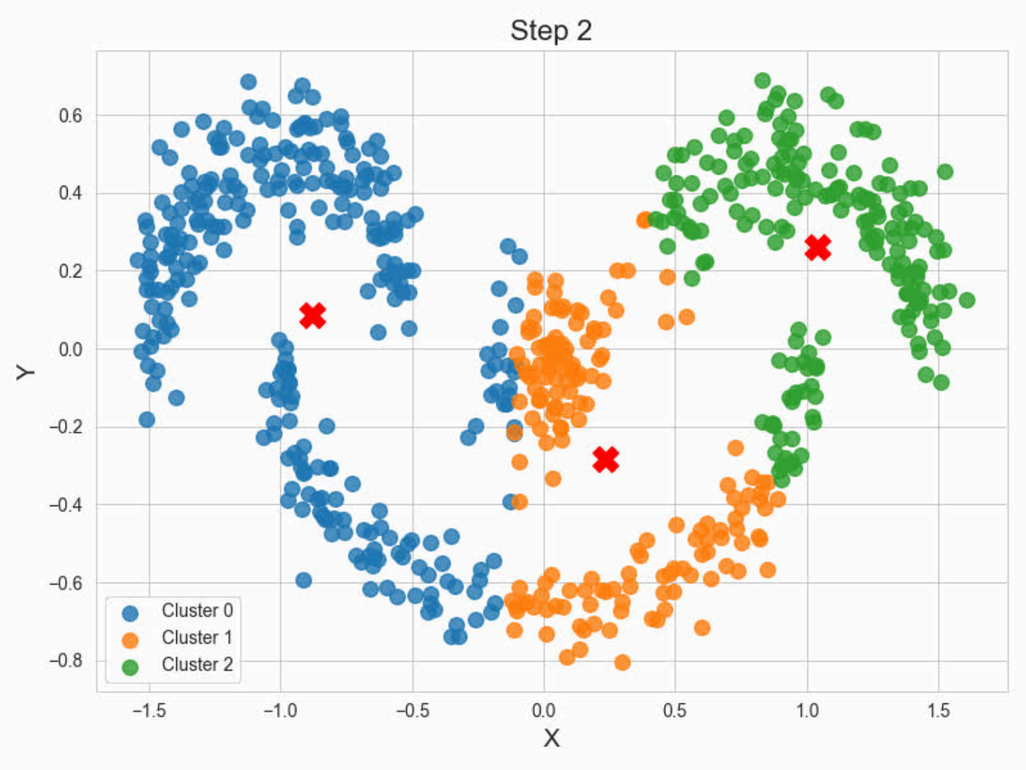


MST

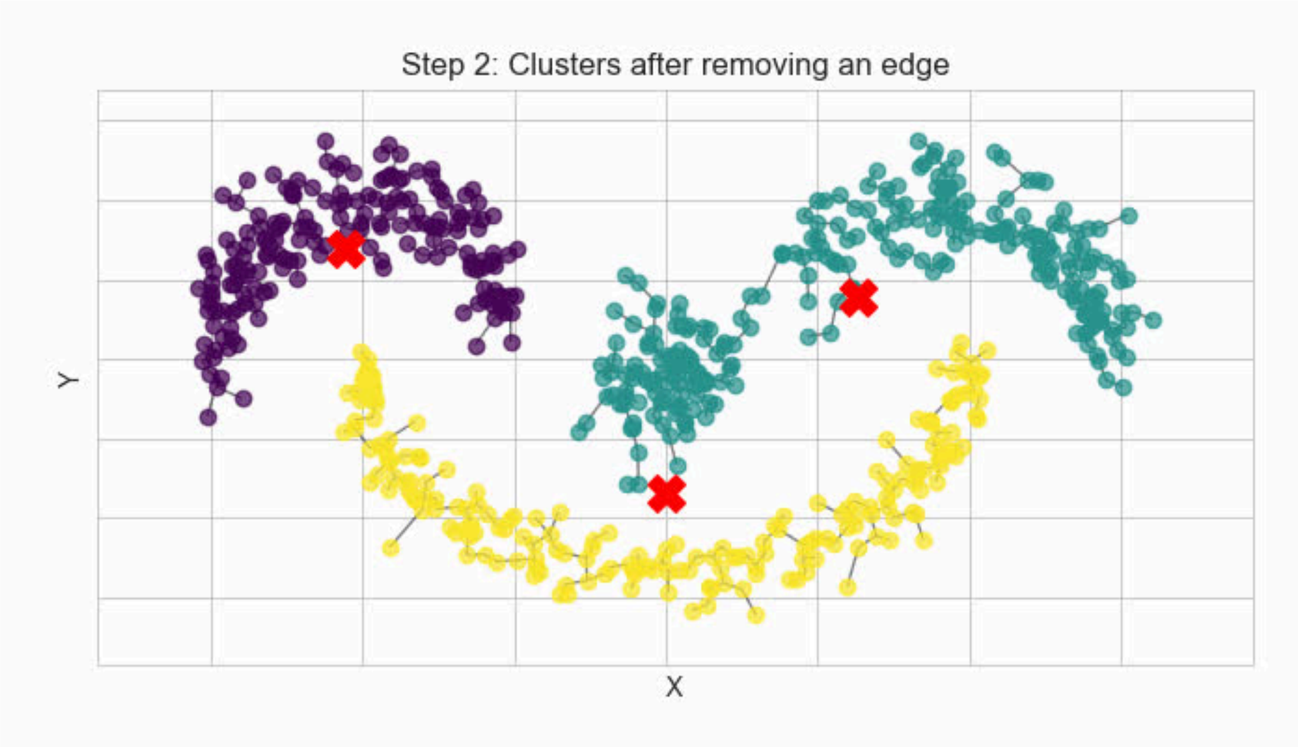


Experiments

BisectingKMeans

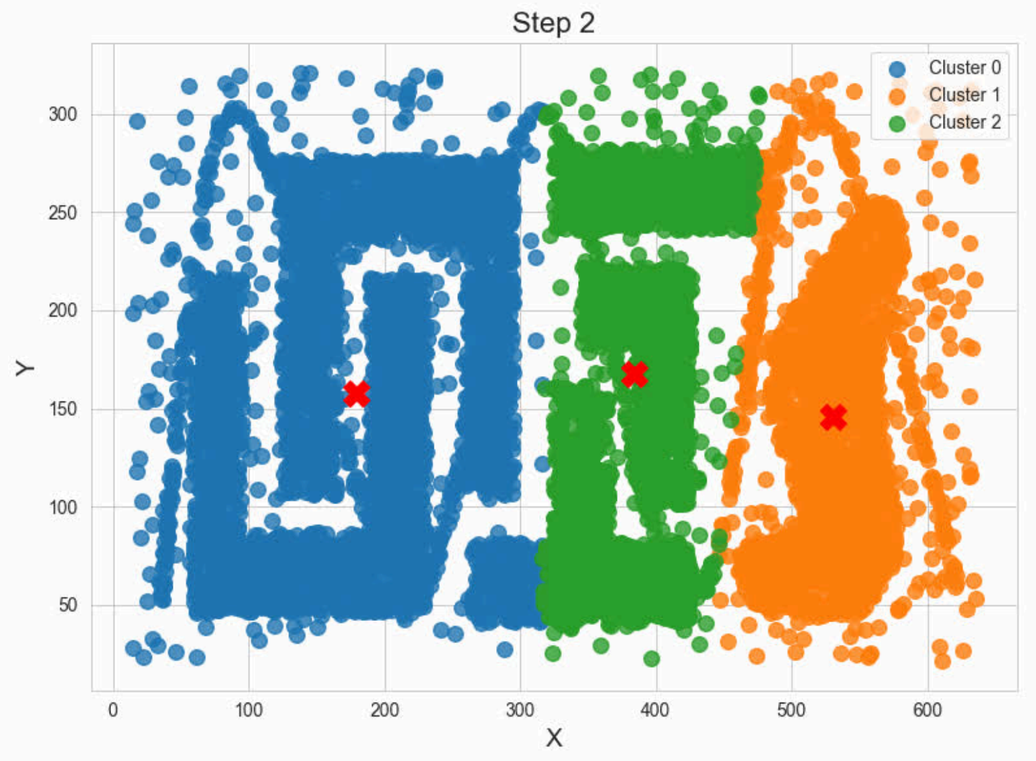


MST

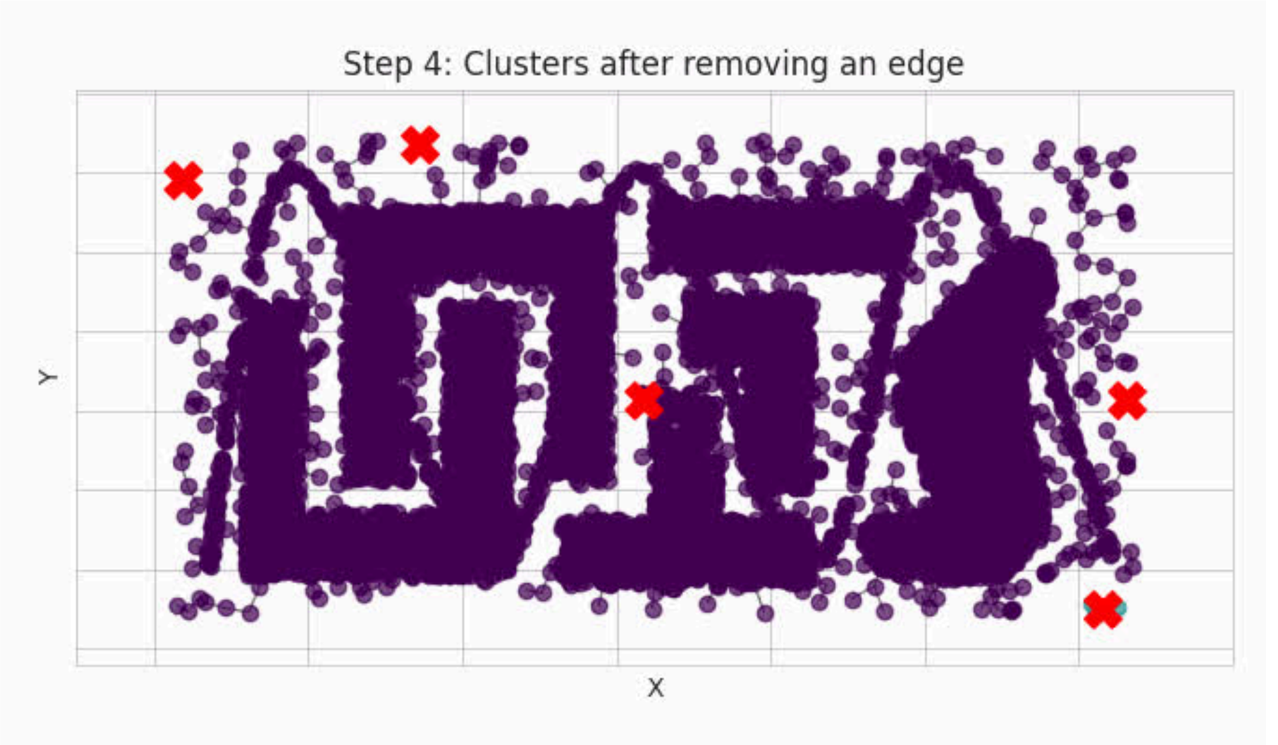


Experiments

BisectingKMeans



MST



BIRCH: Clustering Using Clustering Feature Trees

- BIRCH, developed by Tian Zhang, Raghu Ramakrishnan and Miron Livny in the year 1996.
- BIRCH is designed for clustering a **large amount** of **numeric data** by integrating hierarchical clustering and other clustering methods.
- BIRCH is base on the notation of CF (Clustering Feature) a CF Tree

BIRCH: Clustering Using Clustering Feature Trees

- The clustering feature (CF) of the cluster is a 3-D vector summarizing information about clusters of objects. It is defined as:

$$CF = (n, LS, SS)$$

  - n: Number of data points (d-dimensional data objects)
  - LS: Linear sum of points.
  - SS: Squared sum of points.

$$LS = \sum_{i=1}^{n} x_i \qquad SS = \sum_{i=1}^{n} x_i^2$$

BIRCH: Clustering Using Clustering Feature Trees

- Using a clustering feature, we can easily derive many useful statistics of a cluster. Some key statistic derivations:
  - Centroid: $x_0 = \frac{\sum_{i=1}^{n} x_i}{n} = \frac{LS}{n}$
  - Radius: $R = \sqrt{\frac{\sum_{i=1}^{n}(x_i - x_0)^2}{n}} = \sqrt{\frac{SS}{n} - \frac{LS^2}{n^2}}$
  - Diameter: $D = \sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(x_i - x_j)^2}{n(n-1)}} = \sqrt{\frac{2nSS - 2LS^2}{n(n-1)}}$
- Here, R is the average distance from member objects to the centroid, and D is the average pairwise distance within a cluster.

BIRCH: Clustering Using Clustering Feature Trees

$$R = \sqrt{\frac{\sum_{i=1}^{n}(x_i - x_0)^2}{n}} = \sqrt{\frac{SS}{n} - \frac{LS^2}{n^2}}$$

$$\sum_{i=1}^{n}(x_i - x_0)^2 = \sum_{i=1}^{n}\left(x_i^2 - 2x_i x_0 + x_0^2\right) = \sum_{i=1}^{n} x_i^2 - 2x_0 \sum_{i=1}^{n} x_i + \sum_{i=1}^{n} x_0^2$$

$$\left.\begin{aligned} &\sum_{i=1}^{n} x_i^2 = SS \\ &2x_0 \sum_{i=1}^{n} x_i = 2\frac{LS}{n} \cdot LS = \frac{2LS^2}{n} \\ &\sum_{i=1}^{n} x_0^2 = n \cdot x_0^2 = n \cdot \left(\frac{LS}{n}\right)^2 = \frac{LS^2}{n} \end{aligned}\right\} \sum_{i=1}^{n}(x_i - x_0)^2 = SS - \frac{LS^2}{n}$$

$$\longrightarrow \quad \sqrt{\frac{\sum_{i=1}^{n}(x_i - x_0)^2}{n}} = \sqrt{\frac{SS}{n} - \frac{LS^2}{n^2}}$$

BIRCH: Clustering Using Clustering Feature Trees

$$D = \sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(x_i - x_j)^2}{n(n-1)}} = \sqrt{\frac{2nSS - 2LS^2}{n(n-1)}}$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(x_i - x_j)^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}\left(x_i^2 - 2x_ix_j + x_j^2\right) = \sum_{i=1}^{n}\sum_{j=1}^{n}x_i^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n}x_ix_j + \sum_{i=1}^{n}\sum_{j=1}^{n}x_j^2$$

$$\left.\begin{aligned}
&\sum_{i=1}^{n}\sum_{j=1}^{n}x_i^2 = n\sum_{i=1}^{n}x_i^2 = n\cdot SS \\
&\sum_{i=1}^{n}\sum_{j=1}^{n}x_ix_j = \left(\sum_{i=1}^{n}x_i\right)^2 = LS^2 \\
&\sum_{i=1}^{n}\sum_{j=1}^{n}x_j^2 = n\sum_{j=1}^{n}x_j^2 = n\cdot SS
\end{aligned}\right\} \sum_{i=1}^{n}\sum_{j=1}^{n}(x_i - x_j)^2 = 2nSS - 2LS^2$$

$$\longrightarrow \sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(x_i - x_j)^2}{n(n-1)}} = \sqrt{\frac{2nSS - 2LS^2}{n(n-1)}}$$

BIRCH: Clustering Using Clustering Feature Trees

- Moreover, clustering features are additive.

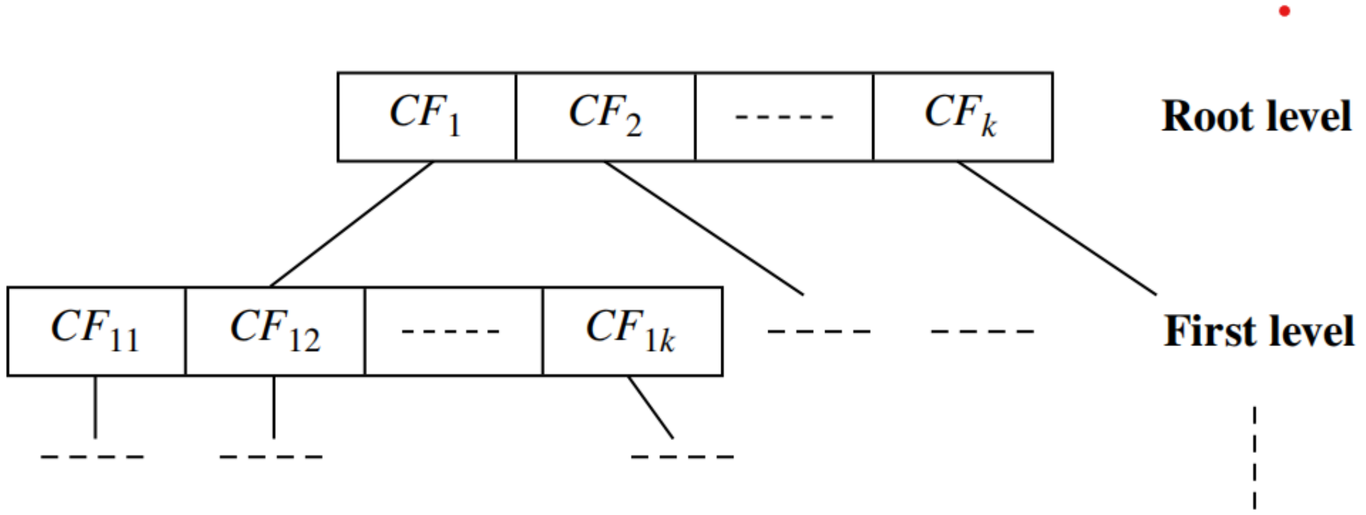
$$CF_1 = (n_1, LS_1, SS_1) \qquad CF_2 = (n_2, LS_2, SS2)$$

$$CF_{12} = CF_1 + CF_2 = (n_1 + n_2, LS_1 + LS_2, SS_1 + SS_2)$$

- The clustering feature for the cluster that formed by merging C1 and C2 is simply.

BIRCH: Clustering Using Clustering Feature Trees

- A CF-tree is a height-balanced tree that stores the clustering features for a hierarchical clustering.
- In a CF-tree, each non-leaf node has "children" or descendants, and it stores the sum of the CFs of these children, providing a summary of their clustering information.

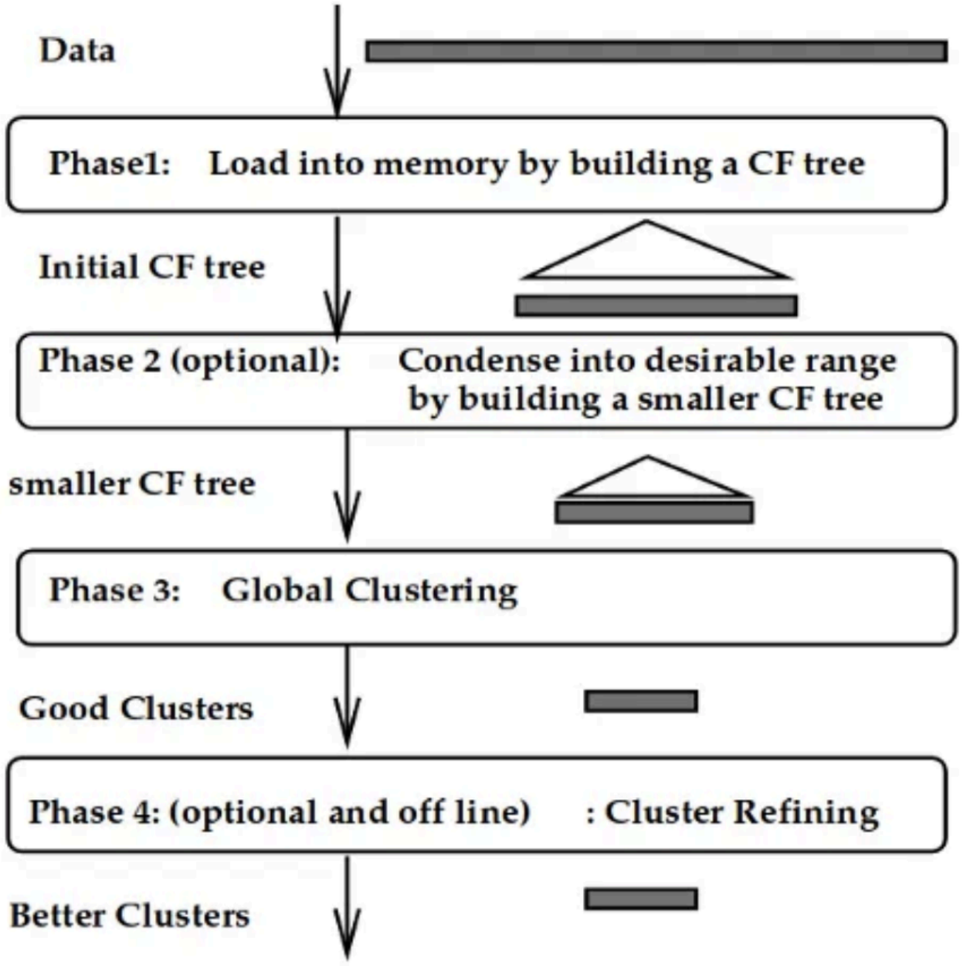


BIRCH: Clustering Using Clustering Feature Trees

- A CF-tree has two parameters: branching factor(B) and threshold(T).
  - The branching factor specifies the maximum number of children per nonleaf node.
  - The threshold parameter specifies the maximum diameter of subclusters stored at the leaf nodes of the tree.

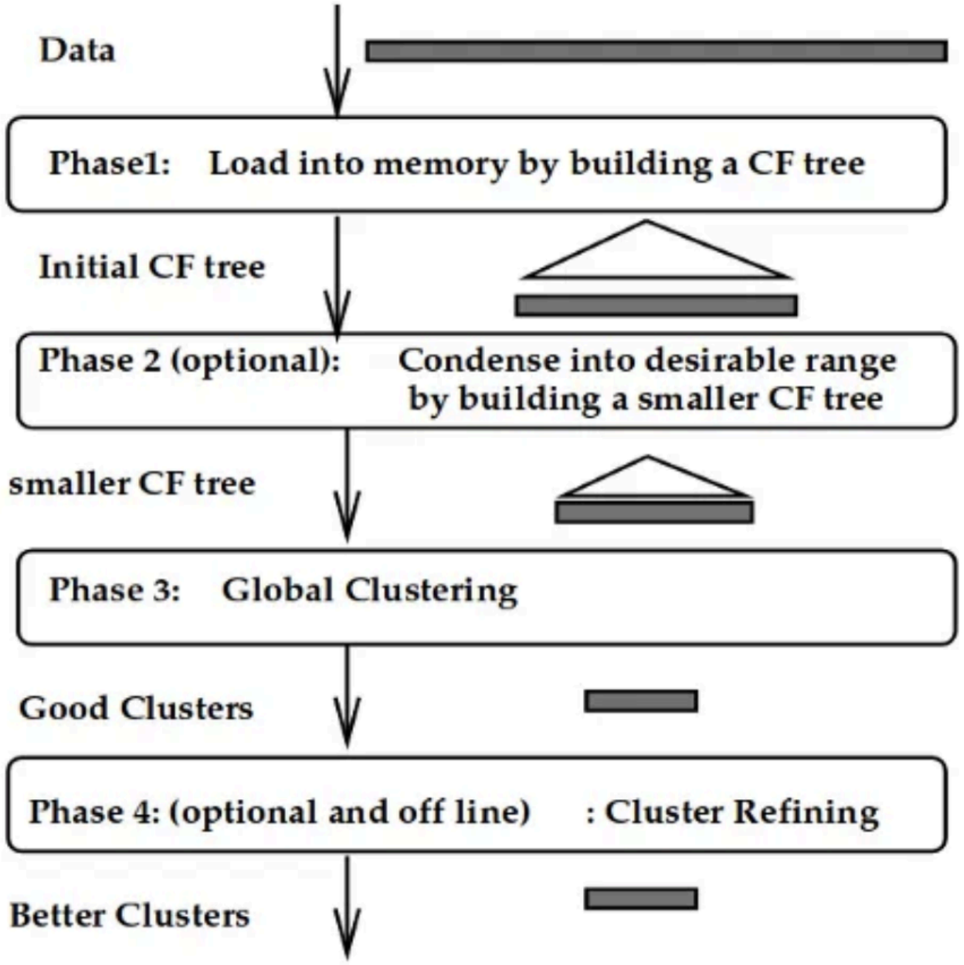
BIRCH: Clustering Using Clustering Feature Trees

- Phase 1:
  - The algorithm scans the data, inserts points into a CF-tree, and rebuilds it with a higher threshold if memory is insufficient. Choosing an optimal threshold reduces rebuilds.



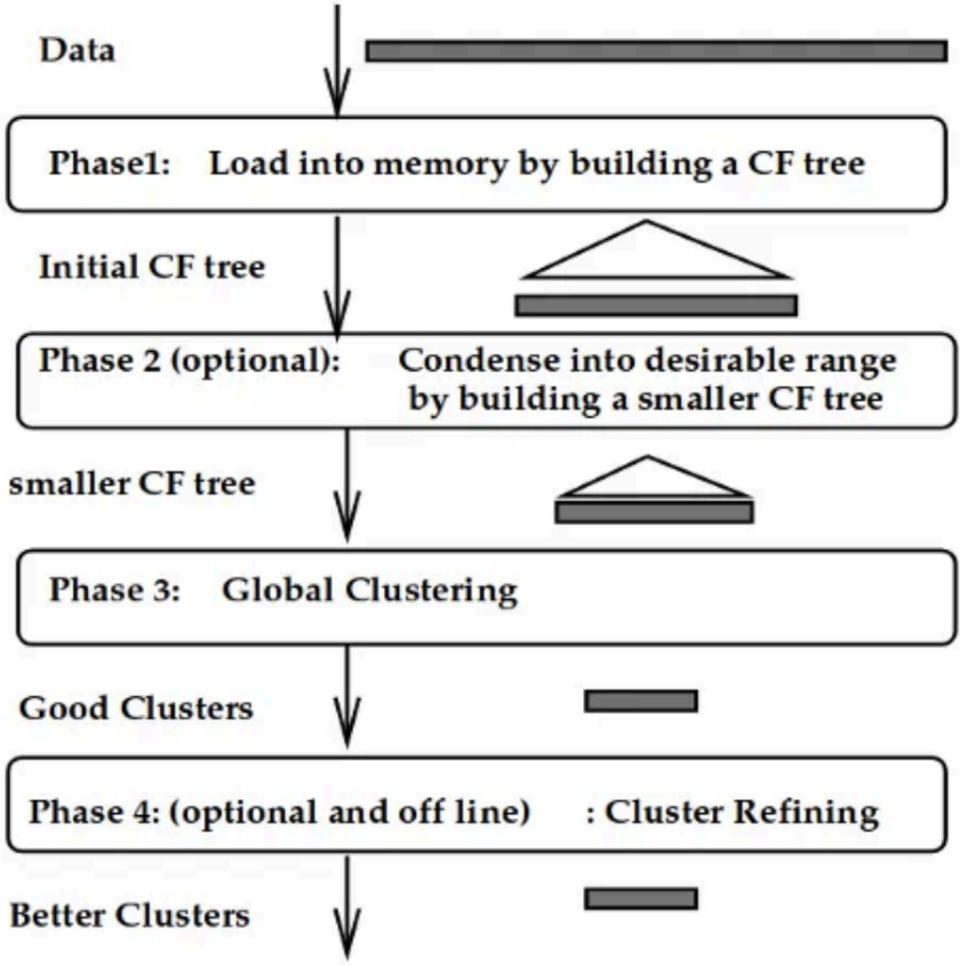
BIRCH: Clustering Using Clustering Feature Trees

- Phase 2:
  Crowded subclusters are grouped into larger clusters to create a more compact CF-tree.



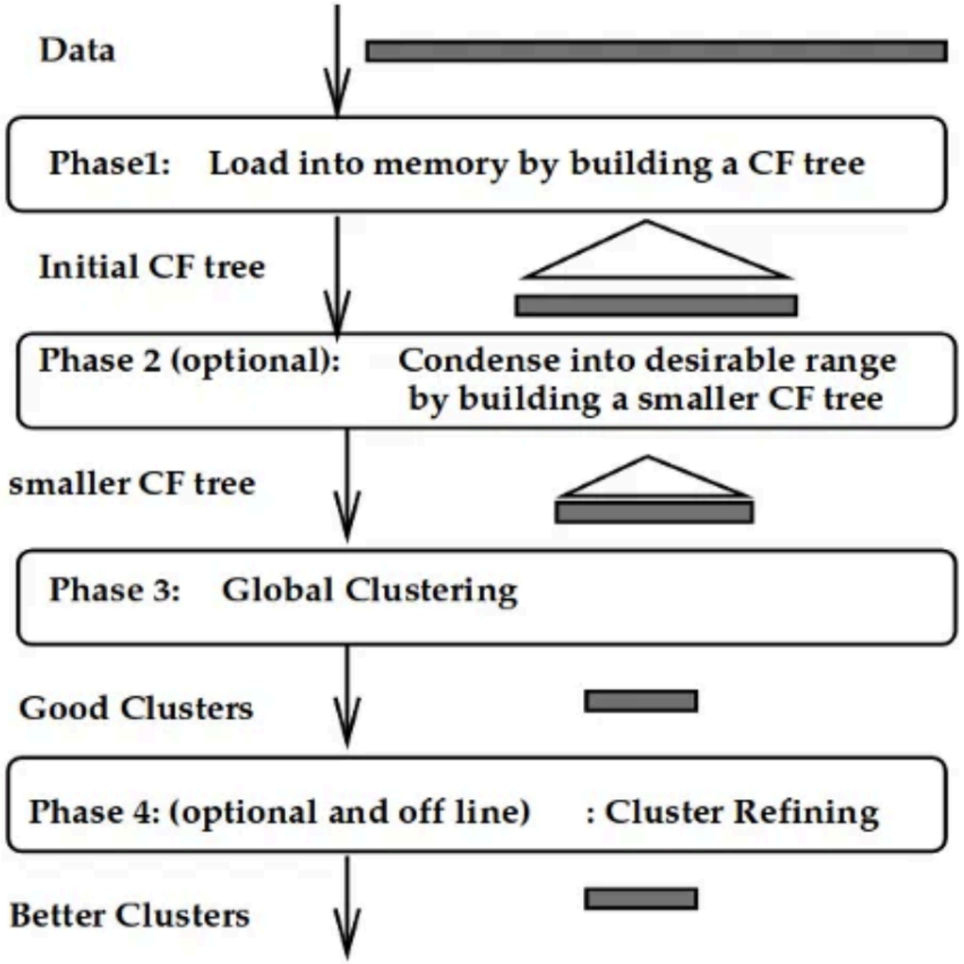
BIRCH: Clustering Using Clustering Feature Trees

- Phase 3:
  A clustering algorithm is applied to clustering features (CFs) rather than data points, minimizing I/O operations.



BIRCH: Clustering Using Clustering Feature Trees

- Phase 4:
  Additional passes refine clustering accuracy and offer the option to discard outliers by correcting course summaries from previous phases.



BIRCH: Clustering Using Clustering Feature Trees

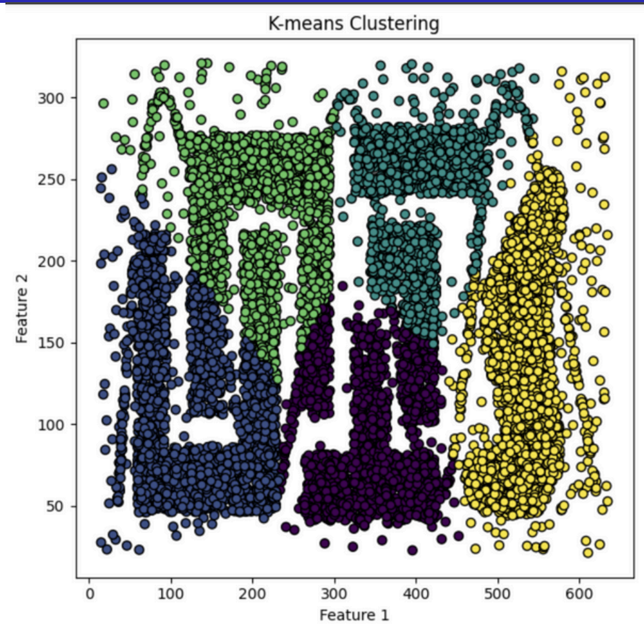
Advantages:

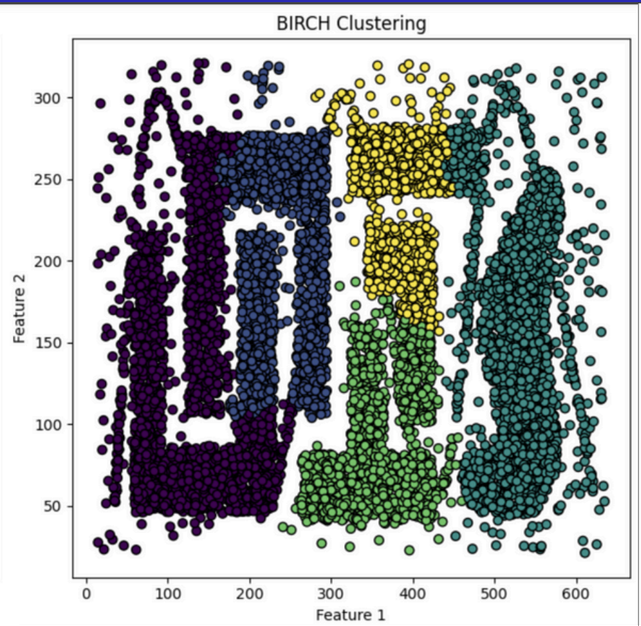
- Efficiently processes **large datasets** with a single scan and optional additional scans.
- Can handle incoming data and adjust clusters without rebuilding from scratch.
- The most important advantage of this algorithm is that its time complexity is only **O(n)**, where n is number of object.

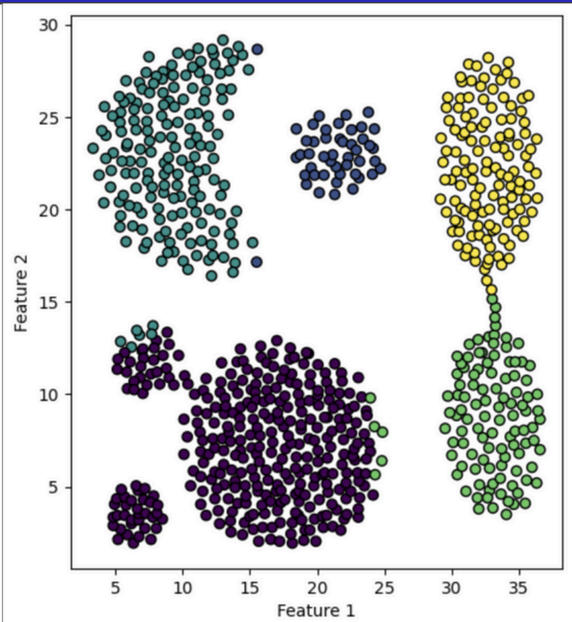
Disadvantages:

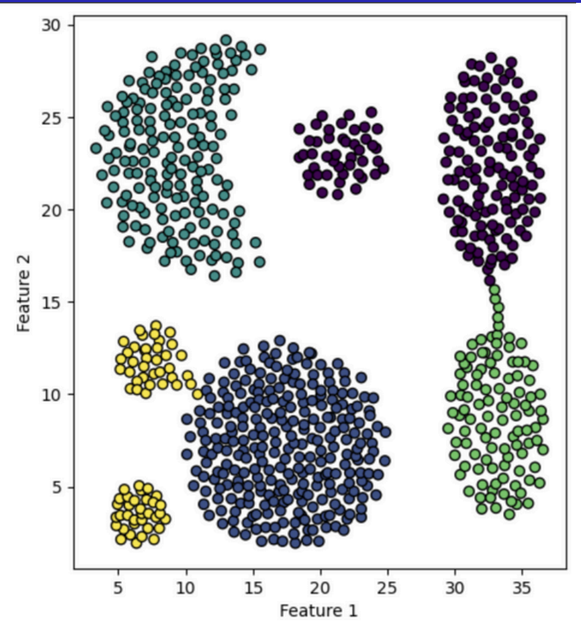
- Does not perform well for **non-spherical clusters** due to the use of **radius/diameter**.
- CF-tree nodes may not always correspond to natural clusters.

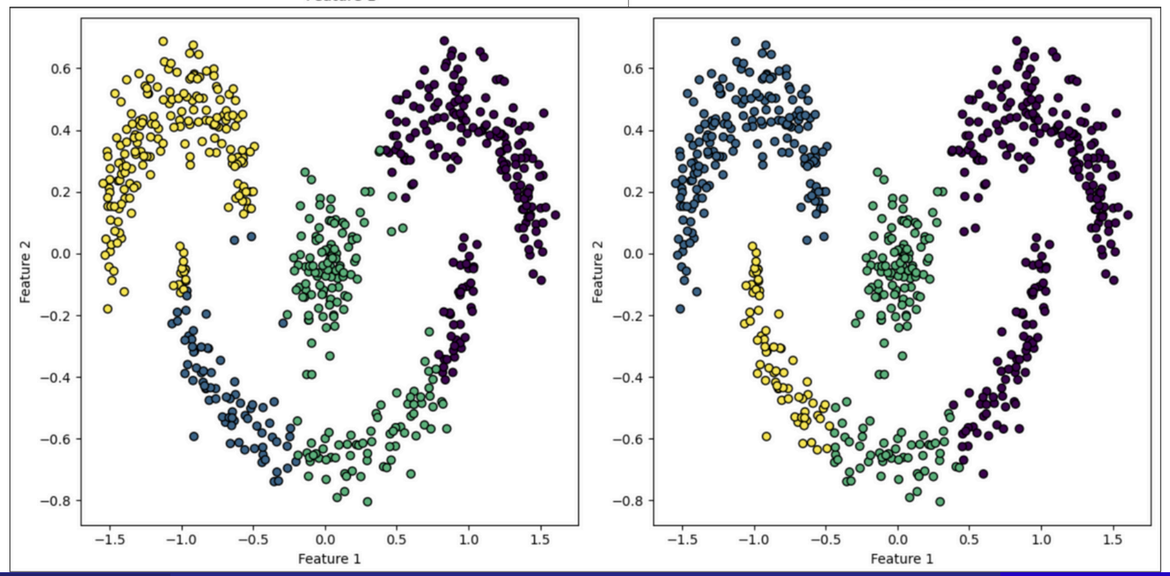
Experiment


K-means Clustering
Feature 1
Feature 2


BIRCH Clustering
Feature 1
Feature 2


Feature 1
Feature 2


Feature 1
Feature 2


Feature 1
Feature 2

Feature 1
Feature 2

Chameleon Clustering

- Traditional method often ignore the **interconnecity** of item of two cluster or **closesness** of two cluster.

  Closesness:
  - Within cluster: how close individual data points are to one another.
  - Between cluster: how close of two cluster.

  Interconnectity:
  - Within cluster: how related individual data points are to one another.
  - Between cluster: how related of two cluster.

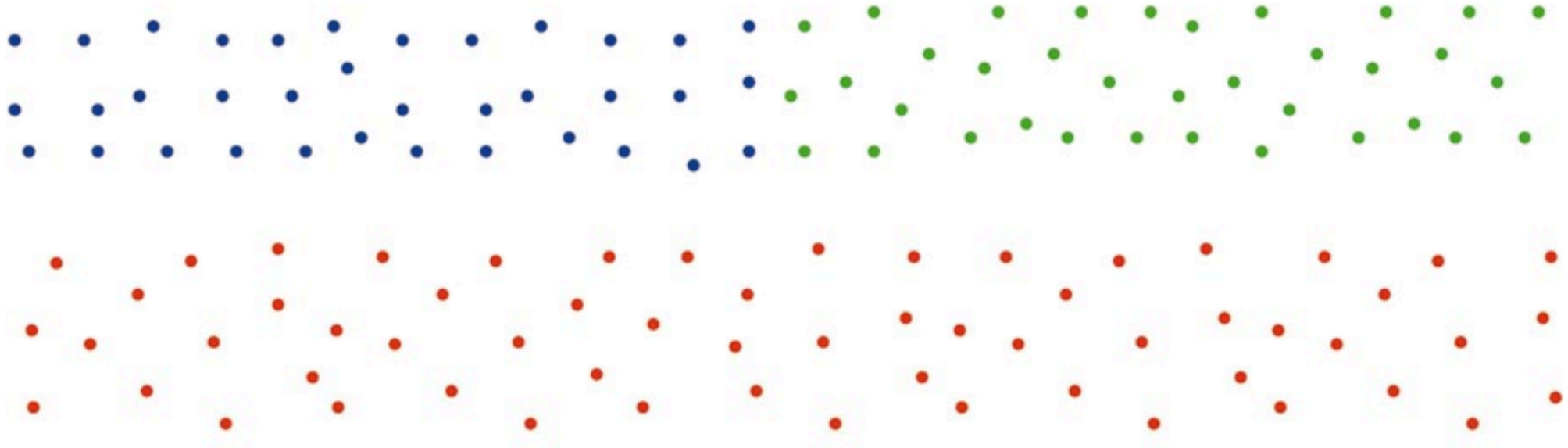
Chameleon Clustering

- Traditional method often ignore the **interconnecity** of item of two cluster or **closesness** of two cluster.

Algorithm incorrectly merge blue and green instead of merging red and cyan cluster

Chameleon Clustering

- Traditional method often ignore the **interconnecity** of item of two cluster or **closesness** of two cluster.

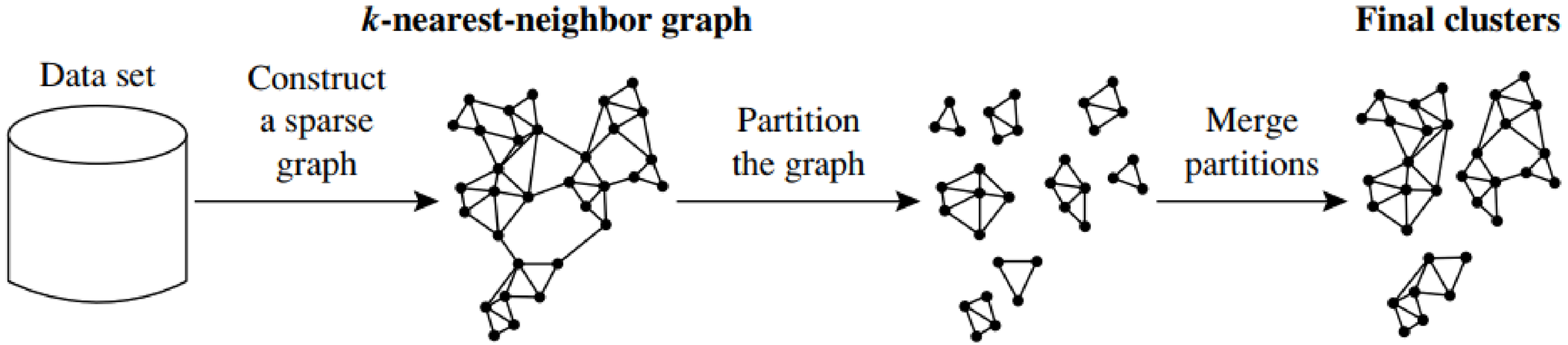


Algorithm incorrectly merge blue and red instead of merging blue and green cluster

Chameleon Clustering

- Traditional method often ignore the **interconnecity** of item of two cluster or **closesness** of two cluster.

- Chameleon is an algorithm that uses **graph-based techniques** and incorporates both **closeness and interconnectivity** to determine whether to merge two clusters.



Chameleon Clustering

- **Relative interconnecity (RI):**

$$RI = \frac{EC(C_i, C_j)}{\frac{1}{2}(EC(C_i) + EC(C_j))}$$

where is $EC(C_i, C_j)$ total weights of the edges that connect two clusters, $EC(C_i)$ is the total weights of the edges that connect two clusters that be bisec cutted of clusters C_i

Chameleon Clustering

- **Relative closeness (RC)**:

$$RC(C_i, C_j) = \frac{S_{EC(C_i,C_j)}}{\frac{m_i}{m_i+m_j} S_{EC(C_i)} + \frac{m_j}{m_i+m_j} S_{EC(C_i)}},$$

where is $S_{EC(C_i,C_j)}$ average weights of the edges that connect two clusters, $S_{EC(C_i)}$ is the total weights of the edges that connect two clusters that be bisec cutted of clusters C_i

Chameleon Clustering

Algorithm 3 Chameleon Clustering with Stopping Conditions

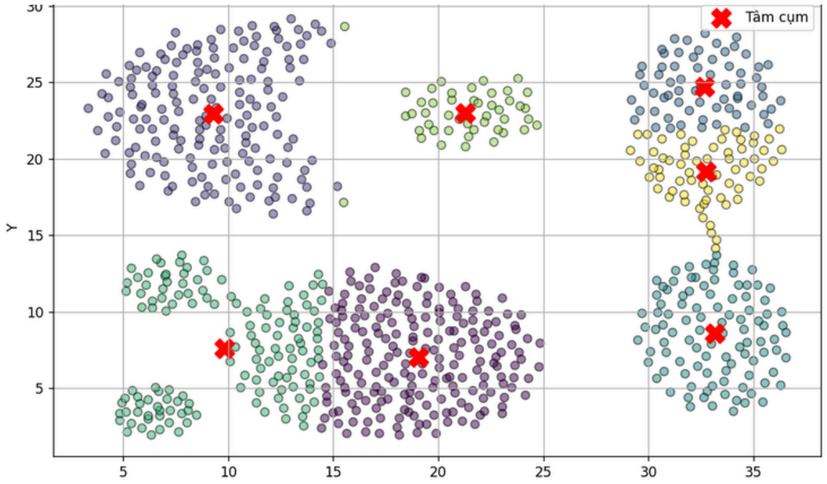
Input: Data D, number of nearest neighbors K
Output: Clusters $C_1, C_2, \ldots, C_k$

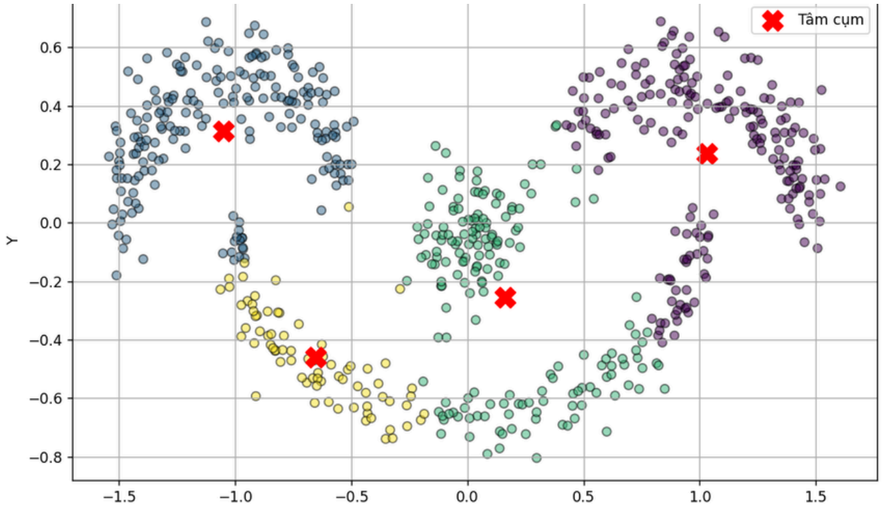
Create a sparse graph G from the data D:
for each point $x_i \in D$ **do**
  Find K nearest neighbors of x_i
  Add edges to the graph
end for

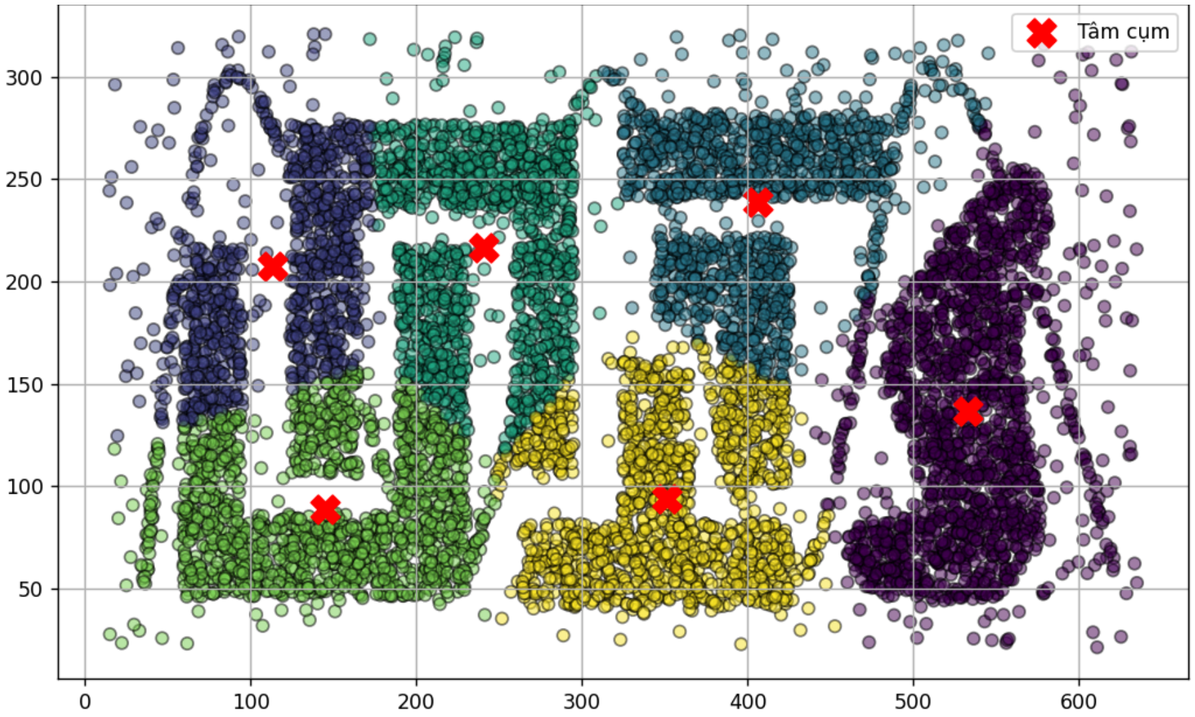
Partition the graph into connected components:
$Clusters \leftarrow$ MinimizeCut(G)

Agglomerative merge
while there are clusters to merge **do**
  Create the relative interconnectivity matrix RI for the clusters
  Create the relative closeness matrix SC for the clusters
  Select the pair of clusters (C_i, C_j) with $\max(RI(C_i, C_j), SC(C_i, C_j))$
  if $\max(RI(C_i, C_j), SC(C_i, C_j))$ is sufficiently high **then**
    Merge C_i and C_j
    Update the interconnectivity and closeness matrices
  else
    Break: No clusters meet the merging criteria
  end if
  if number of clusters reaches desired threshold **then**
    Break: Sufficient number of clusters
  end if
end while
return *Clusters*

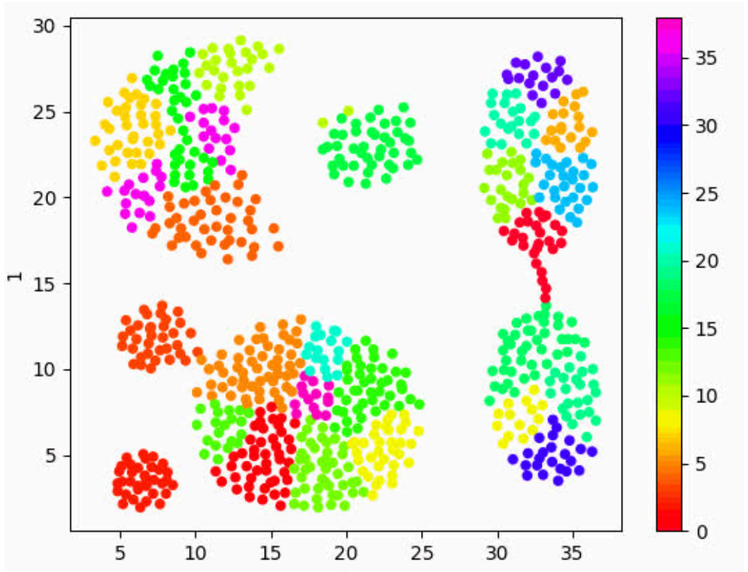
Experiments

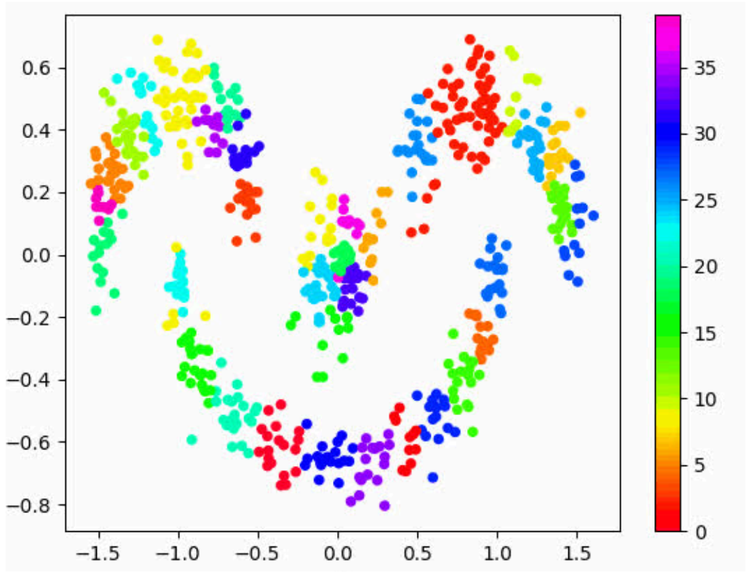


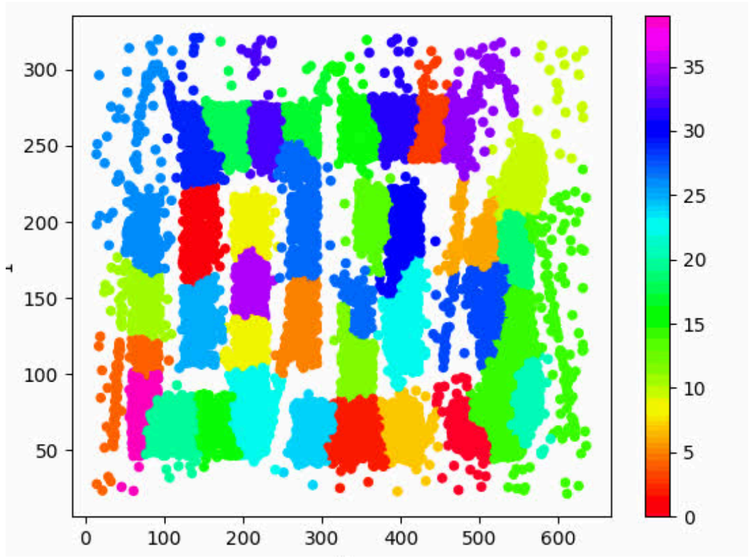




Experiments







Chameleon Clustering

Advantages:

- Don’t need to determine the number of clusters.
- Can takle with complex structural data.

Disadvantages:

- High Complexity

THANKS FOR WATCHING!

[Link Github]