WARSAW UNIVERSITY OF TECHNOLOGY
DEVELOPMENT PROGRAMME

Data Clustering

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HUMAN CAPITAL
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Basic Notions

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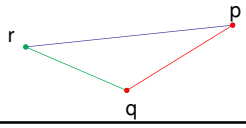
Distance Metric

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

- ∀p,q, distance(p, q) ≥ 0;
- ∀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 */.



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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) = $\sqrt[m]{\sum_{i=1..n}|p_i - q_i|^m}$

(Minkowski function is a distance metric for $m \geq 1$).

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DBSCAN: Density-Based Clustering with Noise

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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,

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

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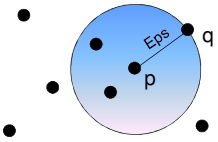
Example: Eps-Neighborhood

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



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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.

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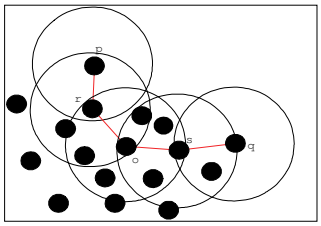
Example: Core Points

For MinPts = 6:

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



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Clusters and Noise 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 unless they were earlier assigned to another cluster.
- A point that is not included in any cluster (that is, does not belong to Eps-neighborhood of any core point) is called a *noise point*.

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Non-Core Points in DBSCAN

- **Property:** A noise point is a non-core point that does not belong to any cluster (that is, which does not belong to Eps-neighborhood of any core point).
- A *border point* is a non-core point that belongs to a cluster (that is, which belongs to Eps-neighbourhood of at least one core point).

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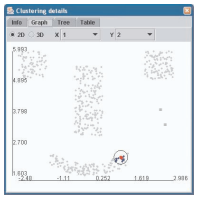
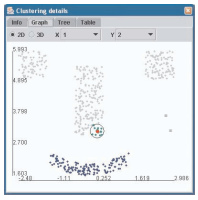
Clusters in DBSCAN…





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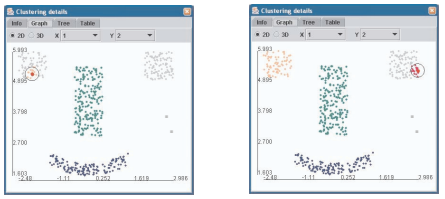
Clusters in DBSCAN…



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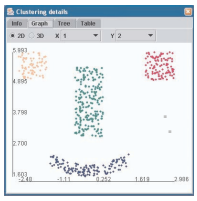
Clusters in DBSCAN



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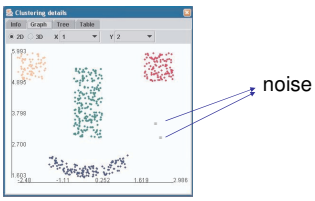
Clusters and Noise in DBSCAN



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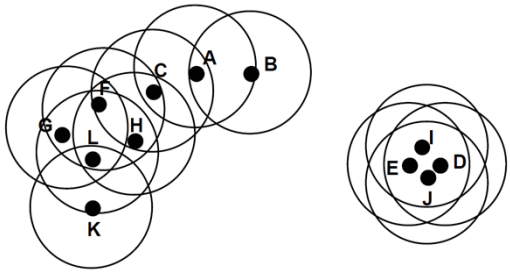
DBSCAN – Definition's Illustration



minPts = 4

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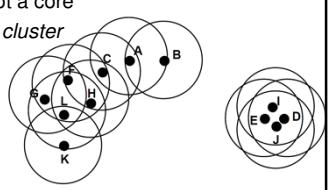
DBSCAN – Extension of a Cluster

- 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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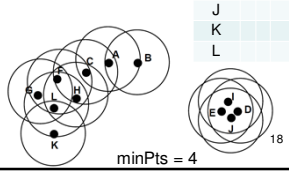
DBSCAN – Example Execution…

- 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

- ClId = 1.
- $N_{Eps}(A)$ = {A, B, C} – A is non-core.

q∈D	x	y	ClId
A			N
B			
C			
D			
E			
F			
G			
H			
I			
J			
K			
L			



minPts = 4

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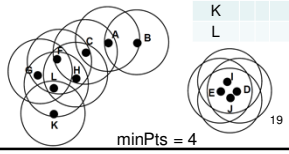
DBSCAN – Example Execution…

- 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

- ClId = 1.
- $N_{Eps}(B) = \{B, A\}$ – B is non-core.

q∈D	x	y	ClId
A			N
B			N
C			
D			
E			
F			
G			
H			
I			
J			
K			
L			



minPts = 4

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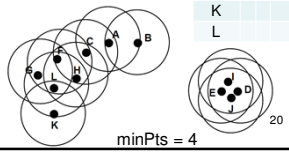
DBSCAN – Example Execution…

- 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

- ClId = 1.
- $N_{Eps}(C) = \{C, A, F, H\}$ – C is a core.
- seeds = {A, F, H}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			
H			1
I			
J			
K			
L			



minPts = 4

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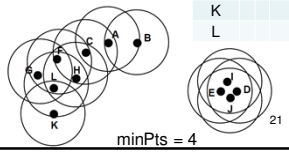
DBSCAN – Example Execution…

- 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

- ClId = 1.
- seeds = {A, F, H}.
- $N_{Eps}(A) = \{A, B, C\}$ – A is non-core.
- Updated seeds = {F, H}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			
H			1
I			
J			
K			
L			



minPts = 4

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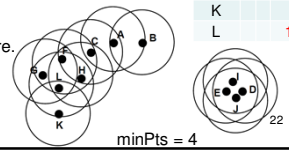
DBSCAN – Example Execution…

- 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

- ClId = 1.
- seeds = {F, H}.
- $N_{Eps}(F) = \{F, C, G, H, L\}$ – F is a core.
- Updated seeds = {H, G, L}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			1
H			1
I			
J			
K			
L			1



minPts = 4

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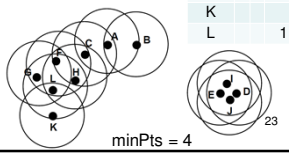
DBSCAN – Example Execution…

- 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

- ClId = 1.
- seeds = {H, G, L}.
- $N_{Eps}(H) = \{H, C, F, L\}$ – H is a core.
- Updated seeds = {G, L}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			1
H			1
I			
J			
K			
L			1



minPts = 4

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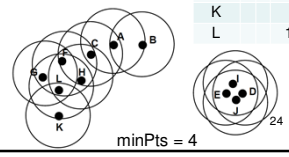
DBSCAN – Example Execution…

- 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

- ClId = 1.
- seeds = {G, L}.
- $N_{Eps}(G) = \{G, F, L\}$ – G is non-core.
- Updated seeds = {L}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			1
H			1
I			
J			
K			
L			1



minPts = 4

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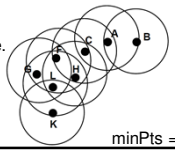
DBSCAN – Example Execution…

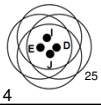
- Dealing with a point q from an analysed neighborhood:

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

- ClId = 1.
- seeds = {L}.
- N_{Eps}(L) = {L, F, G, H, K} – L is a core.
- Updated seeds = {K}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			1
H			1
I			
J			
K			1
L			1





minPts = 4

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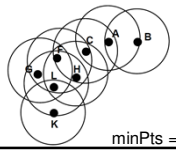
DBSCAN – Example Execution…

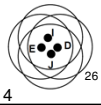
- Dealing with a point q from an analysed neighborhood:

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

- ClId = 1.
- seeds = {K}.
- N_{Eps}(K) = {K, L} – K is non-core.
- Updated seeds = {}.
- Cluster 1 was created.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			
E			
F			1
G			1
H			1
I			
J			
K			1
L			1





minPts = 4

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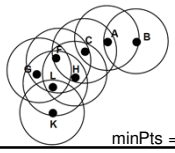
DBSCAN – Example Execution…

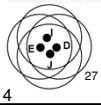
- Dealing with a point q from an analysed neighborhood:

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

- ClId = 2.
- N_{Eps}(D) = {D, E, I, J} – D is a core.
- seeds = {E, I, J}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			2
E			2
F			1
G			1
H			1
I			2
J			2
K			1
L			1





minPts = 4

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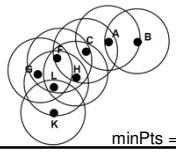
DBSCAN – Example Execution…

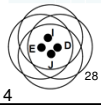
- Dealing with a point q from an analysed neighborhood:

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

- ClId = 2.
- seeds = {E, I, J}.
- N_{Eps}(E) = {E, D, I, J} – E is a core.
- Updated seeds = {I, J}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			2
E			2
F			1
G			1
H			1
I			2
J			2
K			1
L			1





minPts = 4

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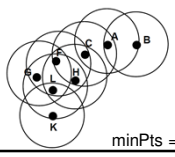
DBSCAN – Example Execution…

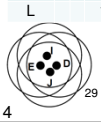
- Dealing with a point q from an analysed neighborhood:

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

- ClId = 2.
- seeds = {I, J}.
- N_{Eps}(I) = {I, D, E, J} – I is a core.
- Updated seeds = {J}.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			2
E			2
F			1
G			1
H			1
I			2
J			2
K			1
L			1





minPts = 4

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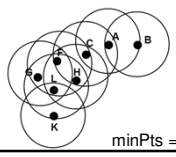
DBSCAN – Example Execution…

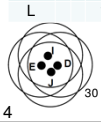
- Dealing with a point q from an analysed neighborhood:

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

- ClId = 2.
- seeds = {J}.
- N_{Eps}(J) = {J, D, E, I} – J is a core.
- Updated seeds = {}.
- Cluster 2 was created.

q∈D	x	y	ClId
A			~~N~~ 1
B			N
C			1
D			2
E			2
F			1
G			1
H			1
I			2
J			2
K			1
L			1





minPts = 4

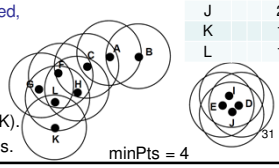
DBSCAN – Example Execution

- 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

q∈D	x	y	Cld
A			~~N~~ 1
B			N
C			1
D			2
E			2
F			1
G			1
H			1
I			2
J			2
K			1
L			1

- All points in dataset D were processed, so the clustering is done.
- The obtained clustering result: 2 clusters and 1 noise point (here: point B).
- Cluster 1 has 3 border points (A, G, K).
- Cluster 2 does not have border points.



minPts = 4

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Properties of Points in DBSCAN

- For given values of Eps and minPts:
  - DBSCAN determines noise points in a deterministic way independently of the order of processing points in dataset D.
  - DBSCAN assigns each core point exactly to one cluster in a deterministic way independently of the order of processing points in dataset D.
  - DBSCAN assigns a border point to one cluster. The cluster to which it will be assigned depends on the order of processing points in dataset D.

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Illustration of Border Point Property

- DBSCAN assigns a border point to one cluster. The cluster to which it will be assigned depends on the order of processing points in dataset D:
- **Example.** Let minPts = 4. Point r belongs to $N_{Eps}(p)$ and $N_{Eps}(q)$, so r will be assigned either to the red cluster or to the blue one by DBSCAN.

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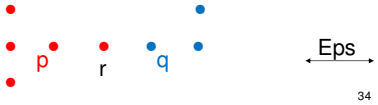
Size of a DBSCAN Cluster

- It may happen that size of a cluster is less than minPts.
- **Example.** Let minPts = 4. Assume that point r, which belongs to $N_{Eps}(p)$ and $N_{Eps}(q)$, was assigned to the red cluster. Then the blue cluster will have only 3 points.



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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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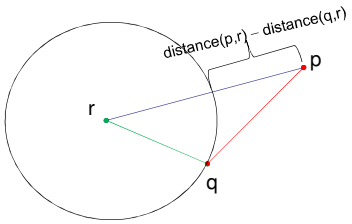
TI for pessimistic estimation of distance

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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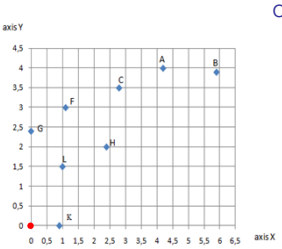
Example: TI & Eps-Neighborhood…



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	∈ $N_{Eps}(F)$
A	4,2	4,0	5,8	
B	5,9	3,9	7,1	

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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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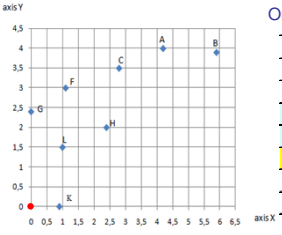
Example: TI & Eps-Neighborhood…



Ordered set of points D; Eps = 0.2

q∈D	X	Y	distance(q,r)	
K	0,9	0,0	0,9	
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	

∈ $N_{Eps}(F)$

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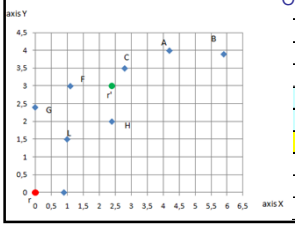
Using Many Reference Points

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 ∉ 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**	∉ N_{Eps}(F)
C	2,8	3,5	4,5	
A	4,2	4,0	5,8	
B	5,9	3,9	7,1	

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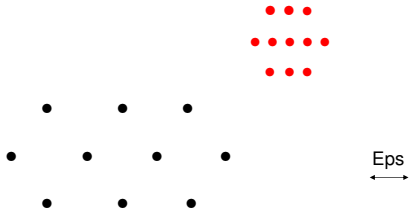
Disadvantages of DBSCAN

- DBSCAN may not be able to discover clusters of different density.
- **Example.** Let minPts = 4. Only red cluster will be found.



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NBC: Neighbourhood Clustering with Nearest Neighbours and Reversed Nearest Neighbours

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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,

$$Rk^+NN(p) = \{q \in D | \ p \in k^+NN(q)\}.$$

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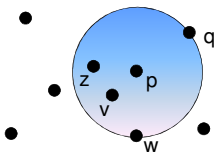
Example: k⁺-neighbourhood and reversed k⁺-neighbourhood

Let k = 3. Then $|k^+\text{-NN}(p)| = 4$ 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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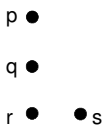
Example: k⁺-neighbourhood and reversed k⁺- neighbourhood

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 ratio of the cardinality of reversed k^+-neighbourhood to the cardinality of k^+-neighbourhood:

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

- Point p plays a role of *a* core point if $NDF(p) \geq 1$.
- A core point is perceived 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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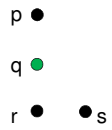
Example: k^+-NN, Rk^+-NN and density factor NDF

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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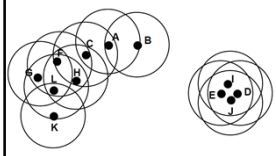
NBC – Calculation of k^+-NN and $|Rk^+$-NN| …



k = 3

q∈D	x	y	k^+-NN	$\|Rk^+$-NN$\|$	NDF	Cld
A	4.2	4.0	B, C, H	0		
B	5.9	3.9		~~0~~ 1		
C	2.8	3.5		~~0~~ 1		
D	12.0	1.3		0		
E	10.0	1.3		0		
F	1.1	3.0		0		
G	0.0	2.4		0		
H	2.4	2.0		~~0~~ 1		
I	11.5	1.8		0		
J	11.0	1.0		0		
K	0.9	0.0		0		
L	1.0	1.5		0		

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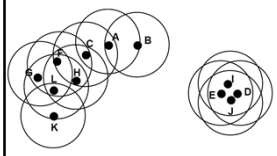
NBC – Calculation of k^+-NN and $|Rk^+$-NN| …



k = 3

q∈D	x	y	k^+-NN	$\|Rk^+$-NN$\|$	NDF	Cld
A	4.2	4.0	B, C, H	~~0~~ 1		
B	5.9	3.9	A, C, H	1		
C	2.8	3.5		~~1~~ 2		
D	12.0	1.3		0		
E	10.0	1.3		0		
F	1.1	3.0		0		
G	0.0	2.4		0		
H	2.4	2.0		~~1~~ 2		
I	11.5	1.8		0		
J	11.0	1.0		0		
K	0.9	0.0		0		
L	1.0	1.5		0		

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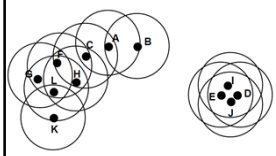
NBC – Calculation of k^+-NN and $|Rk^+$-NN| …



k = 3

q∈D	x	y	k^+-NN	$\|Rk^+$-NN$\|$	NDF	Cld
A	4.2	4.0	B, C, H	~~1~~ 2		
B	5.9	3.9	A, C, H	1		
C	2.8	3.5	A, F, H	2		
D	12.0	1.3		0		
E	10.0	1.3		0		
F	1.1	3.0		~~0~~ 1		
G	0.0	2.4		0		
H	2.4	2.0		~~2~~ 3		
I	11.5	1.8		0		
J	11.0	1.0		0		
K	0.9	0.0		0		
L	1.0	1.5		0		

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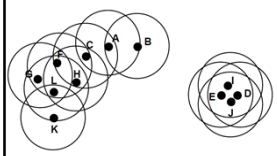
NBC – Calculation of k^+-NN and $|Rk^+$-NN|



k = 3

q∈D	x	y	k^+-NN	$\|Rk^+$-NN$\|$	NDF	Cld
A	4.2	4.0	B, C, H	2		
B	5.9	3.9	A, C, H	1		
C	2.8	3.5	A, F, H	3		
D	12.0	1.3	E, I, J	3		
E	10.0	1.3	D, I, J	3		
F	1.1	3.0	G, H, L	~~3~~ 4		
G	0.0	2.4	F, H, L	~~2~~ 3		
H	2.4	2.0	C, F, L	~~6~~ 7		
I	11.5	1.8	D, E, J	3		
J	11.0	1.0	D, E, I	3		
K	0.9	0.0	G, H, L	~~0~~ 1		
L	1.0	1.5	F, G, H, K	4		

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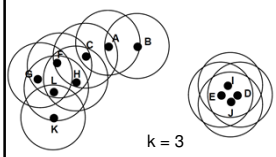
NBC – Calculation of NDF



k = 3

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	
B	5.9	3.9	A, C, H	1	1/3	
C	2.8	3.5	A, F, H	3	3/3	
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	
G	0.0	2.4	F, H, L	3	3/3	
H	2.4	2.0	C, F, L	7	7/3	
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	

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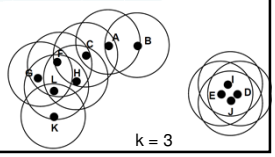
NBC – Looking for first cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	N
B	5.9	3.9	A, C, H	1	1/3	
C	2.8	3.5	A, F, H	3	3/3	
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	
G	0.0	2.4	F, H, L	3	3/3	
H	2.4	2.0	C, F, L	7	7/3	
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	

- Cld = 1.
- NDF(A) < 1, so A is non-core.

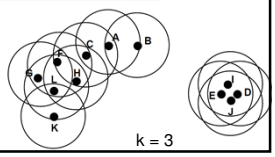


k = 3

NBC – Looking for first cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	N
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	
G	0.0	2.4	F, H, L	3	3/3	
H	2.4	2.0	C, F, L	7	7/3	
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	

- Cld = 1.
- NDF(B) < 1, so B is non-core.

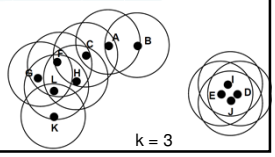


k = 3

NBC – Looking for first cluster

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	N 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	

- Cld = 1.
- NDF(C) ≥ 1, so C is a core.
- Cluster 1 is initialized.
- seeds = {F, H}.

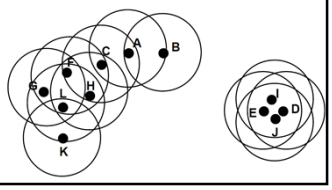


k = 3

NBC – Extension of a Cluster

- Dealing with a point q from an analysed k⁺-NN:

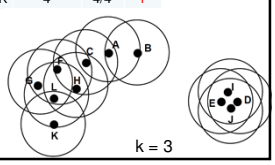
if q.ClusterId = Unclassified **then** // q is not classified
  assign q *to currently created cluster*
  add q *to seeds*
else if q.ClusterId = N // q is not a core
  assign q *to currently created cluster*
else
  do nothing



NBC – Extending first cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	N 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	1

- Cld = 1.
- seeds = {F, H}.
- NDF(F) ≥ 1, so F is a core.
- Updated seeds = {H, G, L}.

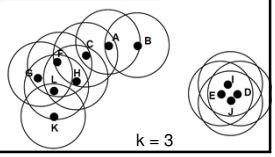


k = 3

NBC – Extending first cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	1

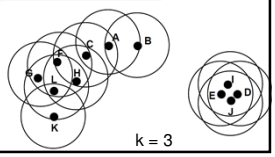
- Cld = 1.
- seeds = {H, G, L}
- NDF(H) ≥ 1, so H is a core.
- Updated seeds = {G, L}.



NBC – Extending first cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	
L	1.0	1.5	F, G, H, K	4	4/4	1

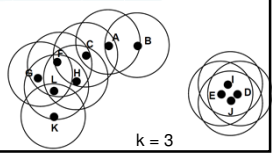
- Cld = 1.
- seeds = {G, L}
- NDF(G) ≥ 1, so G is a core.
- Updated seeds = {L}.



NBC – Extending first cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

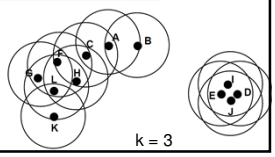
- Cld = 1.
- seeds = {L}
- NDF(L) ≥ 1, so L is a core.
- Updated seeds = {K}.



NBC – Extending first cluster

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	
E	10.0	1.3	D, I, J	3	3/3	
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	
J	11.0	1.0	D, E, I	3	3/3	
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

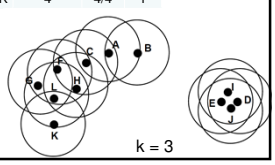
- Cld = 1.
- seeds = {K}
- NDF(K) < 1, so K is non-core.
- Updated seeds = {}.
- Cluster 1 was created.



NBC – Looking for second cluster

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	2
E	10.0	1.3	D, I, J	3	3/3	2
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	2
J	11.0	1.0	D, E, I	3	3/3	2
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

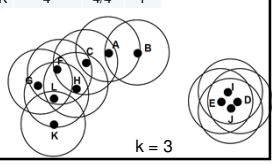
- Cld = 2.
- NDF(D) ≥ 1, so D is a core.
- Cluster 2 is initialized.
- seeds = {E, I, J}.



NBC – Extending second cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	2
E	10.0	1.3	D, I, J	3	3/3	2
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	2
J	11.0	1.0	D, E, I	3	3/3	2
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

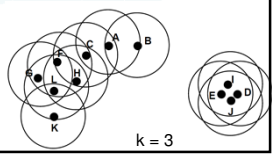
- Cld = 2.
- seeds = {E, I, J}.
- NDF(E) ≥ 1, so E is a core.
- Updated seeds = {I, J}.



NBC – Extending second cluster…

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	2
E	10.0	1.3	D, I, J	3	3/3	2
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	2
J	11.0	1.0	D, E, I	3	3/3	2
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

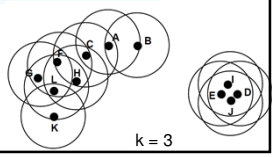
- Cld = 2.
- seeds = {I, J}.
- NDF(I) ≥ 1, so I is a core.
- Updated seeds = {J}.



NBC – Extending second cluster

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	2
E	10.0	1.3	D, I, J	3	3/3	2
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	2
J	11.0	1.0	D, E, I	3	3/3	2
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

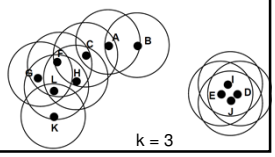
- Cld = 2.
- seeds = {J}.
- NDF(J) ≥ 1, so J is a core.
- Updated seeds = {}.
- Cluster 2 was created.



NBC – Result of Clustering

q∈D	x	y	k⁺-NN	|Rk⁺-NN|	NDF	Cld
A	4.2	4.0	B, C, H	2	2/3	~~N~~ 1
B	5.9	3.9	A, C, H	1	1/3	N
C	2.8	3.5	A, F, H	3	3/3	1
D	12.0	1.3	E, I, J	3	3/3	2
E	10.0	1.3	D, I, J	3	3/3	2
F	1.1	3.0	G, H, L	4	4/3	1
G	0.0	2.4	F, H, L	3	3/3	1
H	2.4	2.0	C, F, L	7	7/3	1
I	11.5	1.8	D, E, J	3	3/3	2
J	11.0	1.0	D, E, I	3	3/3	2
K	0.9	0.0	G, H, L	1	1/3	1
L	1.0	1.5	F, G, H, K	4	4/4	1

- All points in dataset D were processed, so the clustering is done.
- The obtained clustering result: 2 clusters and 1 noise point (here: point B).
- Cluster 1 has 2 border points (A, K).
- Cluster 2 does not have border points.



WARSAW UNIVERSITY OF TECHNOLOGY DEVELOPMENT PROGRAMME

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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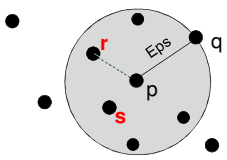
Estimation of the radius of the smallest $N_{Eps}(p)$ that contains k-NN(p) (k⁺-NN(p))

- **Property:** Let Eps denote the greatest distance from p to some other k points. Then:

$$k\text{-NN}(p) \subseteq k^{+}\text{–NN}(p) \subseteq N_{Eps}(p).$$

- **Example.** Let k = 2 and the distances from point p to the (arbitrarily chosen) points r and q have already been calculated. Let Eps equal the greater of these distances. Then:

$$k\text{-NN}(p) = k^{+}\text{–NN}(p) = \{r, s\} \subseteq N_{Eps}(p)$$

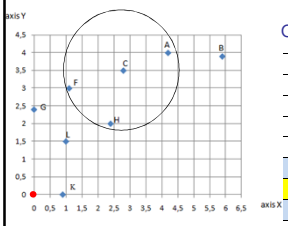


WARSAW UNIVERSITY OF TECHNOLOGY DEVELOPMENT PROGRAMME

TI in Searching k⁺-NN…

Example. Let **r(0, 0)**, k = 2 and first k candidates for k⁺-NN of point C are those with the least pessimistic estimation of its distances to C, that is, *Candidates* = {A, F}.

- Then, Eps = max(distance(C,A), distance(C,F)) = max{1.49, 1.77} = 1.77.



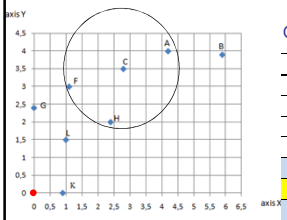
Ordered set of points D

q	X	Y	distance(q,r)	distance(C,q)
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	1.77
C	2,8	3,5	4,5	
A	4,2	4,0	5,8	1.49
B	5,9	3,9	7,1	

TI in Searching k⁺-NN…

Example. **r(0, 0)**, k = 2. *Candidates* = {A, F}.

- distance(B,r) - distance(C,r) = 2.6 > Eps = 1.77.
- So, distance(B,C) > Eps = 1.77 and B ∉ k⁺-NN(C).



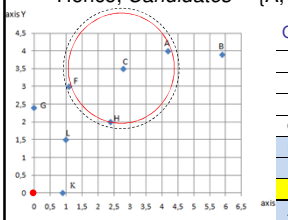
Ordered set of points D; Eps = 1.77

q	X	Y	distance(q,r)	distance(C,q)
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	1.77
C	2,8	3,5	4,5	
A	4,2	4,0	5,8	1.49
B	5,9	3,9	7,1	

TI in Searching k⁺-NN…

Example. Let **r(0, 0)**, k = 2. *Candidates* = {A, F}.

- distance(C,r) - distance(H,r) = 1.4 < Eps = 1.77.
- distance(C,H) = 1.55 < Eps = 1.77.
- Hence, *Candidates'* = {A, H} and Eps' = 1.55.



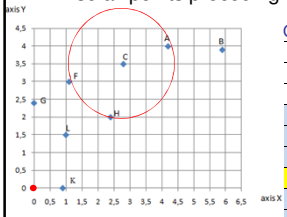
Ordered set of points D; Eps = 1.77

q	X	Y	distance(q,r)	distance(C,q)
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	1.55
F	1,1	3,0	3,2	1.77
C	2,8	3,5	4,5	
A	4,2	4,0	5,8	1.49
B	5,9	3,9	7,1	

TI in Searching k⁺-NN

Example. Let **r(0, 0)**, k = 2. Candidates' = {A, H}.

- distance(C,r) - distance(G,r) = 2.1 > Eps' = 1.55.
- So, distance(C,G) > Eps' = 1.55 and G ∉ k⁺-NN(C).
- Also all points preceding G do not belong to k⁺-NN(C).



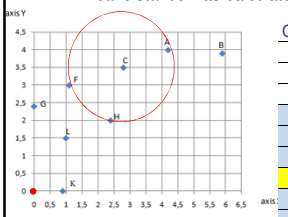
Ordered set of points D; Eps' = 1.55

q	X	Y	distance(q,r)	distance(C,q)
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	1.55
F	1,1	3,0	3,2	1.77
C	2,8	3,5	4,5	
A	4,2	4,0	5,8	1.49
B	5,9	3,9	7,1	

TI in Searching k⁺-NN

Example. Let **r(0, 0)**, k = 2. Candidates' = {A, H}.

- Summary of looking for k⁺-NN(C):
  - k⁺-NN = {A, H}.
  - Pessimistic estimation of distance was calculated for 5 points.
  - Real distance was calculated for 3 points.



Ordered set of points D; Eps' = 1.55

q	X	Y	distance(q,r)	distance(C,q)
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	1.55
F	1,1	3,0	3,2	1.77
C	2,8	3,5	4,5	
A	4,2	4,0	5,8	1.49
B	5,9	3,9	7,1	

Scaling of Attribute Values

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 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.

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External Evaluation of Clustering with Purity

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

C – real clusters,

G – discovered clusters,

n – the number of points.

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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

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External Evaluation of Clustering with Rand

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

- TP – the set of pairs of objects that are in the same real cluster and in the same discovered cluster,
- TN – the set of pairs of objects that are in different real clusters and in different discovered clusters,
- *n* – the number of objects.

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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 the set of pairs of objects that are in the same real cluster and in the same discovered cluster:

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

- Pairs of objects the set of pairs of objects that are in different real clusters and in different discovered clusters:

  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)}.

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

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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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