# Data Mining

— Cluster Analysis —

# What is Cluster Analysis?

- Cluster: a collection of data objects
  - Similar to one another within the same cluster
  - Dissimilar to the objects in other clusters
- Cluster analysis
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- Unsupervised learning: no predefined classes

# Clustering Applications

- **Business Intelligence:** To organize a large no of customers into groups.
- **Image Pattern Recognition:** handwritten character recognition systems to improve overall recognition accuracy using multiple models based on multiple subclasses/clusters.
- **Web Search:** To organize the relevant web pages in a concise and easily accessible way.
- **Biology:** It can be used for classification among different species of plants and animals.
- **Information Retrieval:** cluster documents into topics
- **Marketing:** It can be used to characterize & discover customer segments for marketing purposes.

# Examples of Clustering Applications

- **Libraries:** It is used in clustering different books on the basis of topics and information.
- **Insurance:** Identifying groups of motor insurance policy holders with a high average claim cost and identifying the frauds.
- As a DM function, clustering can be used
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms
- Outlier detection

# Requirements of Clustering in Data Mining

| Requirement | Interpretation / Explanation | Examples / Notes |
|---|---|---|
| **Scalability** | Algorithms should efficiently handle large datasets; clustering on small samples may give biased results. | BIRCH, scalable K-Means variants. |
| **Ability to deal with different types of attributes** | Must work on numerical, categorical, ordinal, spatial, temporal, or mixed attributes; also graphs, sequences, images, documents. | Categorical clustering (k-Modes), text clustering, image segmentation. |
| **Discovery of clusters with arbitrary shape** | Should detect clusters that are not just spherical; ED and MD methods assume globular shapes. | DBSCAN, DENCLUE for irregular cluster shapes. |
| **Noise handling** | Should separate meaningful clusters from noise/outliers; many algorithms are sensitive to noise. | DBSCAN marks noisy points separately. |
| **Incremental clustering & order insensitivity** | Should allow incremental updates when new data arrives, and results should not depend on input order. | BIRCH supports incremental updates. |
| **Capability for high-dimensional data** | High-dimensional data is sparse and distances become less meaningful; algorithm should adapt. | Subspace clustering, PCA + clustering. |
| **Incorporation of user-specified constraints** | Algorithms should consider user/domain rules (e.g., must-link/cannot-link). | Constraint-based clustering (COP-KMeans) |
| **Parameter requirement** | Many algorithms need input parameters (e.g., *k* in K-Means, ε in DBSCAN); hard to determine for unknown datasets. | Adaptive or parameter-free methods preferr |
| **Interpretability and usability** | Results should be understandable and useful to end-users, not just mathematical groupings. | Clusters labeled as “high-value customers” instead of “Cluster 1.” |

# Requirements of Clustering in Data Mining

# Requirements of Clustering in Data Mining

- Scalability:
  - Clustering on only a small sample of a large Dataset can lead to biased results.
- Ability to deal with different types of attributes:
  - Recently many applications need clustering on complex data types like graph, sequences, images and documents.
- Discovery of clusters with arbitrary shape
  - Clusters based on ED and MD are spherical in shape.
- Requirements to provide domain knowledge in the form of input parameters:
  - Hard to determine.(high dimensionality DS and no deep understanding)
  - makes quality of the clustering difficult to control.
  - Clustering results are sensitive to those parameters.

# Requirements of Clustering in Data Mining

- Able to deal with noisy data
  - Clustering algorithms are sensitive to noise and may produce low quality clusters.
- Incremental clustering and insensitivity to input data order.
  - Incorporate incremental updates into existing clustering structures
  - Clustering should allow incremental updates without recalculating everything from scratch, and the results should not depend on the order in which data arrives.
- Capability of clustering high-dimensional data
  - High dimensional data can be very sparse and highly skewed.
- Incorporation of user-specified constraints
  - Clustering algorithms should be able to find clusters that satisfy the specified constraints.
- Interpretability and usability

# Major Clustering Approaches

- Partitioning approach:
  - Given a set of *n* objects, a partitioning method constructs *k* partitions of the data, where each partition represents a cluster and *k* <= *n*.
  - The basic partitioning methods typically adopt ***exclusive cluster separation***
  - Most partitioning methods are distance-based.
  - Given k, this approach creates initial partitioning and then uses Iterative relocation technique to improve it.
  - The general criterion of a good partitioning is that objects in the same cluster are "close" or related to each other, whereas objects in different clusters are "far apart" or very different .
  - Typical methods: k-means, k-medoids, CLARANS

# Major Clustering Approaches

| Approach | Description | Examples / Algorithms |
|---|---|---|
| **Partitioning Methods** | Divide data into *k* non-overlapping clusters, optimizing a criterion (e.g., minimizing distance). Works well for small to medium datasets. | K-Means, K-Medoids (PAM, CLARA, CLARANS) |
| **Hierarchical Methods** | Build a hierarchy of clusters either **bottom-up (agglomerative)** or **top-down (divisive)**. Results are shown using a dendrogram. | AGNES (Agglomerative Nesting), DIANA (Divisive Analysis), BIRCH, CURE |
| **Density-Based Methods** | Clusters are defined as dense regions of points separated by low-density areas. Good for arbitrary-shaped clusters. | DBSCAN, OPTICS, DENCLUE |
| **Grid-Based Methods** | Data space is divided into a finite number of grid cells; clustering is performed on grids instead of individual points. Efficient for large datasets. | STING, CLIQUE, WaveCluster |
| **Model-Based Methods** | Assume data is generated by a model (e.g., probability distribution or mixture of models) and try to fit data to the model. | EM (Expectation-Maximization), Gaussian Mixture Models (GMM), COBWEB |
| **Constraint-Based Methods** | Incorporate user-specified constraints (domain knowledge) into the clustering process. | COP-KMeans, Constrained Hierarchica Clustering |
| **Other Emerging Approaches** | Newer clustering methods designed for special data types. | Spectral Clustering (graph-based), Subspace Clustering (high- dimensiona Deep Clustering (neural networks) |

# The *K-Means* Clustering Method

- A centroid-based partitioning technique uses the ***centroid*** of a cluster, *Ci* , to represent that cluster.
- The quality of cluster *Ci* can be measured by the **within cluster variation**, which is the sum of *squared error* between all objects in *Ci* and the centroid ***ci***, defined as

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} dist(\boldsymbol{p}, \boldsymbol{c_i})^2,$$

where *E* is the sum of the squared error for all objects in the data set; ***p*** is the point in space representing a given object; and ***ci*** is the centroid of cluster *Ci* (both ***p*** and ***ci*** are multidimensional).

- This objective function tries to make the resulting k clusters as compact and as separate as possible.
- Optimizing the within-cluster variation is computationally challenging.
- To overcome the prohibitive computational cost for the exact solution, greedy approaches are often used in practice. e.g k-means algorithm

# The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented as below :
  - First, it randomly selects *k* of the objects in *D*, each of which initially represents a cluster mean or cluster center.
  - For each of the remaining objects, an object is assigned to the cluster to which it is the most similar, based on the Euclidean distance between the object and the cluster mean.
  - The *k*-means algorithm then iteratively improves the within-cluster variation.
    - For each cluster, it computes the new mean using the objects assigned to the cluster in the previous iteration.
    - All the objects are then reassigned using the updated means as the new cluster centers.
    - The iterations continue until the assignment is stable, that is, the clusters formed in the current round are the same as those formed in the previous round.

# The *K-Means* Clustering Method **(5 steps)**

Step 1: Choose the no.of clusters ,k.

Step2: Select at random k points, the centroids(not necessarily from your dataset)

Step3: Assign each data point to the closest centroid as that forms k clusters.

Step4: Compute and place new centroid of each cluster.

Step5: Reassign each data point to the new closest centroid . If any reassignment takes place go to step 4 . Otherwise (if the assignment is stable, i.e. the clusters formed in the current round are the same as those formed in the previous round) then STOP.

- The process of iteratively re assigning objects to clusters to improve the partitioning is referred to as ***iterative relocation technique.***

# K- means Algorithm

**Algorithm: *k*-means.** The *k*-means algorithm for partitioning, where each cluster's center is represented by the mean value of the objects in the cluster.

**Input:**

- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

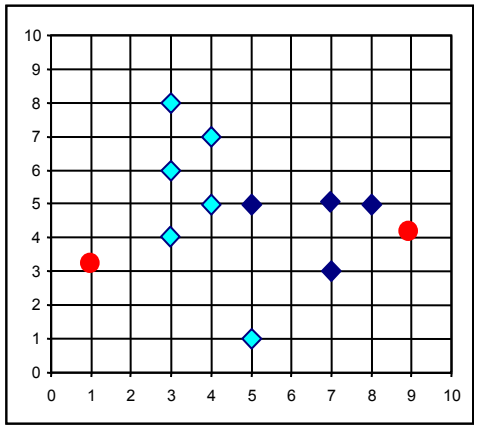
**Output:** A set of *k* clusters.

**Method:**

(1) arbitrarily choose *k* objects from *D* as the initial cluster centers;
(2) **repeat**
(3) (re)assign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster;
(4) update the cluster means, that is, calculate the mean value of the objects for each cluster;
(5) **until** no change;

# The *K-Means* Clustering Method

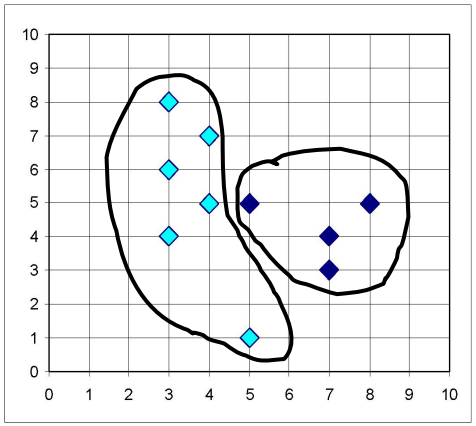
- Example



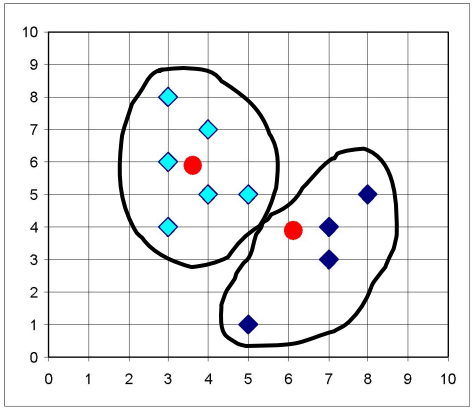

K=2

Arbitrarily choose K object as initial cluster center

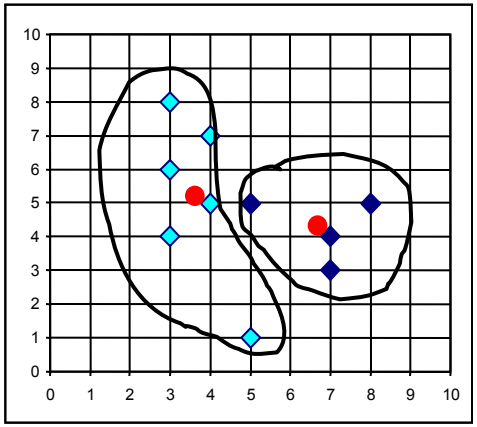
Assign each objects to most similar center



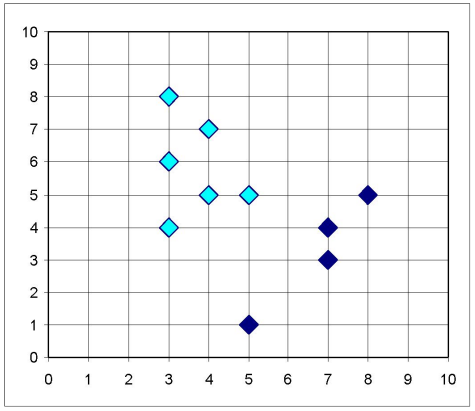

reassign




Update the cluster means




reassign




Update the cluster means

# Example K means

- Given the following 2D data points, perform K-means clustering with K=2. Use Euclidean distance and show the first two iterations.

- Data Points: A(1,2), B(1.5,1.8), C(5,8), D(8,8), E(1,0.5), F(9,11)
- Initial Centroids (chosen randomly):
- $\mu 1 = (1,2)$ (Point A)
- $\mu 2 = (5,8)$ (Point C)

# Example

Iteration 1

- Step 1: Assign Points to Nearest Centroid
- Calculate Euclidean distance (d) from each point to centroids:

| Point | Coordinates | $d$ to $\mu_1$ | $d$ to $\mu_2$ | Cluster |
|---|---|---|---|---|
| A | (1, 2) | 0 | 7.21 | 1 |
| B | (1.5, 1.8) | 0.58 | 6.69 | 1 |
| C | (5, 8) | 7.21 | 0 | 2 |
| D | (8, 8) | 9.22 | 3.00 | 2 |
| E | (1, 0.5) | 1.50 | 8.32 | 1 |
| F | (9, 11) | 13.45 | 5.00 | 2 |

# Example

- Cluster Assignments: Cluster 1: A, B, E Cluster 2: C, D, F
- Step 2: Update Centroids
- Recalculate centroids as the mean of assigned points:

- $\mu_1 = \left(\frac{1+1.5+1}{3}, \frac{2+1.8+0.5}{3}\right) = (1.17, 1.43)$
- $\mu_2 = \left(\frac{5+8+9}{3}, \frac{8+8+11}{3}\right) = (7.33, 9.00)$

# Example

- Iteration 2
- Step 1: Reassign Points to New Centroids

| Point | Coordinates | $d$ to $\mu_1$ | $d$ to $\mu_2$ | Cluster |
|---|---|---|---|---|
| A | (1, 2) | 0.85 | 8.52 | 1 |
| B | (1.5, 1.8) | 0.47 | 8.06 | 1 |
| C | (5, 8) | 6.74 | 2.69 | 2 |
| D | (8, 8) | 8.83 | 1.00 | 2 |
| E | (1, 0.5) | 0.93 | 9.19 | 1 |
| F | (9, 11) | 12.34 | 2.24 | 2 |

# Example

Cluster Assignments:

Cluster 1: A, B, E

Cluster 2: C, D, F

Step 2: Check Convergence

Centroid remain unchanged (no reassignments).

Algorithm converges.

# Example

Final Result

Clusters:

Cluster 1 (Red): A(1,2), B(1.5,1.8), E(1,0.5)

Cluster 2 (Blue): C(5,8), D(8,8), F(9,11)

Final Centroids:

$\mu 1 = (1.17, 1.43)$

$\mu 2 = (7.33, 9.00)$

# Example

- Suppose that the data mining task is to cluster points (with $(x, y)$ representing location) into three clusters, where the points are $A1(2, 10)$,$A2(2, 5)$,$A3(8, 4)$,$B1(5, 8)$,$B2(7, 5)$,$B3(6, 4)$,$C1(1, 2)$,$C2(4, 9)$. The distance function is Euclidean distance. Suppose initially we assign $A1$, $B1$, and $C1$ as the center of each cluster, respectively. Use the *k-means* algorithm to show *only*

  (a) the three cluster centers after the first round of execution.

  (b) the final three clusters.

# Solution

- Suppose that the data mining task is to cluster points (with $(x, y)$ representing location) into three clusters, where the points are $A1(2, 10)$,$A2(2, 5)$,$A3(8, 4)$,$B1(5, 8)$,$B2(7, 5)$,$B3(6, 4)$,$C1(1, 2)$,$C2(4, 9)$. The distance function is Euclidean distance. Suppose initially we assign $A1$, $B1$, and $C1$ as the center of each cluster, respectively. Use the *k-means* algorithm to show *only*

  (a) the three cluster centers after the first round of execution.

  **Answer:**

  After the first round, the three new clusters are: (1) *{A1}*, (2) *{B1,A3,B2,B3,C2}*, (3) *{C1,A2}*, and their centers are (1) (2, 10), (2) (6, 6), (3) (1.5, 3.5).

  (b) the final three clusters.

  **Answer:**

  The final three clusters are: (1) *{A1,C2,B1}*, (2) *{A3,B2,B3}*, (3) *{C1,A2}*.

# Comments on the *K-Means* Method

- Strength: *Relatively efficient*: *O*(nkt), where *n* is # objects, *k* is # clusters, and *t* is # iterations. Normally, *k*, *t* << *n*. Therefore, the method is relatively scalable and efficient in processing large data sets.
-
- Weakness:
  - The *k*-means method is not guaranteed to converge to the global optimum and often terminates at a local optimum
  - The results may depend on the initial random selection of cluster centres.
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance.
  - Unable to handle noisy data and *outliers*
    - A small no. of such data can substantially influence the mean value.
  - Not suitable to discover clusters with *non-convex shapes* or clusters of very different size.

# Comments on the *K-Means* Method

- Strength:

**Simplicity and Ease of Implementation**:
K-Means is one of the simplest and most widely used clustering algorithms. It is easy to understand and implement.
**Scalability**:
K-Means is computationally efficient and works well with large datasets. It has a time complexity of O(n·k·t)O(n \cdot k \cdot t)O(n·k·t), where nnn is the number of data points, kkk is the number of clusters, and ttt is the number of iterations. This makes it scalable for large datasets.
**Convergence**:
K-Means generally converges quickly to a solution, making it suitable for tasks requiring fast results.
**Interpretability**:
The final clusters in K-Means are represented by centroids, which are easy to interpret and visualize, especially in 2D or 3D data.
**Versatility**:
K-Means can be applied to various kinds of data, including image segmentation, market segmentation, anomaly detection, etc.
**Efficient for Spherical Clusters**:
It works very well when the clusters are spherical (i.e., have a similar shape and size).

# Comments on the *K-Means* Method

- Weakness:

**Choice of K**: One of the main drawbacks is that the number of clusters kkk needs to be specified in advance. This can be challenging if you don't know the appropriate number of clusters, and improper choice of kkk may result in poor clustering.

**Sensitivity to Initial Centroids**: The algorithm's outcome can be heavily influenced by the initial placement of centroids. Poor initialization can lead to suboptimal clustering. Techniques like **K-Means++** are used to mitigate this issue.

**Assumption of Spherical Clusters**: K-Means assumes that clusters are spherical and evenly sized, which can be limiting for datasets where clusters have different shapes, densities, or sizes (e.g., elliptical clusters).

**Sensitivity to Outliers** :K-Means is sensitive to outliers, as they can significantly affect the position of centroids, leading to incorrect clustering results.

**Non-Distance-Based Clusters**: It relies on Euclidean distance to assign points to clusters. This means it may not work well with data where clusters are based on non-Euclidean distances (e.g., categorical data).

**Local Optima**: K-Means can converge to local minima rather than the global optimum, depending on the initial centroid positions. Running the algorithm multiple times with different initializations can help mitigate this.

**Not Suitable for Non-Convex Shapes**: K-Means struggles with datasets where clusters are not convex, meaning it can have difficulty correctly identifying clusters that have irregular shapes.

**Scalability Issues with High Dimensional Data**: Although K-Means is scalable for large datasets, it suffers in high-dimensional spaces (curse of dimensionality). In such cases, the distances between points tend to become less informative, making clustering less effective

# Variations of *K-Means* Method

- Handling categorical data: ***k-modes*** (Huang'98)
  - Pick K observations at random and use them as leaders/clusters
  - Calculate the dissimilarities and assign each observation to its closest cluster
  - Define new modes for the clusters
  - Repeat 2–3 steps until there are is no re-assignment required

- Handling mixture of numeric and categorical data: ***k-prototype method***

# K-modes clustering Example

| person | hair color | eye color | skin color |
|---|---|---|---|
| P1 | blonde | amber | fair |
| P2 | brunette | gray | brown |
| P3 | red | green | brown |
| P4 | black | hazel | brown |
| P5 | brunette | amber | fair |
| P6 | black | gray | brown |
| P7 | red | green | fair |
| P8 | black | hazel | fair |

# K-modes clustering Example

| person | hair color | eye color | skin color |
|---|---|---|---|
| P1 | blonde | amber | fair |
| P2 | brunette | gray | brown |
| P3 | red | green | brown |
| P4 | black | hazel | brown |
| P5 | brunette | amber | fair |
| P6 | black | gray | brown |
| P7 | red | green | fair |
| P8 | black | hazel | fair |

k=3.

**Step 1: Lets select P1,P7 and P8 as leaders/cluster**

**Step2 : Calculate the dissimilarities(no. of mismatches) and assign each observation to its closest cluster**

Comparing leader/Cluster P1 to the observation P1 gives 0 dissimilarities.

Comparing leader/cluster P1 to the observation P2 gives 3(1+1+1) dissimilarities.

Likewise, calculate all the dissimilarities and put them in a matrix as shown below and assign the observations to their closest cluster(cluster that has the least dissimilarity)

| | Cluster 1 (P1) | Cluster 2 (P7) | Cluster 3 (P8) | Cluster |
|---|---|---|---|---|
| P1 | 0 ✓ | 2 | 2 | Cluster 1 |
| P2 | 3 ✓ | 3 | 3 | Cluster 1 |
| P3 | 3 | 1 ✓ | 3 | Cluster 2 |
| P4 | 3 | 3 | 1 ✓ | Cluster 3 |
| P5 | 1 ✓ | 2 | 2 | Cluster 1 |
| P6 | 3 | 3 | 2 ✓ | Cluster 3 |
| P7 | 2 | 0 ✓ | 2 | Cluster 2 |
| P8 | 2 | 2 | 0 ✓ | Cluster 3 |

# K-modes clustering Example(Cntd..)

**Step 3: Define new modes for the clusters (Mode is simply the most observed value. )**

**Mark the observations according to the cluster they belong to.** K1: Yellow, Brick Red: K2, Purple: K3

| person | hair color | eye color | skin color |
|---|---|---|---|
| P1 | blonde | amber | fair |
| P2 | brunette | gray | brown |
| P3 | red | green | brown |
| P4 | black | hazel | brown |
| P5 | brunette | amber | fair |
| P6 | black | gray | brown |
| P7 | red | green | fair |
| P8 | black | hazel | fair |

**Considering one cluster at a time, for each feature, look for the Mode and update the new leaders**

Cluster 1 observations(P1, P2, P5) has brunette as the most observed hair color, amber as the most observed eye color, and fair as the most observed skin color.

*Note: If you observe the same occurrence of values, take the mode randomly. In our case, the observations of Cluster 2(P3, P7) have one occurrence of brown, fair skin color. I randomly chose fair as the mode.*

.

| New Leaders | | | |
|---|---|---|---|
| | hair color | eye color | skin color |
| Cluster 1 | brunette | amber | fair |
| Cluster 2 | red | green | fair |
| Cluster 3 | black | hazel | brown |

**Repeat steps 2–3**

| person | hair color | eye color | skin color |
|---|---|---|---|
| P1 | blonde | amber | fair |
| P2 | brunette | gray | brown |
| P3 | red | green | brown |
| P4 | black | hazel | brown |
| P5 | brunette | amber | fair |
| P6 | black | gray | brown |
| P7 | red | green | fair |
| P8 | black | hazel | fair |

| New Leaders | | | |
|---|---|---|---|
| | hair color | eye color | skin color |
| Cluster 1 | brunette | amber | fair |
| Cluster 2 | red | green | fair |
| Cluster 3 | black | hazel | brown |

| | Cluster 1 | Cluster 2 | Cluster 3 | Cluster |
|---|---|---|---|---|
| P1 | 1 ✓ | 2 | 3 | Cluster 1 |
| P2 | 2 ✓ | 3 | 2 | Cluster 1 |
| P3 | 3 | 1 ✓ | 2 | Cluster 2 |
| P4 | 3 | 3 | 0 ✓ | Cluster 3 |
| P5 | 0 ✓ | 2 | 3 | Cluster 1 |
| P6 | 3 | 3 | 1 ✓ | Cluster 3 |
| P7 | 2 | 0 ✓ | 3 | Cluster 2 |
| P8 | 2 | 2 | 1 ✓ | Cluster 3 |

# K-modes clustering Example(Cntd..)

| | Cluster 1 | Cluster 2 | Cluster 3 | Cluster |
|---|---|---|---|---|
| **P1** | 1 ✓ | 2 | 3 | Cluster 1 |
| **P2** | 2 ✓ | 3 | 2 | Cluster 1 |
| **P3** | 3 | 1 ✓ | 2 | Cluster 2 |
| **P4** | 3 | 3 | 0 ✓ | Cluster 3 |
| **P5** | 0 ✓ | 2 | 3 | Cluster 1 |
| **P6** | 3 | 3 | 1 ✓ | Cluster 3 |
| **P7** | 2 | 0 ✓ | 3 | Cluster 2 |
| **P8** | 2 | 2 | 1 ✓ | Cluster 3 |

We stop here as we see there is no change in the assignment of observations.

# K-Medoids Algorithm

- **K-Medoids:** Instead of taking the mean value of the objects in a cluster as a reference point, we can pick actual objects to represent the clusters, using one representative object per cluster(Medoid).

- Each remaining object is assigned to the cluster of which the representative object is the most similar.

- The partitioning method is then performed based on the principle of **minimizing the sum of the dissimilarities** between each object ***p*** and its corresponding representative object.
- An **absolute-error criterion** is defined as $$E = \sum_{i=1}^{k} \sum_{p \in C_i} dist(p, o_i),$$

where *E* is the sum of the absolute error for all objects ***p*** in the data set, and ***oi*** is the representative object of *Ci* .

This is the basis for the ***k*-medoids method**, which groups *n* objects into *k* clusters by minimizing the absolute error

# K-medoids

- A medoid of a finite dataset is a data point from this set, whose average dissimilarity to all the data points is minimal i.e. it is the most centrally located point in the set.

**Algorithm: *k*-medoids.** PAM, a *k*-medoids algorithm for partitioning based on medoid or central objects.

**Input:**

- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

**Output:** A set of *k* clusters.

**Method:**

(1) arbitrarily choose *k* objects in *D* as the initial representative objects or seeds;
(2) **repeat**
(3) assign each remaining object to the cluster with the nearest representative object;
(4) randomly select a nonrepresentative object, $o_{random}$;
(5) compute the total cost, *S*, of swapping representative object, $o_j$, with $o_{random}$;
(6) **if** $S < 0$ **then** swap $o_j$ with $o_{random}$ to form the new set of *k* representative objects;
(7) **until** no change;

PAM, a *k*-medoids partitioning algorithm.

# Example: K-medoids

Given D={1,2,6,7,8,10,15,17,20}  Form 3 clusters using k-medoid algorithm.
Assume initial medoids as 6,7 8 respectively for K1,K2,and K3.
D={1,2,6,7,8,10,15,17,20} with initial medoids 6,7,8.
(I use absolute distance $|x-y|$.)

**Iteration 0 — assign to nearest medoid**

- Medoids = {6, 7, 8}
- Assignments:
  - cluster(6): [1,2,6] (closest to 6)
  - cluster(7): [7]
  - cluster(8): [8,10,15,17,20]
- Recompute medoids (choose the point in each cluster minimizing total intra-cluster distance):
  - for [1,2,6] best medoid = **2**
  - for [7] best medoid = **7**
  - for [8,10,15,17,20]best medoid = **15**
- New medoids = {2, 7, 15}

# Example: K-medoids

D={1,2,6,7,8,10,15,17,20}

**Iteration 1 — reassign**

- Medoids = {2, 7, 15}
- Assignments:
  - cluster(2): [1,2]
  - cluster(7): [6,7,8,10]
  - cluster(15): [15,17,20]
- Recompute medoids:
  - for [1,2]best medoid = **1** (sum distances: 1→1, 2→1)
  - for [6,7,8,10]best medoid = **7**
  - for [15,17,20] best medoid = **17**
- New medoids = {1, 7, 17}

# Example: K-medoids

D={1,2,6,7,8,10,15,17,20}

**Iteration 2 — reassign**

- Medoids = {1, 7, 17}
- Assignments remain:
  - cluster(1): [1,2]
  - cluster(7): [6,7,8,10]
  - cluster(17): [15,17,20]
- Recomputed medoids are still {1,7,17} → **converged**

  **Final result**
- **Medoids:** 1, 7, 17
- **Clusters:**
  - K1K_1K1 (medoid = 1): {1,2}
  - K2K_2K2 (medoid = 7): {6,7,8,10}
  - K3K_3K3 (medoid = 17): {15,17,20}
- **Total clustering cost** (sum of distances of points to their medoids) = **11**

# PAM- Partitioning Around Medoids

**PAM, or Partitioning Around Medoids,** is a k-medoids clustering algorithm that identifies a set of k representative objects (medoids) from a dataset to minimize the total dissimilarity of all data points to their closest medoid. Unlike k-means, which uses cluster means, PAM uses actual data points as medoids, making it more robust to outliers and suitable for various types of non-Euclidean data.

# PAM- Partitioning Around Medoids

The PAM algorithm consists of two main phases:

- **BUILD Phase:**
  - **Initialization:** The algorithm greedily selects k initial medoids from the data points.
  - **Assignment:** Each remaining data point is assigned to the closest medoid, forming k clusters.
- **SWAP Phase:**
  - **Iteration:** The algorithm repeatedly tries to improve the clustering by swapping a medoid with a non-medoid point.
  - **Cost Calculation:** For each possible swap, the change in the total cost (sum of dissimilarities to the closest medoids) is calculated.
  - **Swap Execution:** If a swap results in a decrease in the total cost, it is performed.
  - **Termination:** The algorithm continues until no swap can further reduce the cost, indicating that the optimal set of medoids has been found.

# Example PAM-K Medoids

**Apply PAM K medioits D={1,2,6,7,8,10,15,17,20},k=3 ,**

**Initial medoids are given as {6,7,8}**

**Step 1: Initial assignment**

Medoids = M={6,7,8}

Assign each point to the nearest medoid (absolute distance in 1D):

- Nearest to 6 → {1,2,6}
- Nearest to 7 → {7}
- Nearest to 8 → {8,10,15,17,20}

Clusters:

- C1(6): {1,2,6}
- C2(7): {7}
- C3(8): {8,10,15,17,20}

**Total cost** = $\Sigma|xi - medoid|$

= (|1−6|+|2−6|+0) + (0) + (0+2+7+9+12)

= 5+4+0 + 0 + 30 = **39**

# Example PAM-K Medoids

**Step 2: Try swaps (PAM refinement)**

We test replacing medoids with non-medoids to reduce cost.

**Candidate medoids set {2,7,15}**

D={1,2,6,7,8,10,15,17,20},k=3

- Assign:
  - 2: {1,2}
  - 7: {6,7,8,10}
  - 15: {15,17,20}
- Cost = (1+0) + (1+0+1+3) + (0+2+5)
  = 1 + 5 + 7 = **13** ✅ (much better)

**Candidate medoids set {1,7,17}**

D={1,2,6,7,8,10,15,17,20},k=3

- Assign:
  - 1: {1,2}
  - 7: {6,7,8,10}
  - 17: {15,17,20}
- Cost = (0+1) + (1+0+1+3) + (2+0+3)
  = 1 + 5 + 5 = **11** ✅ (best so far)

# Example PAM-K Medoids

**Step 3: Check further swaps**

Try to swap again — but cost doesn't go below 11.

So PAM converges

**Final PAM Result**

- **Medoids** = {1, 7, 17}
- **Clusters**:
  - C1(1): {1,2}
  - C2(7): {6,7,8,10}
  - C3(17): {15,17,20}
- **Total cost = 11**

# What Is the Problem with PAM?

- Adv: PAM is more robust than k-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean

- Disadv:PAM works efficiently for small data sets but does not **scale well** for large data sets.
  - $O(k(n-k)^2)$ for each iteration : very costly computation for large n and k where n is # of data objects and ,k is # of clusters

→ To deal with large data sets,a sampling based method called CLARA can be used.

# CLARA

- **CLARA** (Clustering Large Applications,is an extension to k-medoids (PAM) methods to deal with data containing a large number of objects (more than several thousand observations) in order to reduce computing time and RAM storage problem. This is achieved using the sampling approach.

- Instead of finding medoids for the entire data set, CLARA considers a small sample of the data with fixed size (*sampsize*) and applies the PAM algorithm to generate an optimal set of medoids for the sample.

- The quality of resulting medoids is measured by the average dissimilarity between every object in the entire data set and the medoid of its cluster, defined as the cost function.

- CLARA repeats the sampling and clustering processes for a pre-specified number of times in order to minimize the sampling bias. The final clustering results correspond to the set of medoids with the minimal cost.
- Instead of using the whole dataset (which is costly), CLARA takes samples of the dataset and applies PAM (Partitioning Around Medoids) on them.

# CLARA Algorithm

1. Create randomly, from the original dataset, multiple subsets with fixed size (sampsize)
2. Compute PAM algorithm on each subset and choose the corresponding k representative objects (medoids). Assign each observation of the entire data set to the closest medoid.
3. Calculate the mean (or the sum) of the dissimilarities of the observations to their closest medoid. This is used as a measure of the goodness of the clustering.
4. Retain the sub-dataset for which the mean (or sum) is minimal. A further analysis is carried out on the final partition.

# CLARA

- The complexity of computing the medoids on a random sample is $O(ks^2 + k.(n-k))$, where $s$ is the size of the sample, $k$ is the number of clusters, and $n$ is the total number of objects.

- The effectiveness of CLARA depends on the sample size.

- If an object is one of the best $k$-medoids but is not selected during sampling, CLARA will never find the best clustering.(Example to demonstrate the same)

# CLARANS

- A randomized algorithm called **CLARANS** (**C**lustering **L**arge **A**pplications based upon **RAN**domized **S**earch) presents a trade-off between the cost and the effectiveness of using samples to obtain clustering.
- Instead of sampling data points, CLARANS improves clustering using a randomized search in the graph of possible solutions.
- Strength: More flexible and usually finds better clusters than CLARA because it doesn't rely only on a fixed sample.
- Weakness: More computationally expensive than CLARA but still better than PAM for large data.
- CLARA = faster, but sample-dependent, CLARANS = more accurate, but slightly slower

Steps of CLARANS algorithm

1. Select ‘k’ random data points and label them as medoids for the time being.
2. Select a random point say ‘a’ from the points picked in step (1), and another point say ‘b’ which is not included in those points.
3. We would already have the sum of distances of point ‘a’ from all other points since that computation is required for selecting the points in step (1). Perform similar computation for point ‘b’.
4. If the sum of distances from all other points for point ‘b’ turns out to be less than that for point ‘a’, replace ‘a’ by ‘b’.
5. The algorithm performs such a randomized search of medoids ‘x’ times where ‘x’ denotes the number of local minima computed, i.e. number of iterations to be performed, which we specify as a parameter. The set of medoids obtained after such ‘x’ number of steps is termed as ‘local optimum’.
6. A counter is incremented every time a replacement of points is made. The process of examining the points for possible replacement is repeated till the counter does not exceed the maximum number of neighbors to be examined (specified as a parameter).
7. The set of medoids obtained when the algorithm stops is the best local optimum choice of medoids.

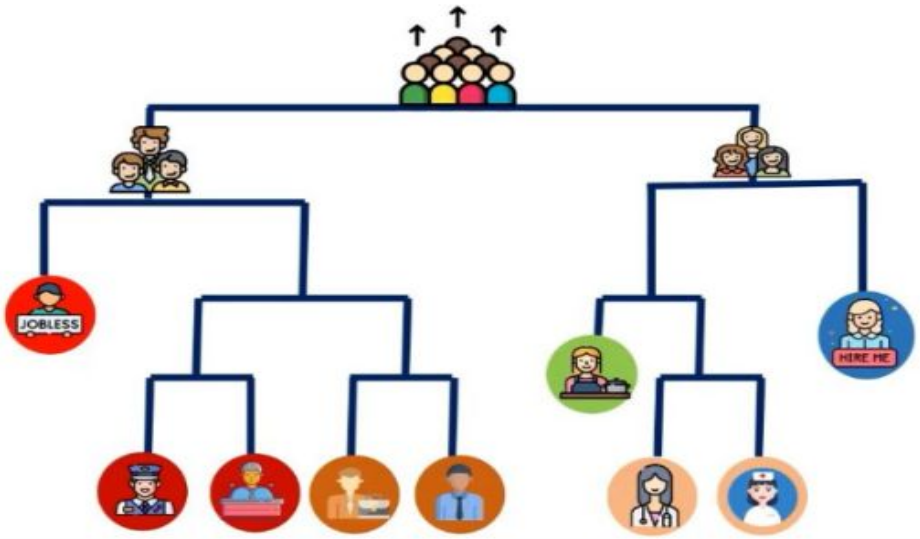
## Comparison between CLARA & CLARANS

- Like CLARA, CLARANS does not check every neighbors of a node.
- Unlike CLARA, CLARANS does not restrict its search to a particular graph. It search the original graph $G_{n,k}$.
- CLARA draws a sample of *nodes* at the beginning of a search, CLARANS draws a sample of *neighbors* in each step of a search.
- CLARANS gives higher quality clustering than CLARA.
- CLARANS requires a very small number of searches than CLARA.

| Feature | CLARA | CLARANS |
| --- | --- | --- |
| Based on | Sampling + PAM | Randomized local search on medoids |
| Efficiency | Fast (works on sample, not full dataset) | Slower than CLARA but better than PAM |
| Accuracy | Can be poor if sample is not representative | Generally better clustering quality |
| Scalability | Good for very large datasets | Moderate, but scalable with optimizations |
| Weakness | Biased if sample is bad | Higher computational cost |

# Hierarchical Clustering

- A **hierarchical clustering method** works by partitioning data objects into groups at different levels like a hierarchy or “tree” of clusters.
- Representing data objects in the form of a hierarchy is useful for data summarization and visualization.
- If necessary, hierarchical partitioning can be continued recursively until a desired granularity is reached.
- It starts with each data point as an individual cluster and successively merges the closest clusters until a single cluster remains.
-



# Hierarchical Clustering (Agglomerative versus Divisive Hierarchical Clustering)

- A hierarchical clustering method can be either *agglomerative* or *divisive*, depending on whether the hierarchical decomposition is formed in a bottom-up (merging) or top-down (splitting) fashion.

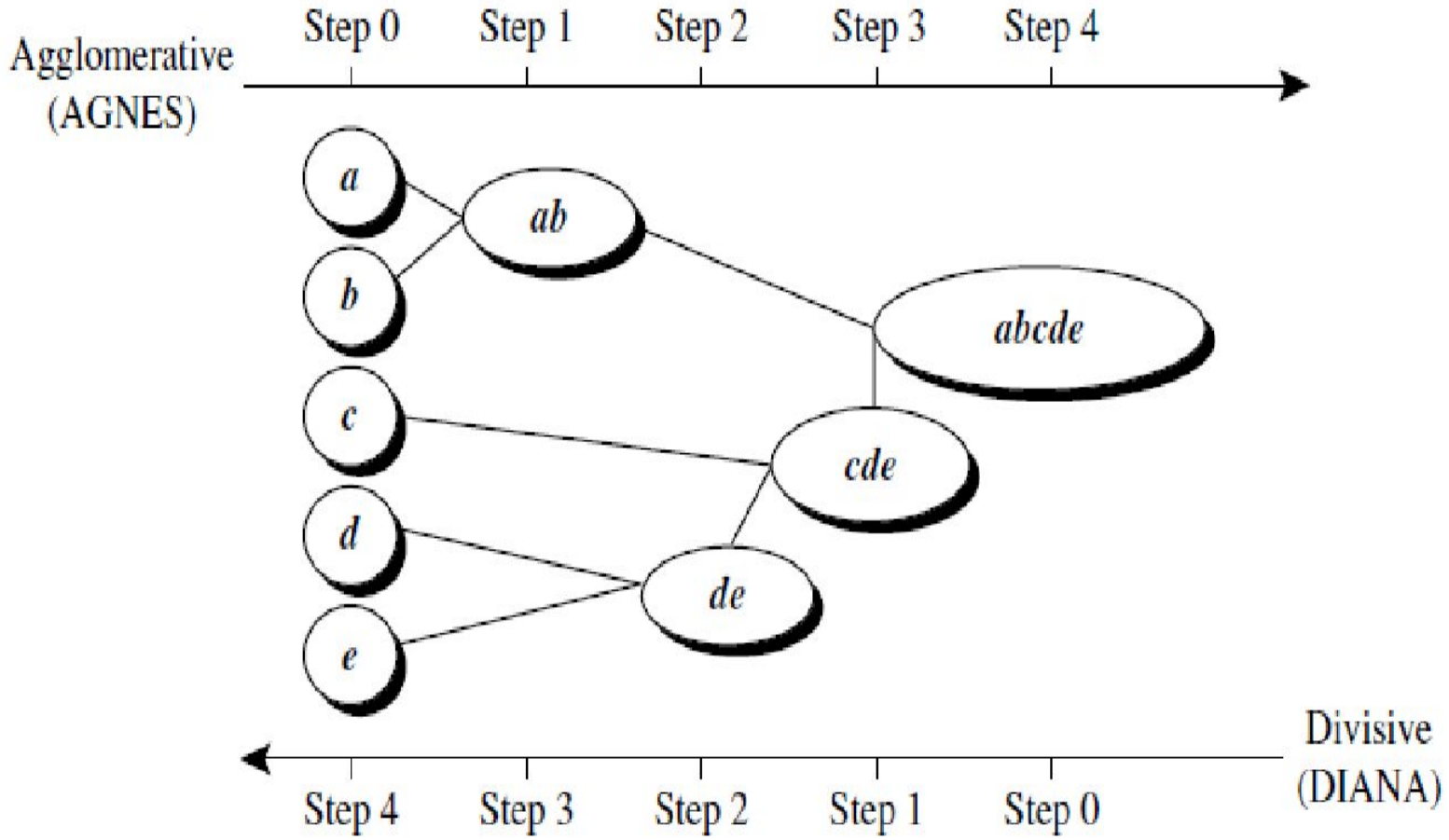
- An **agglomerative hierarchical clustering method :**
  - The hierarchical decomposition is formed in a bottom-up (merging)way

- A **divisive hierarchical clustering method**
  - The hierarchical decomposition is formed in a top-down (splitting)way

- In either agglomerative or divisive hierarchical clustering, a user can specify the desired number of clusters as a termination condition.

- Hierarchical methods suffer from the fact that once a step (merge or split) is done, it can never be undone. So these techniques cannot correct erroneous decisions.

# Example : Application of AGNES(AGglomerative NESting and DIANA(DIvisible ANAlysis)




Agglomerative and divisive hierarchical clustering on data objects $\{a, b, c, d, e\}$.

# Steps in Hierarchical Clustering

1. Start with each data point as a separate cluster.
2. Compute distances between clusters (initially between individual points).
3. Merge the closest clusters.
4. Repeat until only one cluster remains.
5. Generate a dendrogram to visualize the merging process.

# Distance Measures

- There are multiple ways to measure the distance between clusters:
- Single Link Clustering:
  - Distance is defined by the closest pair of points between clusters.
  - May result in long, chain-like clusters.
- Complete Link Clustering:
  - Distance is defined by the farthest pair of points between clusters.
  - Tends to produce compact, well-separated clusters.
- Average Link Clustering:
  - Distance is the average of all pairwise distances betwee points in two clusters.

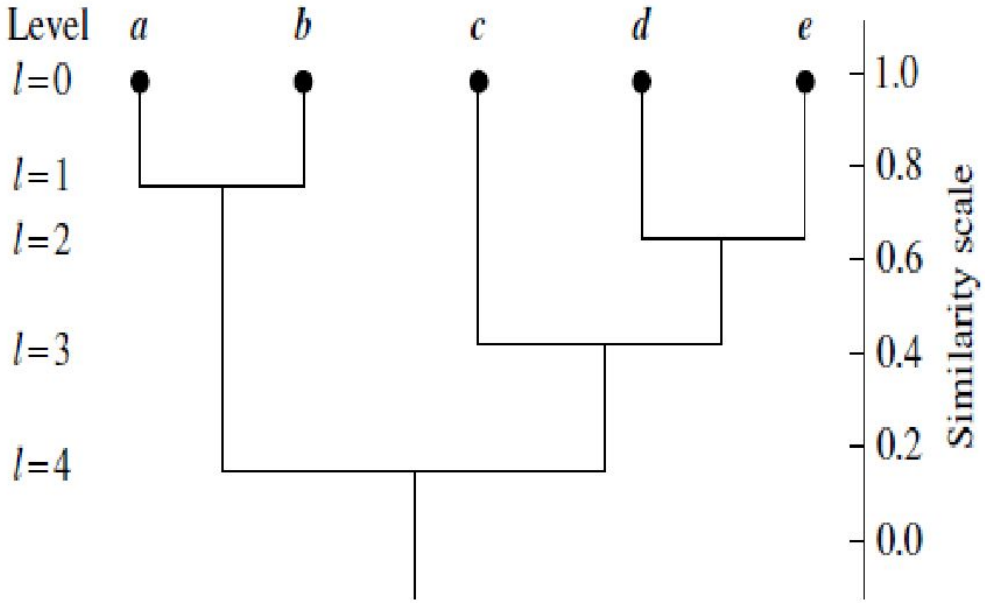
# Distance Measures

Measuring Distance Between Clusters

- Centroid-Based Distance:
  - Distance is measured between the centroids of two clusters.
- Radius-Based Distance:
  - Clusters are merged based on the radius of the combined cluster.
- Diameter-Based Distance:
  - Clusters are merged based on the diameter of the combined cluster.

# Hierarchical Clustering: Dendrogram

- A dendrogram is a tree-like diagram that illustrates the order and levels at which clusters were merged.
- The height at which two clusters are joined represents the distance between them.
- To determine the final clusters, the dendrogram is cut at a chosen threshold.



# Divisive Method Challenges

- How to partition a large cluster into smaller ones is a challenge.
  - $(2^{n-1}-1)$ ways to partition n objects into 2 exclusive clusters.
  - For large n, it is computationally inhibitive to examine all possibilities .
- Also a Divisive method typically uses heuristics in partitioning which can lead to inaccurate results.
- For the sake of efficiency divisive methods typically do not backtrack on the partitioning decisions that have been made.
- Due to these challenges, Agglomerative clustering is mostly used than divisive clustering.

# Distance Measures(*linkage measures*) in Agglomerative Method

- **|p-p' |** is the distance between two objects or points, ***p*** and ***p***';
- ***mi*** is the mean for cluster, *Ci* ;
- ***ni*** is the number of objects in *Ci* .

**Minimum distance:** $dist_{min}(C_i, C_j) = \min_{p \in C_i, p' \in C_j} \{|p - p'|\}$

**Maximum distance:** $dist_{max}(C_i, C_j) = \max_{p \in C_i, p' \in C_j} \{|p - p'|\}$

**Mean distance:** $dist_{mean}(C_i, C_j) = |m_i - m_j|$

**Average distance:** $dist_{avg}(C_i, C_j) = \frac{1}{n_i n_j} \sum_{p \in C_i, p' \in C_j} |p - p'|$

# Distance Measures(*linkage measures)* in Algorithmic Methods

- When an algorithm uses the *minimum distance*, $d_{min}(Ci, Cj)$, to measure the distance between clusters, it is sometimes called a **nearest-neighbor clustering algorithm**.
  - Here if the clustering process is terminated when the minimum distance between nearest clusters exceeds a user-defined threshold, it is called a **single-linkage algorithm**.

- When an algorithm uses the *maximum distance*, $d_{max}(Ci, Cj)$, to measure the distance between clusters, it is sometimes called a **farthest-neighbor clustering algorithm**.
  - Here,If the clustering process is terminated when the maximum distance between nearest clusters exceeds a user-defined threshold, it is called a **complete-linkage algorithm**

# Example: Agglomerative Clustering (Single Linkage)

| | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ |
|---|---|---|---|---|---|
| $P_1$ | 0 | | | | |
| $P_2$ | 9 | 0 | | | |
| $P_3$ | 3 | 7 | 0 | | |
| $P_4$ | 6 | 5 | 9 | 0 | |
| $P_5$ | 11 | 10 | 2 | 8 | 0 |

| | $P_1$ | $P_2$ | $[P_3, P_5]$ | $P_4$ |
|---|---|---|---|---|
| $P_1$ | 0 | | | |
| $P_2$ | 9 | 0 | | |
| $[P_3, P_5]$ | 3 | 7 | 0 | |
| $P_4$ | 6 | 5 | 8 | 0 |

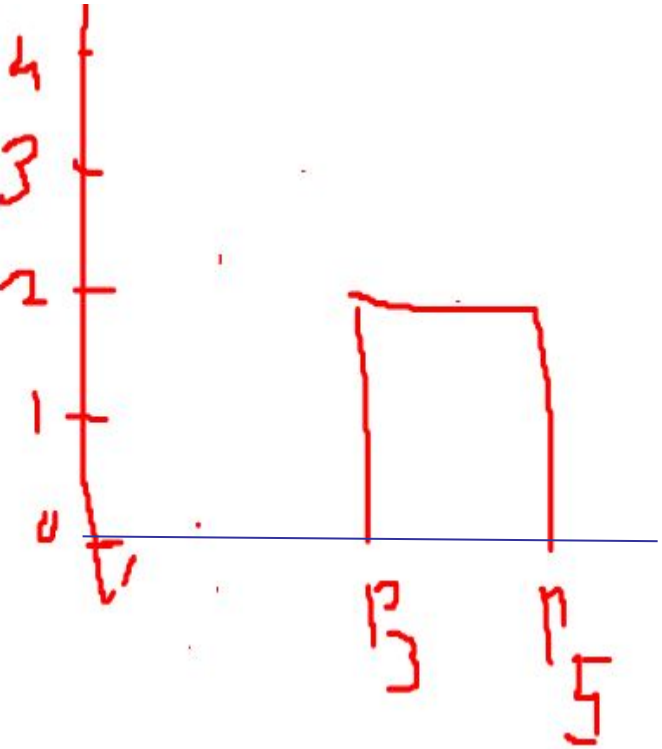
$\Rightarrow d(P_2, [P_3, P_5])$
$\Rightarrow \min(d(P_2, P_3), d(P_2, P_5))$
$\Rightarrow \min(7, 10) \Rightarrow 7$

$\Rightarrow d(P_4, [P_3, P_5])$
$\Rightarrow \min(d(P_4, P_3), d(P_4, P_5))$
$\Rightarrow \min(9, 8) \Rightarrow 8$

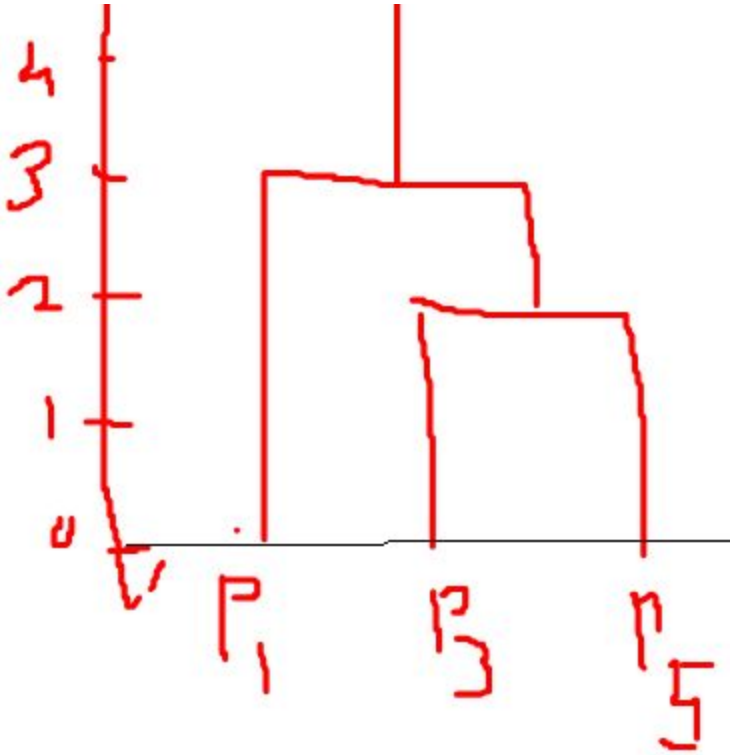
$\Rightarrow d(P_1, [P_3, P_5])$
$\Rightarrow \min(d(P_1, P_3), d(P_1, P_5))$
$\Rightarrow \min(3, 11) \Rightarrow 3$

**As 3 is minimum , combine [P3.P5] and [P1]**

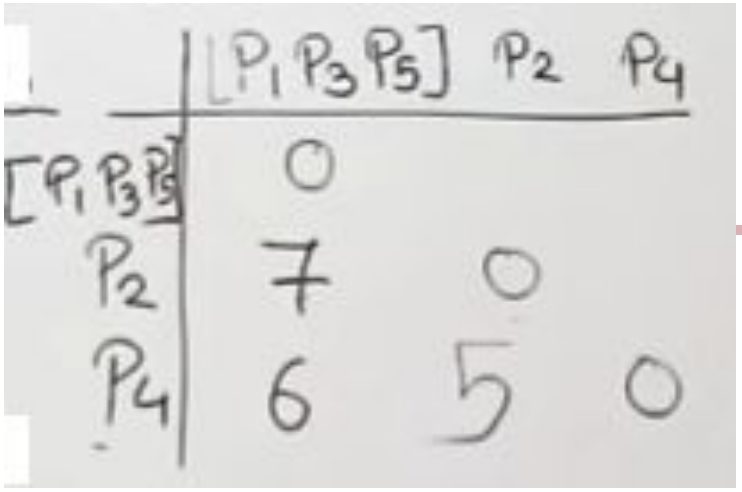
# Dendrogram



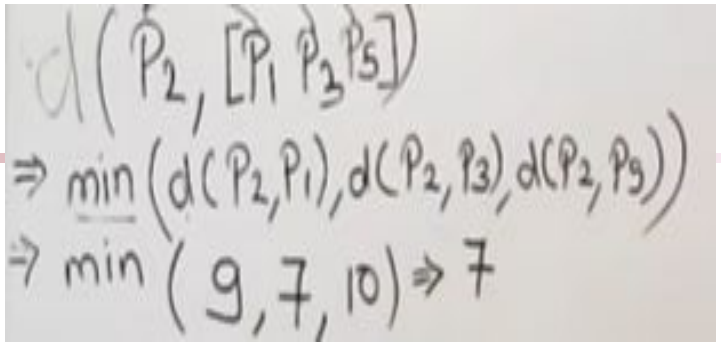

Step 1



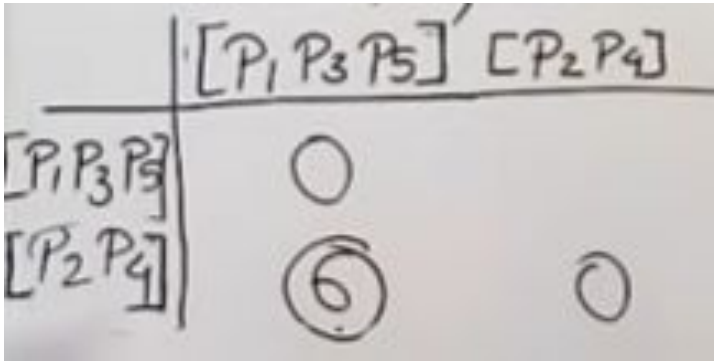

Step 2



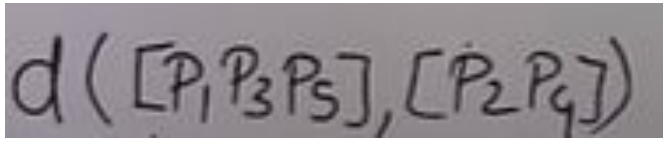
| | [P1 P3 P5] | P2 | P4 |
|---|---|---|---|
| [P1 P3 P5] | 0 | | |
| P2 | 7 | 0 | |
| P4 | 6 | 5 | 0 |




**Combine [P2] and [P4]**



| | [P1 P3 P5] | [P2 P4] |
|---|---|---|
| [P1 P3 P5] | 0 | |
| [P2 P4] | 6 | 0 |




**combine [P1,P3.P5] and [P2,P4]into one cluster**

# Dendrogram Example

# Dendrogram Example

Given the following dataset with five points:

- Perform hierarchical clustering using the Euclidean distance and single linkage.

| Point | X | Y |
|---|---|---|
| A | 1 | 2 |
| B | 2 | 3 |
| C | 3 | 6 |
| D | 8 | 8 |
| E | 9 | 10 |

# Dendrogram Example

- Solution Steps
- Compute the pairwise Euclidean distances:
- Example: Distance between A and B:
- Create an initial distance matrix (distances between all points are computed).
- Find the closest pair: A and B are closest, so merge them into one cluster.
- Recompute the distance matrix:
- Using single linkage, the distance between clusters is the minimum of all pairwise distances.
- Repeat until only one cluster remains.

# Dendrogram Example

Step 1: (A,B)=1.41
—C1- Merge them

Step2: Update distance matrix

| | $A$ | $B$ | $C$ | $D$ | $E$ |
|---|---|---|---|---|---|
| $A$ | 0 | 1.41 | 4.47 | 9.22 | 11.31 |
| $B$ | 1.41 | 0 | 3.16 | 7.81 | 9.90 |
| $C$ | 4.47 | 3.16 | 0 | 5.39 | 7.21 |
| $D$ | 9.22 | 7.81 | 5.39 | 0 | 2.24 |
| $E$ | 11.31 | 9.90 | 7.21 | 2.24 | 0 |

| | $(A,B)$ | $C$ | $D$ | $E$ |
|---|---|---|---|---|
| $(A,B)$ | 0 | 3.16 | 7.81 | 9.90 |
| $C$ | 3.16 | 0 | 5.39 | 7.21 |
| $D$ | 7.81 | 5.39 | 0 | 2.24 |
| $E$ | 9.90 | 7.21 | 2.24 | 0 |

# Dendrogram Example

Step 3: (D,E)=2.24
—C2- Merge them

Step4: Update distance matrix

| | $(A,B)$ | $C$ | $D$ | $E$ |
|---|---|---|---|---|
| $(A,B)$ | 0 | 3.16 | 7.81 | 9.90 |
| $C$ | 3.16 | 0 | 5.39 | 7.21 |
| $D$ | 7.81 | 5.39 | 0 | 2.24 |
| $E$ | 9.90 | 7.21 | 2.24 | 0 |

| | $(A,B)$ | $C$ | $(D,E)$ |
|---|---|---|---|
| $(A,B)$ | 0 | 3.16 | 7.81 |
| $C$ | 3.16 | 0 | 5.39 |
| $(D,E)$ | 7.81 | 5.39 | 0 |

# Dendrogram Example

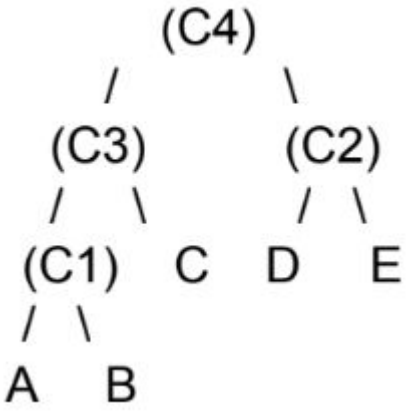
Step 5: (C1,C)=3.16
—C3- Merge them

| | $(A,B)$ | $C$ | $(D,E)$ |
|---|---|---|---|
| $(A,B)$ | 0 | 3.16 | 7.81 |
| $C$ | 3.16 | 0 | 5.39 |
| $(D,E)$ | 7.81 | 5.39 | 0 |

Step 6: Update distance matrix

Step 7: Merge all

| | $(A,B,C)$ | $(D,E)$ |
|---|---|---|
| $(A,B,C)$ | 0 | 5.39 |
| $(D,E)$ | 5.39 | 0 |



# Complete Linkage

| | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ |
|---|---|---|---|---|---|
| $P_1$ | 0 | | | | |
| $P_2$ | 9 | 0 | | | |
| $P_3$ | 3 | 7 | 0 | | |
| $P_4$ | 6 | 5 | 9 | 0 | |
| $P_5$ | 11 | 10 | 2 | 8 | 0 |

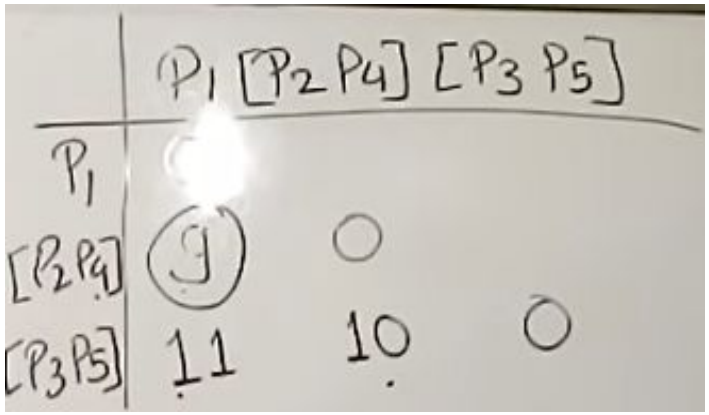
Combine [P3] and [P5]

| | $P_1$ | $P_2$ | $[P_3\ P_5]$ | $P_4$ |
|---|---|---|---|---|
| $P_1$ | 0 | | | |
| $P_2$ | 9 | 0 | | |
| $[P_3\ P_5]$ | 11 | 10 | 0 | |
| $P_4$ | 6 | 5 | 9 | 0 |

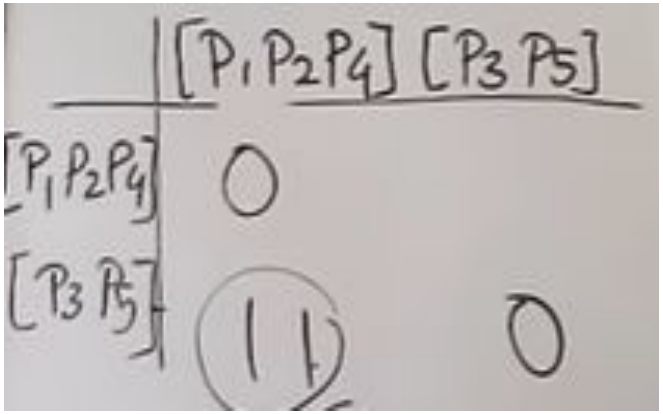
$d(P_2, [P_3\ P_5])$
$\Rightarrow \max(d(P_2, P_3), d(P_2, P_5)) \Rightarrow \max(7, 10) = 10$
$d(P_1, [P_3\ P_5])$
$\Rightarrow \max(d(P_1, P_3), d(P_1, P_5)) \Rightarrow \max(3, 11) = 11$
$d(P_4, [P_3\ P_5])$
$\Rightarrow \max(d(P_4, P_3), d(P_4, P_5)) \Rightarrow \max(9, 8) = 9$

Combine [P4] and [P2]

# Dendrogram Example (Complete Linkage)




Combine [P2,P4] and [P1]




Combine [P1,P2,P4] and [P3.P5 to form a single cluster


Dendogram

# Dendrogram Example

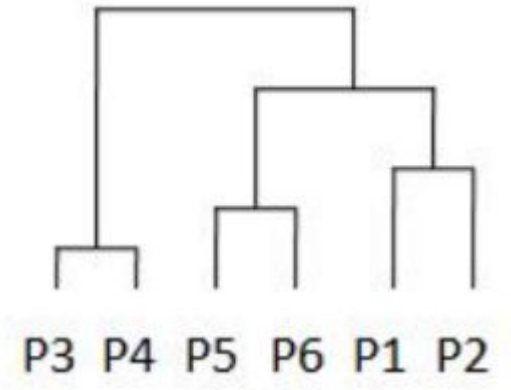
The pairwise distance between 6 points is given below. Draw hierarchy of clusters created by single link clustering algorithm.

| | P1 | P2 | P3 | P4 | P5 | P6 |
|---|---|---|---|---|---|---|
| P1 | 0 | 3 | 8 | 9 | 5 | 4 |
| P2 | 3 | 0 | 9 | 8 | 10 | 9 |
| P3 | 8 | 9 | 0 | 1 | 6 | 7 |
| P4 | 9 | 8 | 1 | 0 | 7 | 8 |
| P5 | 5 | 10 | 6 | 7 | 0 | 2 |
| P6 | 4 | 9 | 7 | 8 | 2 | 0 |

# Dendrogram Example

Step 1: Connect closest pair of points. Closest pairs are:
d(P3, P4) = 1
d(P5, P6) = 2
d(P1, P2) = 3
Step 2: Connect clusters with single link. The cluster pair to combine is bolded:
d({P1, P2}, {P3, P4}) = 8
**d({P1, P2}, {P5, P6}) = 4**
d({P5, P6}, {P3, P4}) = 6
Step 3: Connect the final 2 clusters

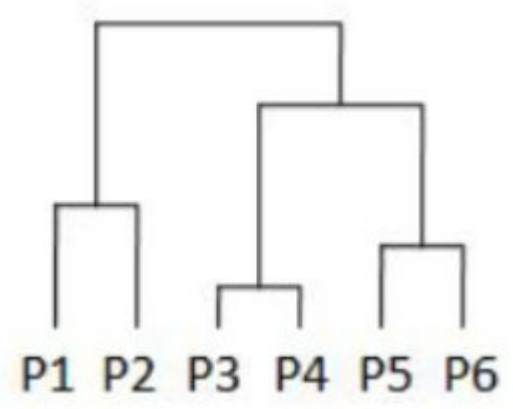
| | P1 | P2 | P3 | P4 | P5 | P6 |
|---|---|---|---|---|---|---|
| P1 | 0 | 3 | 8 | 9 | 5 | 4 |
| P2 | 3 | 0 | 9 | 8 | 10 | 9 |
| P3 | 8 | 9 | 0 | 1 | 6 | 7 |
| P4 | 9 | 8 | 1 | 0 | 7 | 8 |
| P5 | 5 | 10 | 6 | 7 | 0 | 2 |
| P6 | 4 | 9 | 7 | 8 | 2 | 0 |



# Dendrogram Example

The pairwise distance between 6 points is given below. Draw hierarchy of clusters created by the complete link clustering algorithm..

| | P1 | P2 | P3 | P4 | P5 | P6 |
|---|---|---|---|---|---|---|
| P1 | 0 | 3 | 8 | 9 | 5 | 4 |
| P2 | 3 | 0 | 9 | 8 | 10 | 9 |
| P3 | 8 | 9 | 0 | 1 | 6 | 7 |
| P4 | 9 | 8 | 1 | 0 | 7 | 8 |
| P5 | 5 | 10 | 6 | 7 | 0 | 2 |
| P6 | 4 | 9 | 7 | 8 | 2 | 0 |



# BIRCH (1996)

- Balanced Iterative Reducing and Clustering using Hierarchies (BIRCH) is designed for clustering a large amount of numeric data by integrating hierarchical clustering (at the initial *microclustering* stage) and other clustering methods such as iterative partitioning (at the later *macroclustering* stage).
- Small summary of large dataset.
- It overcomes the two difficulties in agglomerative clustering methods: (1) scalability and (2) the inability to undo what was done in the previous step.
- BIRCH uses the notions of *clustering feature* to summarize a cluster, and *clustering feature tree* (*CF-tree*) to represent a cluster hierarchy.
- These structures help the clustering method to achieve good speed and scalability in large DS and also make it effective for incremental and dynamic clustering of incoming data objects.

# BIRCH (1996)

- A clustering feature is essentially a summary of the statistics for the given cluster.
- The **clustering feature** (**CF**) of the cluster is a 3-D vector summarizing information about clusters of objects.
  - *CF* =(*n*,*LS*,*SS*) *where*
    - *LS* is the linear sum of the *n* points i.e., $\sum_{i=1}^{n} x_i$
    - *SS* is the square sum of the data points i.e., $\sum_{i=1}^{n} x_i^2$
- Using a clustering feature, we can easily derive many useful statistics of a cluster.
  - For example, the cluster's centroid, $\boldsymbol{x}\mathbf{0}$, radius, *R*, and diameter, *D*, are

$$x_0 = \frac{\sum_{i=1}^{n} x_i}{n} = \frac{LS}{n}, \quad R = \sqrt{\frac{\sum_{i=1}^{n} (x_i - x_0)^2}{n}} = \sqrt{\frac{nSS - 2LS^2 + nLS}{n^2}}, \quad D = \sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{n} (x_i - x_j)^2}{n(n-1)}} = \sqrt{\frac{2nSS - 2LS^2}{n(n-1)}}.$$

Here, *R* is the average distance from member objects to the centroid, and *D* is the average pairwise distance within a cluster

# Example

**Clustering feature.** Suppose there are three points, $(2,5),(3,2)$, and $(4,3)$, in a cluster, $C_1$. The clustering feature of $C_1$ is

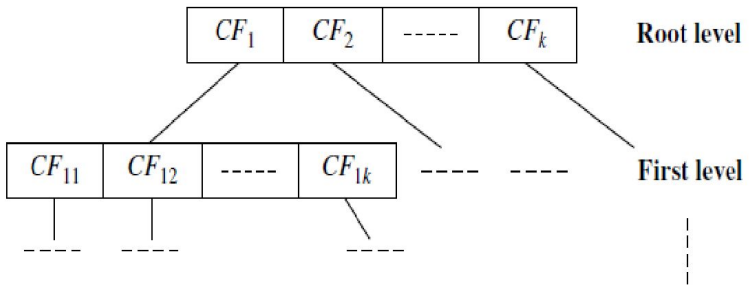
$$CF_1 = \langle 3,(2+3+4,5+2+3),(2^2+3^2+4^2,5^2+2^2+3^2)\rangle = \langle 3,(9,10),(29,38)\rangle.$$

Suppose that $C_1$ is disjoint to a second cluster, $C_2$, where $CF_2 = \langle 3,(35,36),(417,440)\rangle$. The clustering feature of a new cluster, $C_3$, that is formed by merging $C_1$ and $C_2$, is derived by adding $CF_1$ and $CF_2$. That is,

$$CF_3 = \langle 3+3,(9+35,10+36),(29+417,38+440)\rangle = \langle 6,(44,46),(446,478)\rangle. \quad \blacksquare$$

# Clustering Feature Tree (CF Tree)

- A **CF-tree** is a height-balanced tree that stores the clustering features for a hierarchical clustering.




**Each nonleaf node stores sum of CFs of its children**

CF-tree structure.

- A CF-tree has two parameters:
  1. *Branching factor*, *B*, specifies the maximum number of children per nonleaf node.
  2. *The threshold parameter* T, specifies the maximum diameter of subclusters stored at the leaf nodes of the tree.
- These two parameters implicitly control the resulting tree's size.

# Clustering Feature Tree (CF Tree)

- BIRCH applies a *multiphase* clustering technique:

- The primary phases are
  - **Phase 1:** BIRCH scans the database to build an initial in-memory CF-tree, which can be viewed as a multilevel compression of the data that tries to preserve the data's inherent clustering structure.

  - **Phase 2:** BIRCH applies a (selected) clustering algorithm to cluster the leaf nodes of the CF-tree, which removes sparse clusters as outliers and groups dense clusters into larger ones.

# Clustering Feature Tree (CF Treee)

- *"How effective is BIRCH?"*
  - The time complexity of the algorithm is *O(n)*, where *n* is the number of objects to be clustered.
  - Experiments have shown the linear scalability of the algorithm with respect to the number of objects, and good quality of clustering of the data.

- Drawbacks:
  - Since each node in a CF-tree can hold only a limited number of entries due to its size,a CF-tree node does not always correspond to what a user may consider a natural cluster.
  - Moreover, if the clusters are not spherical in shape, BIRCH does not perform well because it uses the notion of radius or diameter to control the boundary of a cluster.
  - It can process only the metric attributes.

- **Implementation of BIRCH in Python: Link**

CF tree is built dynamically as objects are inserted.

- For each point in the input
  - Find closest leaf entry
  - Add point to leaf entry and update CF
  - If entry diameter > max_diameter, then split leaf, and possibly parents

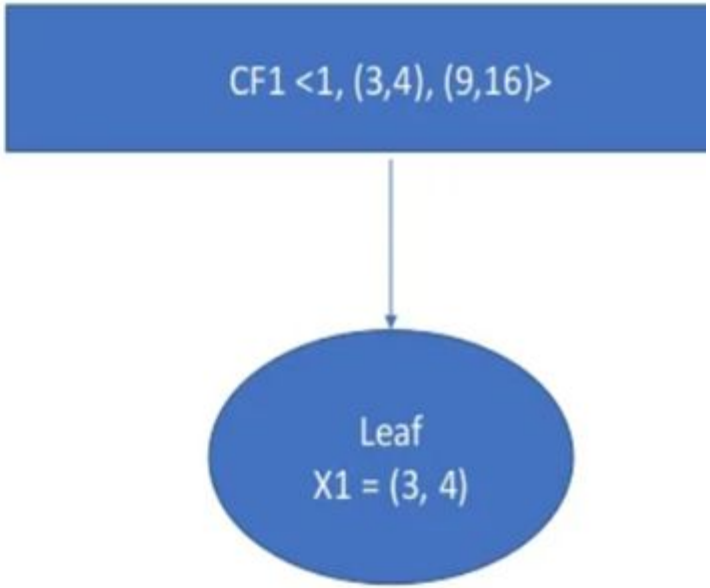
# Example

Let Have Following Data
X1=(3,4), x2= (2,6), x3=(4,5), x4=(4,7), x5=(3,8), x6=(6,2), x7=(7,2), x8=(7,4), x9=(8,4), x10=(7,9)
Cluster the Above Data Using BIRCH Algorithm, , considering T<1.5, and Max Branch = 2

For each Data Point we need to evaluate Radius and Cluster Feature:

->Consider Data Pint (3,4):

As it is alone in the Feature map, Hence
1. Radius = 0
2. Cluster Feature CF1 <N, LS, SS>
   N = 1 as there is now one data point under consideration.
   LS = Sum of Data Point under consideration = (3,4)
   SS = Square Sum of Data Point Under Consideration
   = $(3^2, 4^2)$=(9,16)
3. Now construct the Leaf with Data Point X1 and Branch as CF1.



->Consider Data Pint x2 = (2,6):

1. Linear Sum LS = (3,4) + (2,6) = (5,10)
2. Square Sum SS = $(3^2+2^2 , 4^2+6^2)$ =(13, 52)

Now Evaluate Radius considering N=2

$$R = \sqrt{\frac{SS-LS^2/N}{N}} = \sqrt{\frac{(13,52)-(5,10)^2/2}{2}} = \sqrt{\frac{(13,52)-(25,100)/2}{2}} =$$

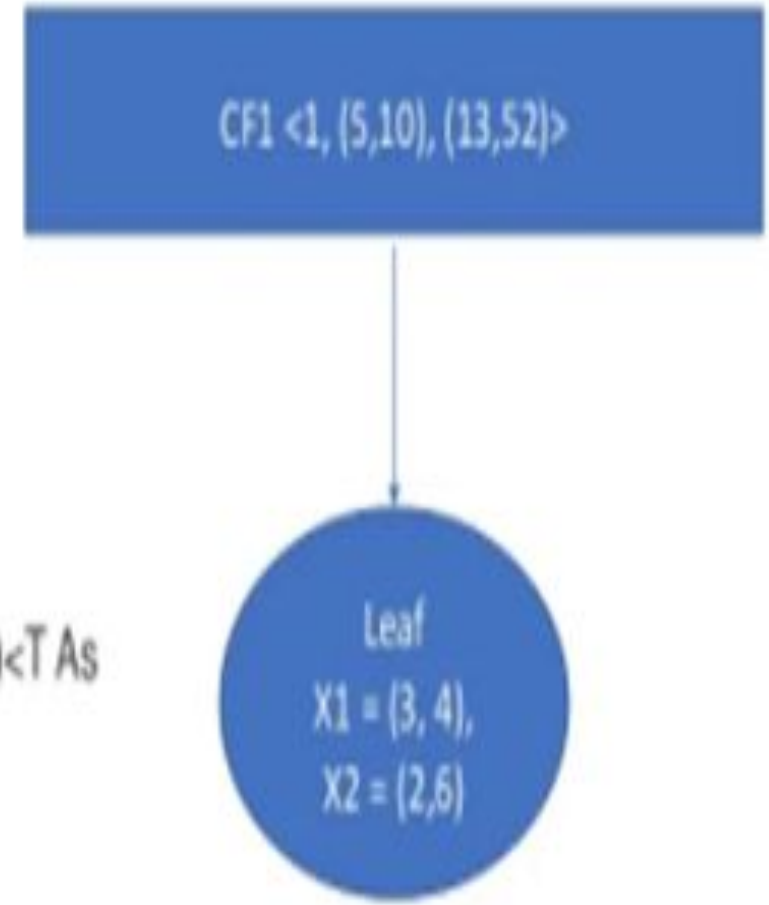
$$\sqrt{\frac{(13,52)-(12.5,50)}{2}} = \sqrt{(6.5,26) - (6.25,25)} = \sqrt{(0.25,1)} = (0.5, 1) < T$$ As (0.25,1) < (T, T), hence X2 will cluster with Leaf X1.

2. Cluster Feature CF1 <N, LS, SS> = <2,(5,10),(13,52)>

   N = 2 as there is now two data point under CF1.

   LS = (3,4) + (2,6) = (5,10)

   SS = $(3^2+2^2 , 4^2+6^2)$ =(13, 52)



->Consider Data Pint x3 = (4,5) on CF1:

1. Linear Sum LS = (4,5) + (5,10) = (9,15)
2. Square Sum SS = ($4^2$+13 , $5^2$ + 52) =(29, 77)

Now Evaluate Radius considering N=3

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(29,77) - (9,15)^2/3}{3}} = (0.47, 0.4714) < T$$

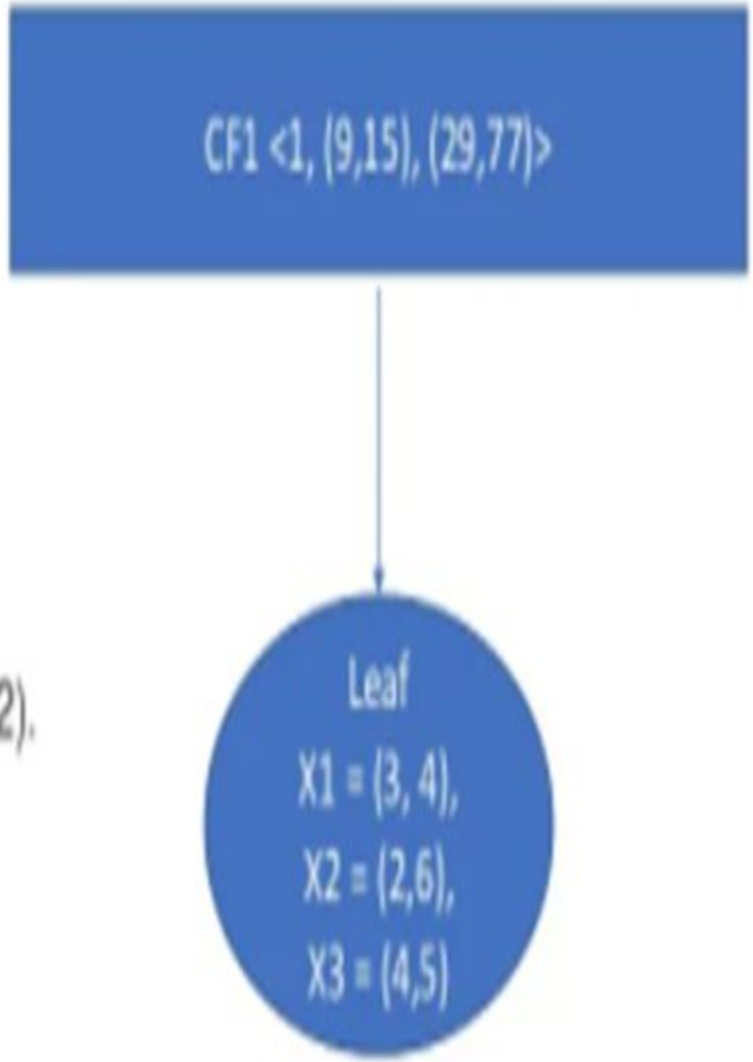
As (0.47, 0.471) < (T, T), hence X3 will cluster with Leaf (X1, x2).

2. Cluster Feature CF1 <N, LS, SS> = <3,(9,15),(29,77)>

N = 3 as there is now Three data point under CF1.

LS = (4,5) + (5,10) = (9,15)

SS = ($4^2$+13 , $5^2$ + 52) =(29, 77)



->Consider Data Pint x4 = (4,7) on CF1:

1. Linear Sum LS = (4,7) + (9,15) = (13,22)
2. Square Sum SS = ($4^2$+29 , $7^2$ + 77) =(45, 126)

Now Evaluate Radius considering N=4

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(45,126) - (13,22)^2/4}{4}} = (0.41, 0.55)$$

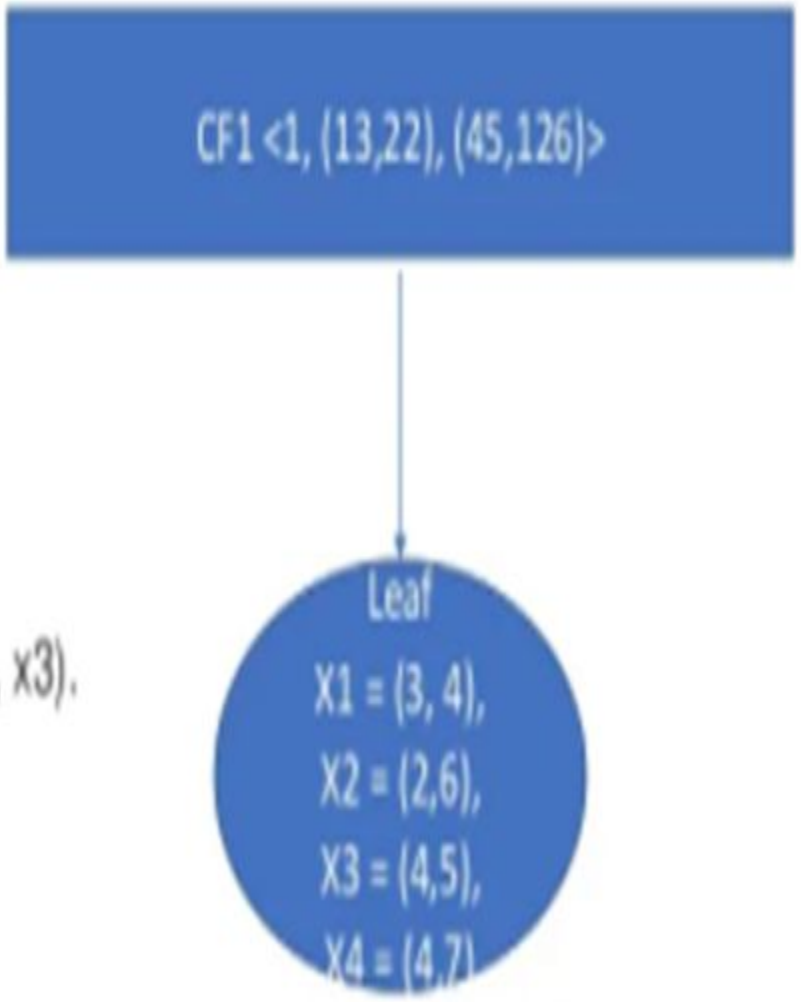
As (0.41, 0.55) < (T, T), hence X4 will cluster with Leaf (X1, x2, x3).

2. Cluster Feature CF1 <N, LS, SS> = <4,(13,22),(45,126)>

N = 4 as there is now four data point under CF1.

LS = (4,7) + (9,15) = (13,22)

SS = ($4^2$+29 , $7^2$ + 77) =(45, 126)



->Consider Data Pint x5 = (3,8) on CF1:

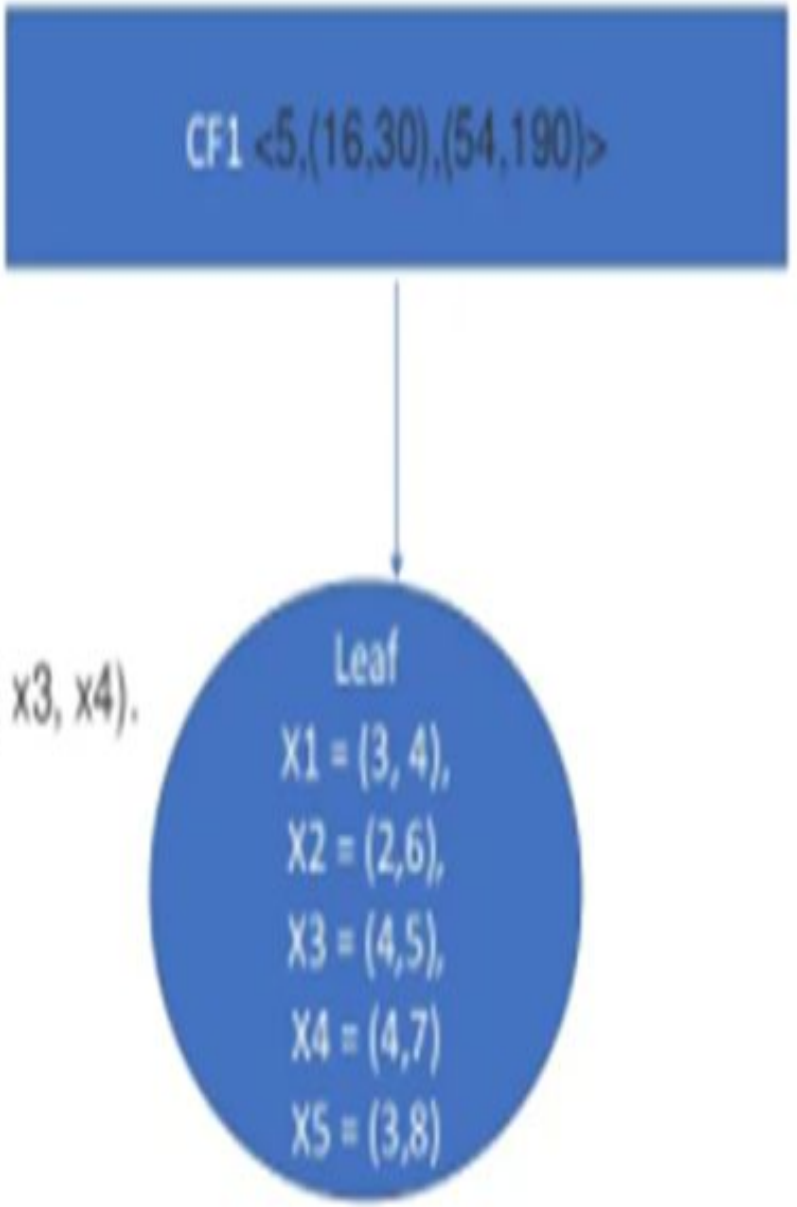
1. Linear Sum LS = (3,8) + (13,22) = (16,30)
2. Square Sum SS = ($3^2$+45 , $8^2$ + 126) =(54, 190)

Now Evaluate Radius considering N=5

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(54,190) - (16,30)^2/5}{5}} = (0.33, 0.63)$$

As (0.33, 0.63) < (T, T), hence X5 will cluster with Leaf (X1, x2, x3, x4).

2. Cluster Feature CF1 <N, LS, SS> = <5,(16,30),(54,190)>
   N = 5 as there is now four data point under CF1.



->Consider Data Pint x6 = (6,2) on CF1:

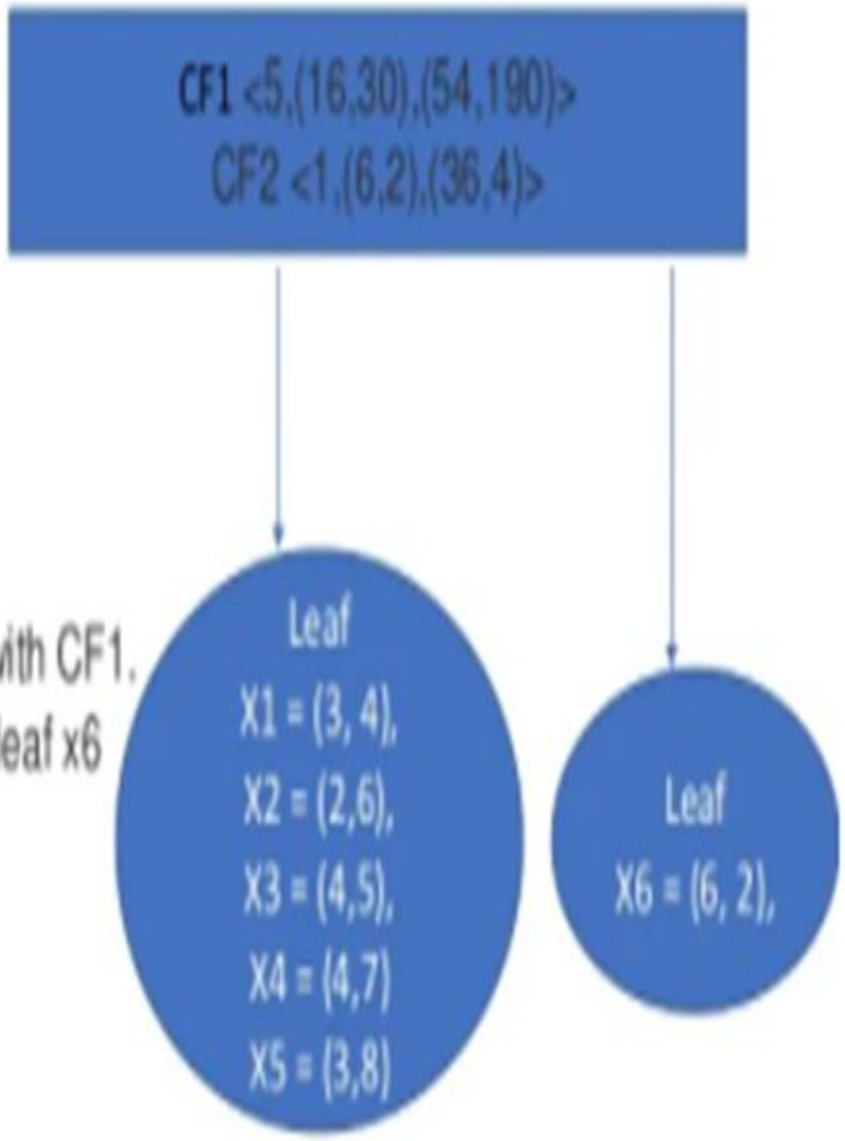
1. Linear Sum LS = (6,2) + (16,30) = (22,32)
2. Square Sum SS = ($6^2$+54 , $2^2$ + 190) =(90, 194)

Now Evaluate Radius considering N=6

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(90,194) - (22,32)^2/6}{6}} = (1.24, 1.97)$$

As (1.24, 1.97) < (T, T), False. hence X6 will Not form cluster with CF1. CF1 will remain as it was in previous step. And New CF2 with leaf x6 will be created.

2. Cluster Feature CF2 <N, LS, SS> = <1,(6,2),(36,4)>
   N = 1 as there is now one data point under CF2.
   LS = (6,2)
   SS = ($6^2$, $2^2$)= (36,4)



->Consider Data Pint x7 = (7,2). As There are Two Branch CF1 and CF2 hence we need to find with which branch X7 is nearer, then with that leaf radius will be evaluated.

With CF1 = LS/N= (16,30)/5=(8,6) As there are N=5 Data Point

With CF2 = LS/N= (6,2)/1=(6,2) As there is N=1 Data Point

Now x7 is closer to (6,2) then (8,6). Hence X7 will calculate radius with CF2.

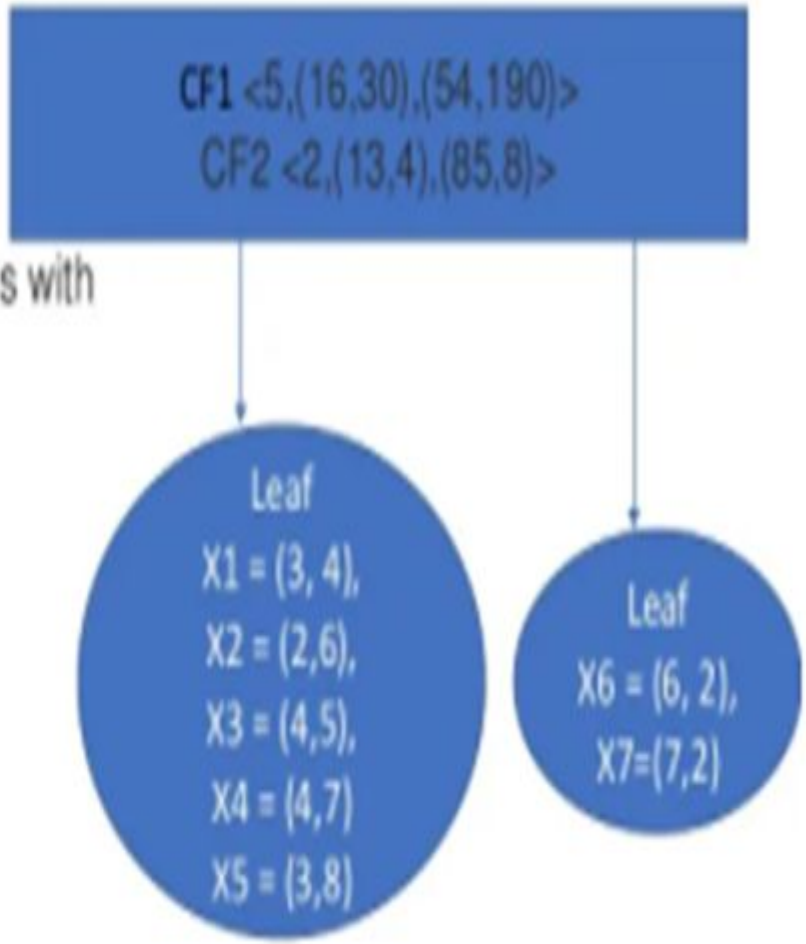
1. Linear Sum LS = (7,2) + (6,2) = (13,4)
2. Square Sum SS = $(7^2+36 , 2^2 + 4)$ =(85, 8)

Now Evaluate Radius considering N=2

$$R = \sqrt{\frac{SS-LS^2/N}{N}} = \sqrt{\frac{(85,8)-(13,4)^2/2}{2}} = (0.5, 0)$$

As (0.5, 0) < (T, T), True. hence X7 will form cluster with CF2

2. Cluster Feature CF2 <N, LS, SS> = <2,(13,4),(85,8)>
   N = 2 as there is now two data point under CF2.
   LS = (7,2) + (6,2) = (13,4)
   SS = $(7^2+36 , 2^2 + 4)$ =(85, 8)



->Consider Data Pint x8 = (7,4). As There are Two Branch CF1 and CF2 hence we need to find with which branch X8 is nearer, then with that leaf, radius will be evaluated.

With CF1 = LS/N= (16,30)/5=(8,6) As there are N=5 Data Point

With CF2 = LS/N= (13,4)/2=(6.5,2) As there is N=2 Data Point

Now x8 is closer to (6.5,2) then (8,6). Hence X8 will calculate radius with CF2.

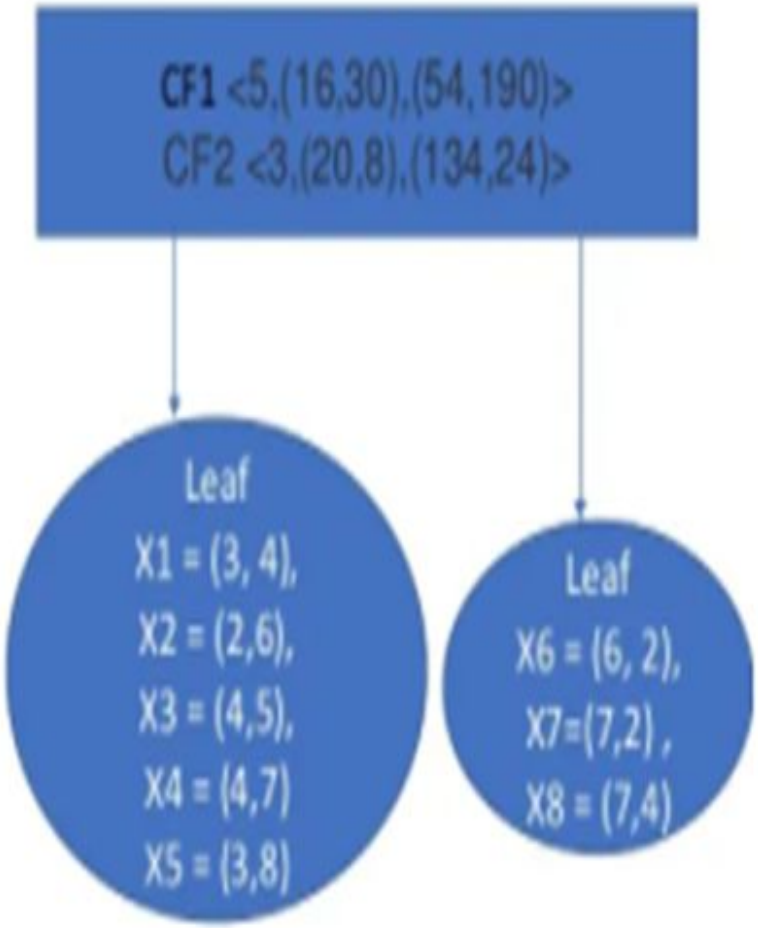
1. Linear Sum LS = (7,4) + (13,4) = (20,8)
2. Square Sum SS = ($7^2$+85 , $4^2$ + 8) =(134, 24)

Now Evaluate Radius considering N=3

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(134,24) - (20,8)^2/3}{3}} = (0.47, 0.94)$$

As (0.47, 94) < (T, T), True. hence X8 will form cluster with CF2

2. Cluster Feature CF2 <N, LS, SS> = <3,(20,8),(134,24)>
   N = 3 as there is now two data point under CF2.
   LS (7,4) + (13,4) = (20,8)
   SS = (134,24)



->Consider Data Pint x9 = (8,4). As There are Two Branch CF1 and CF2 hence we need to find with which branch X9 is nearer, then with that leaf, radius will be evaluated.

With CF1 = LS/N= (16,30)/5=(8,6) As there are N=5 Data Point

With CF2 = LS/N= (20,8)/3=(6.6,2.6) As there is N=3 Data Point

Now x9 is closer to (6.6,2.6) then (8,6). Hence X8 will calculate radius with CF2.

1. Linear Sum LS = (8,4) + (20,8) = (28,12)
2. Square Sum SS = ($8^2$+134 , $4^2$ + 24) =(198, 40)

Now Evaluate Radius considering N=4

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(198,40) - (28,12)^2/4}{4}} = (0.70, 1)$$

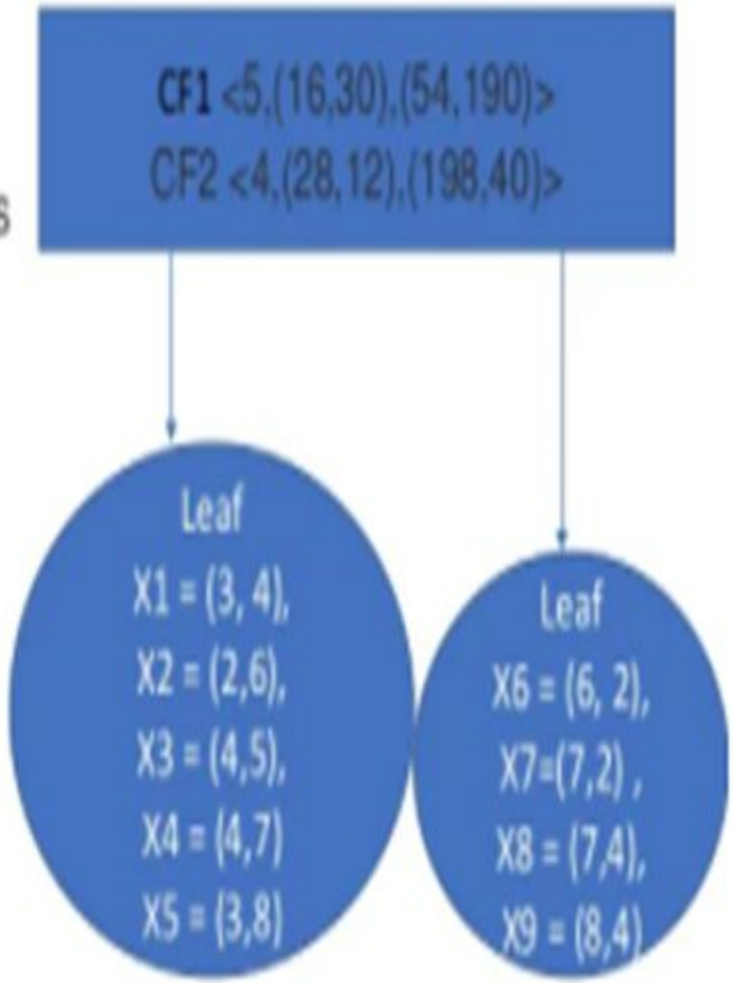
As (0.7, 1) < (T, T), True. hence X9 will form cluster with CF2

2. Cluster Feature CF2 <N, LS, SS> = <4,(28,12),(198,40)>

   N = 4 as there is now four data point under CF2.

   LS = (28,12)

   SS = (198,40)



->Consider Data Pint x10 = (7,9). As There are Two Branch CF1 and CF2 hence we need to find with which branch X9 is nearer, then with that leaf, radius will be evaluated. → 3-2

With CF1 = LS/N= (16,30)/5=(8,6) As there are N=5 Data Point

With CF2 = LS/N= (28,12)/4=(7,3) As there is N=4 Data Point

Now x10 is closer to (8,6) then (7,3). Hence X10 will calculate radius with CF1.

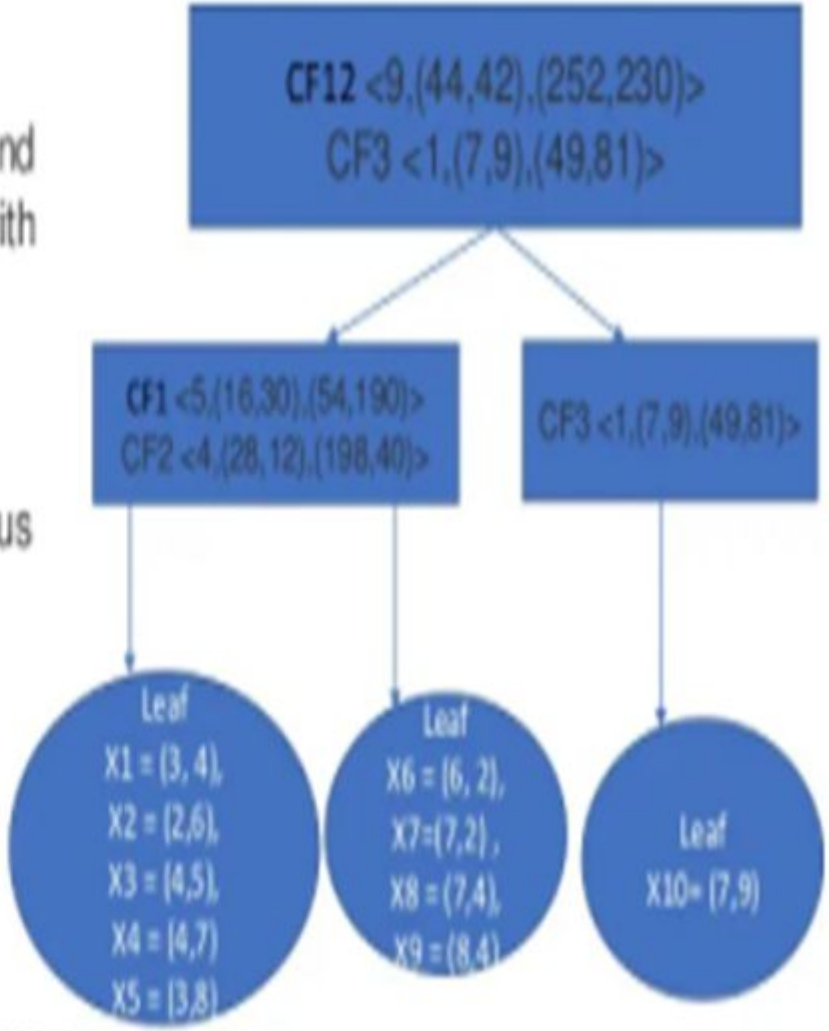
1. Linear Sum LS = (7,9) + (16,30) = (23,39)
2. Square Sum SS = ($7^2$+54 , $9^2$ + 190) =(103, 271)

Now Evaluate Radius considering N=6

$$R = \sqrt{\frac{SS - LS^2/N}{N}} = \sqrt{\frac{(103,271) - (23,39)^2/6}{6}} = (1.57, 1.70)$$

As (1.57, 1.70) < (T, T), False. hence X10 will become new leaf and Create new cluster feature CF3. But in a Branch only two CF is allowed hence Branch will Split.

2. Cluster Feature CF3 <N, LS, SS> = <1,(7,9),(49,81)>



# Density Based Clustering

- Density-based approach:
  - Based on connectivity and density functions.
  - The strategy used is to model the dense clusters separated by sparse clusters.
  - The general idea is to continue growing a given cluster as long as the density (number of objects or data points) in the "neighborhood" exceeds some threshold.
  - Such a method can be used to filter out noise or outliers and discover clusters of arbitrary shape.
    - Major features:
      - Discover clusters of arbitrary shape
      - Handle noise
      - One scan
      - Need density parameters as termination condition

❑ Typical methods: DBSCAN, OPTICS, DenClue

# DBSCAN(Density Based Spatial Clustering of Application with Noise

- Density-Based Clustering Algorithm Based on Connected Regions with High Density.
- The key idea is that for each point of a cluster, the neighborhood of a given radius has to contain at least a minimum number of points.
- **Why DBSCAN?**
  - Real life data may contain irregularities, like:
  1. Clusters can be of arbitrary shape.
  2. Data may contain noise.
  3. K-means: Only convex clusters (fails on non-spherical shapes).
  4. Hierarchical: Computationally expensive (O(n2))

     DBSCAN's Solution:
  5. Density-based: Clusters are dense regions separated by low-density areas.
  6. Noise Handling: Automatically identifies outliers.

# DBSCAN

- **DBSCAN algorithm requires two parameters:**

1. **eps** : It defines the neighborhood around a data point
   - if the distance between two points is <= 'eps' then they are considered as neighbors.
   - If the eps value is chosen too small then large part of the data will be considered as outliers.
   - If it is chosen very large then the clusters will merge and majority of the data points will be in the same clusters.
   - One way to find the eps value is based on the ***k-distance graph***.

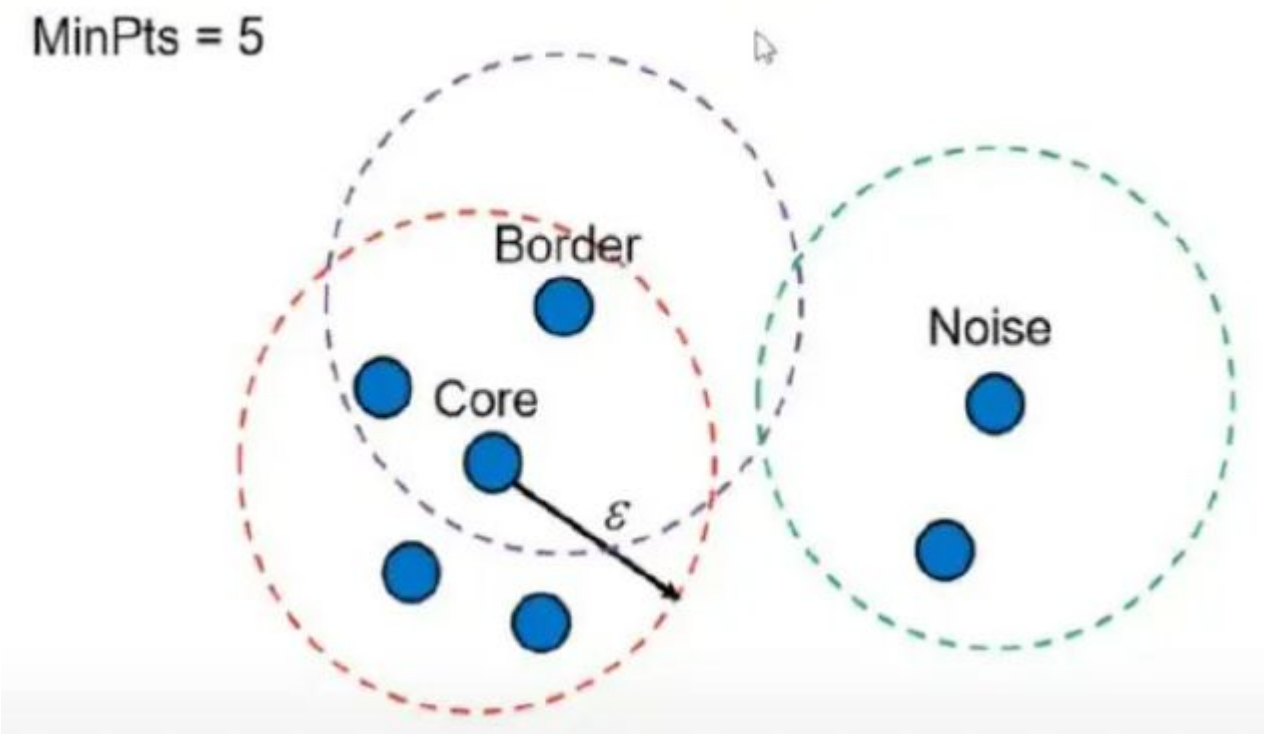
2. **MinPts**: Minimum number of neighbors (data points) within eps radius.
   - Larger the dataset, the larger value of MinPts must be chosen.
   - As a general rule, the minimum MinPts can be derived from the number of dimensions D in the dataset as, MinPts >= D+1.
   - The minimum value of MinPts must be chosen as at least 3.

# DBSCAN: Density-Based Clustering Based on Connected Regions with High Density

- *"How can we find dense regions in density-based clustering?"*
  - The *density* of an object ***o*** can be measured by the number of objects close to ***o***.
  - **DBSCAN** (Density-Based Spatial Clustering of Applications with Noise) finds *core objects*, that is, objects that have dense neighborhoods. It connects core objects and their neighborhoods to form dense regions as clusters.

# DBSCAN

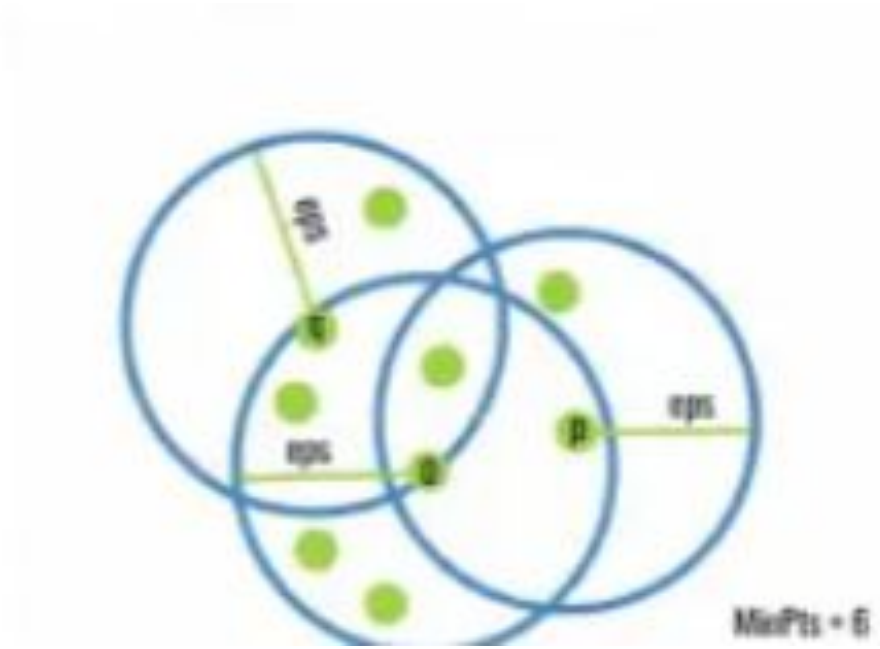
- **In this algorithm, we have 3 types of data points.**
  - **Core Point**: A point is a core point if it has more than MinPts points within eps.
  - **Border Point**: A point which has fewer than MinPts within eps(i.e it is not a core point ) but it is in the neighborhood of a core point.
  - **Noise or outlier**: A point which is not a core point or border point.




MinPts=3

# DBSCAN

- Reachability
- Density Reachable :
  An object q is density-reachable from p w.r.t ε and MinPts if there is a chain of objects $q_1$, $q_2$, …, q□, with $q_1$ = p, q□ = q such that $q_{i+1}$ is directly density-reachable from $q_i$ w.r.t ε and MinPts for all 1 <= i <= n
- Here density reachability is not symmetric. As q is not a core point thus $q_{□-1}$ is not directly density-reachable from q, so object p is not density-reachable from object q.
-

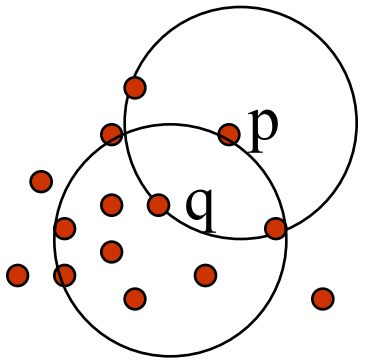



MinPts=3

# Density-Based Clustering: Basic Concepts

- Two parameters*:*
  - *Eps* : Maximum radius of the neighborhood
  - *MinPts* : Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: *{q belongs to D | dist(p,q) <= Eps}*
- Directly density-reachable: A point *p* is directly density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if
  - *p* belongs to $N_{Eps}(q)$
  - core point condition:

$$|N_{Eps}(q)| >= MinPts$$




MinPts = 5

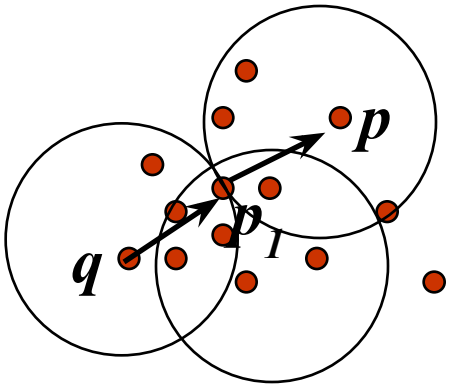
Eps = 1 cm

# Density-Based Clustering: Basic Concepts

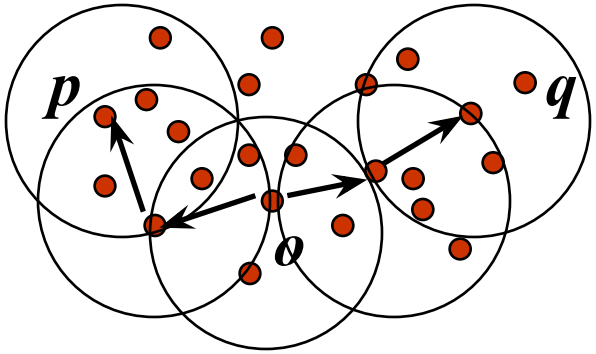
- 

# Density-Reachable and Density-Connected

- Density-reachable:
  - A point *p* is density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if there is a chain of points $p_1, \ldots, p_n, p_1 = q, p_n = p$ such that $p_{i+1}$ is directly density-reachable from $p_i$




- Density-connected
  - A point *p* is density-connected to a point *q* w.r.t. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



# DBSCAN: The Algorithm

- Arbitrarily select a point *p*
- Retrieve all points that are density-reachable from *p* w.r.t. *Eps* and *MinPts*.
- If *p* is a core point, a cluster is formed.
- If *p* is a border point, no points are density-reachable from *p* and DBSCAN visits the next point of the database.
- Continue the process until all of the points have been processed.

# DBSCAN Algorithm

**Algorithm: DBSCAN:** a density-based clustering algorithm.

**Input:**

- $D$: a data set containing $n$ objects,
- $\epsilon$: the radius parameter, and
- *MinPts*: the neighborhood density threshold.

**Output:** A set of density-based clusters.

**Method:**

```
(1)  mark all objects as unvisited;
(2)  do
(3)      randomly select an unvisited object p;
(4)      mark p as visited;
(5)      if the ε-neighborhood of p has at least MinPts objects
(6)          create a new cluster C, and add p to C;
(7)          let N be the set of objects in the ε-neighborhood of p;
(8)          for each point p' in N
(9)              if p' is unvisited
(10)                 mark p' as visited;
(11)                 if the ε-neighborhood of p' has at least MinPts points,
                     add those points to N;
(12)             if p' is not yet a member of any cluster, add p' to C;
(13)         end for
(14)         output C;
(15)     else mark p as noise;
(16) until no object is unvisited;
```

# DBSCAN: Sensitive to Parameters

*Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.*

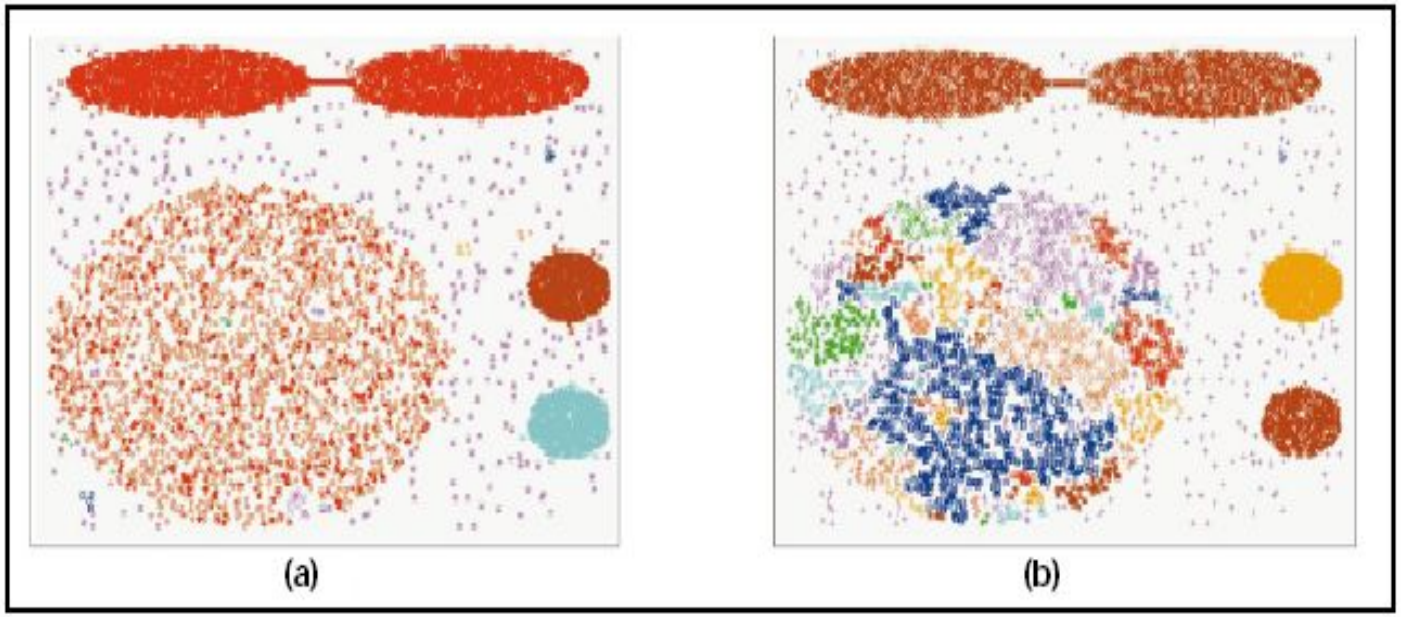
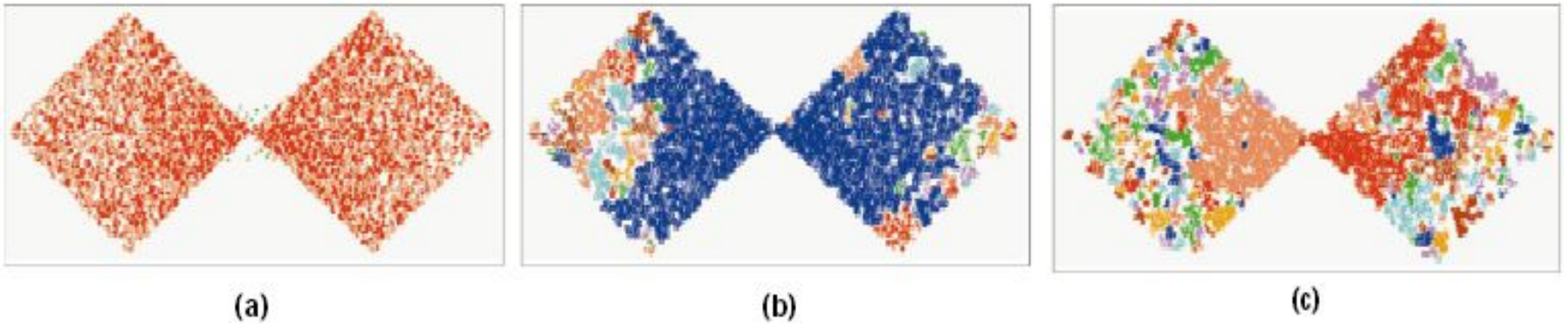



*Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.*



# Example: DBSCAN

**Apply the DBSCAN Algorithm to the given data point and create cluster with:**

**minPts: 4 and**
**eps (ε) : 1.9**

**Data Point's: P1(3,7), P2(4,6), P3(5,5), P4(6,4), P5(7,3), P6(6,2), P7(7,2), P8(8,4), P9(3,3), P10(2,6), P11(3,5), P12(2,4)**

# Example: DBSCAN

## DBSCAN

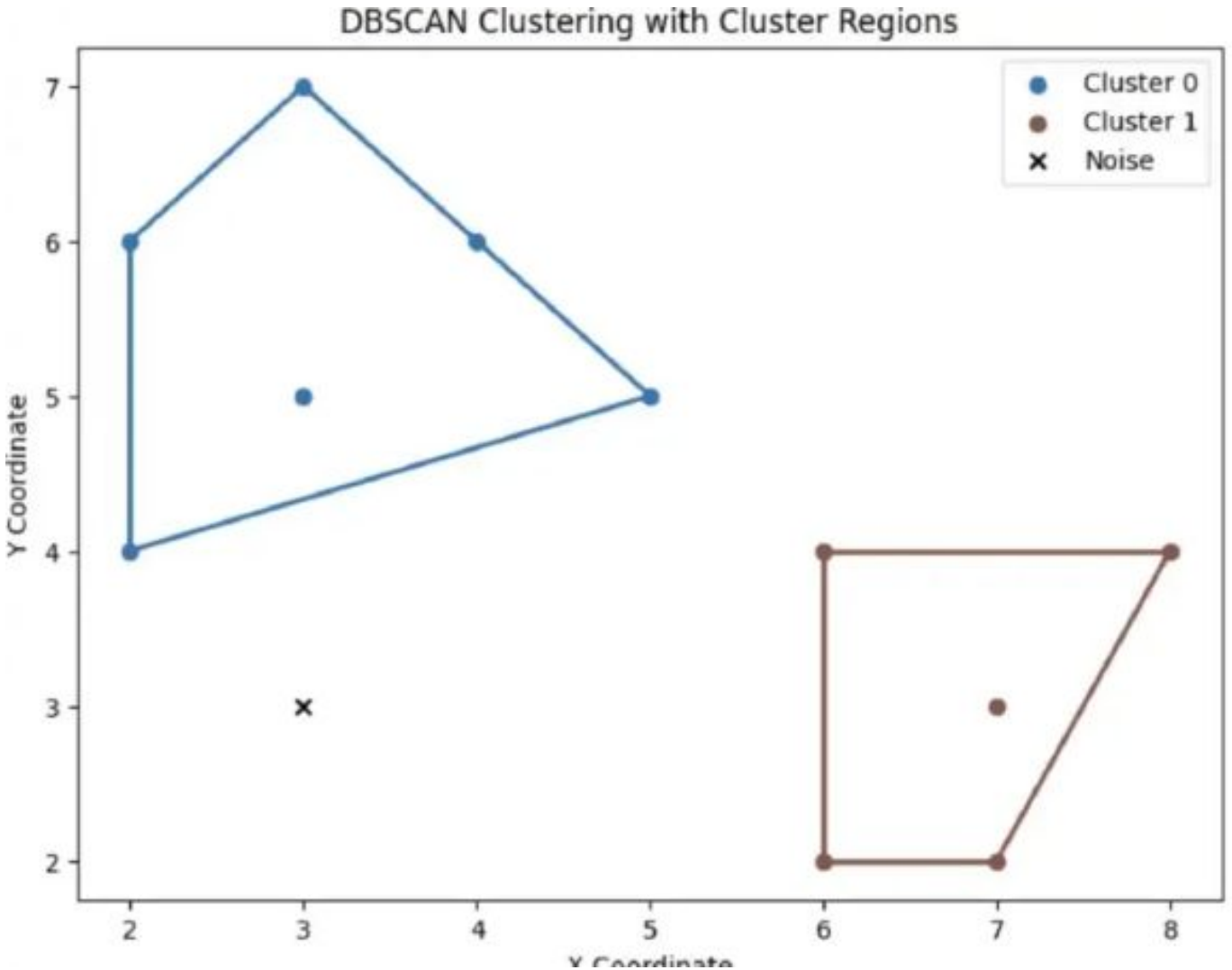
| | $p_1$ | $p_2$ | $p_3$ | $p_4$ | $p_5$ | $p_6$ | $p_7$ | $p_8$ | $p_9$ | $p_{10}$ | $p_{11}$ | $p_{12}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $p_1$ | 0 | | | | | | | | | | | |
| $p_2$ | 1.41 | 0 | | | | | | | | | | |
| $p_3$ | 2.83 | 1.41 | 0 | | | | | | | | | |
| $p_4$ | 4.24 | 2.83 | 1.41 | 0 | | | | | | | | |
| $p_5$ | 5.66 | 4.24 | 2.83 | 1.41 | 0 | | | | | | | |
| $p_6$ | 5.83 | 4.47 | 3.16 | 2.00 | 1.41 | 0 | | | | | | |
| $p_7$ | 6.40 | 5.00 | 3.61 | 2.24 | 1.00 | 1.00 | 0 | | | | | |
| $p_8$ | 5.83 | 4.47 | 3.16 | 2.00 | 1.41 | 2.83 | 2.24 | 0 | | | | |
| $p_9$ | 4.00 | 3.16 | 2.83 | 3.16 | 4.00 | 3.16 | 4.12 | 5.10 | 0 | | | |
| $p_{10}$ | 1.41 | 2.00 | 3.16 | 4.47 | 5.83 | 5.66 | 6.40 | 6.32 | 3.16 | 0 | | |
| $p_{11}$ | 2.00 | 1.41 | 2.00 | 3.16 | 4.47 | 4.24 | 5.00 | 5.10 | 3.16 | 1.41 | 0 | |
| $p_{12}$ | 3.16 | 2.83 | 3.16 | 4.00 | 5.10 | 4.47 | 5.39 | 6.00 | 1.41 | 2.00 | 1.41 | 0 |

# Example: DBSCAN

| |
|---|
| $p_1$:$p_2$, $p_{10}$ |
| $p_2$:$p_1$, $p_3$, $p_{11}$ |
| $p_3$:$p_2$, $p_4$ |
| $p_4$:$p_3$, $p_5$ |
| $p_5$:$p_4$, $p_6$, $p_7$, $p_8$ |
| $p_6$:$p_5$, $p_7$ |
| $p_7$:$p_5$, $p_6$ |
| $p_{12}$:$p_5$ |
| $p_9$:$p_{12}$ |
| $p_{12}$:$p_1$, $p_{11}$ |
| $p_{11}$:$p_2$, $p_{10}$, $p_{12}$ |
| $p_{12}$:$p_9$, $p_{11}$ |

| Point | Status | |
|---|---|---|
| $p_1$ | Noise | Border |
| $p_2$ | Core | |
| $p_3$ | Noise | Border |
| $p_4$ | Noise | Border |
| $p_5$ | Core | |
| $p_6$ | Noise | Border |
| $p_7$ | Noise | Border |
| $p_8$ | Noise | Border |
| $p_9$ | Noise | |
| $p_{10}$ | Noise | Border |
| $p_{11}$ | Core | |
| $p_{12}$ | Noise | Border |

# Example: DBSCAN



# Example: DBSCAN

| | | |
|---|---|---|
| A1 | 2 | 10 |
| A2 | 2 | 5 |
| A3 | 8 | 4 |
| A4 | 5 | 8 |
| A5 | 7 | 5 |
| A6 | 6 | 4 |
| A7 | 1 | 2 |
| A8 | 4 | 9 |

**Find clusters using DBSCAN** Є =2, MinPts=2

**Step1 : Find distance matrix**

| Euclidean Distance | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 8.49 | 3.61 | 7.07 | 7.21 | 8.06 | 2.24 |
| A2 | 5 | 0 | 6.08 | 4.24 | 5 | 4.12 | 3.16 | 4.47 |
| A3 | 8.49 | 6.08 | 0 | 5 | 1.41 | 2 | 7.28 | 6.4 |
| A4 | 3.61 | 4.24 | 5 | 0 | 3.61 | 4.12 | 7.21 | 1.41 |
| A5 | 7.07 | 5 | 1.41 | 3.61 | 0 | 1.41 | 6.71 | 5 |
| A6 | 7.21 | 4.12 | 2 | 4.12 | 1.41 | 0 | 5.39 | 5.39 |
| A7 | 8.06 | 3.16 | 7.28 | 7.21 | 6.71 | 5.39 | 0 | 7.62 |
| A8 | 2.24 | 4.47 | 6.4 | 1.41 | 5 | 5.39 | 7.62 | 0 |

# Example: DBSCAN

**Step2 : Find which data points are core points**

Є =2, MinPts=2

| Euclidean Distance | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 8.49 | 3.61 | 7.07 | 7.21 | 8.06 | 2.24 |
| A2 | 5 | 0 | 6.08 | 4.24 | 5 | 4.12 | 3.16 | 4.47 |
| A3 | 8.49 | 6.08 | 0 | 5 | 1.41 | 2 | 7.28 | 6.4 |
| A4 | 3.61 | 4.24 | 5 | 0 | 3.61 | 4.12 | 7.21 | 1.41 |
| A5 | 7.07 | 5 | 1.41 | 3.61 | 0 | 1.41 | 6.71 | 5 |
| A6 | 7.21 | 4.12 | 2 | 4.12 | 1.41 | 0 | 5.39 | 5.39 |
| A7 | 8.06 | 3.16 | 7.28 | 7.21 | 6.71 | 5.39 | 0 | 7.62 |
| A8 | 2.24 | 4.47 | 6.4 | 1.41 | 5 | 5.39 | 7.62 | 0 |
| Є-neighborhood | A1 | A2 | A3, A5, A6 | A4, A8 | A3, A5, A6 | A3, A5, A6 | A7 | A4, A8 |

Cluster1={A3,A5,A6}
Cluster2={A4,A8}

A1,A2,A7 are outliers

The no. of data points in the Є-neighbourhood of A1= 1(A1 itself) . < MinPts . Hence A1 is not a core point

# Example: DBSCAN

**Find clusters using DBSCAN** $\epsilon$ =2, MinPts=3

| Euclidean Distance | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| A | 0 | 0.7 | 5.7 | 3.6 | 4.2 | 3.2 |
| B | 0.7 | 0 | 4.9 | 2.9 | 3.5 | 2.5 |
| C | 5.7 | 4.9 | 0 | 2.9 | 1.4 | 2.5 |
| D | 3.6 | 2.9 | 2.9 | 0 | 1 | 0.5 |
| E | 4.2 | 3.5 | 1.4 | 1 | 0 | 1.1 |
| F | 3.2 | 2.5 | 2.5 | 0.5 | 1.1 | 0 |

**Find which data points are core points, Boundary points and Outliers.**

# Example: DBSCAN

**Find clusters using DBSCAN** Є =2, MinPts=3

| Euclidean Distance | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| A | 0 | 0.7 | 5.7 | 3.6 | 4.2 | 3.2 |
| B | 0.7 | 0 | 4.9 | 2.9 | 3.5 | 2.5 |
| C | 5.7 | 4.9 | 0 | 2.9 | 1.4 | 2.5 |
| D | 3.6 | 2.9 | 2.9 | 0 | 1 | 0.5 |
| E | 4.2 | 3.5 | 1.4 | 1 | 0 | 1.1 |
| F | 3.2 | 2.5 | 2.5 | 0.5 | 1.1 | 0 |
| Є-neighborhood | A,B | A,B | C,E | D,E,F | C,D,E,F | D,E,F |

**Find which data points are core points, Boundary Points and Outliers**

D,E and F are core points.
A and B are outliers
C is Boundary point as it is in Є-neighborhood of core point E

# Self Learning

- Hierarchical methods :
  - Chameleon, Density based methods: OPTICS,
- Grid based methods: STING, CLIQUE

- Suppose that the data mining task is to cluster points (with $(x, y)$ representing location) into three clusters, where the points are $A1(2, 10)$,$A2(2, 5)$,$A3(8, 4)$,$B1(5, 8)$,$B2(7, 5)$,$B3(6, 4)$,$C1(1, 2)$,$C2(4, 9)$. The distance function is Euclidean distance. Suppose initially we assign $A1$, $B1$, and $C1$ as the center of each cluster, respectively. Use the *k-means* algorithm to show *only*

  (a) the three cluster centers after the first round of execution.

  **Answer:**

  After the first round, the three new clusters are: (1) *{A1}*, (2) *{B1,A3,B2,B3,C2}*, (3) *{C1,A2}*, and their centers are (1) (2, 10), (2) (6, 6), (3) (1.5, 3.5).

  (b) the final three clusters.

  **Answer:**

  The final three clusters are: (1) *{A1,C2,B1}*, (2) *{A3,B2,B3}*, (3) *{C1,A2}*.

- Use an example to show why the $k$-means algorithm may not find the global optimum, that is, optimizing the within-cluster variation.

**Answer:**

Consider applying the $k$-means algorithm on the following points, and set $k = 2$. $A(0, 1)$, $B(0,-1)$, $Ci(100, 50)$ $(i = 1, \ldots, 100)$, and $Dj(100,-50)$ $(j = 1, \ldots, 100)$.

If we use $A$ and $C1$ as the initial cluster centers, then the clustering process will converge to two centers, (0, 0) and (100, 0).

The within-cluster variation is

$E = 12 + 12 + 100 \times 502 + 100 \times 502 = 1 + 1 + 100 \times 2500 + 100 \times 2500 = 500002.$

However, if we use (100, 50) and (100,−50) as the cluster centers, the within-cluster variation is

$E = (1002 + 492) + (1002 + 492) + 100 \times 0 + 100 \times 0 = 24802,$

which is much smaller. This example shows $k$-means may be trapped by a local optimal, and cannot jump out to find the global optimum

Both *k-means* and *k-medoids* algorithms can perform effective clustering.
(a) Illustrate the strength and weakness of *k-means* in comparison with the *k-medoids* algorithm.

**Answer:**

$k$-means vs. $k$ medoids: more efficient but quality deteriorates by noise and outliers.

b) Illustrate the strength and weakness of these schemes in comparison with a hierarchical clustering scheme (such as AGNES).

**Answer:**

Partition: can undo what was done (by moving objects around clusters)—quality is good in general, require the number of clusters to be known; find only spherical shaped clusters.

Hierarchical: cannot undo what was done—quality could be poor, does not require the number of clusters to be known; more efficient and parallel (divide and conquer), may find only arbitrary shaped clusters.

Present conditions under which density-based clustering is more suitable than partitioning-based clustering and hierarchical clustering. Give application examples to support your argument.

---

**Answer:**

Density-based clustering is more suitable if no or very limited domain knowledge is available to determine the appropriate values of the parameters, the clusters are expect of arbitrary shape including non convex shapes, and the efficiency is essential on large data sets.

For example, consider the application of recognizing residential area on a map where buildings and their types are labeled. A user may not have the domain knowledge about how a residential area would look like. Moreover, a residential area may be of arbitrary shape, and may not be in convex, such as those built along a river. In a large city, there are hundreds of thousands of buildings. Efficiency on large data sets is important.

- Give an example of how specific clustering methods can be *integrated*, for example, where one clustering algorithm is used as a preprocessing step for another. In addition, provide reasoning as to why the integration of two methods may sometimes lead to improved clustering quality and efficiency.

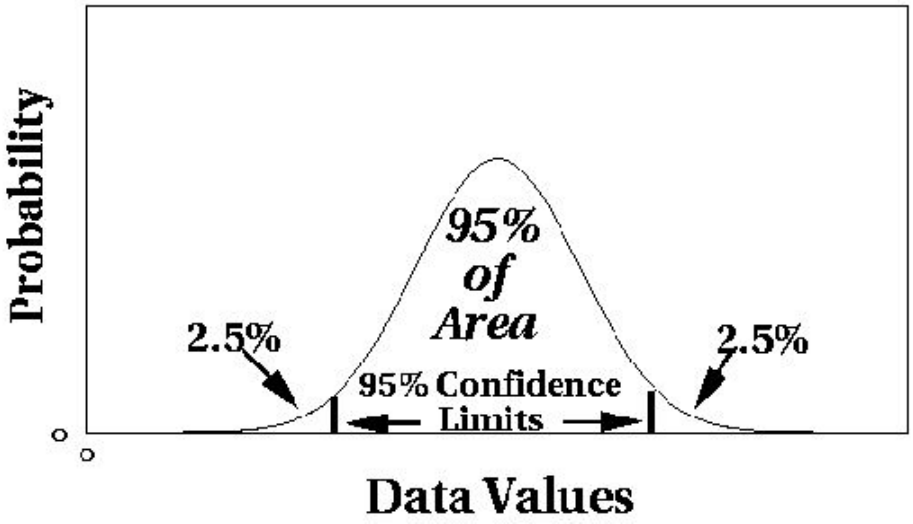
**Answer:**

- Consider building an ontology of queries for information retrieval and web search. A query is associated with a vector of web pages that are clicked when the query is asked. An effective approach is to first conduct density-based clustering to form small clusters as micro-clusters.
- Each micro-cluster is treated as a base unit, sometimes called a concept. Then, a hierarchical clustering method can be applied to build an ontology.
- To use density-based clustering as a pre-processing step can quickly merge synonyms, such as “University of Illinois at Urbana-Champaign” and “UIUC”, into one concept. This preprocessing step can reduce the data so that the ontology built later is more meaningful, and the

# What Is Outlier Discovery?

- What are outliers?
  - The set of objects are considerably dissimilar from the remainder of the data
  - Example:  Sports: Michael Jordon, Wayne Gretzky, ...
- Problem: Define and find outliers in large data sets
- Applications:
  - Credit card fraud detection
  - Telecom fraud detection
  - Customer segmentation
  - Medical analysis

# Outlier Discovery: Statistical Approaches



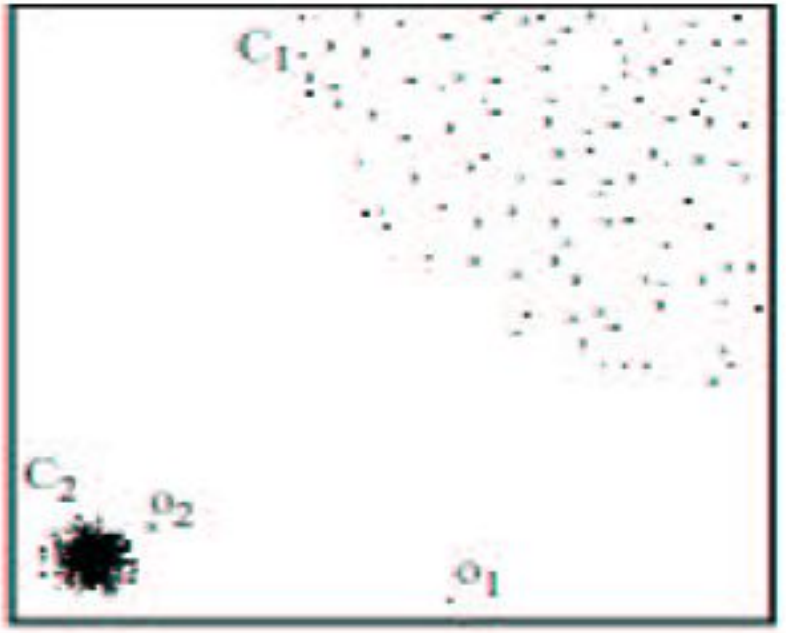

- Assume a model underlying distribution that generates data set (e.g. normal distribution)
- Use discordancy tests depending on
  - data distribution
  - distribution parameter (e.g., mean, variance)
  - number of expected outliers
- Drawbacks
  - most tests are for single attribute
  - In many cases, data distribution may not be known

# Outlier Discovery: Distance-Based Approach

- Introduced to counter the main limitations imposed by statistical methods
  - We need multi-dimensional analysis without knowing data distribution
- Distance-based outlier: A DB(p, D)-outlier is an object O in a dataset T such that at least a fraction p of the objects in T lies at a distance greater than D from O
- Algorithms for mining distance-based outliers
  - Index-based algorithm
  - Nested-loop algorithm
  - Cell-based algorithm

# Density-Based Local Outlier Detection

- Distance-based outlier detection is based on global distance distribution
- It encounters difficulties to identify outliers if data is not uniformly distributed
- Ex. $C_1$ contains 400 loosely distributed points, $C_2$ has 100 tightly condensed points, 2 outlier points $o_1$, $o_2$
- Distance-based method cannot identify $o_2$ as an outlier
- Need the concept of local outlier




- Local outlier factor (LOF)
  - Assume outlier is not crisp
  - Each point has a LOF

# Outlier Discovery: Deviation-Based Approach

- Identifies outliers by examining the main characteristics of objects in a group
- Objects that "deviate" from this description are considered outliers
- Sequential exception technique
  - simulates the way in which humans can distinguish unusual objects from among a series of supposedly like objects
- OLAP data cube technique
  - uses data cubes to identify regions of anomalies in large multidimensional data

# Problems and Challenges

- Considerable progress has been made in scalable clustering methods
  - Partitioning: k-means, k-medoids
  - Hierarchical: AGNES, DIANA, BIRCH,
  - Density-based: DBSCAN,
- Current clustering techniques do not address all the requirements adequately, still an active area of research