MADS-MMS – Mathematics and Multivariate Statistics

Density-Based Clustering

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Moodle (WiSe 24/25)

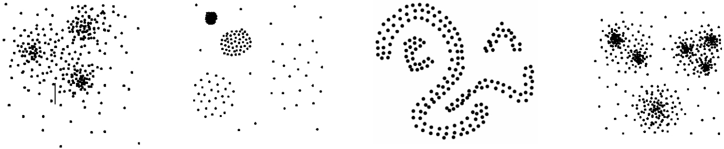
Outline

Motivation

- k-means has various limitations:
  - fixed on Euclidean distance
  - cannot discover outliers/noise
  - discovers compact, round centered shapes
  - needs the number of clusters upfront
- exploit the idea of density rather than of distance to a central entity

Examples

Clusters of different size, form, density, and hierarchical structure



Chapter Goals

- understand the basics of density based clustering
- understand and apply parameters of DBSCAN and their influence on the resulting clustering
- understand the difference between clusters and noise
- understand and apply OPTICS to choose good DBSCAN parameters or to create OPTICS clusterings

Outline

Basics

Idea:

- clusters are regions in space, that are densely populated with data instances
- clusters are separated by regions that are sparsely populated with data instances

Handling Noise:

datasets are rarely clean and contain noise

→ noise detection

Idea: Density Based Clustering

Requirements:

- each object that belongs to a cluster comes from a neighborhood whose data-density exceeds a fixed threshold.
- the set of instances belonging to one cluster is "connected".

Ingredients:

- distinction between noise and valid data
- notion of density
- neighborhoods
- selection of density threshold

Neighborhoods and Core Points

Definition 1 (Neighborhood)

Let D be a dataset and $\mathrm{dist}(\cdot,\cdot)$ a distance function. For an instance $o \in D$ and a given radius ε, the neighborhood of o w.r.t. ε is given as

$$N_\varepsilon(o) = \{p \in D \mid \mathrm{dist}(o,p) \leq \varepsilon\}.$$

Definition 2 (Core Point)

Let D, $\mathrm{dist}(\cdot,\cdot)$, ε and o be as above. Then instance o is called a **core point** w.r.t. the radius ε and the threshold MinPts, if:

$$|N_\varepsilon(o)| \geq \mathrm{MinPts}.$$

With the parameter MinPts, we control the required minimum density of neighborhoods.

Definition 3 (Reachability)

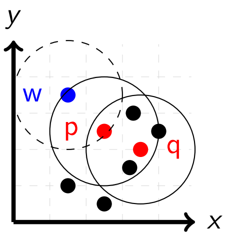
For a dataset D, distance function $\mathrm{dist}(\cdot, \cdot)$, and parameters ε and MinPts:

- a data instance $p \in D$ is called **directly (density-)reachable** from $q \in D$ if $p \in N_\varepsilon(q)$ and q is a core point.
- a data instance $p \in D$ is called **(density-)reachable** if there is a chain of directly reachable objects from q to p.
- two data instances p and q are called **(density-)connected**, if both are reachable from the same instance $o \in D$.

Examples: Reachability

Use Euclidean distance and set $\varepsilon = 1.5cm$, MinPts $= 3$

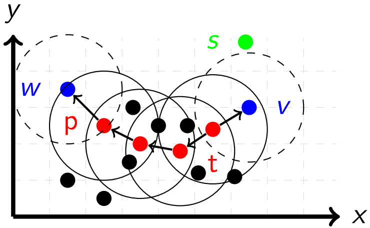
- p and q are core points
- w is not a core point
- w is directly reachable from p but not from q
- w is reachable from q (via p)



Examples: Reachability and Connectedness

Use Euclidean distance and set $\varepsilon = 1.5cm$, $\text{MinPts} = 3$

- s is not reachable from any instance
- w is reachable from t
- t is not reachable from w
- v,w are connected



Remarks on Reachability

- reachability is a parametrized property – depending on the choices of ε and MinPts
- works with any distance function
- reachability is not symmetric!
- reachability implies that all instances in the chain of direct reachability are core points
- if p is reachable from q, then p and q are connected
- reachability gives rise to a notion of noise: everything that is not reachable!

Density-based Clusters

Definition 4 (Density Cluster)

A density cluster C w.r.t. ε and MinPts is a non-empty subset of the data D for which hold:

maximality : $\forall p, q \in D : p \in C \wedge q$ reachable from $p \Rightarrow q \in C$

connectedness : $\forall p, q \in C : p$ and q are connected.

Definition 5 (Density Clustering)

A density clustering $\mathcal{C}$ of the data D w.r.t. ε and MinPts is the set of all density clusters.

Definition 6 (Noise)

With the above definitions, $Noise_{\mathcal{C}}$ is defined as the set of all instances of D that belong to none of the clusters $C \in \mathcal{C}$.

Outline

Basics for DBSCAN

Density-Based Spatial Clustering of Applications with Noise (DBSCAN)

Lemma 7 (Characterization)

Let $p \in D$ be a core point. Then the density cluster C that contains p can be constructed as

$$C = \{q \in D \mid q \textit{ is reachable from } p\}.$$

DBSCAN: For each core-point, add all reachable instances to the same cluster.

DBSCAN: Main Loop

```
DBSCAN (D: dataset, ε: float, MinPts: int):
  mark each instance as unvisited
  C = 0 # ClusterID
  for each instance p in D:
    if (p has been visited):
      continue
    mark p visited
    if (|N_ε(p)| < MinPts):
      mark p NOISE
    else:
      C++;
      expand_cluster(p, N_ε(p) \ p, C, ε, MinPts)
```

DBSCAN: expand_Cluster

```
expand_cluster(p: instance, L: list of instances,
ε: float, MinPts: int):
  mark p with  C
  for each point q in L:
    if (q not visited):
      mark q visited
      if (|N_ε(q)| >= MinPts):
      L = N_ε(q) ∪ L
    if (q is not yet member of any cluster):
      unmark q as NOISE
      mark q with C
```

Notebook 09_1_density_synthetic, Cells 1–12

Discussion of DBSCAN

positive:

- number of clusters must not be set upfront
- clusters can obtain arbitrary geometric shapes
- solution is unique (except for cluster enumeration and non-core-point memberships)
- works with any distance function
- noise is separated from data

negative:

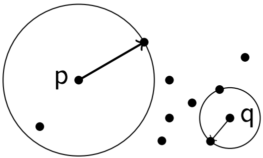
- worst case complexity $O(n^2)$
- computing ε-neighborhoods is expansive
- suitable ε, MinPts must be chosen
- does not allow for differently dense clusters

Exercises 1–2

Outline

Parameters

- determine good values for ε, MinPts
- heuristic approach: order instances by their distance to their k-nearest neighbors



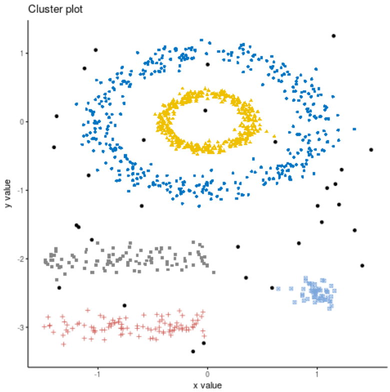
$\longrightarrow$ 2-distance

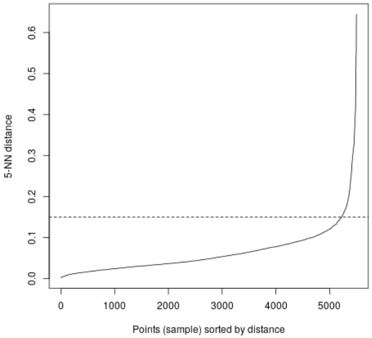
Definition 8 (k-distance)

In the above setting, the **k-distance** of an instance p is:
$\mathrm{dist}_k(p) := \min\{\varepsilon \in \mathbb{R}_{\geq 0} \mid |N_\varepsilon(p)| > k\}$. (Note: p is not counted as its own neighbor.)

- k-distance diagram: the ordered k-distances of all objects

Heuristic Choice of Parameters

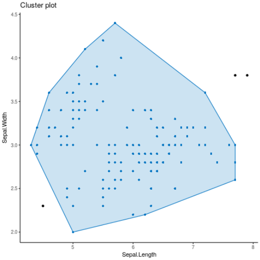


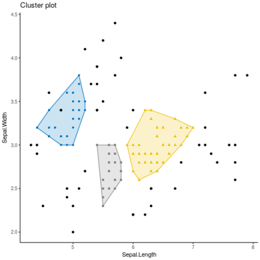


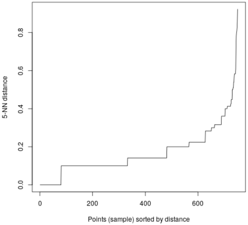
- choose k (rule of thumb $k > d$), and $\text{MinPts} := k + 1$
- compute k-distance diagram
- choose instance o as border object (elbow in graph) and set $\varepsilon := \text{dist}_k(o)$

Problem: Hierarchical Clusters

An example from IRIS







- hierarchical clusters
- strong differences in density in different parts of the space
- clusters and noise are not well separated

Outline

Observation

Theorem 9 (Cluster Monotony)

Let D be a dataset and $\mathcal{C}$ a density based clustering with ε and MinPts. Let $\mathcal{C}'$ be another such clustering with MinPts and $\varepsilon' \geq \varepsilon$. Then, for each $C \in \mathcal{C}$ there exists a $C' \in \mathcal{C}'$ such that $C \subseteq C'$.

Remark:

- lowering ε makes the density constraint harder to meet
- thus, clusters decompose into smaller subsets and noise

Outline

Density based Hierarchical Clustering

Idea

- create a data structure from which one can obtain DBSCAN clusterings for different choices of ε in **linear(!)** time
- Ordering Points To Identify the Clustering Structure ➔ OPTICS

Steps

- fix MinPts
- fix an upper bound for ε
- find a clever ordering of points
- compute the minimum ε for which a point is still reachable from its predecessors
- the upper bound is used to determine whether an instance can be a core point at all (for this or lower values of ε)

The OPTICS Algorithm

Principle: Given fix MinPts and ε, in a DBSCAN-like procedure yield a data structure with three components:

1. the core distance for each instance
2. an order on the dataset
3. a reachability distance for each instance

Visual Representation: a reachability distance diagram, which is readable even for very large datasets with high dimensionality

Core Distance

Definition 10 (Core Distance)

For an instance o of a dataset D with distance dist, the **core distance** of o, given ε and MinPts is

$$\underset{\varepsilon,\text{MinPts}}{core - \text{dist}}(o) := \begin{cases} \textit{undefined} & |N_\varepsilon(o)| < \text{MinPts} \\ \text{dist}_{\text{MinPts}-1}(o) & \text{else} \end{cases}$$

In a clustering with MinPts and $\varepsilon' \leq \varepsilon$, o will be a core point if $core - \text{dist}_{\varepsilon,\text{MinPts}}(o) \leq \varepsilon'$.

Reachability Distance

Definition 11 (Reachability Distance)

For an instances p and o of a dataset D with distance dist, the reachability distance of p from o, given ε and MinPts is

$$\underset{\varepsilon,\mathrm{MinPts}}{reach - \mathrm{dist}}(o, p) := \begin{cases} \textit{undefined} \text{ if } |N_\varepsilon(o)| < \mathrm{MinPts} \\ \max\{core - \mathrm{dist}_{\varepsilon,\mathrm{MinPts}}(o), \mathrm{dist}(o, p)\} \text{ else.} \end{cases}$$

The reachability distance of p from o tells us, for which $\varepsilon' \leq \varepsilon$ is directly reachable, meaning

- o must be a core point and
- p must be in the neighborhood $N_\varepsilon(o) = \{p \in D \mid \mathrm{dist}(o, p) \leq \varepsilon\}$ of o.

Cluster Order

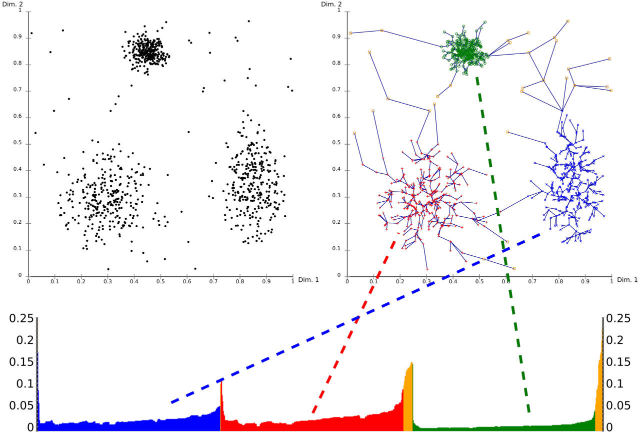
1. start with an arbitrary object
2. as soon as the first object p with defined core distance is found, start an ordered priority list
3. for each neighbor q of p do:
   - if q is not on the list, add it with its reachability distance from p
   - if q is on the list and the reachability distance from p is smaller than the previous reachability distance, replace the previous reachability distance
4. repeat 3 with the first object from from the ordered priority list until the list is empty.
5. repeat 2 with an arbitrary unprocessed instance.

Note that the ordered priority list is updated while it is processed (recursive algorithm).

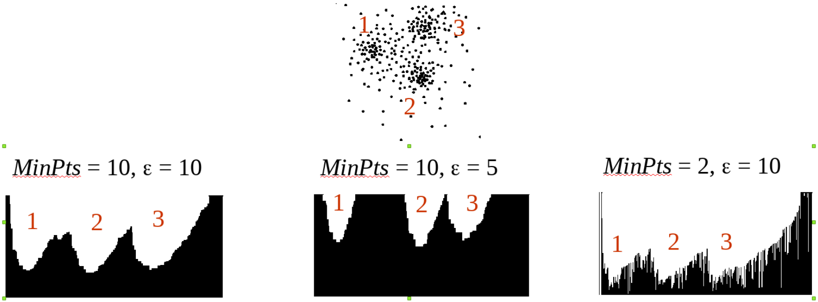
Notebook 09_2_optics_toy_example

Reachability Diagram

- visualize reachability distances of objects, next to each other, ordered by the cluster order
- valleys are clusters
- the deeper the valley, the more dense the cluster



Example: Parameter Sensitivity



Extracting Clusterings

How to determine "a valley"?

Distance Cut :

- select a reachability distance (y-axis) in the reachability diagram
- points between two intersections form a DBSCAN cluster

OPTICS ξ method : (sketch)

- go through cluster order
- start cluster when in an area reachability distance falls ξ-steep
- end cluster when in an area reachability rises ξ-steep
- clusters contain at least MinPts instances

Notebook 09_1_density_synthetic, Cells 13–21

Exercises 3