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Data Clustering

Marzena Kryszkiewicz

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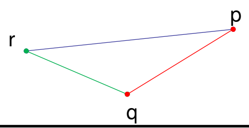
Basic Notions

Distance Metric

A *distance metric* is defined as a measure that satisfies the following conditions:

- ∀p, distance(p, p) = 0;
- ∀p,q, distance(p, q) = distance(q, p);
- ∀p,q,r, distance(p, r) ≤ distance(p, q) + distance(q, r) /* triangle inequality property */.



Example Distance Metrics

- Euclidean(p, q) = $\sqrt{\sum_{i=1..n}(p_i - q_i)^2}$
- Manhattan(p, q) = $\sum_{i=1..n}|p_i - q_i|$
- Minkowski(p, q) = $\sqrt[m]{\sum_{i=1..n}|p_i - q_i|^m}$

DBSCAN: Density-Based Clustering with Noise

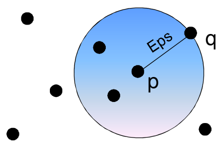
Eps-Neighborhood

- *Eps-neighborhood of a point p* (denoted by $N_{Eps}(p)$) is defined as the set of all points q in dataset D that are distant from p by no more than Eps; that is,

$$N_{Eps}(p) = \{q \in D \mid distance(p,q) \leq Eps\}.$$

Example: Eps-Neighborhood

$|N_{Eps}(p)| = 4$.



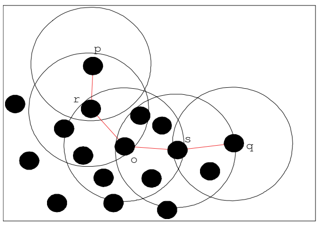
Core Points

- A point p is defined as a *core point* if its *Eps-neighborhood* contains at least MinPts points; that is, if $|N_{Eps}(p)| \geq$ MinPts.

Example: Core Points

For MinPts = 6:

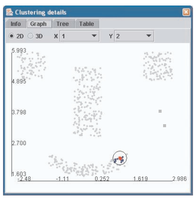
- r is a core point;
- p is not a core.

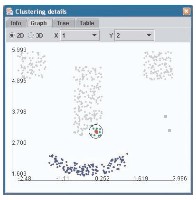


Clusters in DBSCAN…

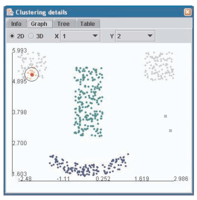
- A core point is treated as a seed from which a cluster is built.
- Whenever any core point is included in the cluster, all points in its Eps-neighborhood are also included in the cluster.

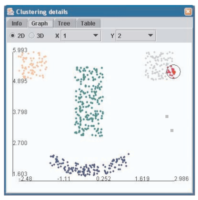
Clusters in DBSCAN…



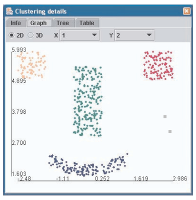


Clusters in DBSCAN…





Clusters in DBSCAN



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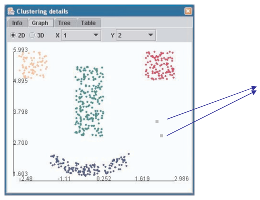
Clusters and Noise in DBSCAN

- The points that are not included in any cluster constitute *noise*.



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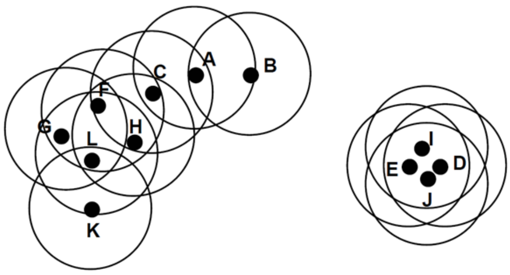
DBSCAN – Definition's Illustration



minPts = 4

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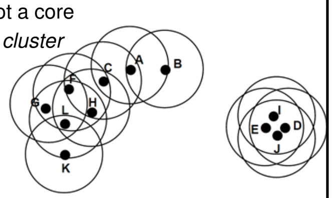
DBSCAN – Example Execution

- Dealing with a point q from an analysed neighborhood:

if q.ClusterId = Unclassified **then** // q is not classified
  assign q *to currently created cluster*
  add q *to seeds*
else if q.ClusterId = N // q is not a core
  assign q *to currently created cluster*
else
  do nothing



minPts = 4

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Major Challenges in DBSCAN

- Efficient calculation of Eps-neighborhood for each point.
- To this end, DBSCAN uses the R*-tree index.
- The use of such indices helps in the case of low dimensional data only.

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TI-DBSCAN: DBSCAN with Efficient Calculation of Eps-Neighboorhoods

- Use the triangle inequality property (TI) to reduce the number of candidates for being a member of Eps-neighboorhood of a given point.

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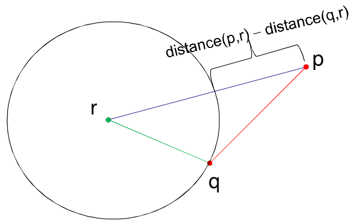
TI for pessimistic estimation of distance

For any three points p, q, r:

- distance(p,q) + distance(q,r) ≥ distance(p,r).
- **distance(p,q)** ≥ distance(p,r) – distance(q,r).



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TI & Eps-Neighborhood…

Lemma. Let D be a set of points. For any two points p, q in D and any point r:

distance(p,r) – distance(q,r) > Eps ⇒

distance(p,q) ≥ distance(p,r) – distance(q,r) > Eps ⇒

by TI

$q \notin N_{Eps}(p) \wedge p \notin N_{Eps}(q)$.

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TI & Eps-Neighborhood…

Theorem. Let:

- r be any point,
- D be a set of points ordered in a non-decreasing way wrt. their distances to r;
- p be any point in D;
- q be a point following point p in D such that distance(q,r) – distance(p,r) > Eps.

Then q and all points following q in D do not belong to $N_{Eps}(p)$.

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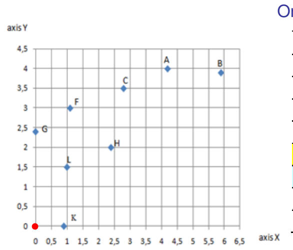
Example: TI & Eps-Neighborhood…



Ordered set of points D; Eps = 0.2

q∈D	X	Y	distance(q,r)
K	0,9	0,0	0,9
L	1,0	1,5	1,8
G	0,0	2,4	2,4
H	2,4	2,0	3,1
F	1,1	3,0	3,2
C	2,8	3,5	4,5
A	4,2	4,0	5,8
B	5,9	3,9	7,1

$\notin N_{Eps}(F)$

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TI & Eps-Neighborhood…

Theorem. Let:

- r be any point,
- D be a set of points ordered in a non-decreasing way wrt. their distances to r;
- p be any point in D;
- q be a point preceding point p in D such that distance(p,r) – distance(q,r) > Eps.

Then q and all points preceding q in D do not belong to $N_{Eps}(p)$.

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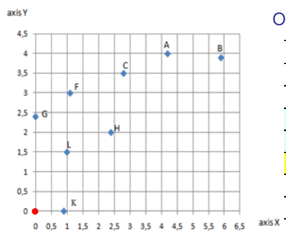
Example: TI & Eps-Neighborhood…



Ordered set of points D; Eps = 0.2

q∈D	X	Y	distance(q,r)
K	0,9	0,0	0,9
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G	0,0	2,4	2,4
H	2,4	2,0	3,1
F	1,1	3,0	3,2
C	2,8	3,5	4,5
A	4,2	4,0	5,8
B	5,9	3,9	7,1

$\notin N_{Eps}(F)$

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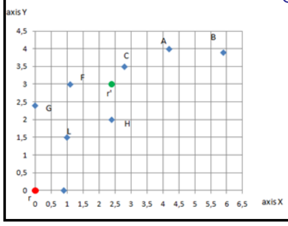
Using Many Reference Points

Example. Let r(0, 0), r'(2.4, 3.0), Eps = 0.2. Then:
distance(F,r) – distance(H,r) = 3.2 – 3.1 = 0.1 ≤ Eps.
distance(F,r') – distance(H,r') = 1.3 – 1.0 = 0.3 > Eps.
Hence, H $\notin$ N_{Eps}(p).



Ordered set of points D; Eps = 0.2

q∈D	X	Y	distance(q,r)
K	0,9	0,0	0,9
L	1,0	1,5	1,8
G	0,0	2,4	2,4
H	2,4	2,0	3,1
F	**1,1**	**3,0**	**3,2**
C	2,8	3,5	4,5
A	4,2	4,0	5,8
B	5,9	3,9	7,1

$\notin N_{Eps}(F)$

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NBC: Clustering Based on k+-neighbours and Reversed k+- neighbours

- *k+-neighbourhood of a point p* (k+NN(p)) is the set of all points in D that are distant from p by no more than any k-neighbour of p.
- A reversed *k+-neighbourhood of a point p* (Rk+NN(p)) is the set of all points in D having p as their k+-neighbour,

Rk+NN(p) = {q ∈ D| p ∈ k+NN(q)}.

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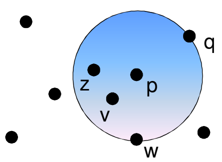
Example: k+-neighbourhood and reversed k+-neighbourhood

Let k = 3. Then |k+-NN(p)| = 4 and:

- Point q is a k+-neighbour of point p (i.e., q∈k+NN(p)).
- Point p is a reversed k+- neighbour of q (i.e., p∈Rk+NN(q)).



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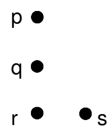
Example: k+-neighbourhood and reversed k+- neighbourhood

Let k = 2. Then:

- k+-NN(p) = {q, r}; k+-NN(q) = {p, r}; k+-NN(r) = {q, s}; k+-NN(s) = {r, q}
- Rk+-NN(p) = {q}
- Rk+-NN(q) = {p,r,s}



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Clusters generated by NBC

- Density of a subspace is expressed by means of density factor NDF understood as the ration of the cardinality of k+-neighbourhood to the cardinality of reversed k+-neighbourhood :

$$\mathrm{NDF}(p) = \frac{|Rk^{+}NN(p)|}{|k^{+}NN(p)|}.$$

- Point p playes a role of a core point if NDF(p) ≥ 1.
- A core point is understood as a seed that together with its k+-neighbourhood represents a dense space, which can be regarded as a cluster or its part.

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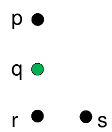
Example: k+-NN, Rk+-NN and density factor NDF

Let k = 2. Then:

- k+-NN(p) = {q, r}; k+-NN(q) = {p, r}; k+-NN(r) = {q, s}; k+-NN(s) = {r, q}
- Rk+-NN(p) = {q}; NDF(p) = 1/2
- Rk+-NN(q) = {p,r,s}; NDF(q) = 3/2



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TI-NBC: NBC Clustering with Efficient Calculation of k+-neighboorhood

By applying:

- multiple estimation of a decreasing radius within which k+-neighbourhood is guaranteed to be found
- triangle inequality property (TI)

in order to reduce the number of distance calculations.

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Hierarchical Clustering

Hierarchical Clustering

- Agglomerative:
  Initially, each point is treated as a different cluster.
- Divisive:
  Initially, the whole dataset is treated as one cluster.
- Note: Both approaches use measures of *dis(similarities) between clusters.*

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Measuring Dissimilarity of Clusters

- Single link:
  $d(C1,C2) = \min\{d(x,y) \mid x \in C1, y \in C2\}$.
- Average link:
  $d(C1,C2) = \text{avg}\{d(x,y) \mid x \in C1, y \in C2\}$.
- Complete link:
  $d(C1,C2) = \max\{d(x,y) \mid x \in C1, y \in C2\}$.
- Based on representatives of clusters:
  $d(C1,C2) = d(R1,R2)$, where
  - R1 is *a representative* (*a set of representatives*) of C1,
  - R2 is *a representative* (*a set of representatives*) of C2.

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Iterative-Optimization Clustering

Partitioning Algorithm: k-Means

1) Randomly choose k data points in D to play a role of centroids of k distinct clusters.
2) Each point p in D assign to the cluster represented by p’s closest centroid.
3) Recompute the centroids of obtained clusters.
4) If stopping criterion is not met, go to 2.

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Alternative Stopping Criteria

- No point is reassigned to a different cluster.
- There is no (or minimal) change of centroids.
- In iteration j:

$$\frac{E_{j-1}-E_j}{E_j} < \varepsilon,$$

  - $E_j = \sum_{i=1}^{k} \sum_{X \in C_i} d(X, M_i)$, where
    C_i is the i-th cluster, M_i is the centroid of C_i;
  - ε is a user-defined threshold value.

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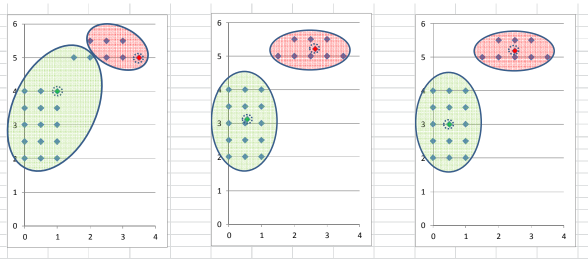
Example: Algorithm k-means



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Scaling of Attribute Values

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Scaling of Continuous Attributes: range

Let:

- v be a value of a continuous attribute A,
- v_{min} be the least value of A,
- v_{max} be the greatest value of A.

Then:

$$range(v) = \frac{v - v_{min}}{v_{max} - v_{min}}.$$

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Scaling of Continuous Attributes: Z-score

Let D consist of *n* data points that have values $v_1, \ldots, v_n$, for a continuous attribute A. Then:

$$Z - score(v) = \frac{v - \mu}{s}, \text{ where}$$

- the mean for A:

$$\mu = \frac{1}{n}(v_1 + \cdots + v_n),$$

- the mean absolute deviation for A:

$$s = \frac{1}{n}(|v_1 - \mu| + \cdots + |v_n - \mu|).$$

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Quality of Clustering

Evaluation of Clustering

- Evaluation based on external information: calculated clusters can be compared with real clusters (e.g. determined by a knowledgeable user).
- Evaluation based on internal information.

External Evaluation of Clustering with Purity

$Purity = \frac{1}{n}\sum_{g \in G} max_{c \in C} |g \cap c|$, where

C – real clusters,

G – discovered clusters,

n – the number of points.

Example: External Evaluation of Clustering with Purity

Real clusters	Discovered clusters	Correct assignment of points to clusters
L	1	
L	3	
L	2	Yes (L)
L	2	Yes (L)
L	2	Yes (L)
H	2	
H	1	Yes (H)
H	1	Yes (H)
H	3	Yes (H)
H	3	Yes (H)

Purity = 7/10

External Evaluation of Clustering with Rand

$Rand = \frac{|TP| + |TN|}{\binom{n}{2}}$, where

- TP – the set of pairs of objects each of which is contained in some real cluster and is contained in some discovered cluster,
- TN – the set of pairs of objects each of which is neither contained in any real cluster nor is contained in any discovered cluster,
- *n* – the number of objects.

Example: External Evaluation of Clustering with Rand

Id	Real clusters	Discovered clusters
1	L	1
2	L	3
3	L	2
4	L	2
5	L	2
6	H	2
7	H	1
8	H	1
9	H	3
10	H	3

- Pairs of objects each of which is contained in some real cluster and is contained in some discovered cluster:

  TP = {(3,4), (3,5), (4,5), (7,8), (9,10).}

- Pairs of objects each of which is neither contained in any real cluster nor is contained in any discovered cluster:

  TN = {(1,6), (1,9), (1,10), (2,6), (2,7), (2,8), (3,7), (3,8), (3,9), (3,10), (4,7), (4,8), (4,9), (4,10), (5,7), (5,8), (5,9), (5,10)}.

$Rand = \frac{|TP| + |TN|}{\binom{10}{2}} = \frac{5+18}{45} \approx 0.51$

Internal Evaluation of Clustering with Davies-Bouldin

$Davies\text{−}Bouldin = \frac{1}{n}\sum_{i=1}^{n} \max_{j \neq i}\left(\frac{\sigma_i+\sigma_j}{d(c_i,c_j)}\right)$, where

- n – the number of discovered clusters,
- c_k – the centroid of cluster k,
- σ_k – the average distance of points in cluster k to its centroid c_k,
- $d(c_i, c_j)$ – the distance between centroids c_i, c_j.

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Internal Evaluation of Clustering with Silhouette Coefficient

Quality of assigning a point *i* to its cluster:

$$s(i) = \frac{b(i)-a(i)}{\max\{b(i),a(i)\}}, \text{ where}$$

- $a(i)$ – the average distance of point *i* to all other points in its cluster,
- $b(i)$ – the least average distance of point *i* to all points of a cluster that does not contain point *i*.

Quality of a cluster *C* – the average $s(i)$ over all points *i* in *C*.

Quality of clustering – the average $s(i)$ over all points *i* in the whole data set.

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