DATA MINING 1 Density-based Clustering

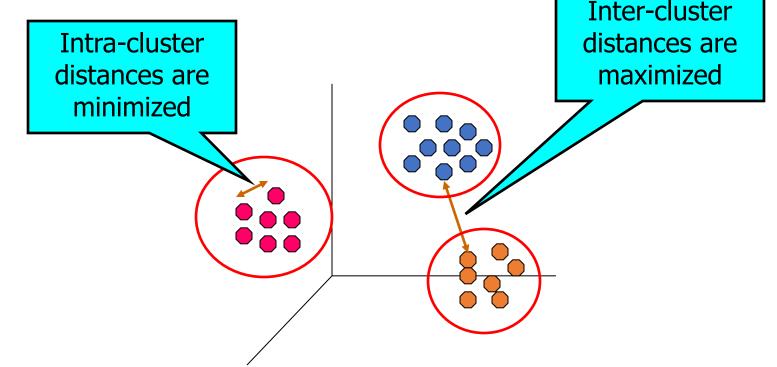
Riccardo Guidotti

Revisited slides from Lecture Notes for Chapter 7 "Introduction to Data Mining", 2nd Edition by Tan, Steinbach, Karpatne, Kumar



What is Cluster Analysis?

 Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups

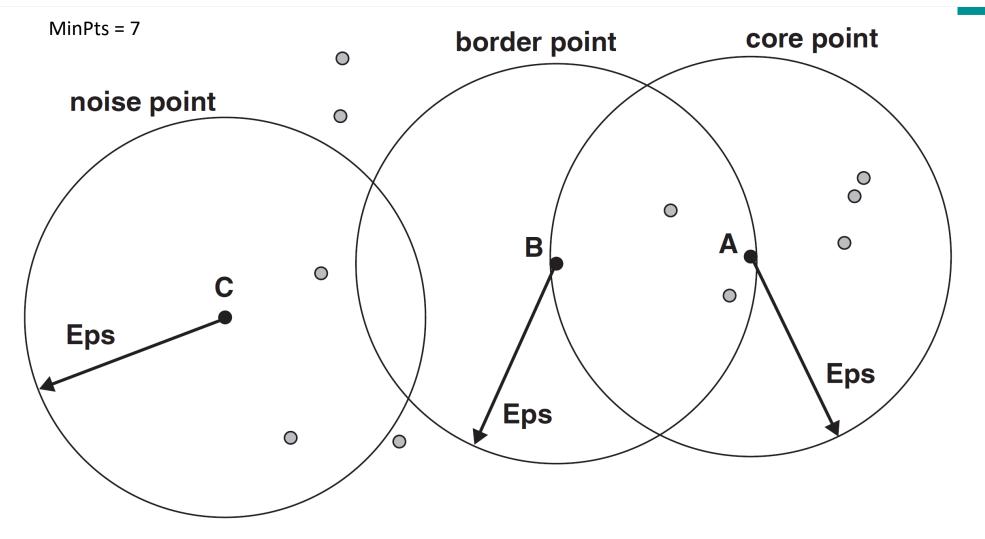


DBSCAN

DBSCAN

- DBSCAN is a density-based algorithm.
 - Density = number of points within a specified radius (Eps)
 - A point is a core point if it has at least a specified number of points (MinPts) within Eps
 - These are points that are at the interior of a cluster
 - Counts the point itself
 - A border point is not a core point, 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

DBSCAN: Core, Border, and Noise Points



DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points
 - $current_cluster_label \gets 1$

 $\mathbf{for} \ \mathrm{all} \ \mathrm{core} \ \mathrm{points} \ \mathbf{do}$

 ${\bf if}$ the core point has no cluster label ${\bf then}$

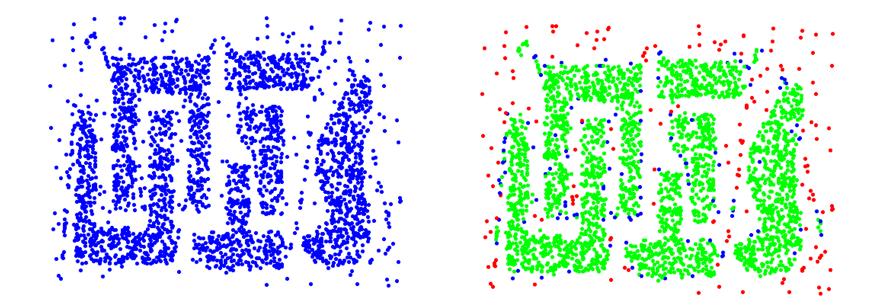
 $current_cluster_label \leftarrow current_cluster_label + 1$

Label the current core point with cluster label *current_cluster_label* end if

for all points in the Eps-neighborhood, except ith the point itself do
 if the point does not have a cluster label then
 Label the point with cluster label current_cluster_label
 end if
end for

end for

DBSCAN: Core, Border and Noise Points

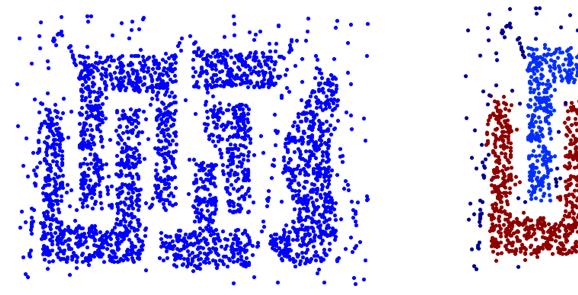


Original Points

Point types: core, border and noise

Eps = 10, **MinPts = 4**

When DBSCAN Works Well

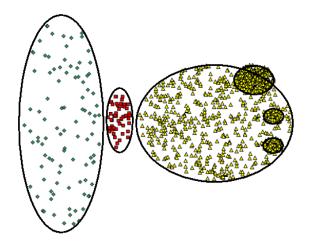


Original Points

Clusters

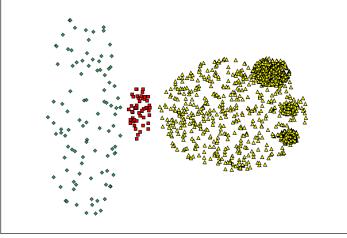
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN Does NOT Work Well

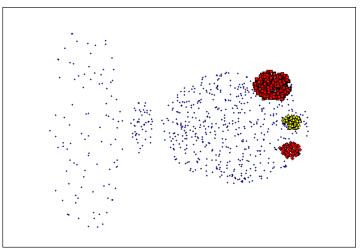


Original Points

- Varying densities
- High-dimensional data



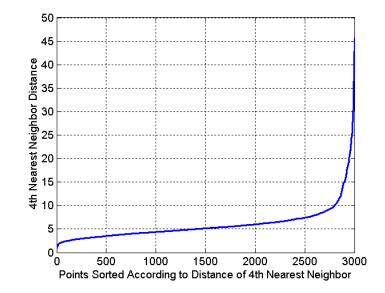
(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

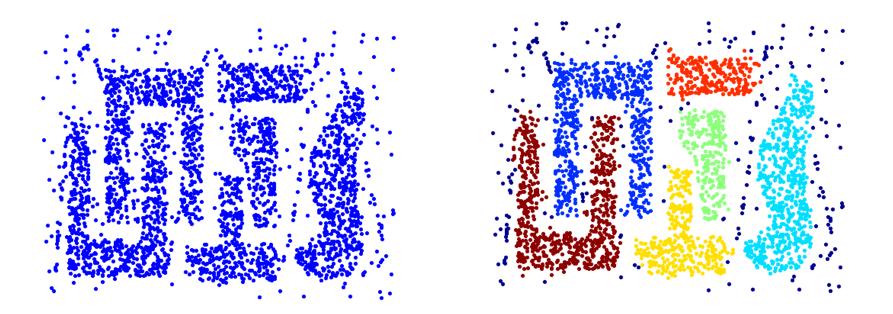
DBSCAN: Determining EPS and MinPts

- Idea is that for points in a cluster, their kth nearest neighbors are at roughly the same distance
- Noise points have the kth nearest neighbor at farther distance
- So, plot sorted distance of every point to its kth nearest neighbor



DBSCAN Evolution OPTICS

When DBSCAN Works Well

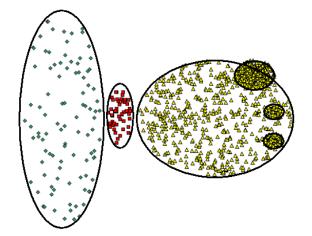


Original Points

Clusters

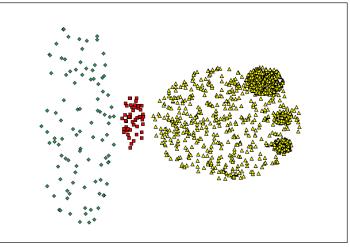
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN Does NOT Work Well

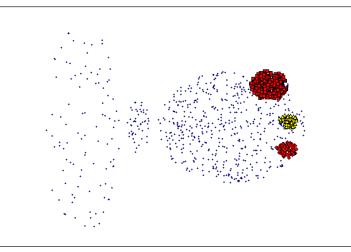


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).



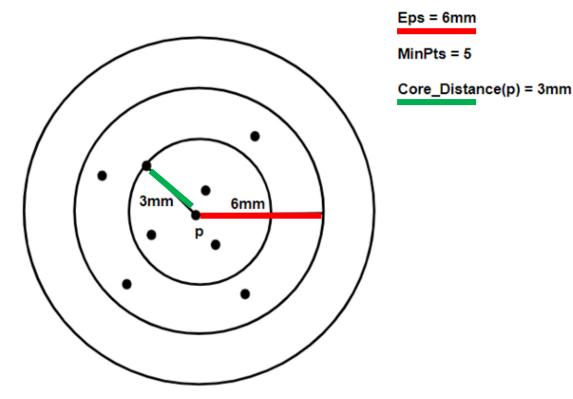
(MinPts=4, Eps=9.92)

OPTICS

- OPTICS: Ordering Points To Identify the Clustering Structure
 - Produces a special order of the dataset wrt its density-based clustering structure.
 - This cluster-ordering contains info equivalent to the density-based clusterings corresponding to a broad range of parameter settings.
 - Good for both automatic and interactive cluster analysis, including finding intrinsic clustering structure.
 - Can be represented graphically or using visualization techniques.

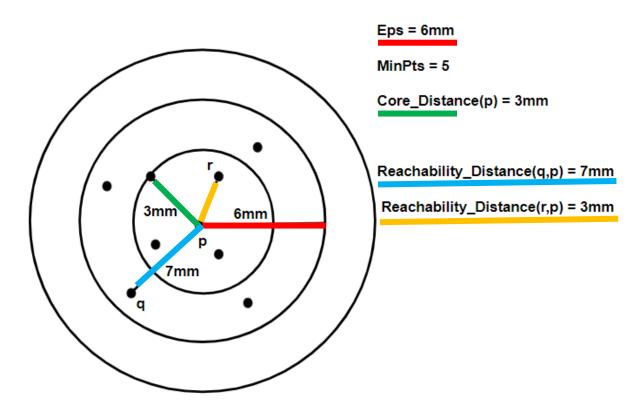
OPTICS: Extension from DBSCAN

- OPTICS requires two parameters:
 - ε, which describes the maximum distance (radius) to consider,
 - MinPts, describing the number of points required to form a cluster
- Core point. A point *p* is a core point if at least MinPts points are found within its εneighborhood.
- **Core Distance**. It is the **minimum** value of radius required to classify a given point as a core point. If the given point is not a Core point, then it's Core Distance is undefined.



OPTICS: Extension from DBSCAN

- Reachability Distance. The reachability distance between a point *p* and *q* is the maximum of the Core Distance of *p* and the Distance between p and q.
- The Reachability Distance is not defined if *q* is not a Core point. Below is the example of the Reachability Distance.
- In other words, if q is within the core distance of p then use the core distance, otherwise the real distance.



OPTICS Pseudo-Code

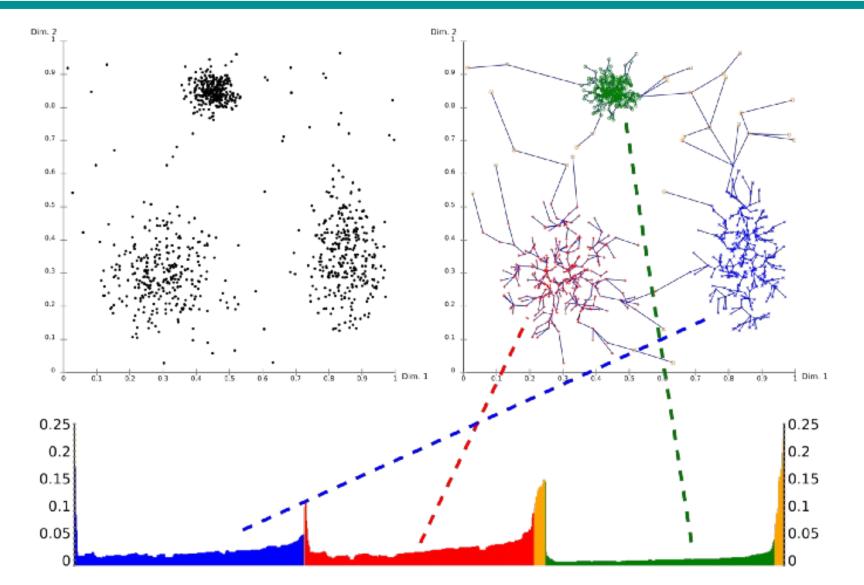
- For each point *p* in the dataset
 - Initialize the reachability distance of *p* as undefined
- For each unprocessed point *p* in the dataset
 - Get the neighbors N of p
 - Mark *p* as processed and output to the *ordered list*
 - If *p* is a core point
 - Initialize a priority queue Q to get the closest point to p in terms of reachability
 - Call the function update(N, p, Q)
 - For each point q in Q
 - Get the neighbors N' of q
 - Mark q as processed and output to the ordered list
 - If q is a core point Call the function update(N', q, Q)

OPTICS Pseudo-Code

- Function *update(N, p, Q)*
 - Calculate the core distance for *p*
 - For each neighbor q in N (update the reachability)
 - If q is not processed
 - *new_rd* = reachability distance between *p* and *q*
 - If q is not in Q
 - Q.insert(q, new_rd)
 - Else
 - If new_rd < q.rd
 - Q.move_up(q, new_rd)

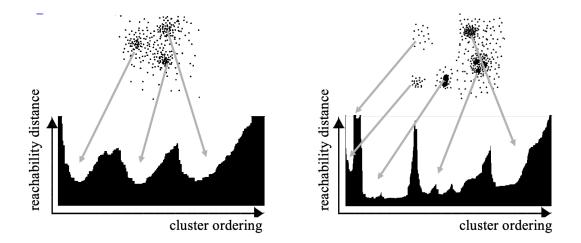
- OPTICS outputs the points in a particular ordering, annotated with their smallest reachability distance.
- A reachability-plot (a special kind of dendrogram), the hierarchical structure of the clusters can be obtained easily.
- x-axis: the ordering of the points as processed by OPTICS
- y-axis: the reachability distance
- Points belonging to a cluster have a low reachability distance to their nearest neighbor, the clusters show up as valleys in the reachability plot. The deeper the valley, the denser the cluster.

OPTICS Output

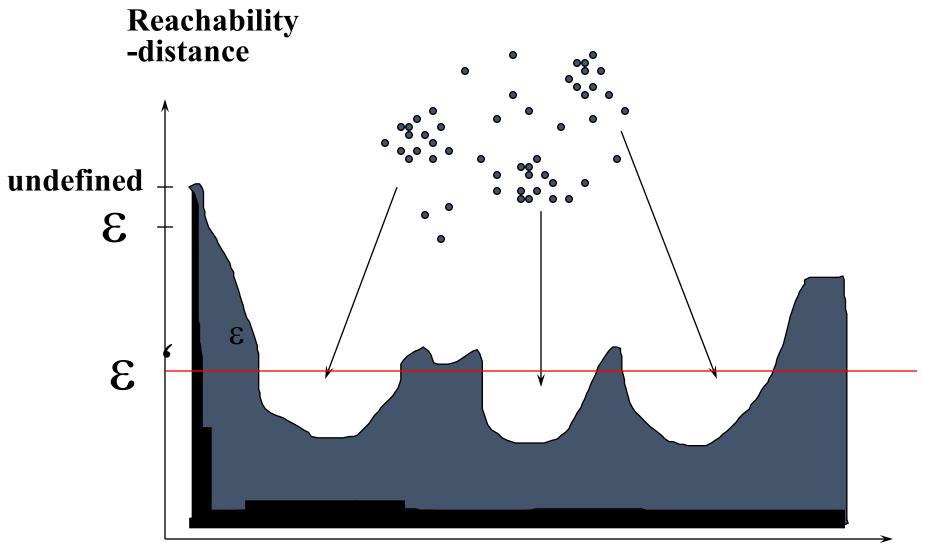


OPTICS Output

- Clusters are extracted
 - 1. by selecting a range on the x-axis after visual inspection,
 - 2. by selecting a threshold on the y-axis
 - 3. by different algorithms that try to detect the valleys by steepness, knee detection, or local maxima. Clustering obtained this way usually are hierarchical, and cannot be achieved by a single DBSCAN run.



https://scikit-learn.org/stable/auto_examples/cluster/plot_optics.html#sphx-glr-auto-examples-cluster-plot-optics-py



Cluster-order of the objects

OPTICS: The Radius Parameter

- Both core-distance and reachability-distance are undefined if no sufficiently dense cluster (w.r.t. ε) is available.
- Given a sufficiently large ε, this never happens, but then every εneighborhood query returns the entire database.
- Hence, the ε parameter is required to cut off the density of clusters that are no longer interesting, and to speed up the algorithm.
- The parameter ε is, strictly speaking, not necessary.
- It can simply be set to the maximum possible value.
- When a spatial index is available, however, it does play a practical role with regards to complexity.
- OPTICS abstracts from DBSCAN by removing this parameter, at least to the extent of only having to give the maximum value.

References

- Clustering. Chapter 7. Introduction to Data Mining.
- Mihael Ankerst; Markus M. Breunig; Hans-Peter Kriegel; Jörg Sander (1999). OPTICS: Ordering Points To Identify the Clustering Structure.

