Clustering

Density based and grid based approaches

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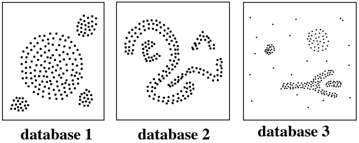
Density-based clustering methods

- Clustering based on density (local cluster criterion), such as density-connected points



(Data sets from DBSCAN paper)

- Motivation:
  - Discover clusters of arbitrary shape
  - Handle noise
- Requirement:
  - Need density parameters as termination condition

Density-based clustering methods

- Several interesting studies
  - DBSCAN: Ester, et al. (KDD96)
  - OPTICS: Ankerst, et al (SIGMOD99).
  - DENCLUE: Hinneburg & D. Keim (KDD98)
  - CLIQUE: Agrawal, et al. (SIGMOD98) (more grid-based)

DBSCAN: Density Based Spatial Clustering of Applications with Noise

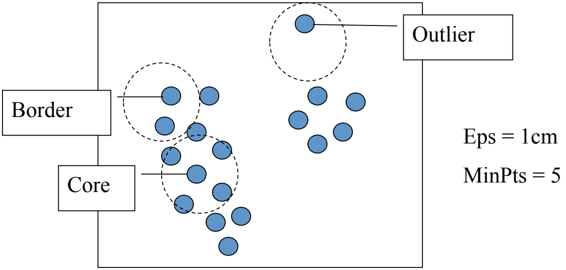
- Relies on a density-based notion of cluster
- A cluster is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise

DBSCAN – basic concepts

- Dataset D of points in k-dimensional space
- $dist(p, q)$: distance of two objects p and q
- Two parameters
  - Eps ϵ: Maximum radius of the neighbourhood
  - *MinPts*: Minimum number of points in an Eps-neighbourhood of that point
- The Eps-neighborhood of a point p:
  $N_\epsilon(p) = \{q | q \in D \wedge dist(p, q) \leq \epsilon\}$

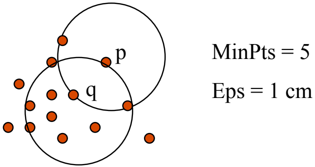
DBSCAN – basic concepts

- Core point: points inside a cluster. $|N_\epsilon(q)| \geq MinPts$
- Border point: points on the border of a cluster.



DBSCAN – basic concepts – directly density-reachable

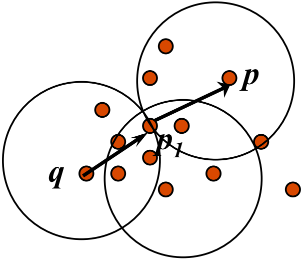
- Directly density-reachable: A point p is directly density-reachable from a point q w.r.t. *Eps* ϵ, *MinPts* if
  - $p \in N_\epsilon(q)$
  - q is a core point, i.e., $|N_\epsilon(q)| \geq MinPts$
- Directly density-reachable is symmetric for pairs of core points; NOT symmetric if one core point and one border point are involved.



p is directly density reachable from q; q is not directly density reachable from p.

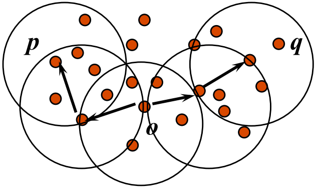
DBSCAN – basic concepts

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



DBSCAN – density-connected

- There must be a core point in a cluster C from which two border points of C are density-reachable.
  - A point p is density-connected to a point q w.r.t. *Eps* ϵ, *MinPts* if there is a point o such that both p and q are density-reachable from o w.r.t. *Eps* ϵ, *MinPts*.
  - Symmetric



DBSCAN – cluster

- Let D be a database of points. A cluster C w.r.t. *Eps* and *MinPts* is a non-empty subset of D satisfying the following conditions:
  - 1) $\forall p, q$: if $p \in C$ and q is density-reachable from p w.r.t. *Eps* and *MinPts*, then $q \in C$. (Maximality)
  - 2) $\forall p, q \in C$: p is density-connected to q w.r.t. *Eps* and *MinPts*. (Connectivity)
- Let $C_1, \cdots, C_k$ be the clusters of the database D w.r.t. parameters Eps_i and $MinPts_i$, $i = 1, \cdots, k$. Then we define the noise as the set of points in the database D not belonging to any cluster C_i, i.e. $noise = \{p \in D | \forall i : p \notin C_i\}$.

DBSCAN – the algorithm

- Initialize all points to be UNCLASSIFIED
- Loop
  - Arbitrarily select an UNCLASSIFIED point p
  - Calculate $N_\epsilon(p)$ and put the points to *SeedSet*
  - If *SeedSet* contains less than *MinPts* points, mark every point in this set to be NOISE.
  - Else (i.e., *SeedSet* contains more than *MinPts* points)
    - Loop every point $q \in SeedSet$
      – (1) Change q's cluster id, remove q from *SeedSet*
      – (2) If q is a core point, do further expansion by adding the density reachable points to *SeedSet*
      – (3) If q is a border point, no need to further expand q
- Continue the process until all of the points have been processed.

DBSCAN – determining the parameters – concepts

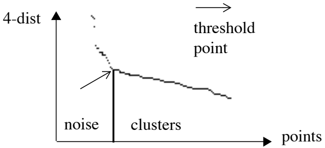
- *k*-dist: For a given k, we define a function k-dist from the database D to real numbers, mapping each point to the distance from its k-th nearest neighbor.
- Object p's k-dist: the distance between p and its k-th nearest neighbor.
- Observation 1: let $d = k$-dist of p, then the d-neighborhood of p contains exactly $k + 1$ points for almost all points p.
  - Very unlikely, the d-neighborhood of p contains more than $k + 1$ points, which means several points have *exactly* the same distance d from p. (k-dist is generally different for different objects).
- Observation 2: k-dist of p does not change dramatically when k changes gradually from 1, to 2, to $\cdots$.

DBSCAN – determining the parameters – procedure

- Calculate the k-dist for each point
- Sorted k-dist graph: sort the points in D in descending order of their k-dist
- User can estimate percentage of noise, from this percentage to derive a threshold.
- Given a threshold point
  - All points with a higher k-dist value (left of the threshold) are considered to be noise
  - All other points (right of the threshold) are assigned to some cluster.
- Set $MinPts = k$ and $Eps = k$-dist

DBSCAN – determining the parameters – thinnest cluster

- Thinnest cluster: least dense cluster in the dataset.
- The threshold point for the thinnest cluster: the first point in the first "valley" of the sorted k-dist graph.



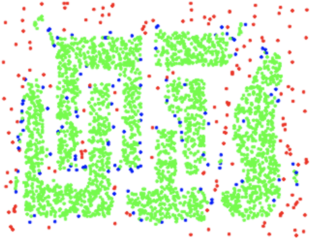
sorted 4-dist graph for sample database 3

DBSCAN – determining the parameters – further discussion

- How to decide the valley? Interactive interface.
- How to decide k: Experimentally, it has shown that k-dist graphs for $k > 4$ do not significantly differ from the 4-dist graph

DBSCAN: Core, Border and Noise Points

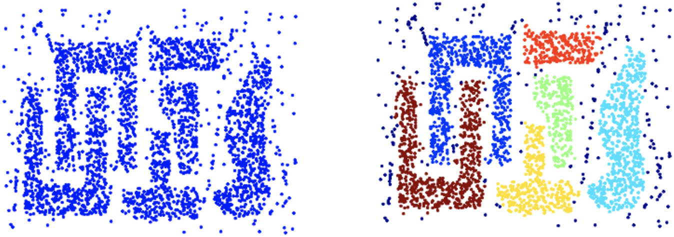
Original Points



Point types: core, border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well

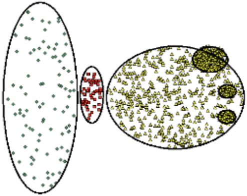


Original Points

Clusters

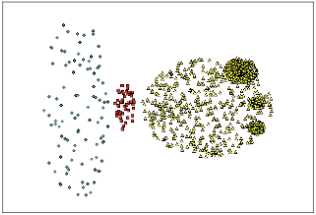
- **Resistant to Noise**
- **Can handle clusters of different shapes and sizes**

When DBSCAN Does NOT Work Well

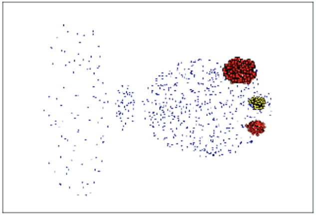


Original Points

- **Varying densities**
- **High-dimensional data**



(MinPts=4, Eps=9.92).



(MinPts=4, Eps=9.75)

Clustering in High Dimensional Space

- In high dimensional space, not all dimensions are relevant to a given cluster.
- Idea: pick the closely related dimensions and find clusters in the corresponding subspace.

Subspace Clustering Method

- Data are in high-dimensional space.
  – Distance function that uses all the dimensions of the data may be ineffective.
- Search various subspaces to find clusters
- Bottom-up approaches
  - Start from low-D subspaces and search higher-D subspaces only when there may be clusters in such subspaces
  - Various pruning techniques to reduce the number of higher-D subspaces to be searched
  - Eg. CLIQUE in *Rakesh Agrawal, Johannes Gehrke, Dimitrios Gunopulos, Prabhakar Raghavan: Automatic Subspace Clustering of High Dimensional Data for Data Mining Applications. SIGMOD 1998:94-105*.

Subspace Clustering Method

- Top-down approaches
  - Start from full space and search smaller subspaces recursively
  - Eg. PROCLUS in *Charu C. Aggarwal, Cecilia Magdalena Procopiuc, Joel L. Wolf, Philip S. Yu, Jong Soo Park: Fast Algorithms for Projected Clustering. SIGMOD 1999:61-72.*

CLIQUE (Clustering In QUEst)

- Targets:
  - Process data in high dimensions
  - Get easy-to-interpret results
  - Achieve better scalability and usability: scale well with the number of dimensions and the size of input; insensitive to the input order of data records;
  - WEKA has implementation of CLIQUE

CLIQUE – Intuitive ideas

- Subspace: automatically identify subspaces of high dimensions
  – Do not consider new dimensions: e.g., linear combination of original dimensions, which is hard to interpret
- Density-based approach
  – A cluster is a region that has a higher density of points than its surrounding region.
- Grid-based method
  – To approximate density, partition the data space to cells/units/grids
- Find clusters in the corresponding projections/subspaces/dimensions
  – A cluster is a union of connected high density units within a subspace
  – Clusters are constrained to be axis-parallel hyper-rectangles

References

- Chapter 7: Introduction to Data Mining (2nd Edition) by Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar
- Scikit-learn DBSCAN algorithm: https://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html
- CLIQUE algorithm: https://pyclustering.github.io/docs/0.9.0/html/d2/d4f/classpyclustering_1_1cluster_1_1clique_1_1clique.html