Clustering algorithms

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ISIMA / LIMOS

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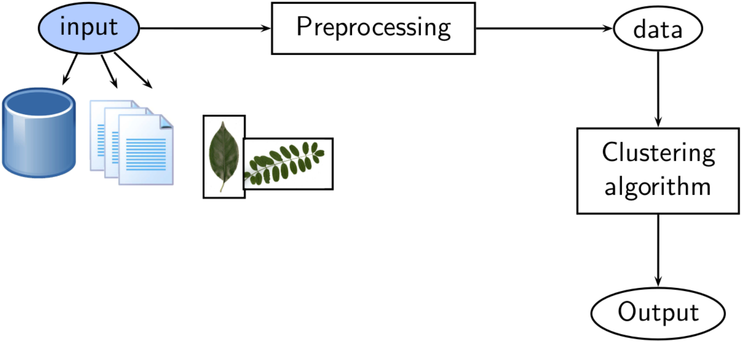
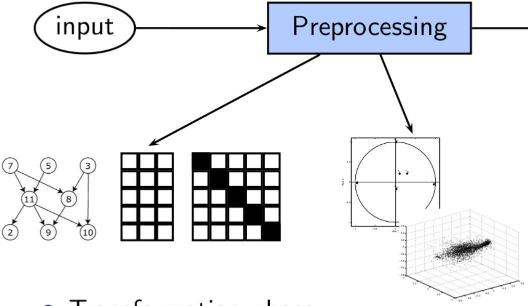
Outline

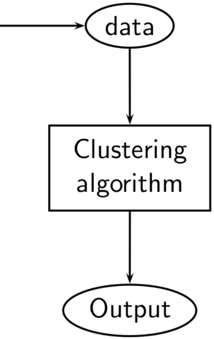
Outline

Global scheme



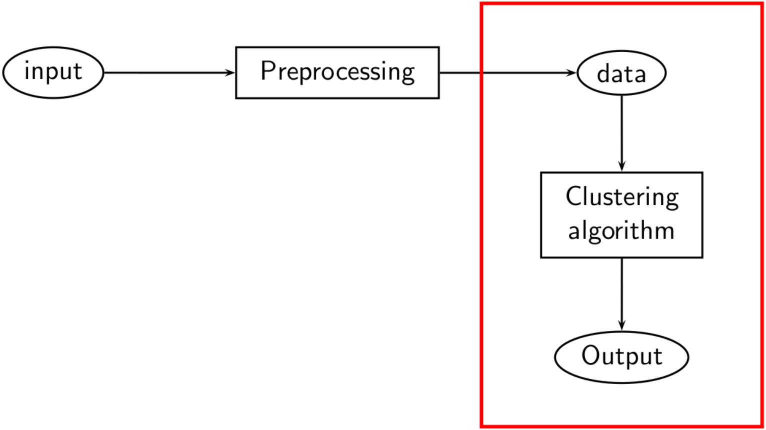
Global scheme





- Transformation phase
- Data analysis
  - PCA, CA, correlation measures, . . .
- normalization, feature selection, . . .

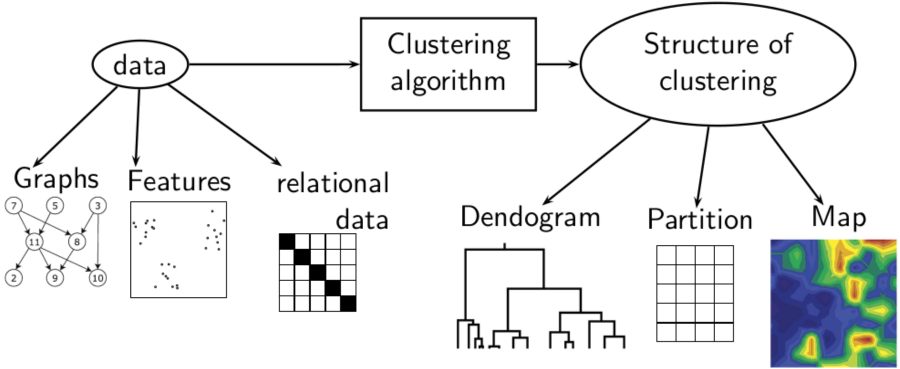
Global scheme



Clustering process

Clustering

Grouping objects into cluster following a similarity notion



Clustering process

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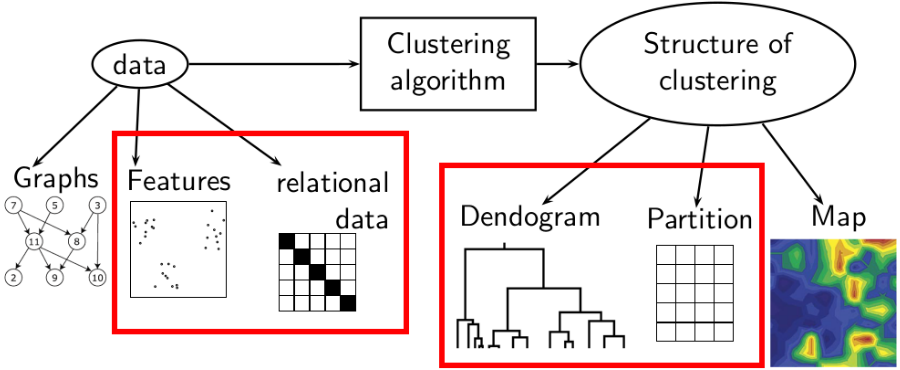
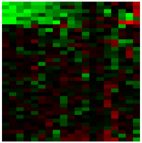
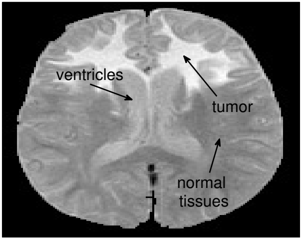


Applications

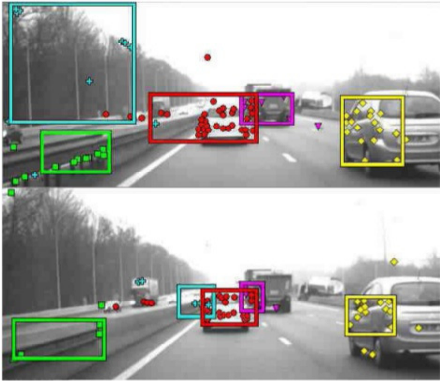
- Biology and bioinformatics
  - grouping genes with related expression patterns using DNA microarray [?]
  - clustering plants or animals
- Medicine [?]





Applications

- Detection of objects
  - robotics
  - video surveillance
  - automotive driving assistance [?]



Applications

- Geology
  - earth-quake and volcanoes studies
- Social network analysis
- Market research
  - Findind groups of customers
  - Predicting behavior of shopping
- World wide web [**?**]
  - documents engine search
  - images engine search

Problematic : the background knowledge

Clustering

Grouping objects into cluster following a similarity notion

Which similarity/dissimilarity definition should be chosen ?

Problematic : the background knowledge

Clustering

Grouping objects into cluster following a similarity notion

Which similarity/dissimilarity definition should be chosen ?

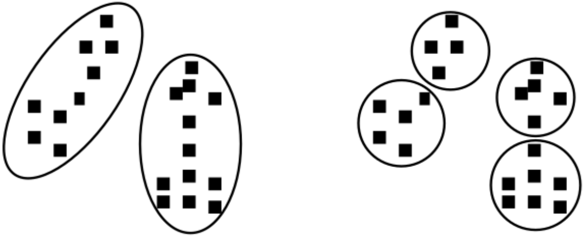
Distance measures

Two major family of distances :

- Euclidean distances
  - Mahalanobis distance : $d(\mathbf{x}, \mathbf{y}) = \sqrt{\mathbf{x} - \mathbf{y})^\top \Sigma (\mathbf{x} - \mathbf{y})}$
  - Manhattan distance : $d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{p} |x_i - y_i|$
- Non-Euclidean distances
  - Edit distance : measures difference between 2 strings
  - Jaccard index : measures dissimilarity between sample sets

Problematic : clustering or subclustering

Which clusters retains ?



Other problematics

- How to measure the correctness of a partition ?
- How to deal with noise in the feature vectors ?
- What to do if we have uncertain data ?
- How to detect outliers ?
- ...

Notations

Input notations

- $\mathbf{x}_i \in \{\mathbf{x}_1 \dots \mathbf{x}_N\}$ the set of objects with p attributes

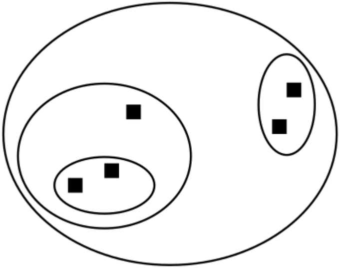
Clustering notations

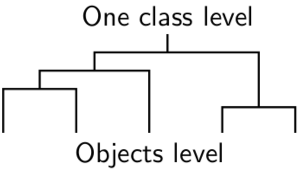
- $\omega_k \in \Omega = \{\omega_1 \dots \omega_c\}$ the set of clusters
- $n_1, n_2, \dots n_c$ the number of objects belonging to $\omega_1, \omega_2, \omega_c$

Outline

Hierarchical clustering

Produces a set of nested cluster organised as a dendrogram.





Two categories of hierarchical clustering

- Agglomerative methods
- Divise methods

Hierarchical clustering

Advantages

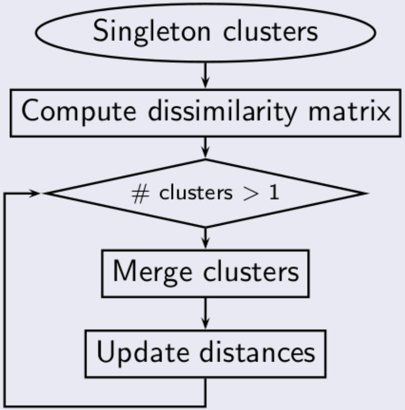
- No assumptions on the number of clusters
- Visualization of subclusterings
- Deterministic methods

Disadvantages

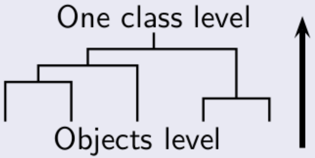
- Interpretation of the hierarchy can be complex
- Considerable amount of data implies large dendrogram

Agglomerative clustering

Basic scheme

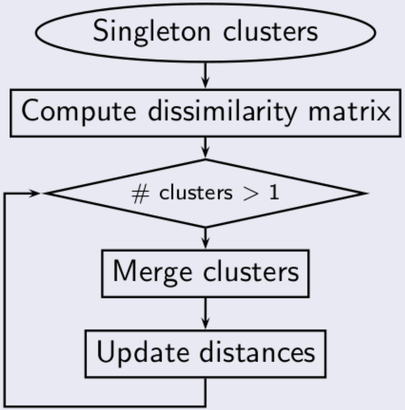


Bottom-up hierarchy

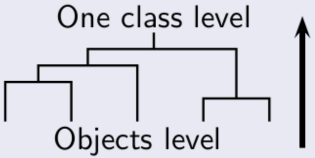


Agglomerative clustering

Basic scheme



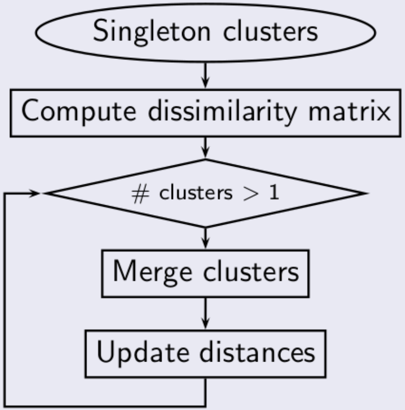
Bottom-up hierarchy



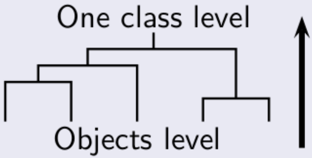
- Merge criterion : distance minimum

Agglomerative clustering

Basic scheme



Bottom-up hierarchy



- Merge criterion : distance minimum
- Update distances
  - single-link
  - complete-link
  - average-link

The single-link algorithm [? ?]

Distance calculation

Let c_i and c_j be two clusters

- The distance between c_i and c_j is the minimum distance between any object in c_i and any object in c_j

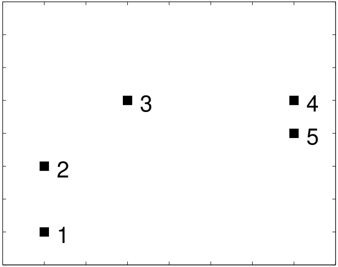
$\Rightarrow$ The distance is defined by the two most similar objects

Underlying idea

- Importance is given to regions where clusters are closed
- Overall structure of the cluster is negliged

$\Rightarrow$ local similarity-based clustering method

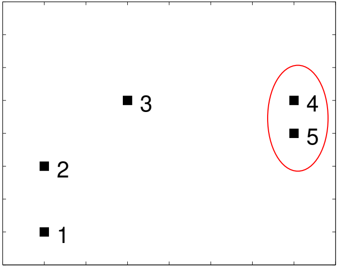
Single-link example



	1	2	3	4	5
1	0	1	2.2	3.6	3.4
2	1	0	1.4	3.2	3
3	2.2	1.4	0	2	2.1
4	3.6	3.2	2	0	0.5
5	3.4	3	2.1	0.5	0

1 2 3 4 5

Single-link example



	1	2	3	4	5
1	0	1	2.2	3.6	3.4
2	1	0	1.4	3.2	3
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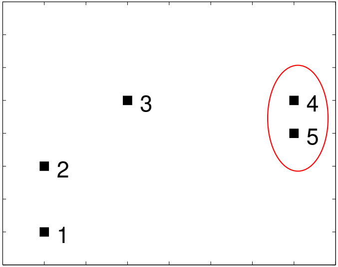
5	3.4	3	2.1	0.5	0

Single-link example



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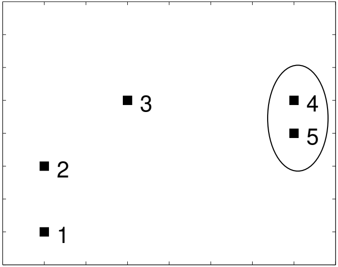
2	1	0	1.4	3.2	3
3	2.2	1.4	0	2	2.1
4	3.6	3.2	2	0	0.5
5	3.4	3	2.1	0.5	0

Update distances

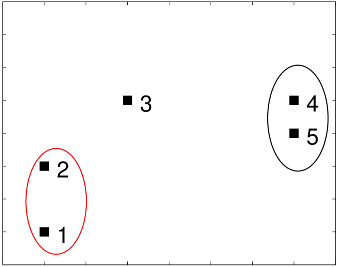
d((4,5),1) = min(d(4,1),d(5,1)) = 3.4
d((4,5),2) = min(d(4,2),d(5,2)) = 3
d((4,5),3) = min(d(4,3),d(5,3)) = 2

Single-link example



	1	2	3	(4,5)
1	0	1	2.2	3.4
2	1	0	1.4	3
3	2.2	1.4	0	2
(4,5)	3.4	3	2	0

Single-link example



	1	2	3	(4,5)
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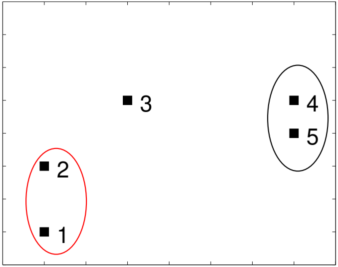
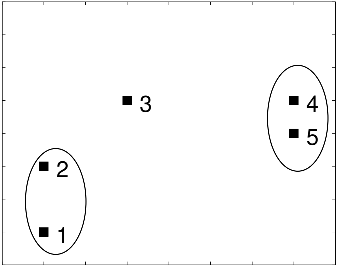


	1	2	3	(4,5)
1	0	1	2.2	3.4
2	1	0	1.4	3
3	2.2	1.4	0	2
(4,5)	3.4	3	2	0

Update distances

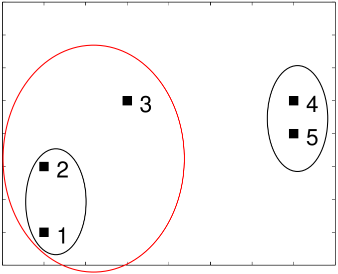
$$d((1,2),3) = \min(d(1,3),d(2,3)) = 1.4$$
$$d((1,2),(4,5)) = \min(d(1,(4,5)), d(2,(4,5))) = 3$$

Single-link example

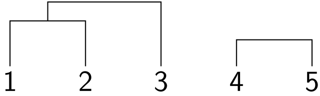


	(1,2)	3	(4,5)
(1,2)	0	1.4	3
3	1.4	0	2
(4,5)	3	2	0

Single-link example



	(1,2)	3	(4,5)
(1,2)	0	1.4	3
3	1.4	0	2
(4,5)	3	2	0



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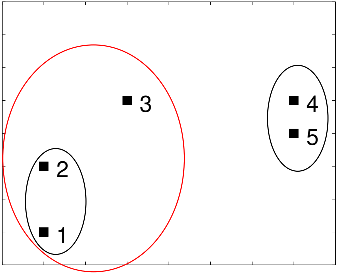
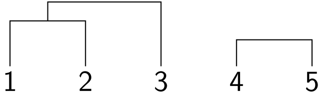


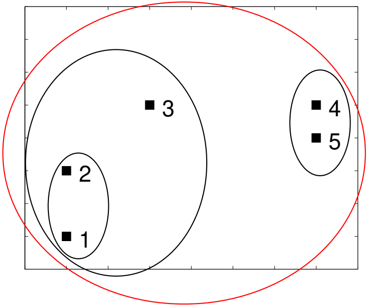


	(1,2)	3	(4,5)
(1,2)	0	1.4	3
3	1.4	0	2
(4,5)	3	2	0

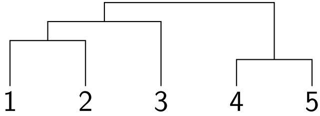
Update distances

d((1,2,3),(4,5)) $=$
min(d(3,(4,5)),d((1,2)(4,5))) $= 2$

Single-link example



	(1,2)	3	(4,5)
(1,2)	0	1.4	3
3	1.4	0	2
(4,5)	3	2	0

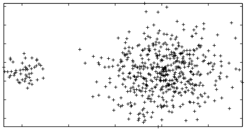


Update distances

d((1,2,3),(4,5)) =
min(d(3,(4,5)),d((1,2)(4,5))) = 2

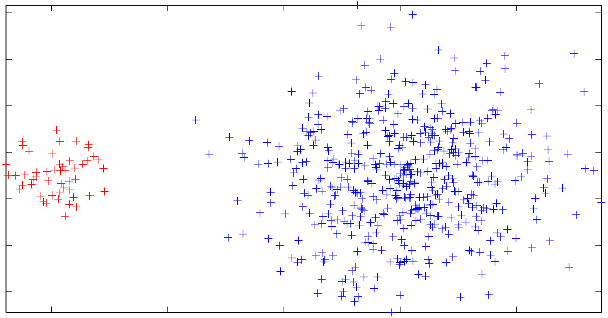
Strengths of the single-link clustering

Original data



Enable to find :

- non elliptical shaped groups
- unbalanced groups



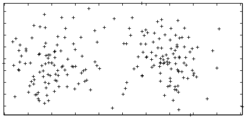
Single-link algorithm

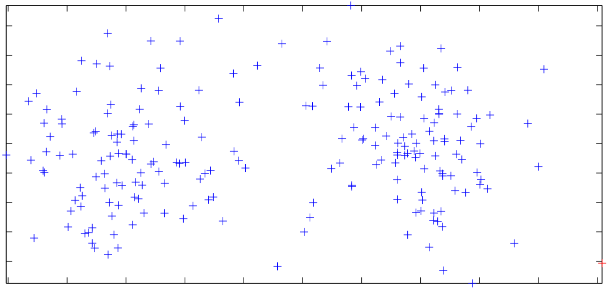
Limitations of the single-link clustering

Sensitive to

- noise
- outliers

Original data





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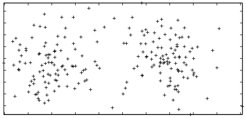
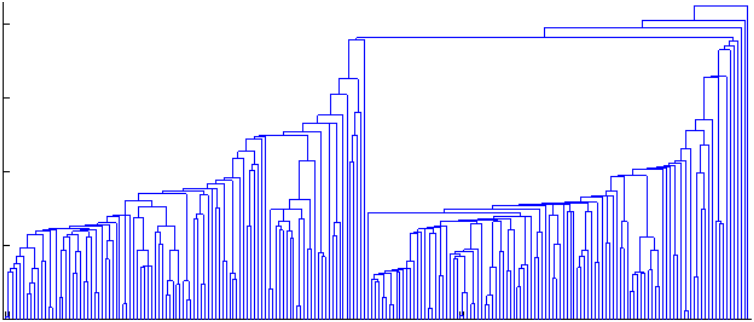




dendrogram

The complete-link algorithm [?]

Distance calculation

Let c_i and c_j be two clusters

- The distance between c_i and c_j is the maximum distance between any object in c_i and any object in c_j

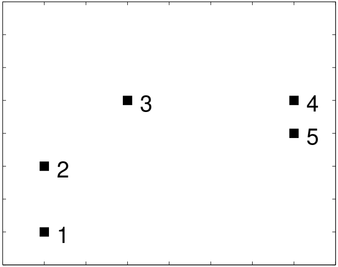
$\Rightarrow$ The distance is defined by the two most dissimilar objects

Underlying idea

- Merge cluster with the smallest diameter
- Importance is given to the cluster structure

$\Rightarrow$ global similarity-based clustering method

Complete-link example



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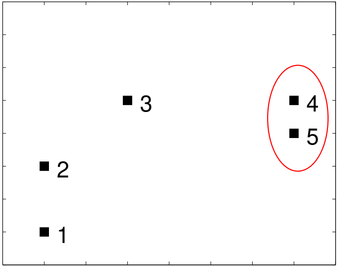
2	1	0	1.4	3.2	3
3	2.2	1.4	0	2	2.1
4	3.6	3.2	2	0	0.5
5	3.4	3	2.1	0.5	0

1 2 3 4 5

Complete-link example



	1	2	3	4	5
1	0	1	2.2	3.6	3.4
2	1	0	1.4	3.2	3
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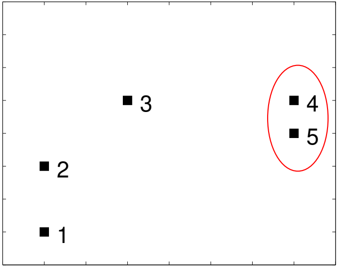
4	3.6	3.2	2	0	0.5
5	3.4	3	2.1	0.5	0

Complete-link example

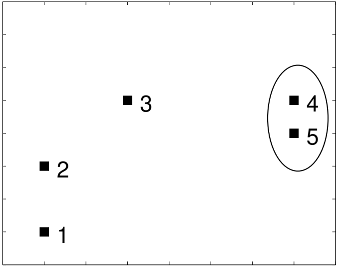


	1	2	3	4	5
1	0	1	2.2	3.6	3.4
2	1	0	1.4	3.2	3
3	2.2	1.4	0	2	2.1
4	3.6	3.2	2	0	0.5
5	3.4	3	2.1	0.5	0

Update distances

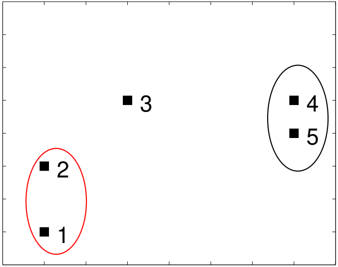
d((4,5),1)=max(d(4,1),d(5,1))=3.6
d((4,5),2)=max(d(4,2),d(5,2))=3.2
d((4,5),3)=max(d(4,3),d(5,3))=2.1

Complete-link example



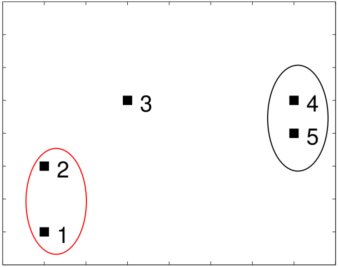
	1	2	3	(4,5)
1	0	1	2.2	3.6
2	1	0	1.4	3.2
3	2.2	1.4	0	2.1
(4,5)	3.6	3.2	2.1	0

Complete-link example



	1	2	3	(4,5)
1	0	1	2.2	3.6
2	1	0	1.4	3.2
3	2.2	1.4	0	2.1
(4,5)	3.6	3.2	2.1	0

Complete-link example

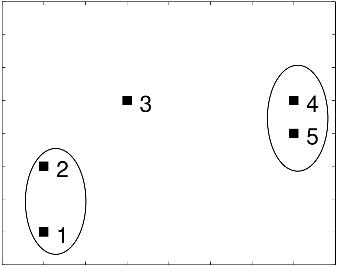


	1	2	3	(4,5)
1	0	1	2.2	3.6
2	1	0	1.4	3.2
3	2.2	1.4	0	2.1
(4,5)	3.6	3.2	2.1	0

Update distances

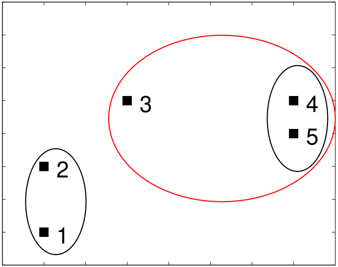
$$\begin{aligned} d((1,2),3) &= \max(d(1,3),d(2,3)){=}2.2 \\ d((1,2),(4,5)) &= \max(d(1,(4,5)), \\ &\qquad d(2,(4,5))){=}3.6 \end{aligned}$$

Complete-link example

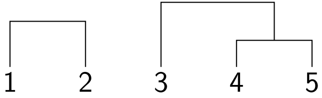


	(1,2)	3	(4,5)
(1,2)	0	2.2	3.6
3	2.2	0	2.1
(4,5)	3.6	2.1	0

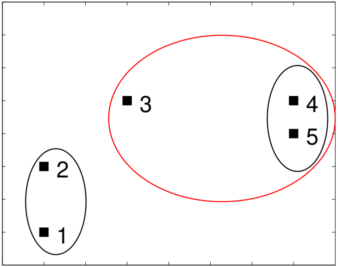
Complete-link example



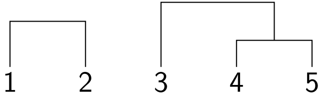
	(1,2)	3	(4,5)
(1,2)	0	2.2	3.6
3	2.2	0	2.1
(4,5)	3.6	2.1	0



Complete-link example



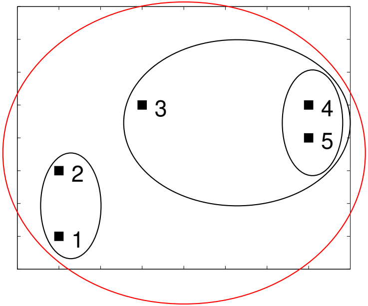
	(1,2)	3	(4,5)
(1,2)	0	2.2	3.6
3	2.2	0	2.1
(4,5)	3.6	2.1	0



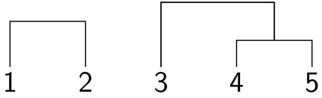
Update distances

d((1,2),(3,4,5))=
max(d((1,2),3),d((1,2),(4,5)))=3.6

Complete-link example



	(1,2)	3	(4,5)
(1,2)	0	2.2	3.6
3	2.2	0	2.1
(4,5)	3.6	2.1	0

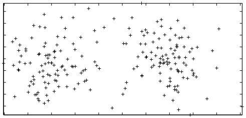


Update distances

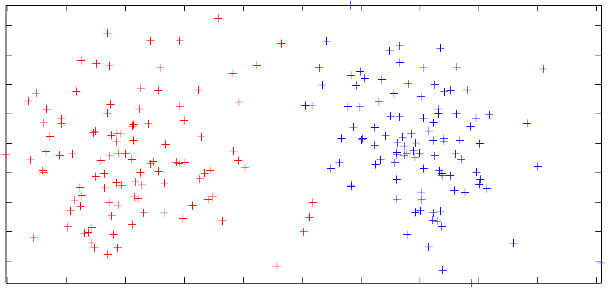
d((1,2),(3,4,5))=
max(d((1,2),3),d((1,2),(4,5)))=3.6

Strengths of the complete-link clustering

Original data



- Enable to find compact shaped cluster
- Less sensitive to noise



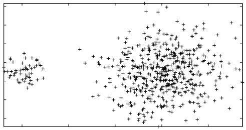
Complete-link algorithm

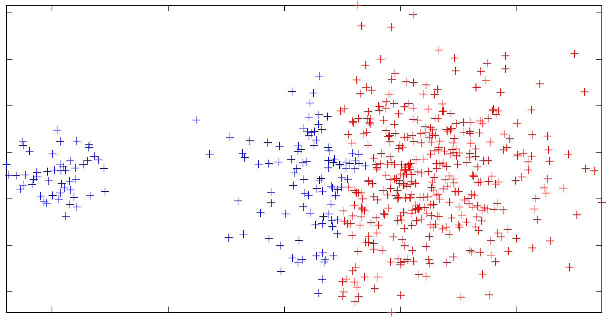
Limitations of the complete-link clustering

Sensitive to

- unbalanced cluster

Original data





Complete-link algorithm

Average-link algorithm [?]

Distance calculation

Let c_i and c_j be two clusters

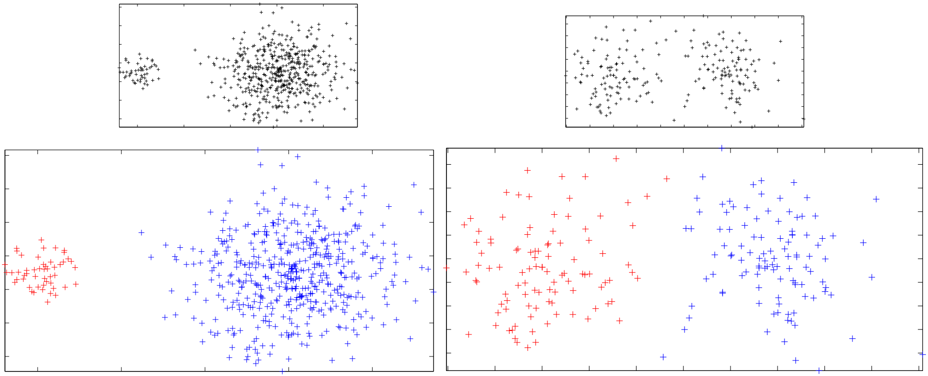
- The distance between c_i and c_j is the average distance between any object in c_i and any object in c_j

$$\Rightarrow d(c_i, c_j) = \frac{1}{|c_i||c_j|} \sum_{x_i \in c_i, x_j \in c_j} d(x_i, x_j)$$

Underlying idea

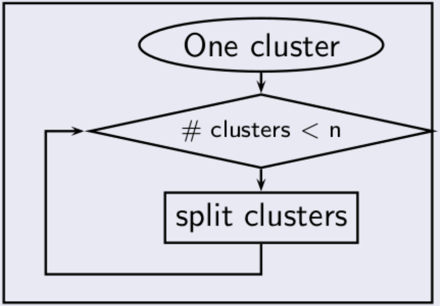
Reducing drawbacks associated to single and complete link

Strengths of the average-link clustering

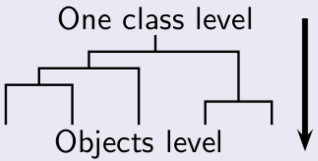


Divise clustering

Basic scheme

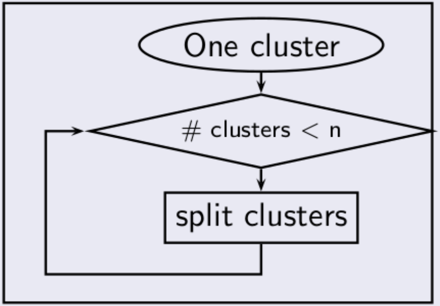


Top-down hierarchy



Divise clustering

Basic scheme



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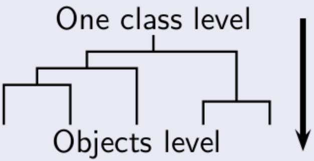
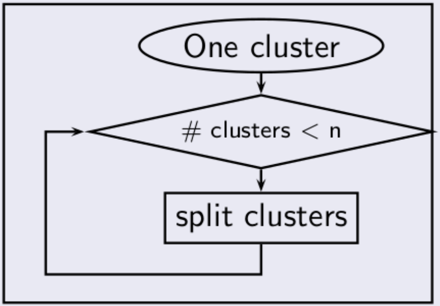


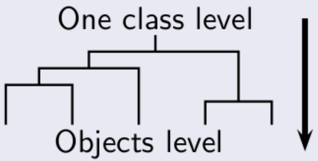
- Split criterion :
  - using one/several attributes for a specific split
  - intercluster distances

Divise clustering

Basic scheme



Top-down hierarchy



- Split criterion :
  - using one/several attributes for a specific split
  - intercluster distances

⇒ computationally intensive

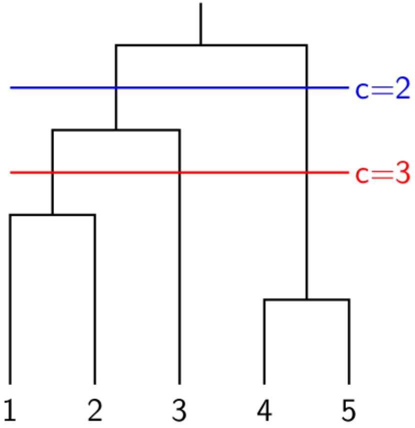
⇒ less widely used than agglomerative methods

The cut of dendrogram

Getting a crisp partition

Goal : Find the α-cut that

- select c groups
- find balanced clusters
- minimize a clustering validation measure
- select the maximum distance between two merges
- ...



Outline

Partitional clustering

Produces a hard or fuzzy partition.

Types of partition

- Hard partition
  - Each object $\mathbf{x}_i$ belongs to an exclusive class ω_k
  - $p_{ik} = \{0, 1\}$, $\sum p_{ik} = 1$
- Fuzzy partition
  - $\mathbf{x}_i$ has a degree of membership for each class ω_k
  - $u_{ik} \in [0, 1]$, $\sum_{k=1}^{c} u_{ik} = 1$

Density-based clustering methods

Basic idea

Clusters are dense regions in the data space.

Important notions

- The density
- The connectivity between objects

Advantages

Non-parametric methods, i.e. no assumption about :

- the number of clusters
- their distribution

The DBSCAN algorithm

Neighborhood definition

The neighborhood of an object $\mathbf{x}_i$ is :

$$N_\varepsilon(\mathbf{x}_i) = \{\mathbf{x}_j \quad s.t. \quad d_{ij} \leq \varepsilon\}$$

Ddr definition

$\mathbf{x}_j$ is directly density-reachable from $\mathbf{x}_i$ if

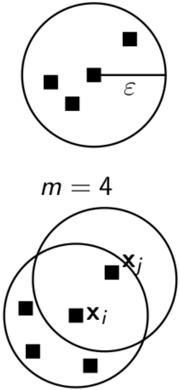
$\rightarrow$ $\mathbf{x}_j \in N_\varepsilon(\mathbf{x}_i)$

$\rightarrow$ $|N_\varepsilon(\mathbf{x}_i)| \geq m$

Consequence

Carefull ! The definition is non symmetric :

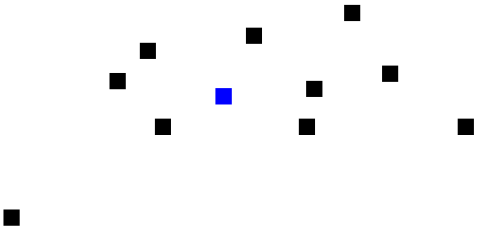
$$\mathbf{x}_j \text{ is ddr from } \mathbf{x}_i \nRightarrow \mathbf{x}_i \text{ is ddr from } \mathbf{x}_j$$



The DBSCAN algorithm

Expansion rule

If $\mathbf{x}_i \in \omega_k$ and $\mathbf{x}_j$ is ddr from $\mathbf{x}_i$ then $\mathbf{x}_j \in \omega_k$



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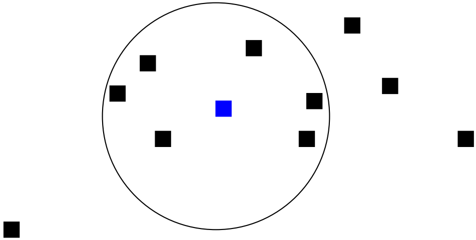

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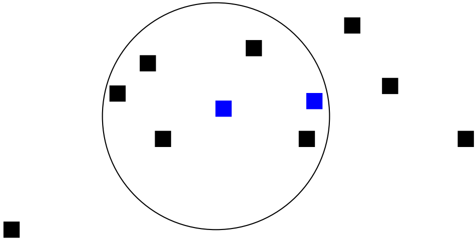

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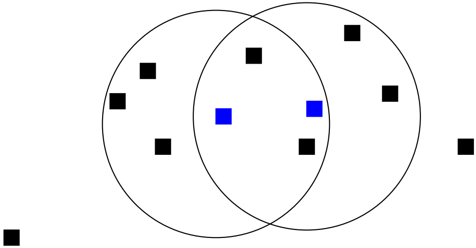

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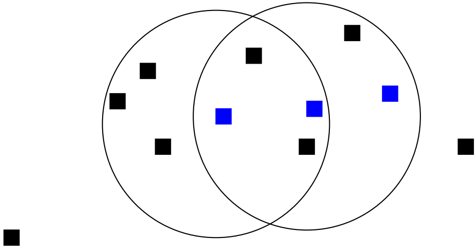

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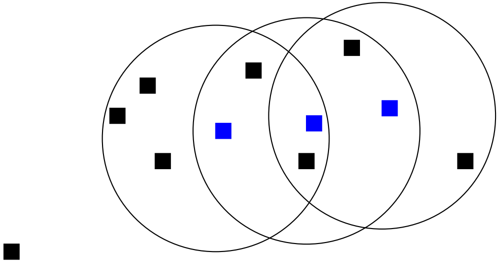

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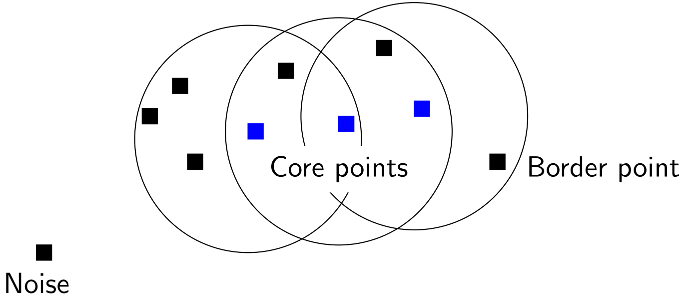
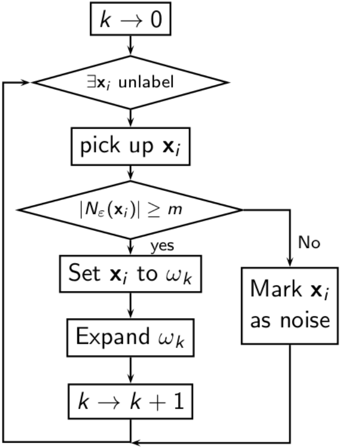
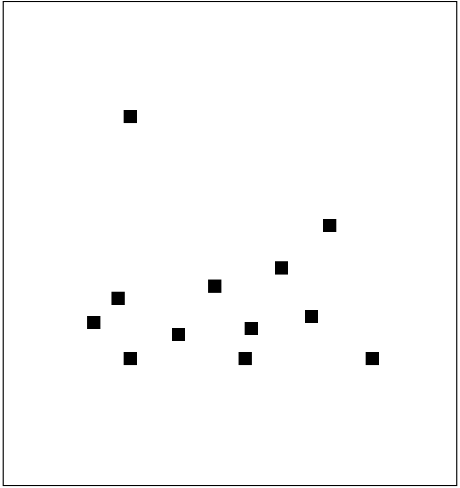
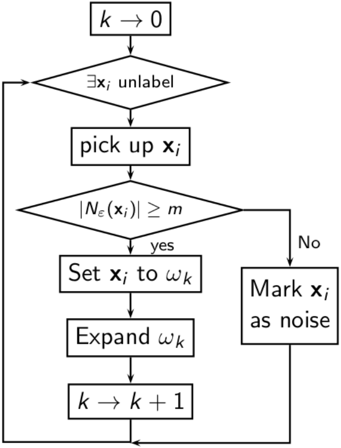


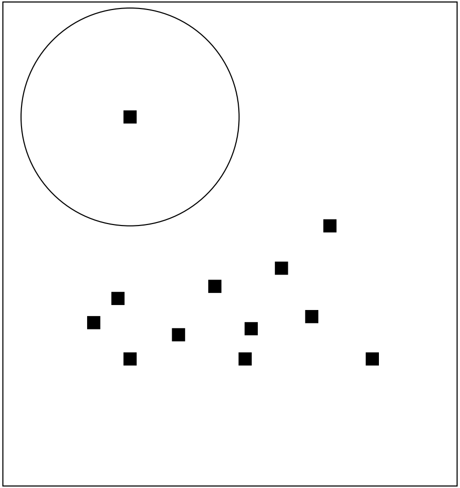
The DBSCAN algorithm





The DBSCAN algorithm





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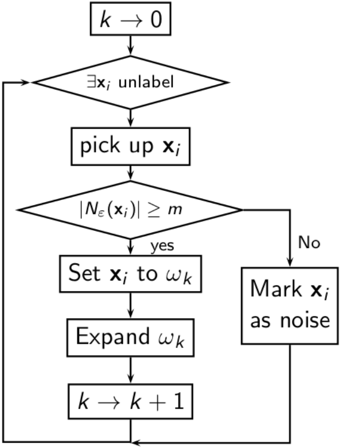

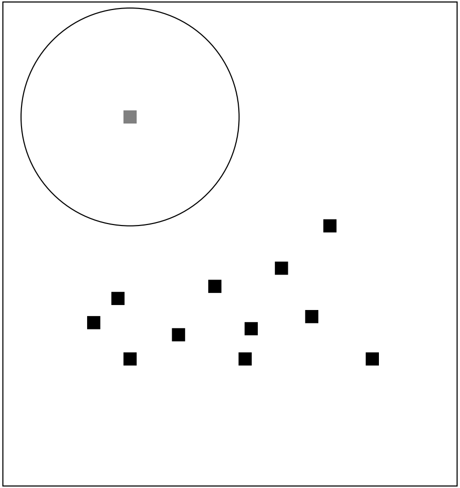

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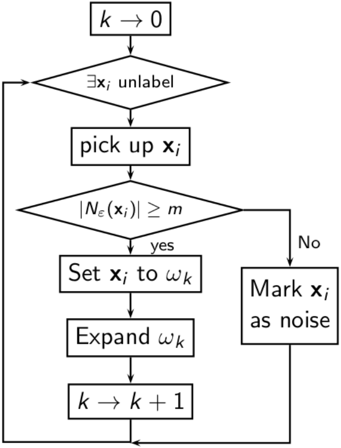

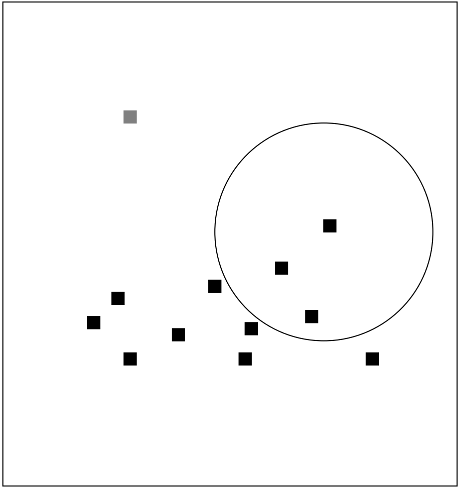

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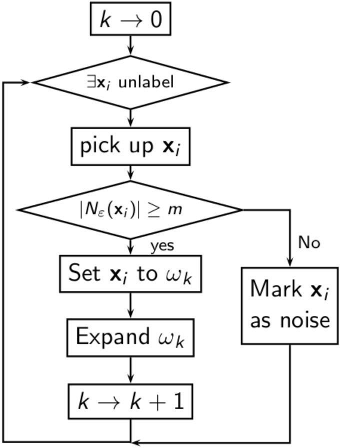

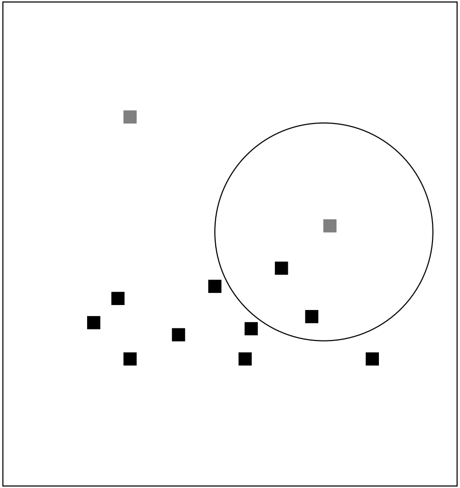

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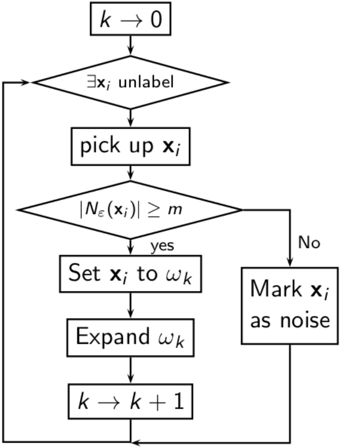

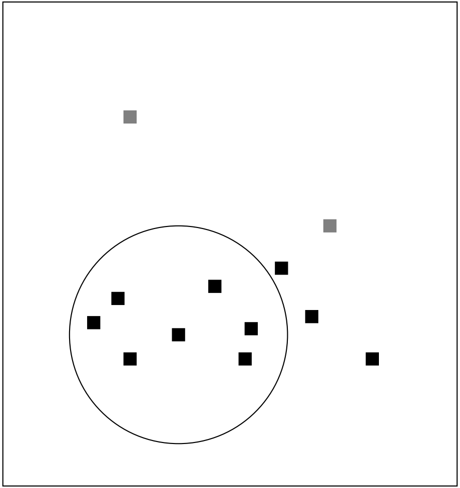

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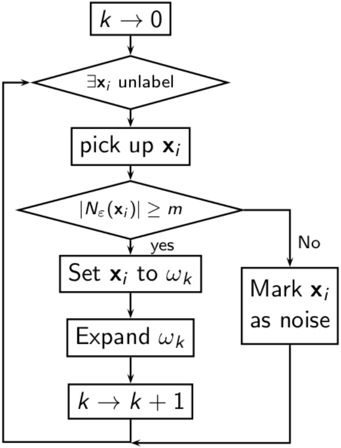
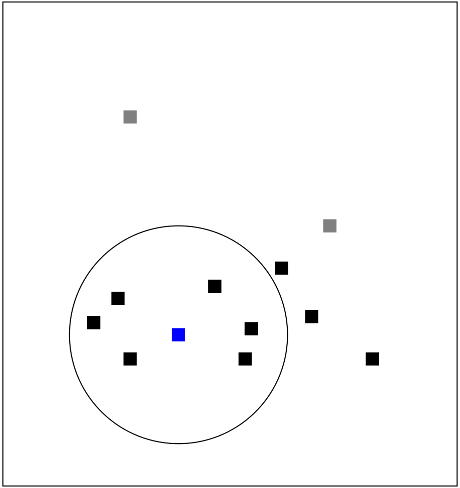
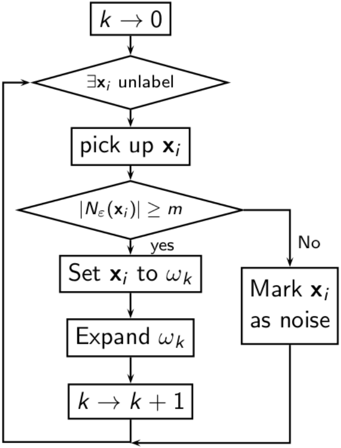
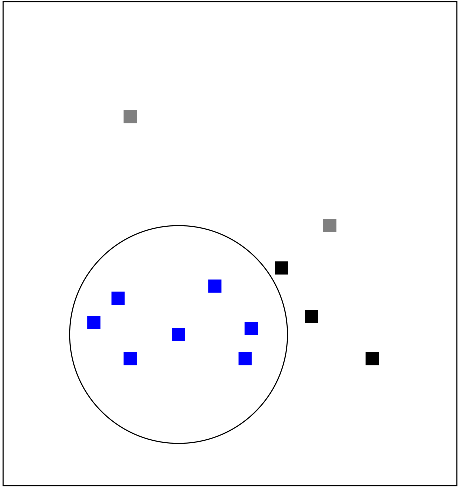




The DBSCAN algorithm





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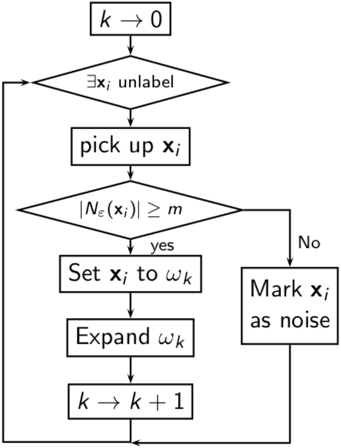

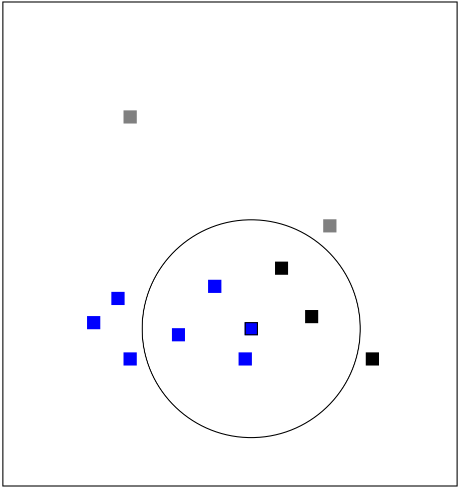

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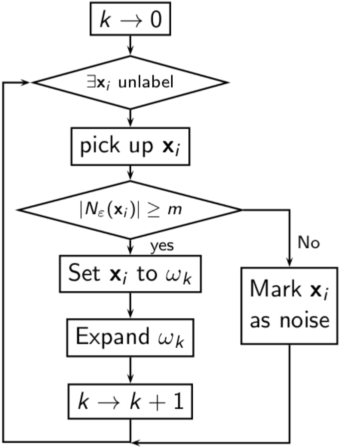

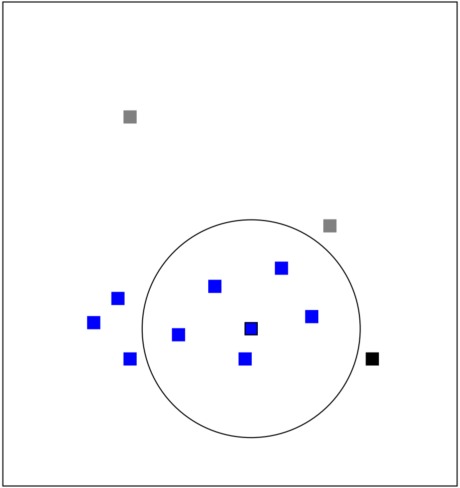

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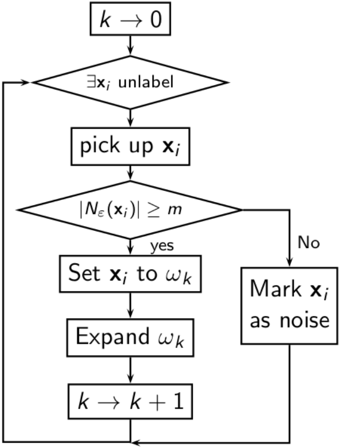

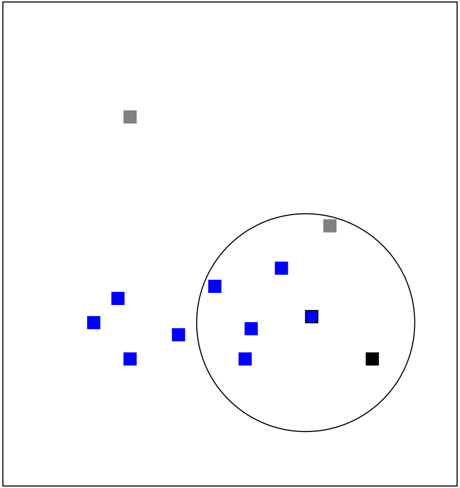

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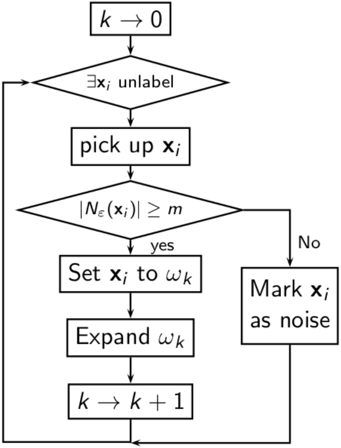

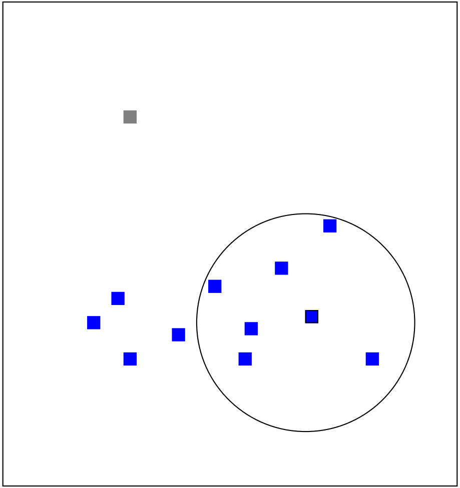

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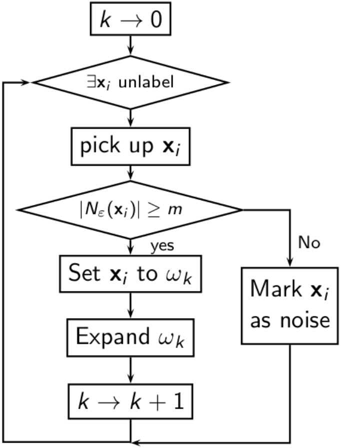
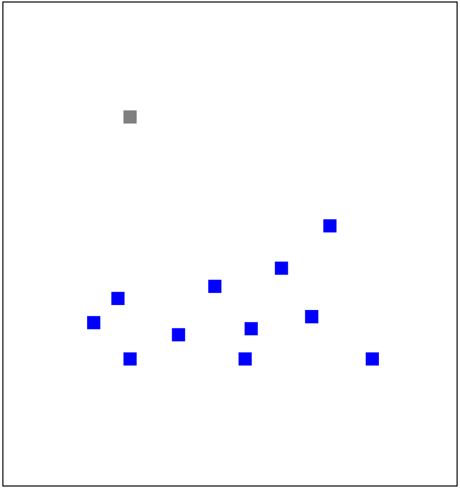
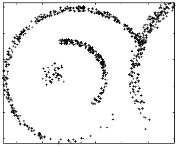




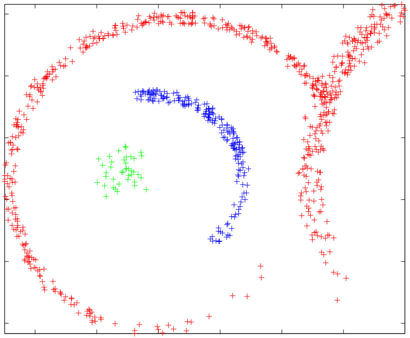
Strengths of DBSCAN

Original data



Enable to :

- find arbitrary shapes and unbalanced groups
- deal with noise



DBSCAN (m=5, $\varepsilon = 3$)

Strengths of DBSCAN

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- deal with noise

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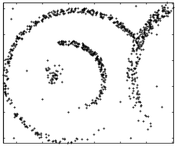
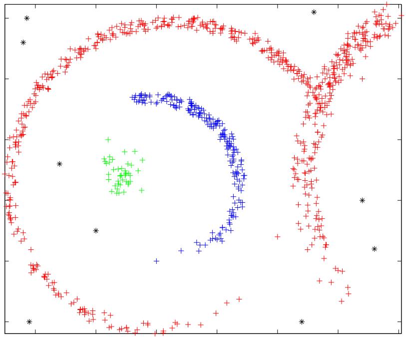




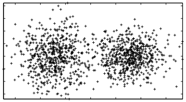
DBSCAN (m=5, $\varepsilon = 3$)

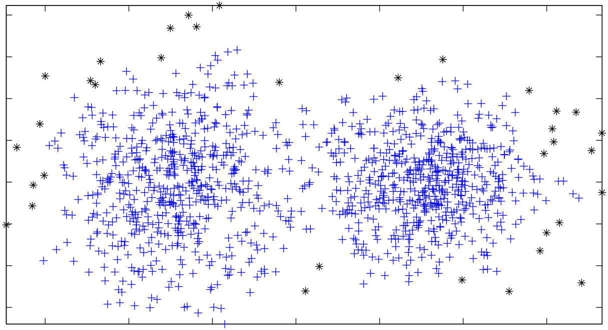
Limitations of DBSCAN

Unable to :

- split overlapped cluster
- cluster with large difference densities

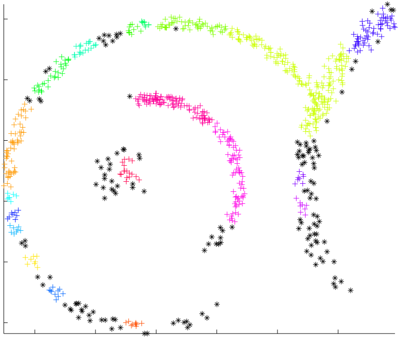
Original data



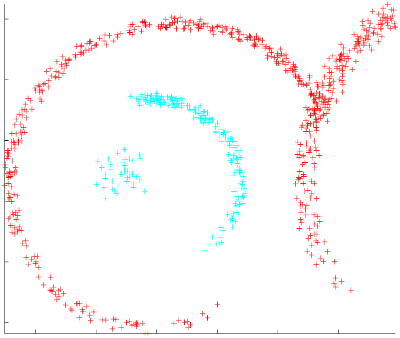


DBSCAN (m=5, $\varepsilon = 0.5$)

DBSCAN : sensitivity to parameters



$\varepsilon = 0.5$



$\varepsilon = 4$

The parameters determination

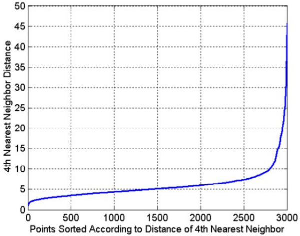
Basic idea

For one object $\mathbf{x}_i$ in a cluster :

- Neighbors are roughly at the same distance of $\mathbf{x}_i$
- Outliers have more distance with $\mathbf{x}_i$ than other neighbors

Suppose m fixed.

To set ε, plot sorted distance of every points to its 4^{th} nearest neighbor :



Geometrical clustering methods

Basic idea

A cluster ω_k is represented by a centroid $\mathbf{v}_k$
$\Rightarrow$ The number of cluster is known

Geometrical clustering methods

Basic idea

A cluster ω_k is represented by a centroid $\mathbf{v}_k$

$\Rightarrow$ The number of cluster is known

Notations

$\mathbf{V} = \{\mathbf{v}_1 \dots \mathbf{v}_c\}$

$d_{ik} = d(\mathbf{x}_i, \mathbf{v}_j) = \|\mathbf{x}_i - \mathbf{v}_k\|$

k-means and its variants

k-means [?]

Objective function

min J_{KM} s.t.

$$J_{KM} = \sum_{i=1}^{N} \sum_{\mathbf{x}_i \in \omega_k}^{C} \|\mathbf{x}_i - \mathbf{v}_k\|^2$$

Optimization

NP-Hard $\Rightarrow$ minimization using an iterative procedure :

$$\min J_{KM} \text{ w.t.r to clusters} \quad \rightleftarrows \quad \min J_{KM}(\mathbf{V})$$

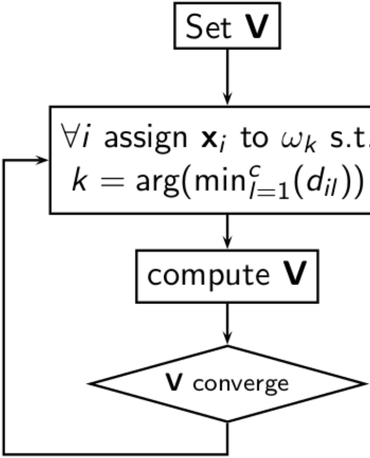
Advantage

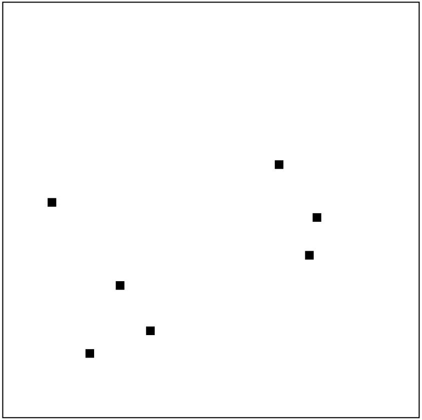
Fast

Disadvantage

Risk of local minimum

Optimization





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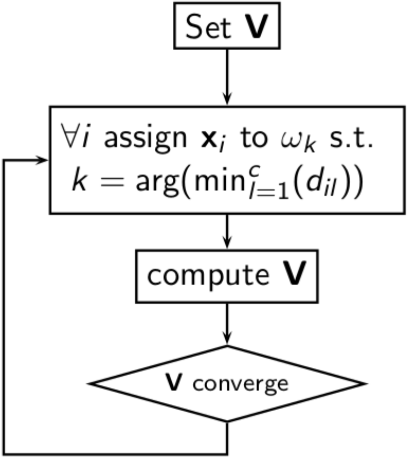

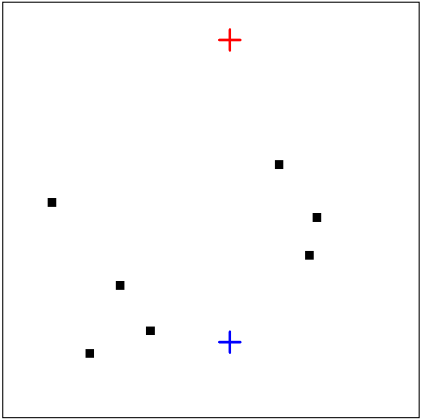

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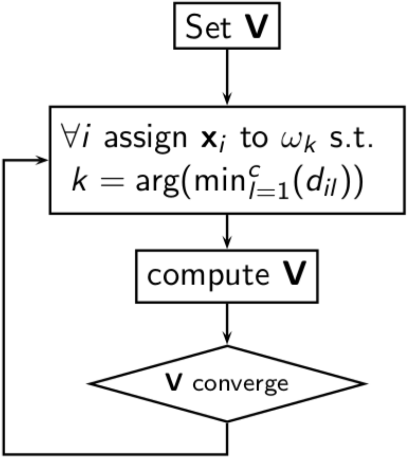
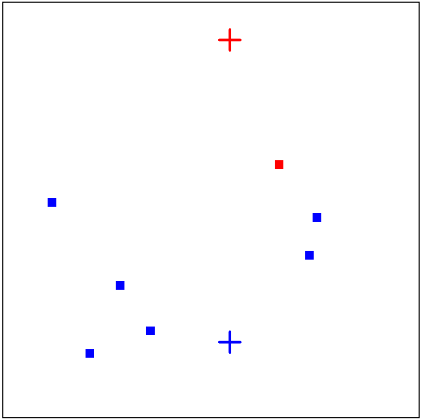
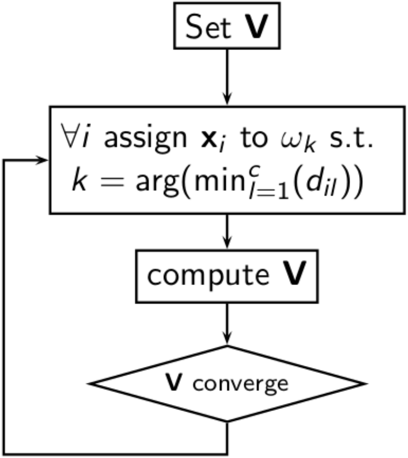
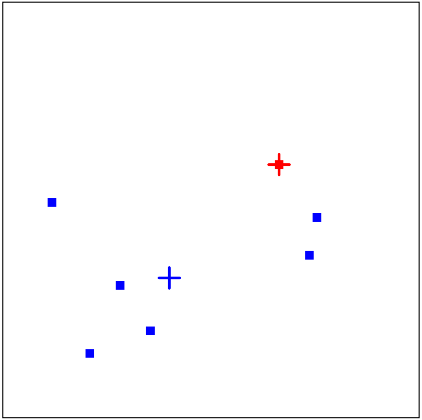


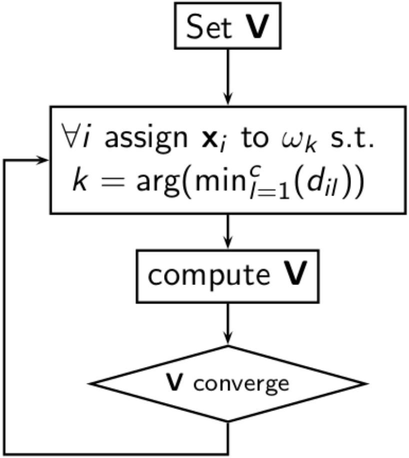


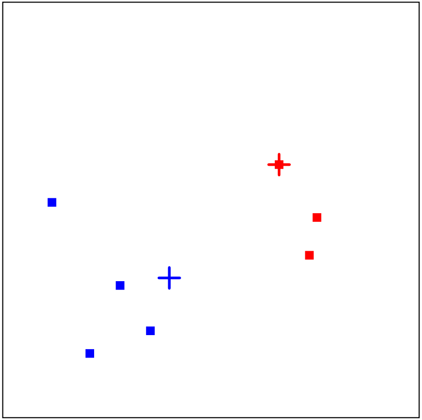
Optimization





Optimization





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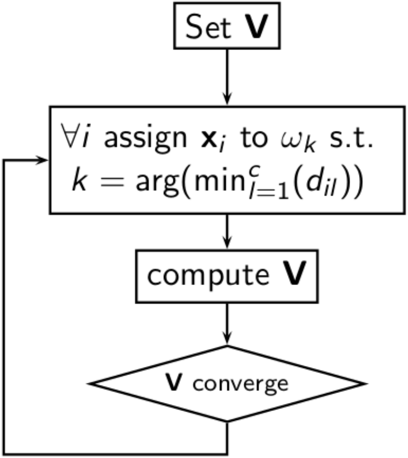
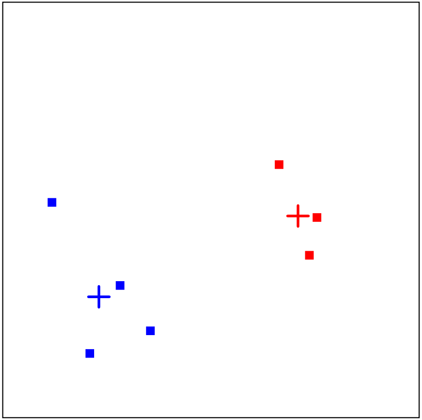


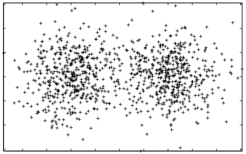


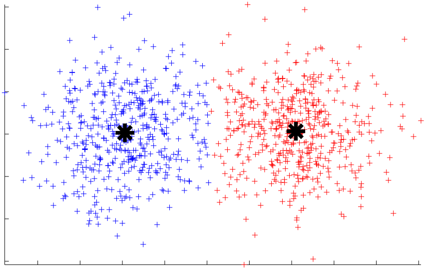
Strengths of *k*-means

Enable to deal with :

- globular shapes
- overlapped cluster

Original data

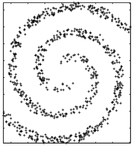




k-means (k=2)

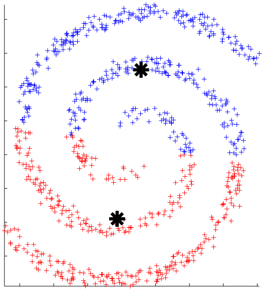
Limitations of *k*-means

Original data



Sensitive to :

- non geometrical shapes
- unbalanced cluster



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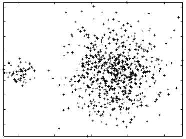
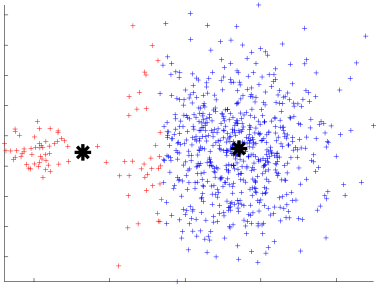
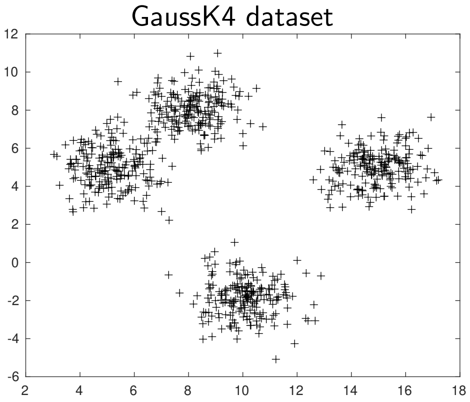




k-means (k=2)

Determination of the number of clusters



Basic idea

For c=1 to 10

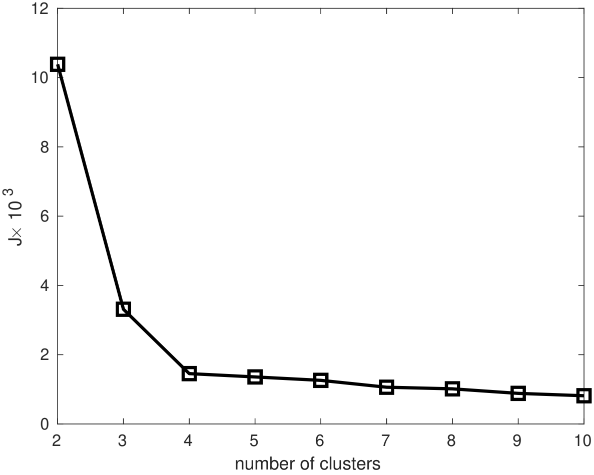
- run kmeans
- evaluate the partition

Plot evaluation measure vs number of clusters

Possible measures

- Gap Statistic
- AIC / BIC criterions
- Silhouette coefficients

Determination of the number of clusters



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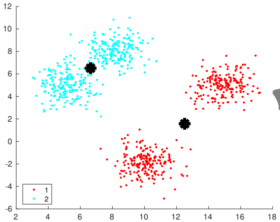

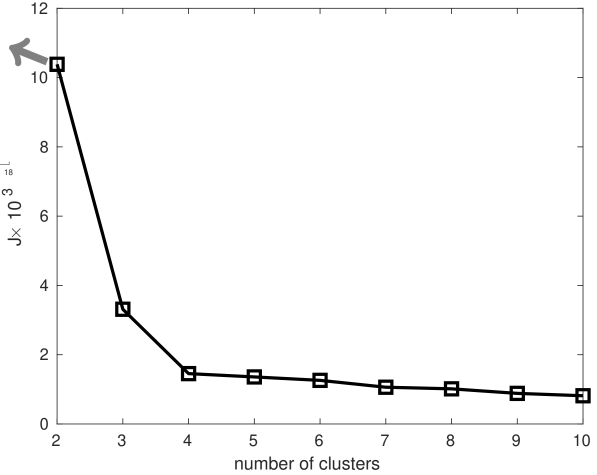

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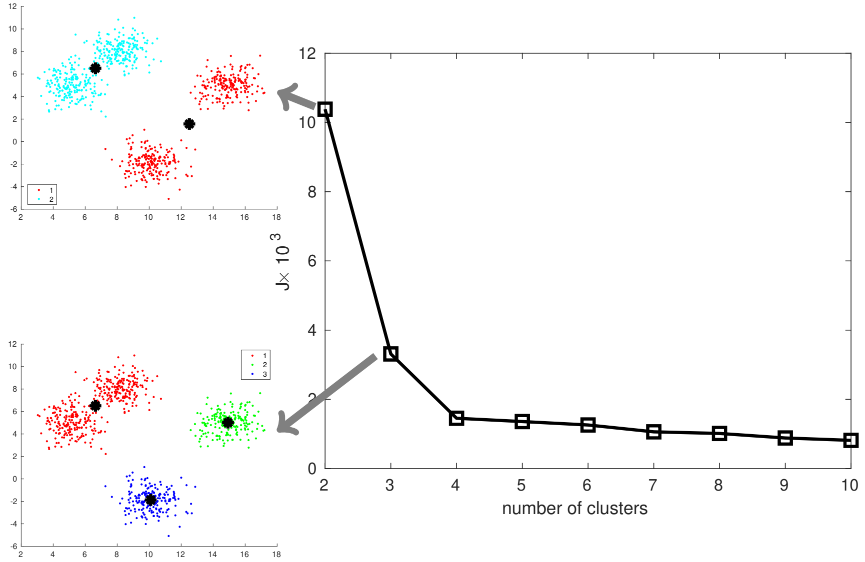

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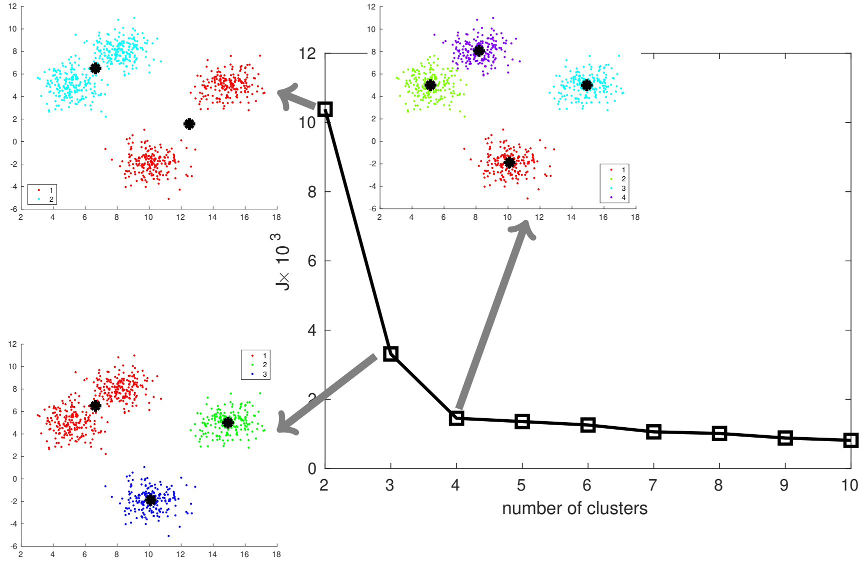

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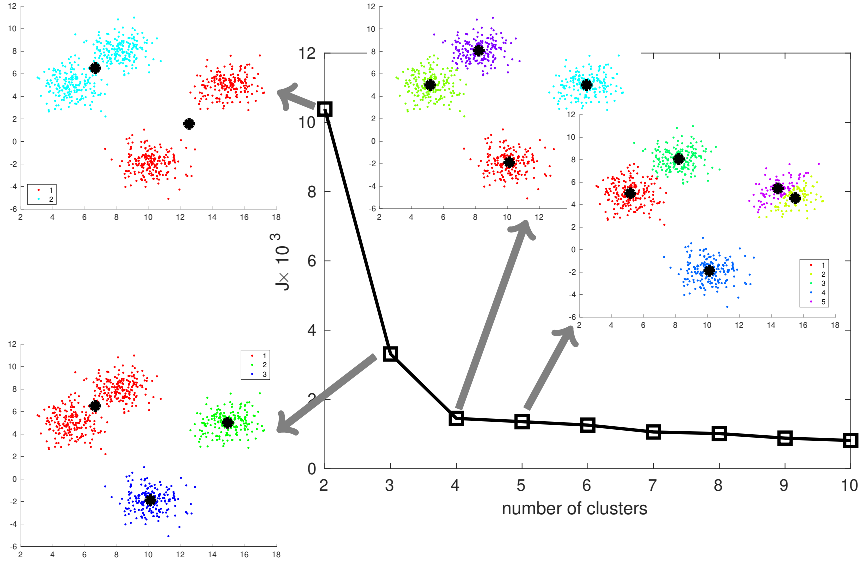

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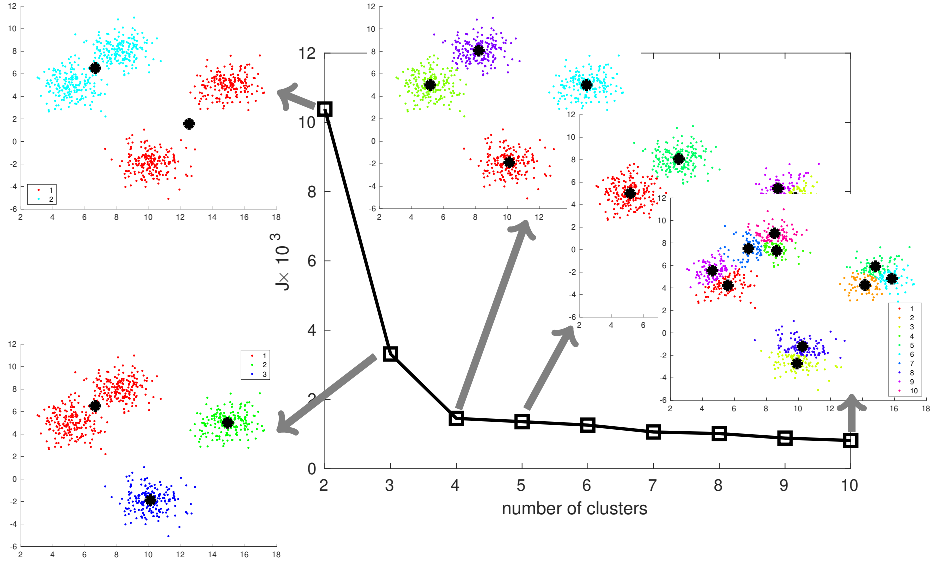
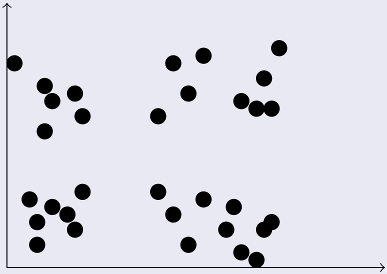


The choice of initial centroids

The farthest-first method [?]

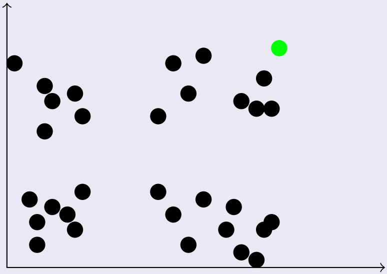


Other methods

- Nearest neighbor density
- Agglomerative hierarchical clustering

The choice of initial centroids

The farthest-first method [?]



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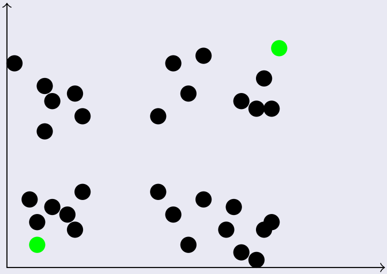

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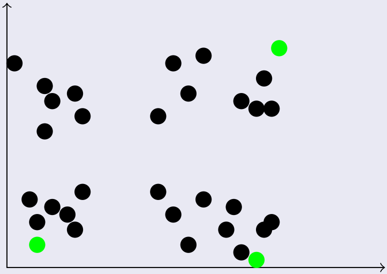


Other methods

- Nearest neighbor density
- Agglomerative hierarchical clustering

Variants of k-means

Different choice of centroids

- k-Medoids
- k-Medians
- k-Modes

Automatically handling c

- Competitive Agglomeration
- Bisecting k-means

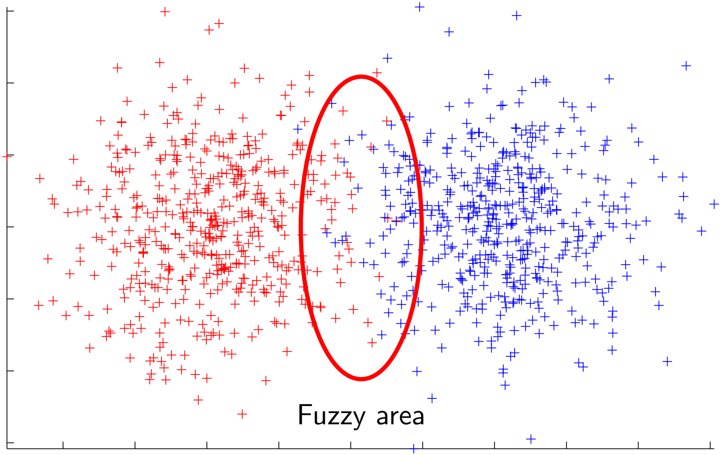
Returning non crisp partition

- Fuzzy c-means
- Evidential c-means

Algorithms returning fuzzy partition

Goal

Express uncertainty about the clustering result



Fuzzy c-means (FCM) [? ?]

Geometrical model

Each object x_i has a degree of membership in each cluster ω_k : u_{ik}

Aternate optimization

$$opt(u_{ik}) \rightleftarrows opt(\mathbf{v}_k)$$

Objective function

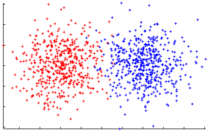
$$J_{FCM} = \sum_{i=1}^{N} \sum_{k=1}^{C} u_{ik}^{\beta} d_{ik}^{2}$$

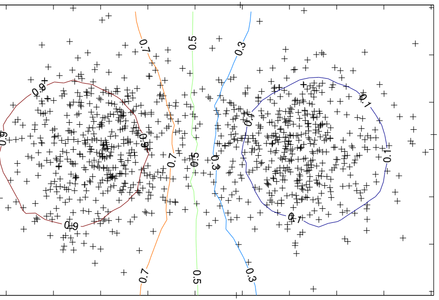
Subject to

$$\sum_{k=1}^{C} u_{ik} = 1 \text{ and } u_{ik} \geq 0 \quad \forall i, k$$

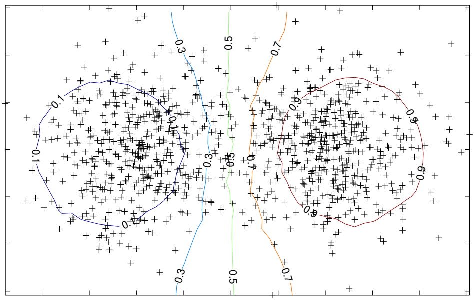
Fuzzy c-means

Original data





ω_1



ω_2

Variants of FCM

The Noise Clustering algorithm [?]

Add a noise cluster ω_* associated to a fixed δ :

$$J_{NC}(U, V) = \sum_{i=1}^{N} \sum_{k=1}^{C} u_{ik}^{\beta} d_{ik}^{2} + \sum_{k=1}^{C} u_{i*}^{\beta} \delta$$

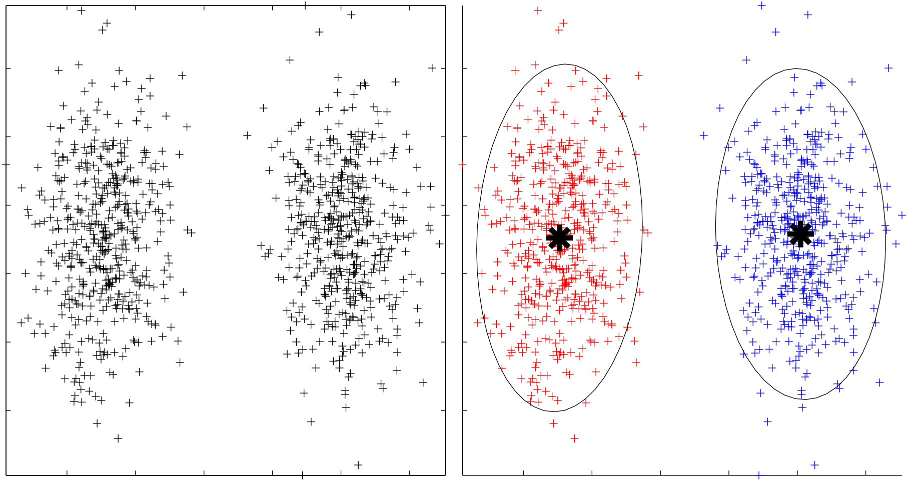
FCM with Mahalanobis distance [?]

Add a Mahalanobis distance between each $\mathbf{x}_i$ and ω_k :

$$d_{ik}^2 = (\mathbf{x}_i - \mathbf{v}_k)^\top S_k (\mathbf{x}_i - \mathbf{v}_k)$$

Minimize $J_{GK}(U, V, S)$ s.t. $|S_k| = 1 \quad \forall k = 1, C$

GK clustering [?]



original data GK algorithm

Outline

Measures

Two types of clustering validation measures :

External measures

External information are available (e.g. class label)

$\Rightarrow$ evaluation of the behavior of a clustering algorithm

$\Rightarrow$ expert assessment on few objects

Internal measures

No background knowledge

$\Rightarrow$ most of the real world applications

Internal measures

Depend on the output structure.

Goals

- Comparaison with different clustering algorithms
- Parameters determination for a specific algorithm
- Evaluation of the uncertainty of the clustering result

Internal measures

Depend on the output structure.

Goals

- Comparaison with different clustering algorithms
- Parameters determination for a specific algorithm
- Evaluation of the uncertainty of the clustering result

Example

Validity index for

- Crisp partitions
- Fuzzy partitions
- Evidential partitions

Measures for crisp partitions

Based on the combination of two criteria :

Compactness

Separation

Measures for crisp partitions

Based on the combination of two criteria :

Compactness

- Variance cluster

  $\Rightarrow$ low value $\equiv$ good density

Separation

Measures for crisp partitions

Based on the combination of two criteria :

Compactness

- Variance cluster

  $\Rightarrow$ low value $\equiv$ good density
- Intra-cluster distance
  - max or avg center-based distance
  - max or avg pairwise distance

$$d_{intra}(\omega_k) = \max_{x_i, x_j \in \omega_k} d_{ij}$$

$\Rightarrow$ d_{intra} low $\equiv$ good compactness

Separation

Measures for crisp partitions

Based on the combination of two criteria :

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Separation

- Inter-cluster distance
  - min or avg center-based distance
  - min or avg pairwise distance

$$d_{inter}(\omega_k, \omega_l) = \min_{\substack{x_i \in \omega_k, \\ x_j \in \omega_l}} d_{ij}$$

$\Rightarrow$ d_{inter} high $\equiv$ large separation

Dunn's indice

Definition

$$D = \min_{\omega_k} \left[\min_{\omega_l \neq \omega_k} \left(\frac{d_{inter}(\omega_k, \omega_l)}{\max\limits_{k=1\ldots c} d_{intra}(\omega_k)} \right) \right]$$

D should be maximized

Properties

Robust to :

- Various density
- Unequal size of cluster

Sensitive to :

- Noise
- Subclusters
- Arbitrary shapes

Silhouette index

Definition

$$S = \frac{1}{c} \sum_{\omega_k} \frac{1}{n_k} \sum_{x_i \in \omega_k} \frac{d_{ma}(x_i) - d_{intra}(x_i)}{\max(d_{ma}(x_i), d_{intra}(x_i))}$$

s.t. $d_{ma}(x_i) = \min_{l \neq k} d_{avg}(x_i, \omega_l)$

S should be maximized

Properties

Enable to handle :

- Noise
- Various density
- Unequal size of cluster

Affected by :

- Subclusters
- Arbitrary shapes

Other measures

RMSSD (Root Mean Square Standard Deviation)

- Consider only the compactness of a cluster
- Close to k-means objective function

Index

- A combination between Compactness and Separation
- Handle subclusters

CVNN

- Based on nearest neighbor
- Handle arbitrary shapes of cluster

And still several other measures [**?**].

Measures for fuzzy partitions

Only based on fuzzy memberships

Measure the amount of overlap between clusters

The partition coefficient

$$PC = \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{c} u_{ik}^2$$

Should be maximized

The partition entropy

$$PE = \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{c} u_{ik}^2 \log(u_{ik})$$

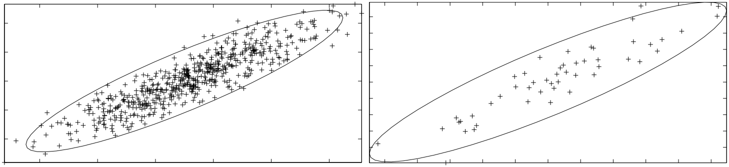
Should be minimized

Measures mainly used to determine c in FCM.

Measures for fuzzy partitions

Basic idea

High concentration of points in a small spatial volume
$\Rightarrow$ measures compactness



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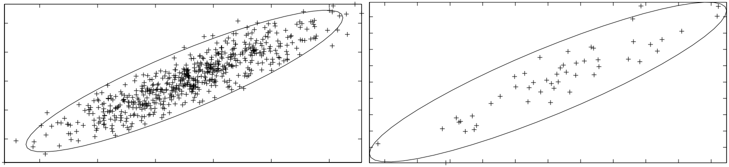

Fuzzy HyperVolume

$$FHV = \sum_{k=1}^{c} \det(F_k)^{1/2}, \text{ s.t. } F_k = \frac{\sum_{i=1}^{n} u_{ik}^{\beta}(\mathbf{x}_i - \mathbf{v}_k)(\mathbf{x}_i - \mathbf{v}_k)^T}{\sum_{i=1}^{n} u_{ik}^{\beta}}$$

is the fuzzy covariance matrix of ω_k

FHV should be lowered

Outline

Conclusion

Most popular clustering algorithm

- hierarchical clustering
- k-means
- dbscan

Conclusion

Most popular clustering algorithm

- hierarchical clustering
- k-means
- dbscan

Advantages

Simple and fast

Disadvantages

Parameters to set (similarity notion, number of cluster, etc.)
$\Rightarrow$ Little background knowledge is a necessity !

Conclusion

Which clustering algorithm chose ?

Guideline

Dataset characteristics	Algorithms
unbalanced groups	single-link, DBSCAN
subclusters	hierarchical clustering
arbitrary shapes	DBSCAN
elliptic shapes	k-means, GK
overlapped cluster	k-means and variants

Conclusion

Other dataset characteristics

- High-dimensional data (p high)
- Big data (n high)
- categorical data
- uncertain data

Other interesting clustering techniques

- ensemble clustering
- constrained clustering

Conclusion

Clustering for special data

- documents
- multimedia
- time-series
- biological
- network

References I