Clustering

Data Science with Python
CS677

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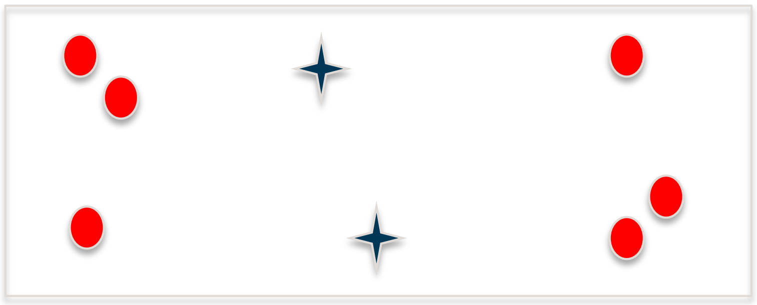
K-means Initialization

Problem: K-means is sensitive to initial points, and initial points can result to a sub-optimum solution.

Example:



K-Mean Initialization Solutions

- Random selection of initial points. In this case run the algorithm multiple times and select the best answer

- Question – What is the best solution?

It is the model with the lowest Mean Squared distance between data points and their centroids.

This is called *“intertia”*

- A kmeans object has ”inertia_”

  *Kmeans_object.inertia_*

Initialization Solution – K-means++

- K-means++ is a suggestion to smart initialization of K-means.

The idea is as follows

If a center point is C_i and distance between a point and its centroid is $D(x_i, C_i)$

1. Choose the first random point
2. Choose point x_i as the next centroid with probability
$$D(x_i, C_i) \Big/ \textstyle\sum_{j=1}^{M} D(x_j, C_j)$$
3. Go to step 2 until K centroids have been selected

K-means++

- Adds extra computation
- But it reduces number of iterations dramatically
- Most of the time find optimum or very close to optimum solution

Note that K-means function in python uses this method by default.

Note "init" parameter in kmeans object instantiation chooses initialization method.

How to Set K?

- Looking at the "Inertia" for a range of K values and decide the elbow point
- Silhouette score,
  - Silhouette coefficient is $^{(b-a)}/_{\max(b,a)}$
    - *a* is the mean distance to the other instances in the same cluster
    - b is the mean distance to the nearest cluster instances
  - The mean silhouette coefficient over all the instances.
- Silhouette score varies between -1 and 1
  - +1 means good separation between clusters
  - 0 means cluster boundaries are fuzzy
  - -1 means clusters are merged to the same space

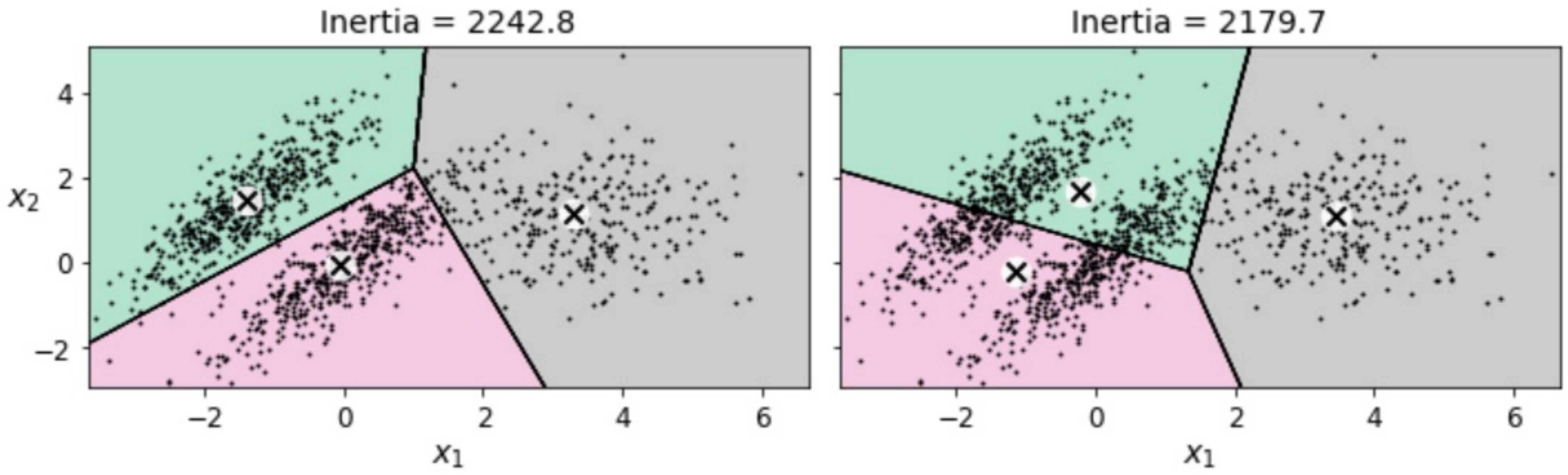
- Scikit learn function

  Silhouette_score(data, kmeans_obj.labels_)

K-means

- Fast
- Scalable
- But
  - Sometimes provide sub-optimum solutions
  - Need K!
  - K-means doesn’t work well with clusters with different size and density
  - K-means doesn’t behave well in non-spherical shapes
  - Scaling of variables of observations is suggested
  - Distance function is important

K-means example



Reference: Hands-on Machine learning with Sci_kit learn Keras & Tensorflow by A. Geron

OPTICS

Optics: Ordering Points to Identify Clustering Structure

- Proposed by the same inventors of DBSCAN in 1999
- DBSCAN:
  - Sensitive to parameter selection (eps, minPoints)
  - One global eps doesn't work
- It is based on the following observation:

  high density clusters are contained by low density clusters
- Idea is processing higher density clusters first

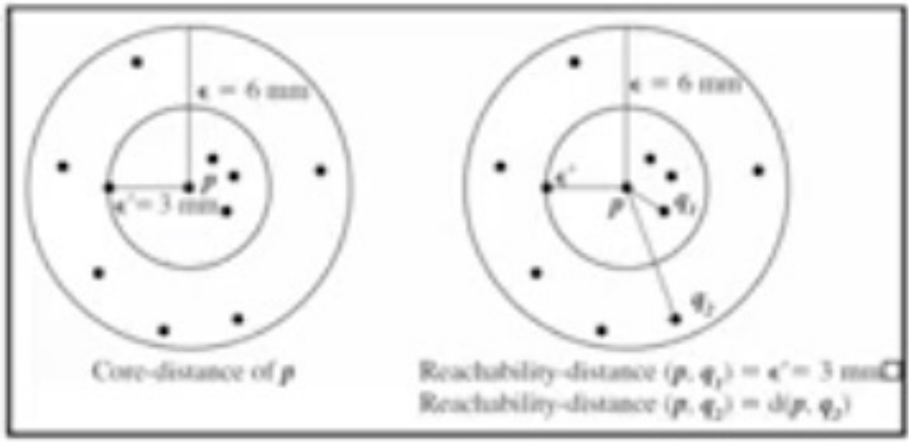
OPTICS

- Optics introduces two parameter
  - Core distance: is the smallest eps distance from a core point *p* to cover at least minPoints

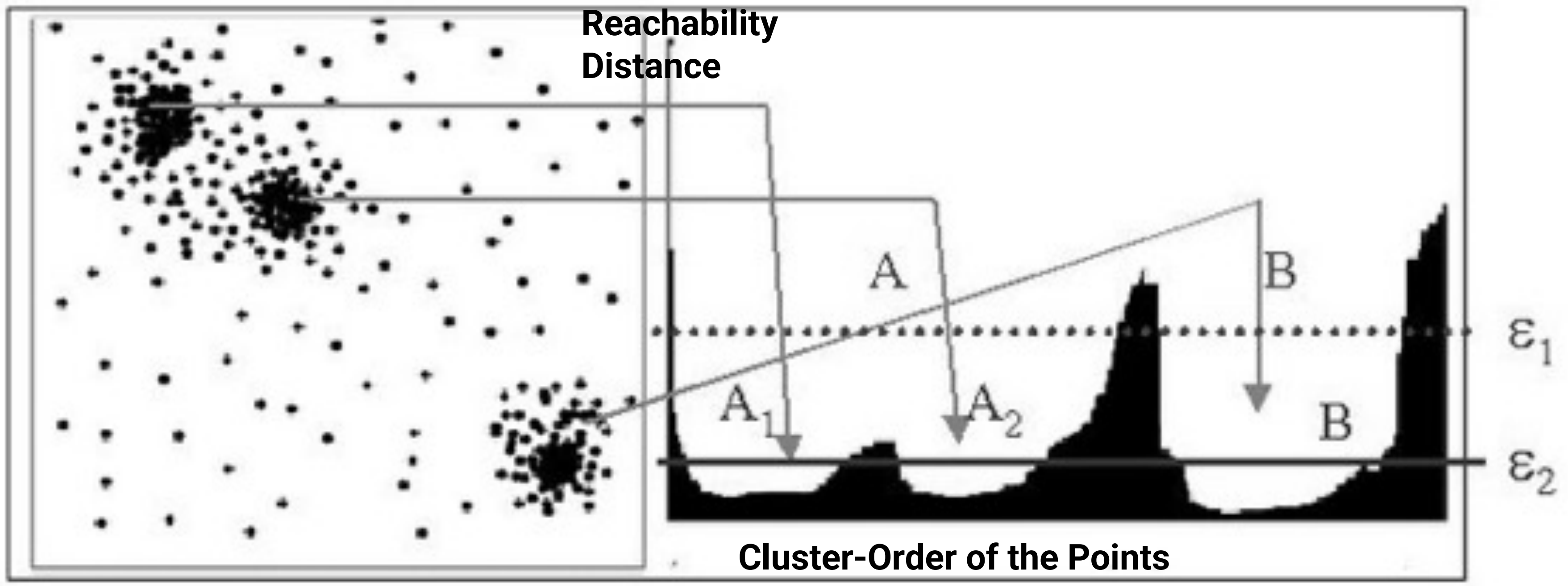
$$core\ dis(p) = \begin{cases} Min(eps)\ cover\ minPoints \\ Not\ defined\ if\ p\ isn't\ core \end{cases}$$

  - Reachability distance:

$$Max[core\ dis(q), dis(p,q)]$$


ε = 6 mm
p
ε′ = 3 mm
Core-distance of p
ε = 6 mm
ε′
p
q1
q2
Reachability-distance (p, q1) = ε′ = 3 mm
Reachability-distance (p, q2) = d(p, q2)

Ref: Prof Han course in University of Illinois Urbana Champaign



Ref: Effective Similarity Search on Voxelized CAD Object.by: P. Kroger, and Et. Al.

- The smaller reachability, the denser the cluster

OPTICS Algorithm

1. Set eps (which can be set to a high number)
2. Start with a random point, *p (*Set reachability of *p* to undefined).
3. Choose all neighbors within eps distance of *p.* If *p* is not a core object select next random point
4. If *p* is a core point, order points in ascending reachability order
5. Go to step 3 until all the data points are covered

- Initial eps and MinPoints identifies core points
- Core distance helps to choose high density points
- Ascending order helps to have a flat valley
- Reachability distance helps to have different eps

OPTICS

- Allows a range of eps to get explored
- Orders points to identify clusters
- Trying to produce an order of points based on density
  - In way - It is a hierarchical clustering
- It can be used for interactive and automatic analysis of clusters
- It can use clusters with different size, shapes, and density
- Can be used to detect outliers
- It does have a good visualization by-product
- Complexity O(N *log*N)

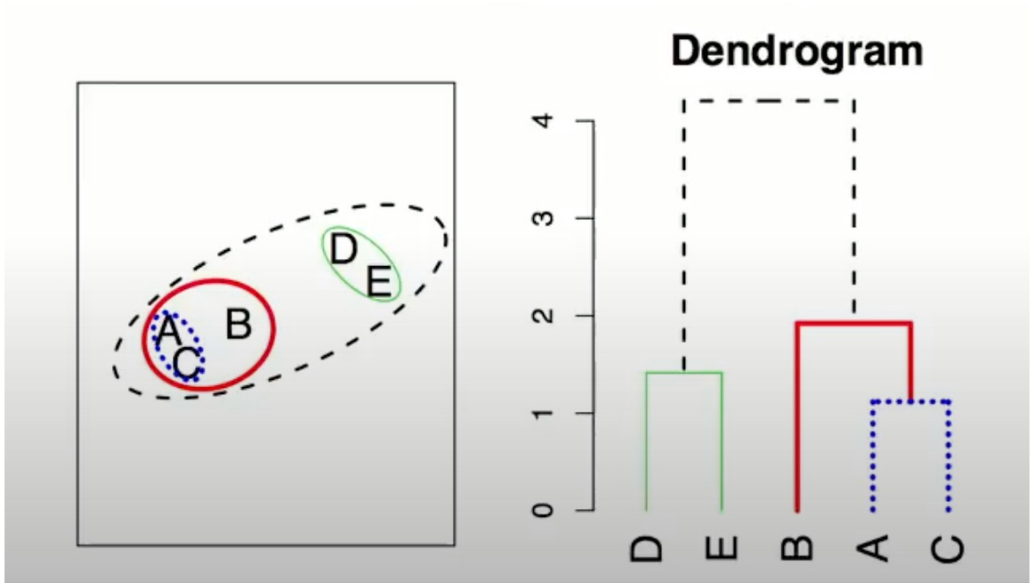
Hierarchical Clustering

Agglomerative and BIRCH

Hierarchical Clustering

- Attractive approach since no need to decide on K in advance.
- Bottom-up or agglomerative Hierarchical clustering

Example



Reference: Tibshirani and Hastie – Intro to statistical learning

BIRCH – Balanced Iterative Reducing and Clustering Using Hierarchies

BIRCH Main Purpose

- Create a tree in the memory, when the entire data set is big and cannot fit in memory
- The tree contains all the information that we need. Therefore, we don't need to go back to data again and again
- It is an incremental construct of the tree
- It scales linearly

BIRCH

- Incremental construct of CF (clustering features) tree, holding information for the rough hierarchical clustering & fine clustering later

  phase 1: Scan the data one by one and build CF tree in-memory. Rough clustering.

  Phase 2: Use any clustering algorithm to cluster the leaf nodes of the tree, merge clusters or remove outliers

Let us start with BIRCH Cluster Features(CF)

- Clustering features – a summary of data to build the CF-tree, and also the final clustering
  1. N: number of points
  2. LS: Linear sum of N points: $\sum_{i=1}^{N} x_i$
  3. SS: Sum of square of N points: $\sum_{i=1}^{N} \overrightarrow{x_i}^{\,2}$

Note: CFs are 0^{th}, 1^{st}, and 2nd moments of a cluster

BIRCH – Measures of a Cluster

- Centroid: middle of a cluster

$$C_k = \frac{\sum_{i=1}^{N} x_i}{N}$$

- Radius: average distance of members to centroid

$$\sqrt{\frac{\sum_{i=1}^{N}(x_i - C_k)^2}{N}}$$

- Diameter: Average pairwise distance

$$\sqrt{\frac{\sum_{i=1}^{N}\sum_{j=1}^{N}(x_i - x_j)^2}{N(N-1)}}$$

Clustering Computations Based on CF

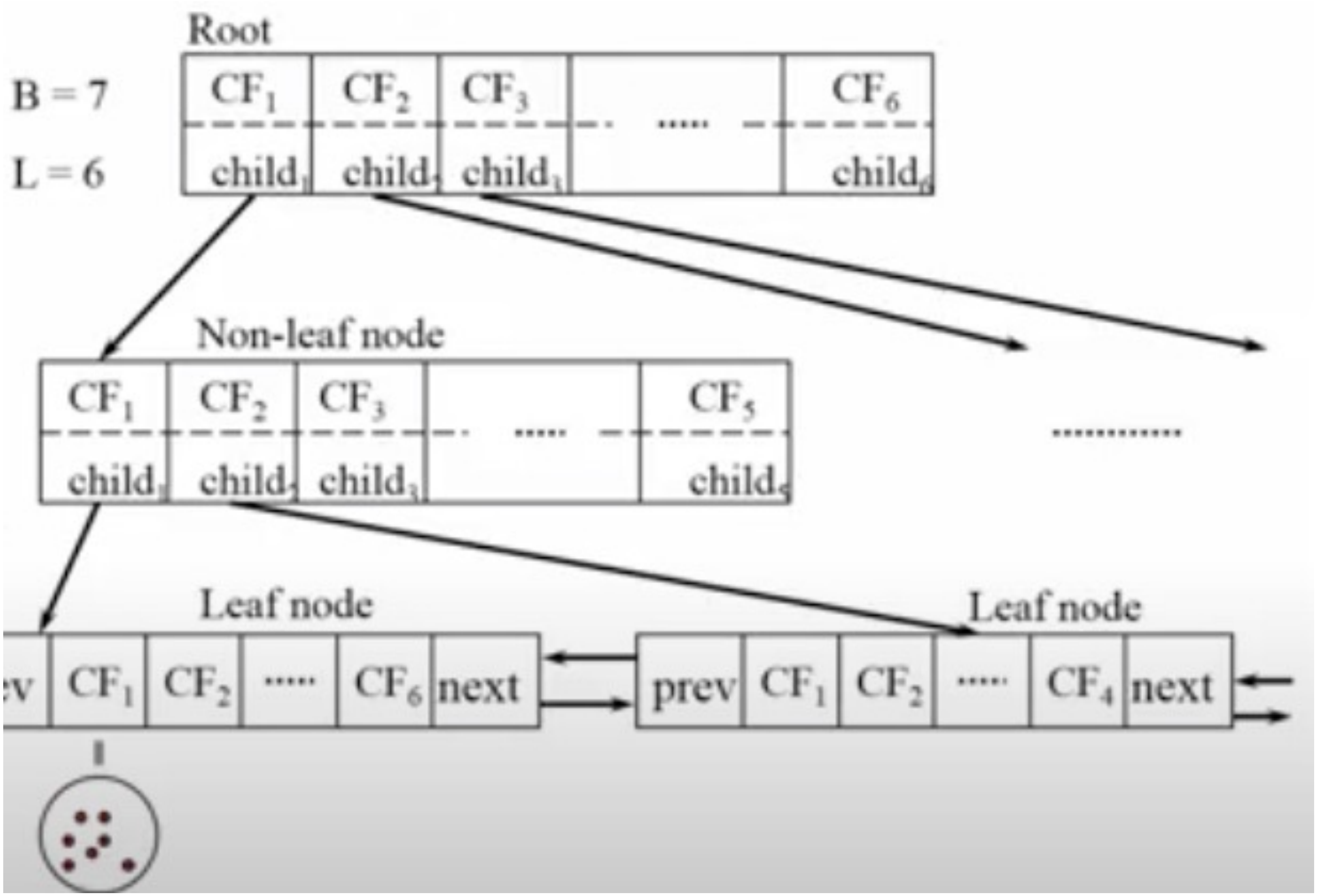
- Centroid: C = LS/N
- Radius R =

$$\sqrt{\frac{\sum_{i=1}^{N}(x_i - C_k)^2}{N}} = \sqrt{\frac{N.C^2 + SS - 2C.LS}{N}} = \sqrt{\frac{SS}{N} + \left(\frac{LS}{N}\right)^2}$$

- Diameter D = $\sqrt{\frac{\sum_{i=1}^{N}\sum_{j=1}^{N}(x_i - x_j)^2}{N(N-1)}} = \sqrt{\frac{2N.SS - 2LS^2}{N(N-1)}}$

- CF merge = CF1 + CF2 = (N1+N2, LS1 + LS2, SS1+SS2)

Note: LS is a vector and SS is a scalar



Ref: Prof Han course in University of Illinois Urbana Champaign

BIRCH Hyperparameters

How To build a CF tree

Note: CFs are 0th, 1st, and 2nd moments of a cluster

- BRICH Important parameters
  - T: Maximum diameter of a leaf node
  - B: max number of branches
  - L: Max length of leaf node
- CF (non leaf node) = sum of CF of nodes below

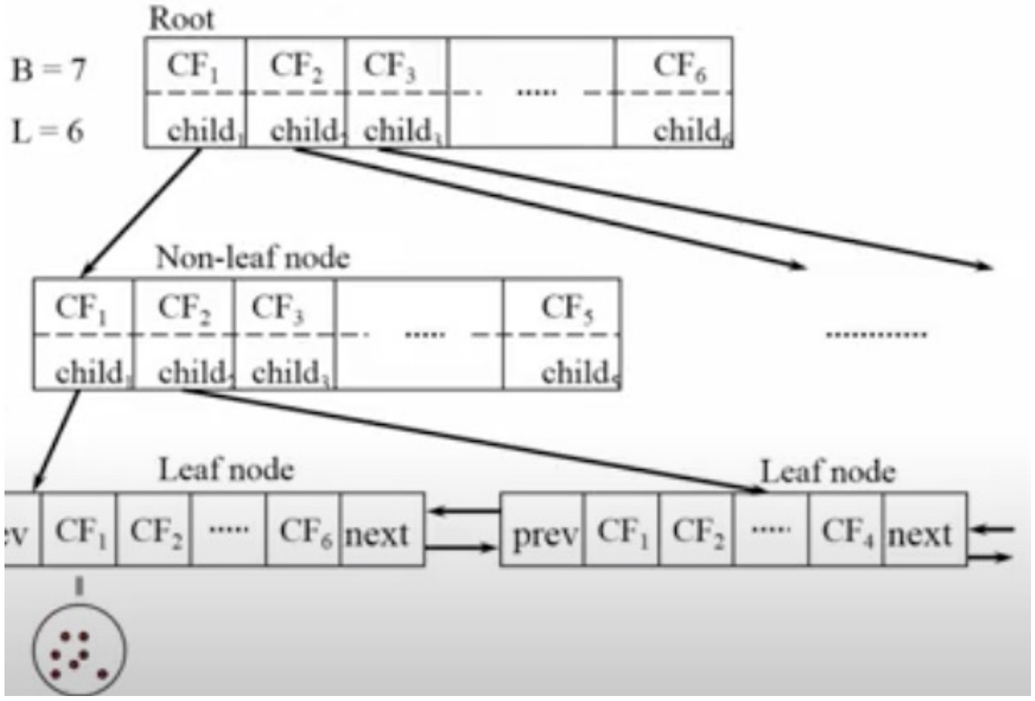
How to Build a Cluster

Assume T=L=2, and B=3. Let us use Manhattan dis.

Data points

(3,4), (2,6), (4,5), (4,7), (8,4)

1. (3,4) -> CF1(1,(3,4),25)
2. (2,6)-> (D>T)=> CF2(1,(2,6),40)
3. (4,5)->(D<T)=>merge with into CF1 => CF1(2,(7,9),66)
4. (4,7)->(D>T)->CF3(1,(4,7),55)
5. (8,4)->(D>T) & (B>3)=> two non-leaf nodes. One CF2&CF3 and one CF1&CF4(1,(8,4),80)


Root
B = 7
L = 6
CF1 CF2 CF3 ..... CF6
child1 child2 child3 child6
Non-leaf node
CF1 CF2 CF3 ..... CF5
child1 child2 child3 child5
Leaf node
prev CF1 CF2 ..... CF6 next
Leaf node
prev CF1 CF2 ..... CF4 next

BIRCH

- Add new points to the tree incrementally, by adding the point to the closest leaf
- Update CF values
- Check two criterias
  1. If (New Diameter > max_diameter) split the leaf and possibly parents
  2. If (# of leafs > max_children) split the parent

BIRCH Concerns

Pros:

- Efficient for clustering large data which doesn’t fit in memory
- Different clustering algorithms can be used on the “tight” clusters on the leaf nodes
- Outlier removal which can be any algorithm or use leaf size as a criteria
- It grows linearly

Cons:

- Need numerical data
- Sensitive to insertion order of data points
  - Duplicates might end up in different clusters
  - Solution:
    - Randomized reading
    - Reading the data again with knowing centroids and make assignments based on distance to centroids
- Ceiling on number of leaf nodes is an artificial restriction
- Clusters are expected to be spherical because of D criteria

Probabilistic Hierarchical Clustering

Probabilistic Hierarchical Clustering

- Non-probabilistic hierarchical clustering /algorithmic clustering
  - Good distance measure is critical and hard to choose
  - Cannot handle missing attributes
  - Optimization goal is heuristic
  - Relies on local search
- Probabilistic approach
  - Generative model
  - Easy to generalize

Note: any model can be used as a base of the generative models

Gaussian Generative Model

- Probability of a point Xi generated by a Gaussian distribution $N(\mu, \sigma)$

$$P(x_i|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Then for probability of a set of X is generated by the Gaussian model is product of probabilities

Goal: Finding Gaussian distributions, which maximizes probability

Probabilistic Clustering Algorithm

Goal: Finding Gaussian distributions, which the best explains the existing data set

- Criteria is maximizing aggregate probabilities that the data set is generate by a Gaussian distribution

$$Max\ [P(X|\mu,\sigma)]$$

- And

$$P(X|\mu,\sigma) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- Therefore, merge/split clusters if it results to increase the probability of getting generated by a Gaussian model.

CLIQUE – Clustering in QUEst

What problem is getting addressed?

- Curse of Dimensionality: Clustering in a high dimension is hard, since the data becomes sparse
  - Example: One dimension expansion to two dimension

CLIQUE

- It is a bottom up approach
- It is an algorithm which combines grid based and density based ideas
- It identifies sparse and dense areas in space
- Based on the idea that data is not uniformly distributed in a high-dimensional space
- Data in a high-dimensional space is sparse

Grid Based Clustering

- Divide the data space into finite number of cells
- Find dense cells in the grid structure

Features

- It is efficient and scalable
- Limited by cell size and borders, and the density threshold

Basic Definitions

- Partition:
  - non-overlapping units, which divides a K dimensional space
- Unit:
  - A unit rectangle in the K-dimension space
- Dense unit:
  - A unit with points more than a threshold
- Minimal Cluster
  - The largest area with dense samples – or the largest continues dense area

Idea Behind CLIQUE

- Based on Apriori Principle
  - If an area is dense in K-dimensional space, it is also dense on K-1 dimensional space
  - If an area is not dense in K-1 dimensional space, it is also not dense in K dimensional space.
    - If an area is dense on K-1 dimension space, it might not be dense in K dimension space
- Identify sparse and dense areas on the multi-dimensional space
- By looking at the lower dimensional space, identify candidate dense areas/units
- This result to much smaller search space

Example (Ref: Original Paper)

- Clusters may exist only in some subspaces.
- Subspace-clustering: find clusters in all the subspaces.

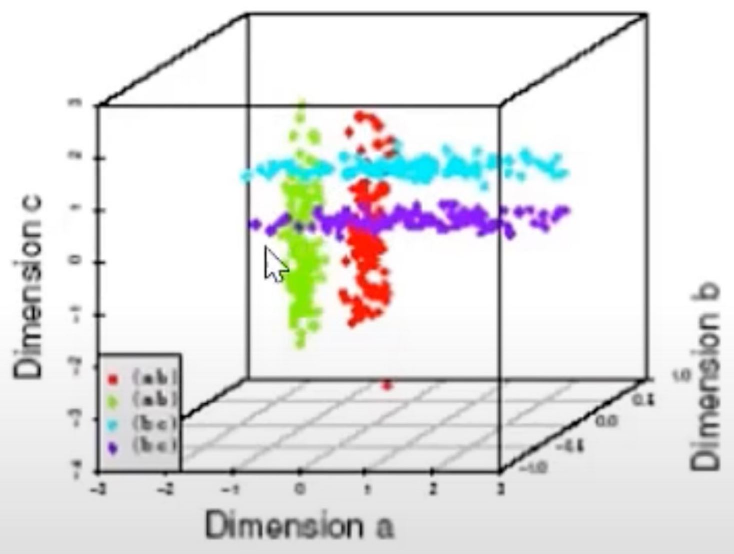
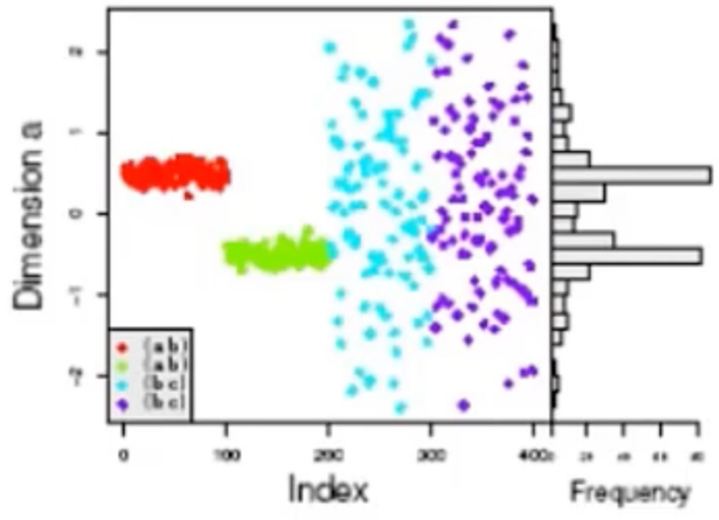
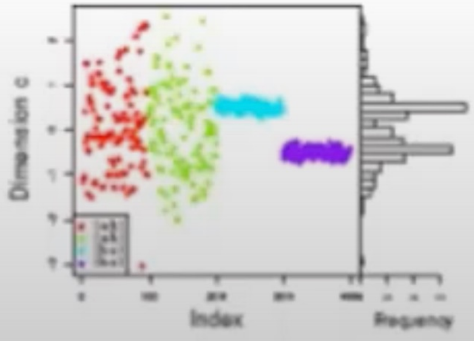


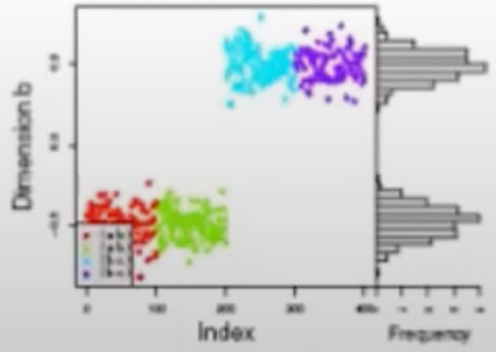
Figure 2: Sample dataset with four clusters, each in two dimensions with the third dimension being noise. Points from two clusters can be very close together, confusing many traditional clustering algorithms.



(a) Dimension *a*



(c) Dimension *c*



(b) Dimension *b*

CLIQUE Algorithm – High Level

- Partition – partition each dimension to girds/intervals
- Identify dense units of increasing dimension using Apriori principle
- Generate a cluster, which is a maximal set of connected dense units

CLIQUE - Algorithm

- Create a grid in all the dimensions
- (K = 1) Find all the dense areas in the one-dimensional spaces for all the attributes. This is a set of dense one-dim cells.
- Consider a dimension with largest dense units

1. (K=K+1) Add the next high density dimension
2. Find all candidate dense units in the K-dimension from the K-1 dimension candidate units
3. Eliminate units with low density from the candidate set
4. If there is no dimension left, go to 5. Otherwise go to 1.
5. Merge adjacent dense units
6. Identify clusters of high density areas

CLIQUE

<u>Pros</u>

- Performs well in a high-dimension
- Scales linearly with the size
- Doesn’t need to know number of clusters
- Can cluster any shape
- Automatically finds high density clusters in a subspaces, since clusters can exist in lower dimensions!

<u>Cons</u>

- Grid size
- Density threshold
- Can merge overlapping clusters, if density threshold not set correctly.