Course. Introduction to Machine Learning

Work 1. Clustering Exercise

Session 2

Course 2023-2024

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Contents

1. Introduction (session 1)
2. Preprocess the data (session 1)
3. DBSCAN with sklearn (session 2)
4. BIRCH with sklearn (session 2)
5. K-Means + K-Modes (your own code) (session 2)
6. K-Medoids or K-Prototypes (your own code) (session 2)
7. Fuzzy clustering (your own code) (session 3)
8. Validation techniques (using sklearn validation metrics) (session 3)

Taxonomy of Clustering Algorithms

- *Clustering Techniques*
  - *Partitioning methods*
    - ***k-Means algorithm*** *[1957, 1967]*
    - ***k-Medoids algorithm***
      - *PAM [1990]*
      - *CLARA [1990]*
      - *CLARANS [1994]*
    - ***k-Modes*** *[1998]*
    - *Fuzzy c-means algorithm [1999]*
  - *Hierarchical methods*
    - *Divisive*
      - *DIANA [1990]*
    - *Agglomerative methods*
      - *AGNES [1990]*
      - ***BIRCH [1996]***
      - *CURE [1998]*
      - *ROCK [1999]*
      - *Chamelon [1999]*
  - *Density-based methods*
    - *STING [1997]*
    - ***DBSCAN [1996]***
    - *CLIQUE [1998]*
    - *DENCLUE [1998]*
    - *OPTICS [1999]*
    - *Wave Cluster [1998]*
  - *Graph based methods*
    - *MST Clustering [1999]*
    - *OPOSSUM [2000]*
    - *SNN Similarity Clustering [2001, 2003]*
  - *Model based clustering*
    - *EM Algorithm [1977]*
    - *Auto class [1996]*
    - *COBWEB [1987]*
    - *ANN Clustering [1982, 1989]*

DBSCAN
Density-Based Clustering

Using sklearn

Some Links

- http://www2.cs.uh.edu/~ceick/7363/Papers/dbscan.pdf
- https://youtu.be/sKRUfsc8zp4
- https://youtu.be/6jl9KkmgDIw
- https://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html#sklearn.cluster.DBSCAN

Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as **density-connected points** or based on an explicitly constructed density function
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  - DENCLUE: Hinneburg & D. Keim (KDD'98/2006)
  - OPTICS: Ankerst, et al (SIGMOD'99).
  - CLIQUE: Agrawal, et al. (SIGMOD'98)

DBSCAN: Density-Based Clustering

- DBSCAN is a Density-Based Clustering algorithm
- Reminder: In density based clustering we partition points into dense regions separated by not-so-dense regions.
- Important Questions:
  - How do we measure density?
  - What is a dense region?
- DBSCAN:
  - Density at point p: number of points within a circle of radius Eps
  - Dense Region: A circle of radius Eps that contains at least MinPts points

DBSCAN: Preliminary concepts

Characterization of points

- Density = number of points within a specified radius (Eps)
- A point is a **core point** if it has more than a specified number of points (*MinPts*) within Eps
  - These points belong in a dense region and are at the interior of a cluster
- A **border point** has fewer than *MinPts* within Eps, but is in the neighborhood of a core point
- A **noise point** is any point that is not a core point or a border point

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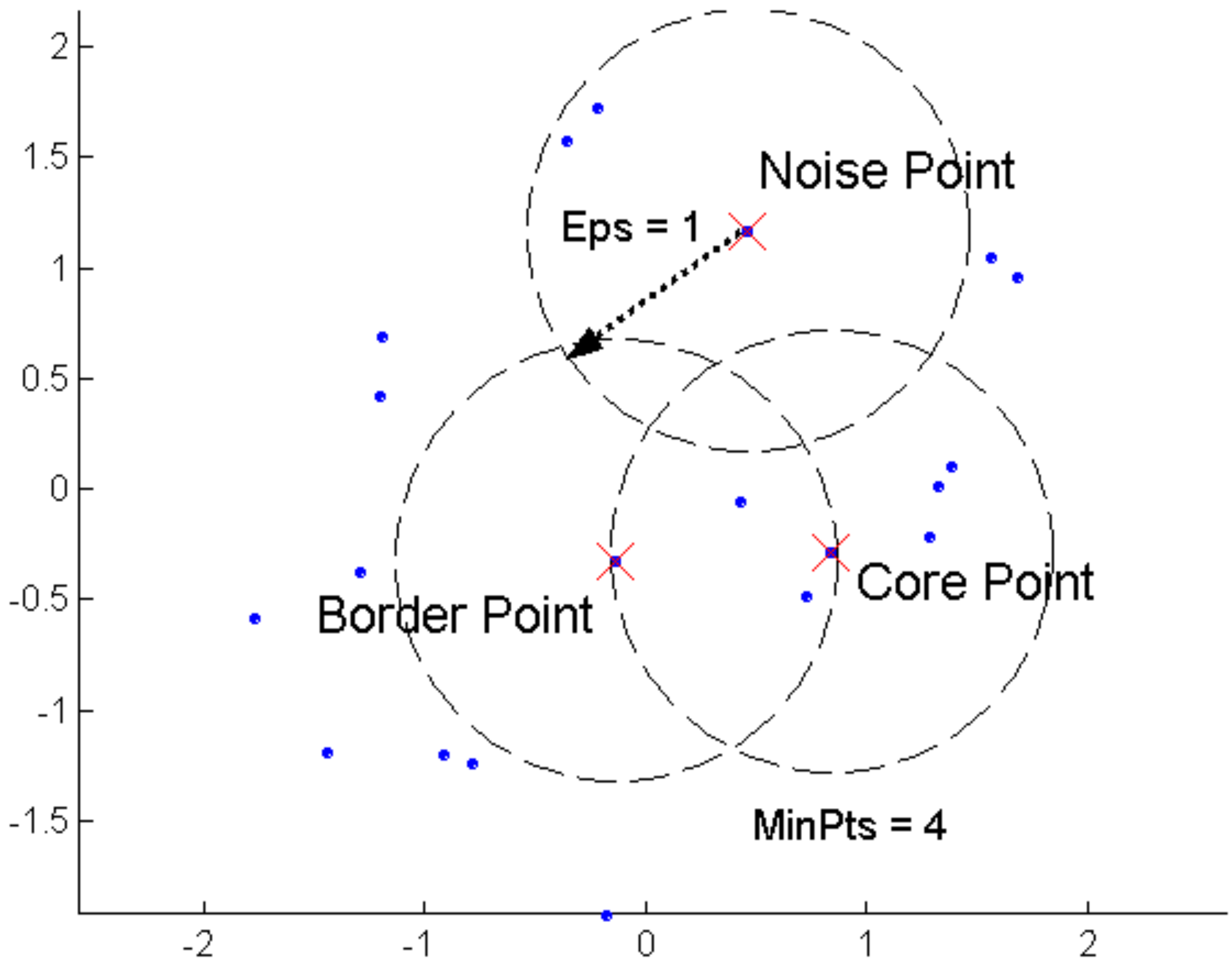
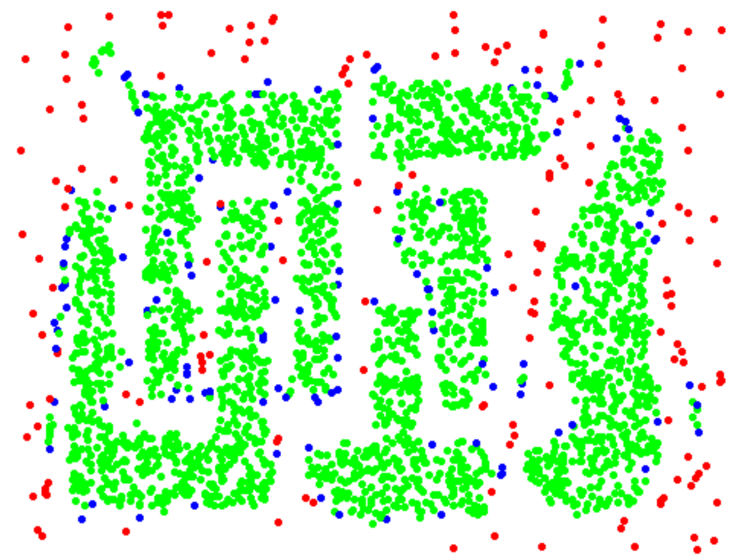
DBSCAN: Core, Border, and Noise Points



DBSCAN: Core, Border and Noise Points

Original Points



Point types: core, border and noise

Eps = 10, MinPts = 4

Parameter Estimation

- Parameters must be specified by the user
  - Ɛ = physical distance (radius),
  - *minPts* = desired minimum cluster size

minPts

- derived from the number of dimensions *D* in the data set, as *minPts* ≥ *D* + *1*
- *minPts* = *1* does not make sense, as then every point on its own will already be a cluster
- *minPts* must be chosen at least 3. Larger is better.
- larger the dataset, the larger the value of *minPts* should be chosen

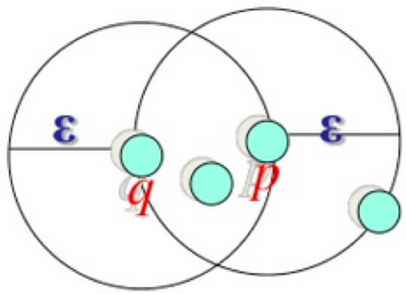
Ɛ

- value can be chosen by using a k-distance graph
- If Ɛ is chosen much too small, a large part of the data will not be clustered
- If too high value, majority of objects will be in the same cluster
- In general, small values of Ɛ are preferable

Concepts: Ɛ-Neighborhood

- Ɛ-Neighborhood: Objects within a radius of Ɛ from an object (epsilon-neighborhood)

- Core objects: Ɛ-Neighborhood of an object contains at least *MinPts* of objects



ε-Neighborhood of *p*
ε-Neighborhood of *q*
p is a core object (MinPts = 4)
q is not a core object

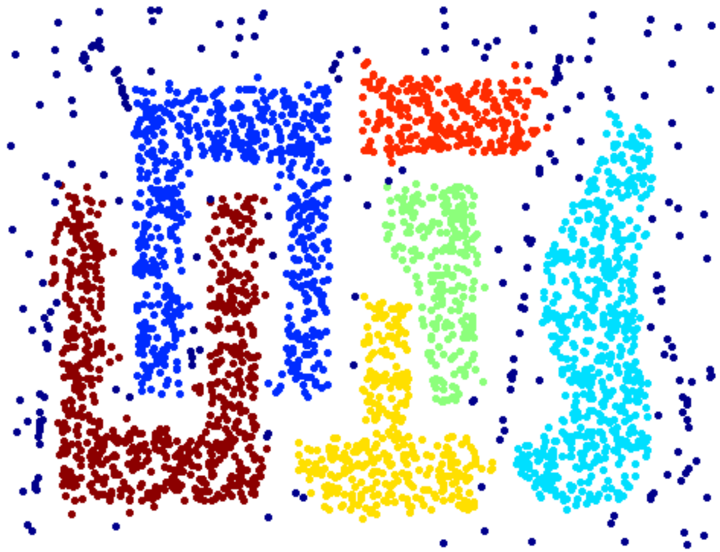
DBSCAN Algorithm (simplified view for teaching)

1. Create a graph whose nodes are the points to be clustered
2. For each core-point c create an edge from c to every point p in the **ε-neighborhood** of c
3. Set N to the nodes of the graph;
4. If N does not contain any core points terminate
5. Pick a core point c in N
6. Let X be the set of nodes that can be reached from c by going forward;
    1. create a cluster containing $X \cup \{c\}$
    2. $N = N / (X \cup \{c\})$
7. Continue with step 4

Remark: points that are not assigned to any cluster are outliers;

When DBSCAN Works Well

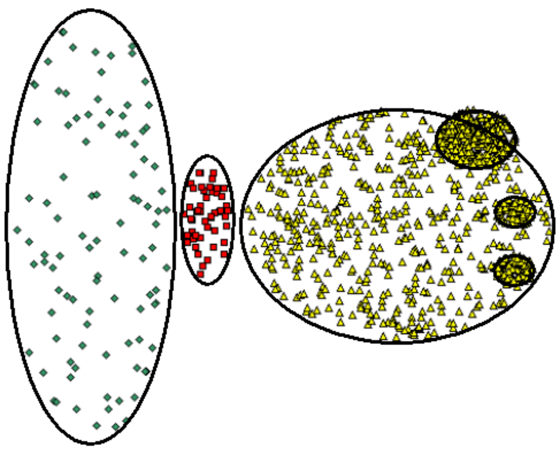
Original Points



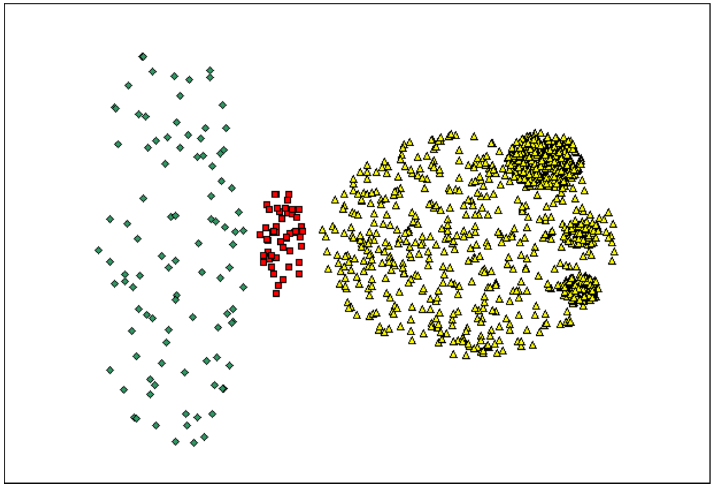
Clusters

- Resistant to Noise
- Can handle clusters of different shapes and sizes

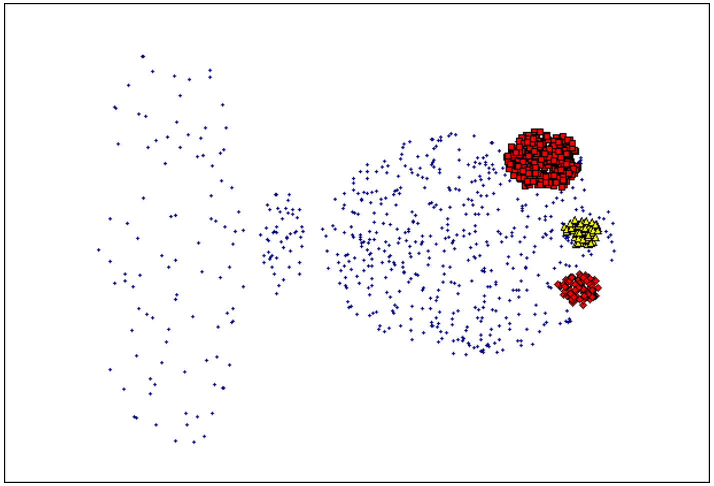
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

- Varying densities
- High-dimensional data

Complexity DBSCAN

- Time Complexity: `O(n²)`
  - For each point it has to be determined if it is a core point
  - Can be reduced to `O(n*log(n))` in lower dimensional spaces by using efficient data structures (where n is the number of objects to be clustered);

- Space Complexity: `O(n)`

Birch

Balanced Iterative Reducing and Clustering Using Hierarchies

Using sklearn

Some Links

- https://youtu.be/xw3RwYs7fUM
- https://scikit-learn.org/stable/modules/generated/sklearn.cluster.Birch.html

Extensions to Hierarchical Clustering

- Major weakness of agglomerative clustering methods
  - Can never undo what was done previously
  - Do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects
- Integration of hierarchical & distance-based clustering
  - BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

BIRCH

- Zhang, Ramakrishnan & Livny, SIGMOD'96
- Incrementally construct a CF (Clustering Feature) tree, a hierarchical data structure for multiphase clustering
  - **Phase 1**: scan DB to build an initial in-memory CF tree (a multi-level compression of the data that tries to preserve the inherent clustering structure of the data)
  - **Phase 2**: use an arbitrary clustering algorithm to cluster the leaf nodes of the CF-tree
- *Scales linearly*: finds a good clustering with a single scan and improves the quality with a few additional scans
- *Weakness:* handles only numeric data, and sensitive to the order of the data record

Clustering Feature Vector in BIRCH

Clustering Feature (CF): CF = (N, LS, SS)

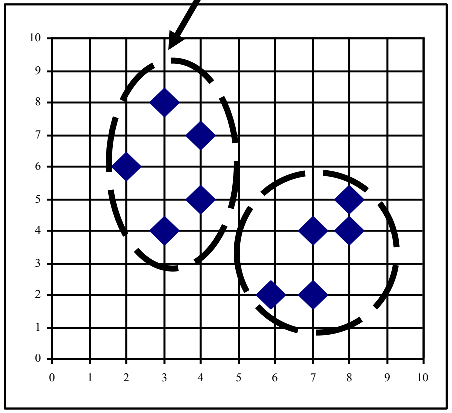
***N**: Number of data points*

***LS**: linear sum of N points:* $\sum_{i=1}^{N} X_i$

***SS**: square sum of N points*

$$\sum_{i=1}^{N} X_i^{\,2}$$

CF = (5, (16,30),(54,190))

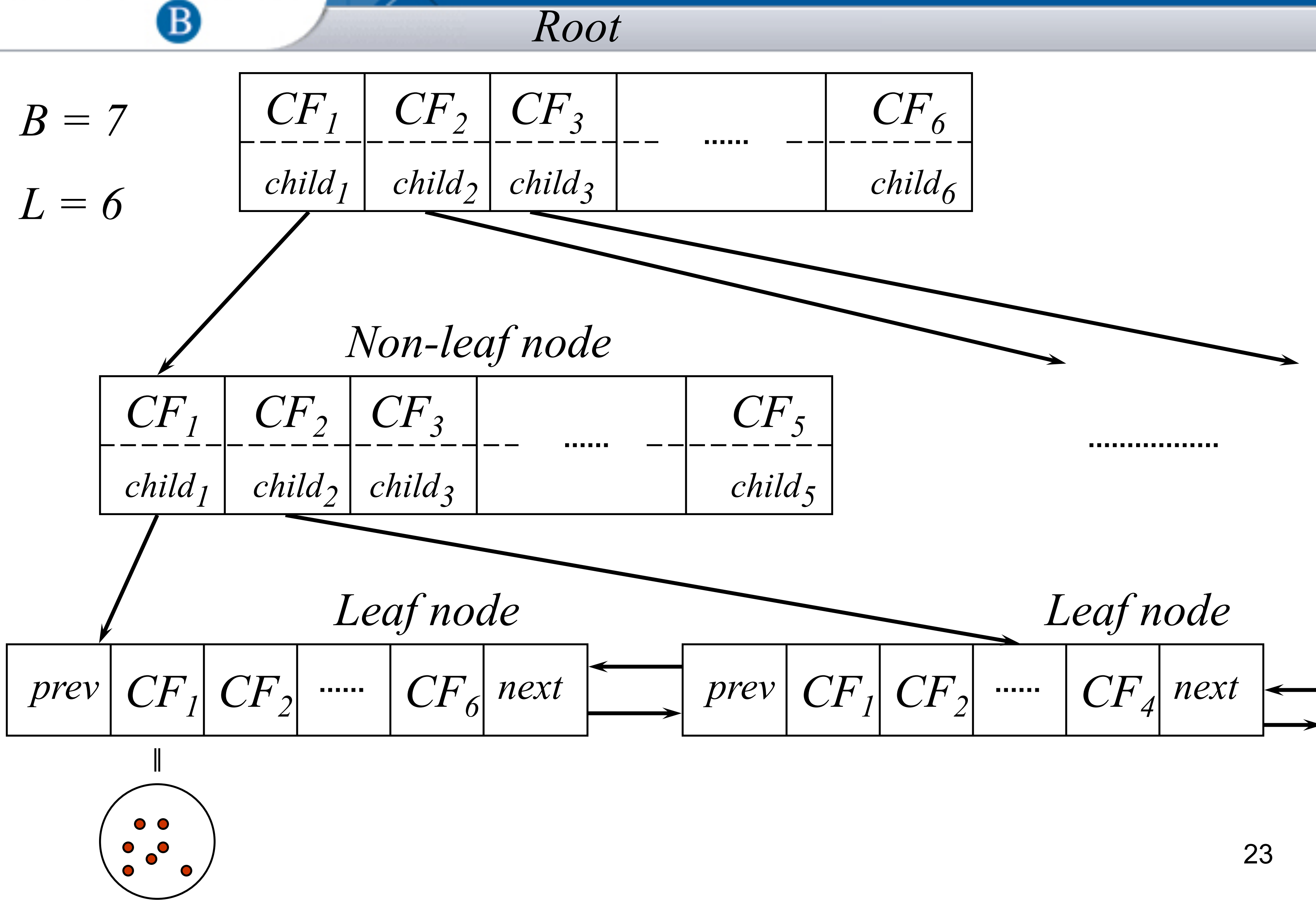


(3,4)
(2,6)
(4,5)
(4,7)
(3,8)

CF-Tree in BIRCH

- Clustering feature:
  - Summary of the statistics for a given subcluster: the 0-th, 1st, and 2nd moments of the subcluster from the statistical point of view
  - Registers crucial measurements for computing cluster and utilizes storage efficiently
- A CF tree is a **height-balanced** tree that stores the clustering features for a hierarchical clustering
  - A nonleaf node in a tree has descendants or "children"
  - The nonleaf nodes store sums of the CFs of their children
- A CF tree has two **parameters**
  - **Branching factor**: max # of children
  - **Threshold**: max diameter of sub-clusters stored at the leaf nodes

The CF Tree Structure



The Birch Algorithm

- Cluster Diameter $$\sqrt{\frac{1}{n(n-1)}\sum(x_i - x_j)^2}$$
- 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
- Algorithm is O(n)
- **Concerns**
  - Sensitive to insertion order of data points
  - Since we fix the size of leaf nodes, so clusters may not be so natural
  - Clusters tend to be spherical given the radius and diameter measures

K-Means

Implement your own code

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K-Means basis

- It is a partitional algorithm that …
  - Assumes instances are **real-valued vectors**
  - Clusters based on ***centroids, center of gravity***, or **mean of points** in a cluster, ***c***:

$$\vec{\mu}(\mathrm{c}) = \frac{1}{|c|} \sum_{\vec{x} \in c} \vec{x}$$

  - Reassignment of instances to clusters is **based on distance** to the current cluster centroids
    - Manhattan distance (L_1 norm), Euclidean distance (L_2 norm), Cosine similarity

K-Means basis

Algorithm	Basic K-means algorithm.

1: Select K points as initial centroids.
2: **repeat**
3:     Form K clusters by assigning each point to its closest centroid.
4:     Recompute the centroid of each cluster.
5: **until** Centroids do not change.

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Discussion on the K-Means method

- K-Means clustering often **terminates at a local optimal**
  - Initialization can be important to find high-quality clusters
- **Need to specify K**, the number of clusters, in advance
  - There are ways to automatically determine the "*best*" K
  - In practice, one often runs a range of values and selected the "*best*" K value
- **Sensitive to noisy data and outliers**
  - Variations: Using K-medians, K-medoids, etc.
- K-Means is applicable only to objects in a **continuous n-dimensional space**
  - Using the K-Modes for **categorical data**
- Non suitable to discover clusters with **non-convex shapes**
  - Using density-based clustering, kernel k-means, etc.

Variations of K-Means

- There are many variants of the K-Means methods, varying different aspects
  - Choosing better initial centroid estimates
    - K-Means++, Intelligent K-Means, Genetic K-Means
  - Choosing different representatives for the clusters
    - K-Medoids, K-Medians, K-Modes
  - Applying feature transformation techniques *(explained at the supervised part of the course)*
    - Weighted K-Means, Kernel K-Means

Initialization of K-Means

- Different initializations may generate rather different clustering results
- Original proposal (MacQueen,1967): selects the k seed randomly
  - Need to run the algorithm multiple times using different seeds
- There are many methods proposed for better initialization of K seeds
  - **K-Means++** (Arthur and Vassilvitskii,2007):
    - The first centroid is selected randomly
    - The next centroid selected is the one that is farthest from the currently selected (selection is based on a weighted probability score).
    - The selection continues until K centroids are obtained

k-Means++

- K-Means algorithm is sensitive to the initialization of the centroids or the mean points
- K-Means++ ensures a smarter initialization of the centroids and improves the quality of the clustering
  – The initialization is different
  – The remaining of the algorithm is the same as standard k-Means

Arthur, D.; Vassilvitskii, S. (2007). **K-means++: the advantages of careful seeding**. Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms. Society for Industrial and Applied Mathematics Philadelphia, PA, USA. pp. 1027–1035.

Some k-Means references

- MacQueen, J. B. (1967). **Some Methods for classification and Analysis of Multivariate Observations**. Proceedings of 5th Berkeley Symposium on Mathematical Statistics and Probability. University of California Press. pp. 281–297.

- Celebi, M. E., Kingravi, H. A., and Vela, P. A. (2013). **A comparative study of efficient initialization methods for the k-means clustering algorithm**. Expert Systems with Applications. 40 (1): 200–210.
- Arthur, D.; Vassilvitskii, S. (2007). **K-means++: the advantages of careful seeding**. Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms. Society for Industrial and Applied Mathematics Philadelphia, PA, USA. pp. 1027–1035.

Note **all the documents with this icon are in a zip file in campus virtual**

K-Modes

K-Modes for categorical data

- K-Means cannot handle non-numerical (categorical) data
  - Mapping categorical value to 1/0 cannot generate quality clusters for high-dimensional data
- K-Modes is a variation of the *K-Means* Method (Huang'98)
  - Replacing means of clusters with <u>modes</u>
  - Using new dissimilarity measures to deal with categorical objects
  - Using a <u>frequency</u>-based method to update modes of clusters

K-Modes basis

- K-Modes: an extension to K-Means by replacing means with **modes**

$$\Phi(x_j, z_j) = 1 - n_j^r/n_l \text{ when } x_j = z_j \text{ ; } 1 \text{ when } x_j \neq z_j$$

where z_j is the categorical value of attribute j in Z_l, n_l is the number of objects in cluster l, and n_j^r is the number of objects whose attribute value is r

- Dissimilarity measure between object X and the center of a cluster Z
- The dissimilarity measure (distance function) is **frequency-based**

$$d(X_i, X_l) \equiv \sum_{j=1}^{m} \delta(x_{i,j}, x_{l,j})$$

where

$$\delta(x_{i,j}, x_{l,j}) = \begin{cases} 0, & x_{i,j} = x_{l,j} \\ 1, & x_{i,j} \neq x_{l,j} \end{cases}$$

K-Modes algorithm

- K-Modes deals with categorical attributes

```
Insert the first K objects into K new clusters.
Calculate the initial K modes for K clusters.
Repeat {
    For (each object O) {
       Calculate the similarity between object O and the
       modes of all clusters.
       Insert object O into the cluster C whose mode is the
       least dissimilar to object O.
    }
       Recalculate the cluster modes so that the cluster
       similarity between mode and objects is maximized.
} until (num_iterations or few objects change clusters).
```

K-Modes

- Algorithm is still based on iterative object cluster assignment and centroid update

- A **fuzzy k-modes** method is proposed to calculate a **fuzzy cluster membership** value for each object to each cluster

- A mixture of categorical and numerical data: Using a **K-prototype** method

References of K-Modes

- Zhexue Huang and Michael K. Ng. 2003. **A Note on K-Modes Clustering**. J. Classif. 20, 2 (September 2003), 257-261. DOI=http://dx.doi.org/10.1007/s00357-003-0014-4
- Anil Chaturvedi, Paul E. Green, and J. Douglas Caroll. 2001. **K-Modes Clustering**. J. Classif. 18, 1 (January 2001), 35-55. DOI=http://dx.doi.org/10.1007/s00357-001-0004-3
- Zengyou He, **Approximation algorithms for K-Modes clustering**. https://arxiv.org/pdf/cs/0603120.pdf
- Fuyuan Cao, Jive Liang, Deyu Li, Liang Bai, Chuangyin Dang. **A dissimilarity measure for the K-Modes clustering algorithm**. Knowledge-based Systems, Volume 26, 2012, ISSN 0950-7051.DOI= https://doi.org/10.1016/j.knosys.2011.07.011.

http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.652.5571&rep=rep1&type=pdf

K-Medoids

K-Medoids basis

- The **k-Means algorithm is sensitive to outliers**!!
  - since an object with an extremely large value may substantially distort the distribution of the data
- **K-Medoids**:
  - Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located object** in a cluster

K-Medoids

- The K-Medoids clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial k-Medoids)
  - Repeat
    - Assigning each point to the cluster with the closest medoid
    - Randomly select a non-representative object o_i
    - Compute the total cost S of swapping the medoid m with o_i
    - If S<0, then swap m with o_i to form the new set of medoids

Discussion on K-Medoids Clustering

- **K-Medoids Clustering**: find representative objects (**medoids**) in clusters
- **PAM (Partitioning Around Medoids)**
  - Starts from an initial set of medoids, and
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) of the resulting clustering
  - PAM works effectively for small data sets but does not scale well for large data sets (due to the computational complexity)
  - Computational Complexity: PAM $O(K(n-K)^2)$ (quite expensive!)
- Efficiency improvements on PAM
  - **CLARA** (Kaufmann & Rousseeuw, 1987)
    - PAM on samples; $O(Ks^2 + K(n-k))$, s is the sample size
  - **CLARANS** (ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality

References K-Medoids

- R. T. Ng and Jiawei Han (2002), "**CLARANS: a method for clustering objects for spatial data mining**" in *IEEE Transactions on Knowledge and Data Engineering*, vol. 14, no. 5, pp. 1003-1016, Sep/Oct 2002. doi: 10.1109/TKDE.2002.1033770

- Kaufman, L. and Rousseeuw, P.J. (1987), **Clustering by means of Medoids**, in Statistical Data Analysis Based on the L_1 –Norm and Related Methods, edited by Y. Dodge, North-Holland, 405–416

- H.S. Park , C.H. Jun, **A simple and fast algorithm for K-medoids clustering**, Expert Systems with Applications, 36, (2) (2009), 3336–3341

- J. Xie and S. Jiang, "**A Simple and Fast Algorithm for Global K-means Clustering**", 2010 Second International Workshop on Education Technology and Computer Science, Wuhan, 2010, pp. 36-40. doi: 10.1109/ETCS.2010.347

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K-Prototypes

K-prototypes Algorithm

- To integrate the k-means and k-modes algorithms into the k-prototypes algorithm that is used to cluster the mixed-type objects

- The dissimilarity between two mixed-type objects X and Y, which are described by attributes $A_1^r, A_2^r, \ldots, A_p^r, A_{p+1}^c, \ldots, A_m^c$ (*m* is the attribute numbers the first *p* means numeric data, the rest means categorical data), can be measured by::

$$d_2(X,Y) = \sum_{j=1}^{p}(x_j - y_j)^2 + \gamma \sum_{j=p+1}^{m} \delta(x_j, y_j)$$

K-prototypes Algorithm(cont.)

$$d_2(X,Y) = \sum_{j=1}^{p}(x_j - y_j)^2 + \gamma \sum_{j=p+1}^{m}\delta(x_j, y_j)$$

- The first term is the Euclidean distance measure on the numeric attributes and the second term is the simple matching dissimilarity measure on the categorical attributes
- The weight γ is used to avoid favoring either type of attribute

References of K-prototypes

- Zhexue Huang, **Clustering large datasets with mixed numerical and categorical values**. https://pdfs.semanticscholar.org/d42b/b5ad2d03be6d8fefa63d25d02c0711d19728.pdf
- Byoungwook Kim. **A Fast K-prototypes Algorithm Using Partial Distance Computation**. https://www.researchgate.net/publication/316348009_A_Fast_K-prototypes_Algorithm_Using_Partial_Distance_Computation

Course. Introduction to Machine Learning

Work 1. Clustering Exercise

Session 2

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