Lecture 11

Clustering

Information Systems (Machine Learning)

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06.12.2018

Lecture plan

- Clustering Problem
- Graph-based clustering
- Hierarchical clustering
- EM clustering
- Density-based clustering
- Non-parametric clustering
- Semi-supervised learning

- The presentation is prepared with materials of the K.V. Vorontsov's course "Machine Leaning"

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Problem statement

Problem: split set of objects of the same type to archive groups, such that object in these group have similar properties.

"Similarity" is formalized with an abstract measure.

X^m is training set consisting of objects from X

$\rho: X \times X \to [0; +\infty)$ is metric measure on X.

Find algorithm $a: X \to Y$, where Y is cluster set.

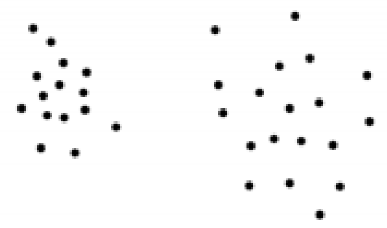
Problem formulation incorrectness

- No correct problem statement
- No universal quality criterion
- No universal metric measure (consequence of the Kleinberg theorem)
- Number of clusters is usually unknown

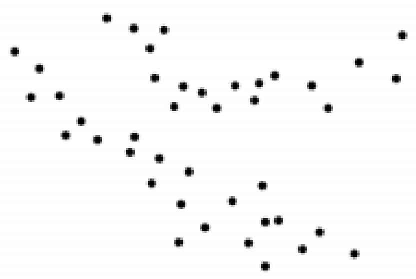
Goals of clustering

- Decrease data volume
- Find groups of similar objects
- Find unusual object
- Find hierarchy of objects (groups)

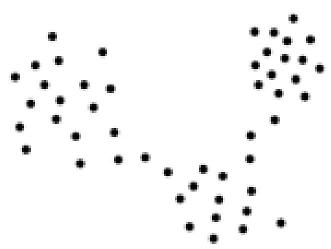
Примеры кластеров(1/2)



Explicitly separable



Stripes



With bridges

Примеры кластеров(2/2)

With regular noise

Distribution mixture

No clusters

Clustering applications

- Biology and medicine
  - Sequence analysis
  - Medical imaging (PET scans)
- Social science
  - Crime analysis
- Computer science
  - Image segmentations
- Marketing
  - Target groups
- Text analysis
- Social networks

Evaluation

- **External** – based on data that was not used for clustering, such as known class labels and external benchmarks.
- **Internal** – forbid using any external information, based on the structure of partition.

Metric space quality functional

Mean inner cluster distances:

$$F_0 = \frac{\sum_{i<j}[y_i = y_j]\rho(x_i, x_j)}{\sum_{i<j}[y_i = y_j]} \to \min.$$

Mean outer cluster distance:

$$F_1 = \frac{\sum_{i<j}[y_i \neq y_j]\rho(x_i, x_j)}{\sum_{i<j}[y_i \neq y_j]} \to \max.$$

Relation:

$$F_0/F_1 \to \min.$$

Vector space quality functional

Mean inner cluster distances:

$$\Phi_0 = \sum_{y \in Y} \frac{1}{|K_y|} \sum_{i: y_i = y} \rho^2(x_i, c_y) \to \min.$$

Sum of outer cluster distances:

$$\Phi_1 = \sum_{y \in Y} \rho^2(c_y, c) \to \max.$$

Relation:

$$\Phi_0 / \Phi_1 \to \min.$$

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Graph-based approach

Main idea: we will work with graphs, its vertices are objects and its edge lengths are equal to distances between the corresponding objects.

Clusters can be well-represented in graph description.

Connected component selection

Fix a radius R.

Delete edges $\{x, y\}$: $\rho(x, y) > R$.

Clusters are equal to connected components.

Fix K_1, K_2.

Change R until number of clusters is in interval $[K_1, K_2]$.

Shortest path

Fix number of clusters K.

Find minimum spanning tree (Kruskal, Boruvka, MST).

Delete $K-1$ edges with maximal lengths.

We can change for each K.

FOREL

Input: $U = X^m -$ set of unclusterized points.

1. Repeat
2. Choose a random point x from U
3. Repeat
4. $B \leftarrow$ sphere with radius R and center x
5. $c \leftarrow$ mass center of B
6. Until the sphere does not change
7. $U \leftarrow U \backslash B$
8. Until $U \neq \emptyset$

Return set of clusters

FOREL properties

Depends on *R*

How to choose mass center?

- Mass center in (vector space)
- Object, such that sum of distances from it to all the other objects in minimal
- Object, which in sphere of radius *R* contains maximum number of objects from the sample
- Object, which in sphere of radius *r* contains maximum number of object from sphere of radius *R*

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Hierarchical approach

Main idea: build cluster hierarchy.

You can build beautiful pictures (**dendrograms**). And then you can think about number of clusters as about height of this tree.

Two approaches:

Division (split clusters)

Agglomeration (join clusters)

Lance-Williams algorithms

1. 1-element clusters:

   $t = 1, C_t = \{x_1, \dots, x_l\};$

   $R(\{x_i\}, \{x_j\}) = \rho(x_i, x_j);$

2. For all $t = 2 \dots l$ $(t -$ iteration number):
3. In C_{t-1} find 2 *closest* clusters:

   $(U, V) = argmin_{U \neq V} R(U, V)$;R(U,V);

   $R_t = R(U, V);$

4. Merge them to one cluster:

   $W = U \cup V;$

   $C_t = C_{t-1} \cup \{W\} \setminus \{U, V\};$

5. For all $S \in C_t$ count $R(W, S)$.

Lance-Williams distance

Distance $R(W, S)$ between clusters

$W = U \cup V$ and S

Lance-Williams distance:

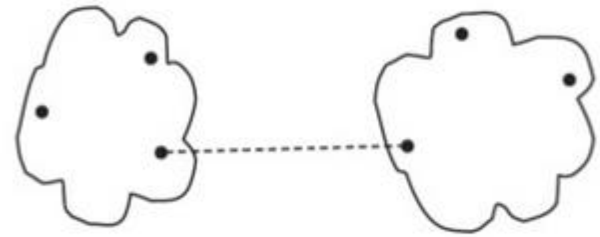
$$R(U \cup V, S) = \alpha_U R(U, S) + \\ + \alpha_V R(V, S) + \\ + \beta R(U, V) + \\ + \gamma |R(U, S) - R(V, S)|$$

Options of $R(W, S)$ (1/2)

1. Nearest neighbor distance

$$R^N(W,S) = \min_{w \in W, s \in S} \rho(w,s);$$

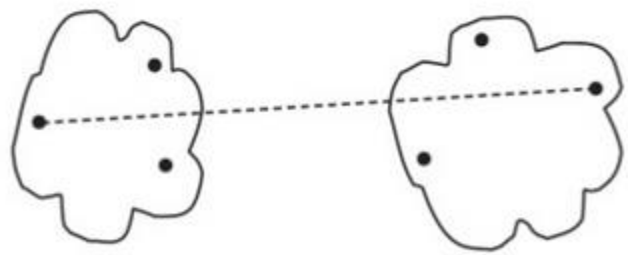
$$\alpha_U = \alpha_V = \tfrac{1}{2}, \ \ \beta = 0, \ \ \gamma = -\tfrac{1}{2}.$$



2. Most distant neighbor distance

$$R^D(W,S) = \max_{w \in W, s \in S} \rho(w,s);$$

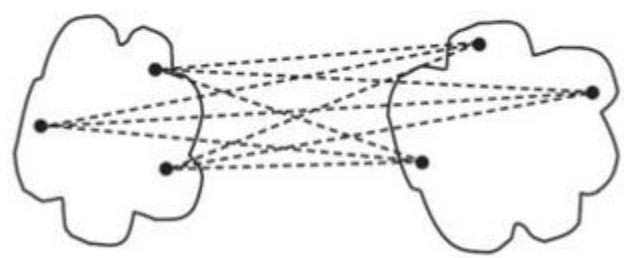
$$\alpha_U = \alpha_V = \tfrac{1}{2}, \ \ \beta = 0, \ \ \gamma = \tfrac{1}{2}.$$



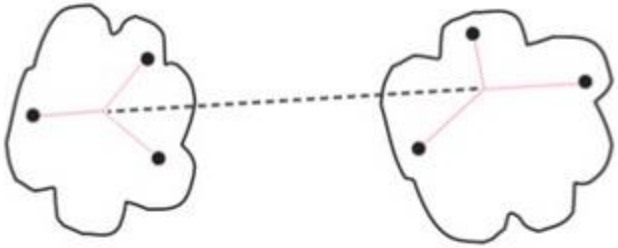
3. Mean group distance

$$R^G(W,S) = \frac{1}{|W||S|} \sum_{w \in W} \sum_{s \in S} \rho(w,s);$$

$$\alpha_U = \frac{|U|}{|W|}, \ \ \alpha_V = \frac{|V|}{|W|}, \ \ \beta = \gamma = 0.$$



Options of $R(W,S)$ (2/2)



4. Distance between centres

$$R^c(W,S) = \rho^2\Big(\sum_{w\in W}\frac{w}{|W|}, \sum_{s\in S}\frac{s}{|S|}\Big);$$

$$\alpha_U = \frac{|U|}{|W|},\quad \alpha_V = \frac{|V|}{|W|},$$

$$\beta = -\alpha_U\alpha_V,\quad \gamma = 0.$$

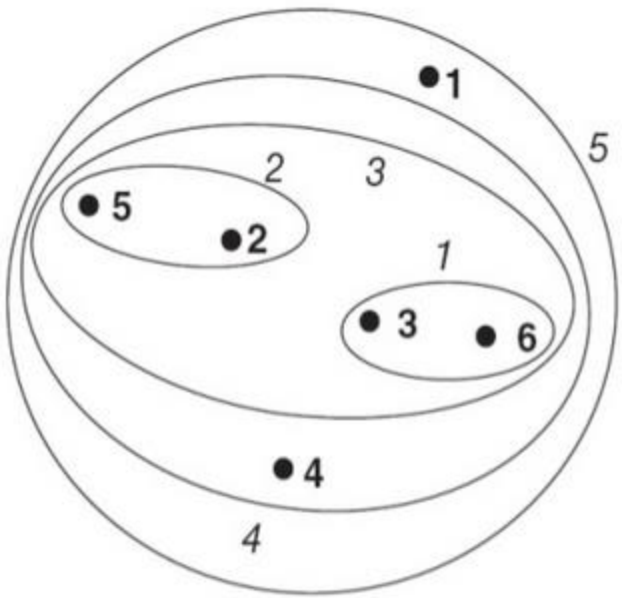
5. Ward's distance

$$R^w(W,S) = \frac{|S||W|}{|S|+|W|}\rho^2\Big(\sum_{w\in W}\frac{w}{|W|}, \sum_{s\in S}\frac{s}{|S|}\Big);$$

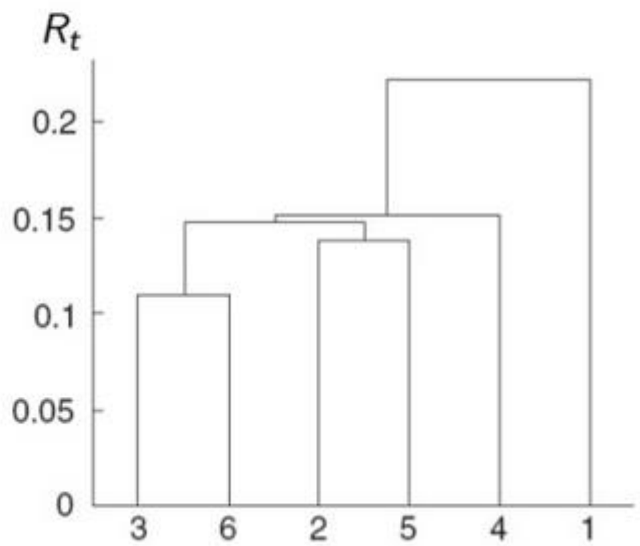
$$\alpha_U = \frac{|S|+|U|}{|S|+|W|},\quad \alpha_V = \frac{|S|+|V|}{|S|+|W|},\quad \beta = \frac{-|S|}{|S|+|W|},\quad \gamma = 0.$$

Nearest neighbor visualization

Inclusion plot

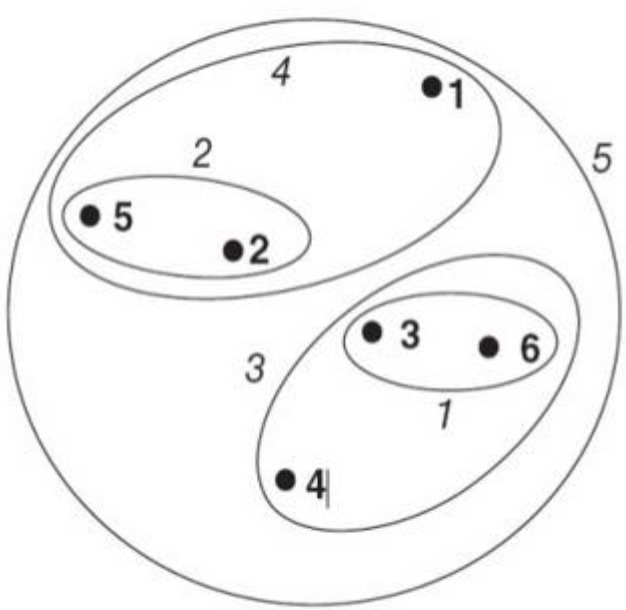


Dendrogram

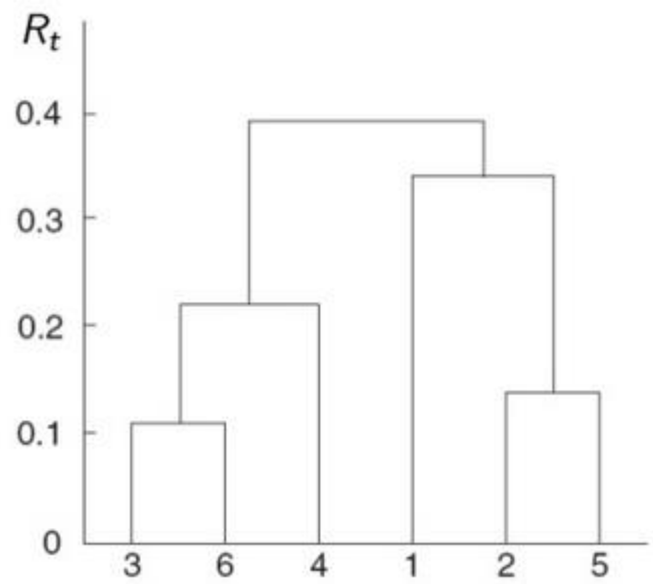


Most distant neighbor visualization

Inclusion plot



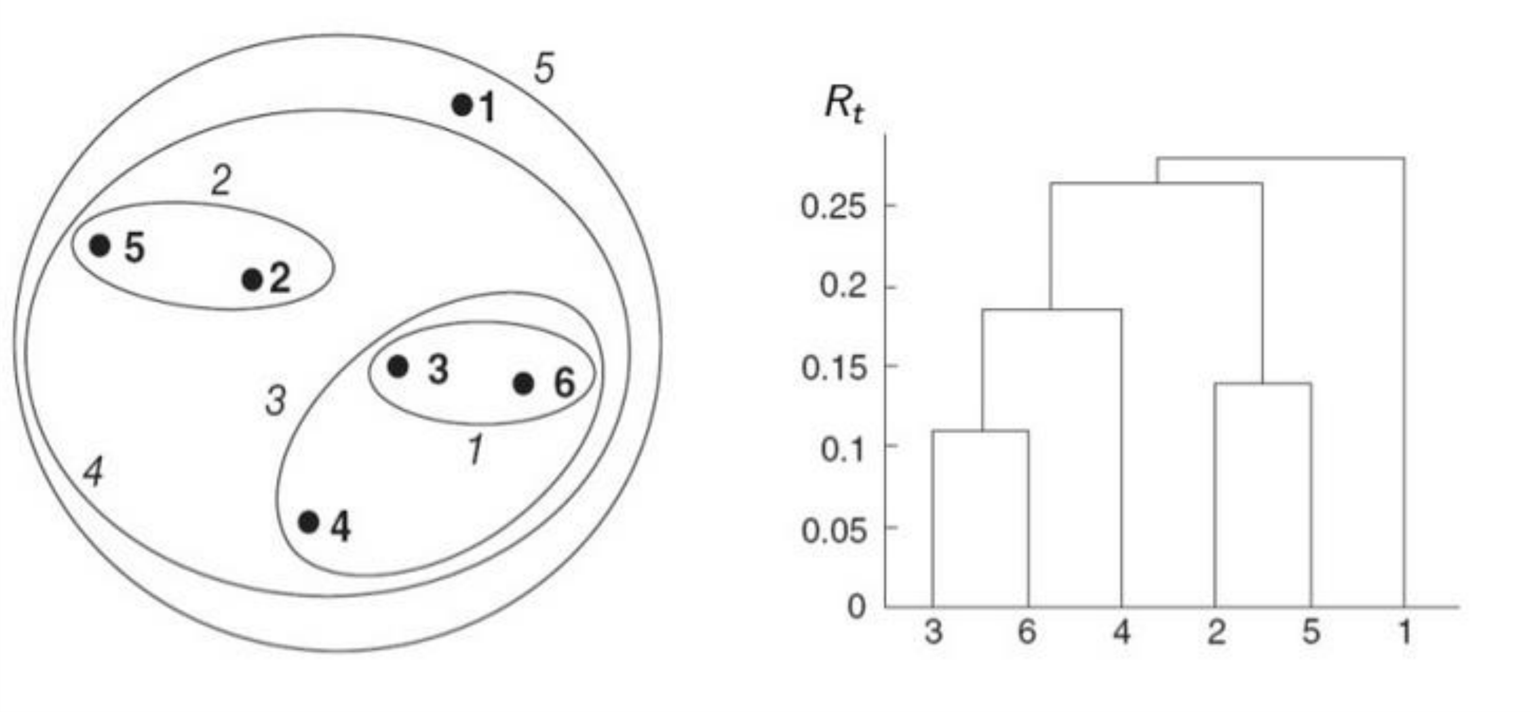
Dendrogram



Group mean visualization

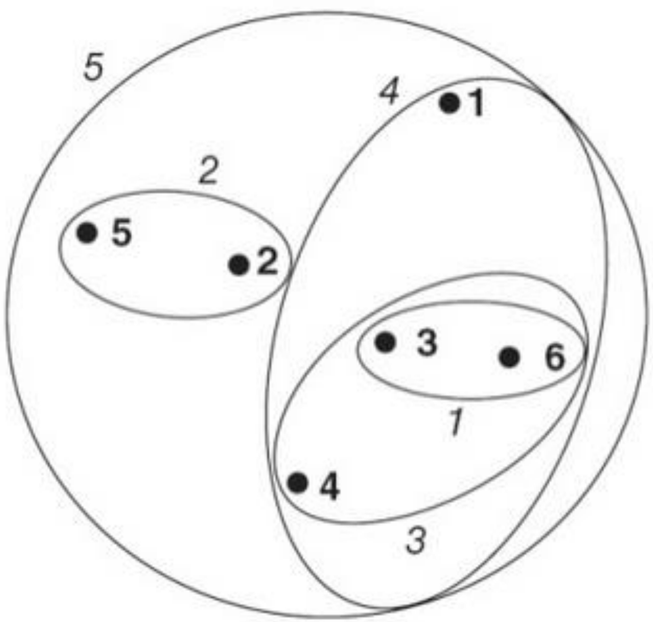
Inclusion plot

Dendrogram

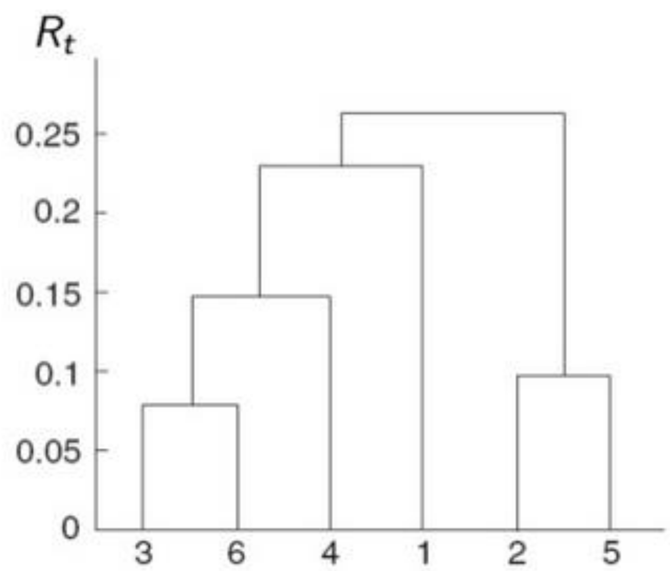


Ward’s distance visualization

Inclusion plot



Dendrogram



Monotonic clustering

Clustering is **monotonic** if cluster distance do not decrease with after joining.

Theorem (Milligan, 1979)

Clustering is monotonic, if

$\alpha_U \geq 0, \alpha_V \geq 0, \alpha_U + \alpha_V + \beta \geq 1, \min\{\alpha_U, \alpha_V\} + \gamma \geq 0.$

If clustering is monotonic, dendrogram has no intersections.

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If clustering is monotonic, dendrogram has no intersections.

R^C is not monotonic.

General recommendation

- Ward's distance is more preferable;
- Accelerate algorithms: join locally close clusters.
- Choose number of clusters by minimizing $|R_{t+1} - R_t|$.

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EM

Works in the same way as original EM

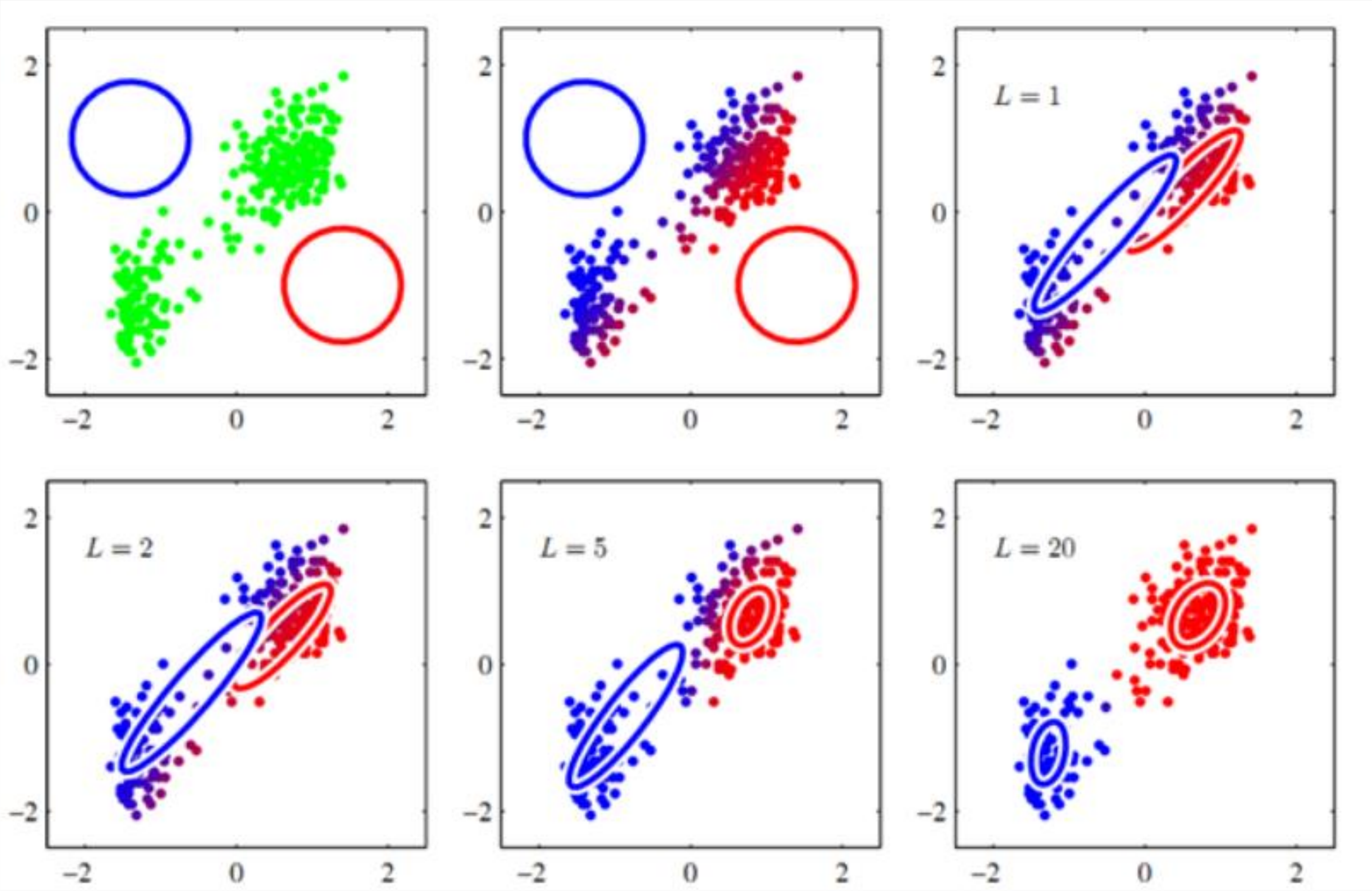
Assumption: simple sample.

w_y is prior probability of class y.

Approximate with Gaussians.

Each class is described with d-dimensional Gaussian density with diagonal covariance matrix.

EM example



k-means

- ***k*-means** is an iterative algorithm that splits sets on k parts.
- Mass center of a cluster (mean intercluster distance by each feature) C_j is called *centroid*

$$c_j = \frac{1}{|C_j|}\sum_{i \in C_j} x_i \in C_j$$

k-means

It is EM-algorithm simplification with strong association with only one class.

1. Chose k points (**centroids**) $\{c_i\}_{i=1}^{k}$ from sample.
2. Repeat
3. For each x find nearest centroid $n(x)$.

$$C_i = \{x|n(x) = c_i\}$$

4. For each C_i find central point and claim it to be centroid.
5. Until centroid set do not change.

c-means (fuzzy clustering)

Imprecise degree of cluster belonging $u_i(x)$ of object x to cluster C_i, having $\sum_i u_i(x) = 1$.

Cluster center is chosen with

$$c_i = \frac{\sum_{x \in X^m} u_i^{\;d}(x)x}{\sum_{x \in X^m} u_i^{\;d}(x)}.$$

Re-estimate degree of belonging:

$$u_i(x) = \frac{1}{\sum_j \left(\frac{\rho(c_i, x)}{\rho(c_j, x)}\right)^{2/(d-1)}}.$$

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Density-based approach

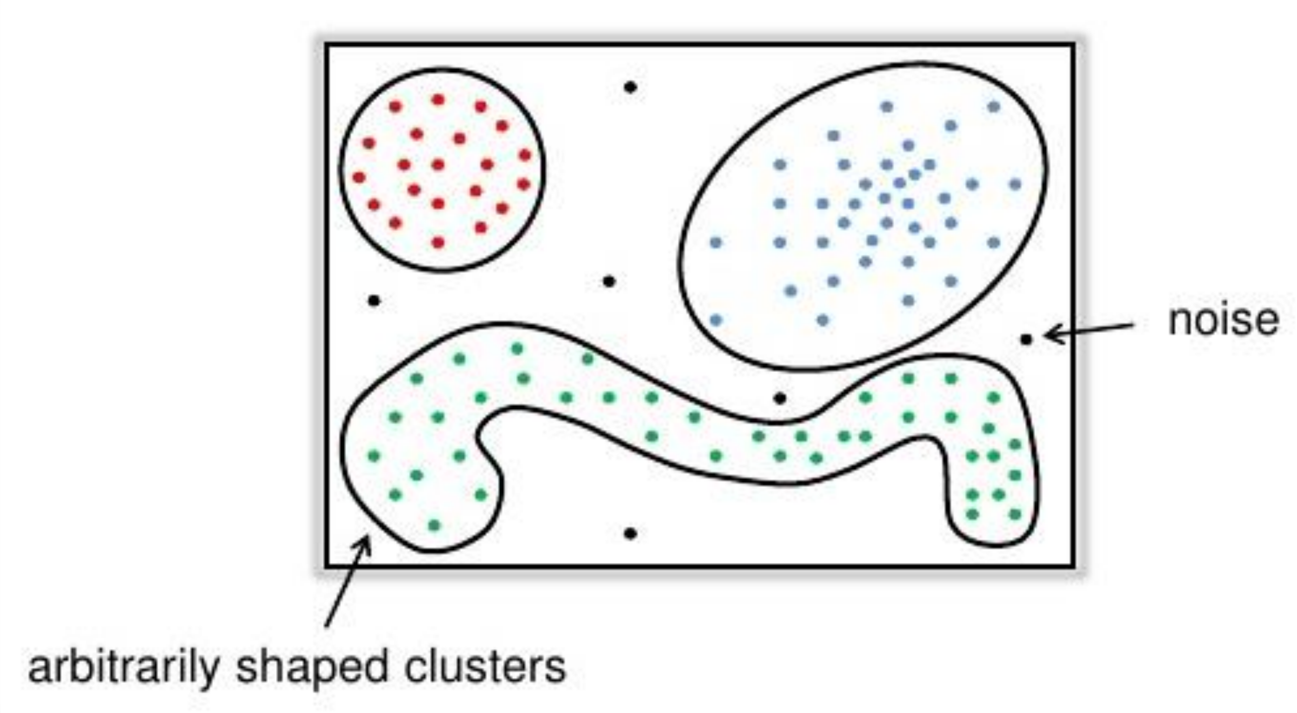
Main idea: each p point of cluster contains more than M points within eps distance:

$N_{eps}(p)$ – set of points around p within distance eps. $|N_{eps}(p)| \geq M$.

Problem with border points.

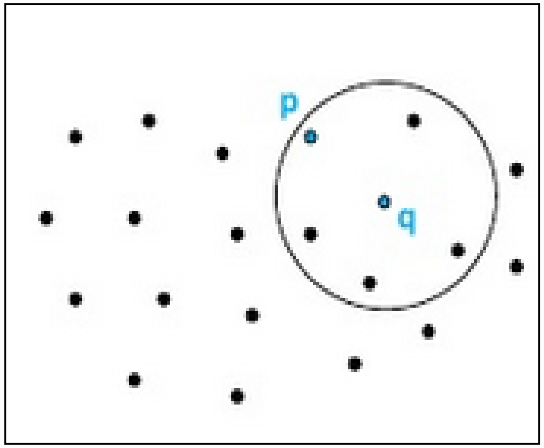
DBSCAN

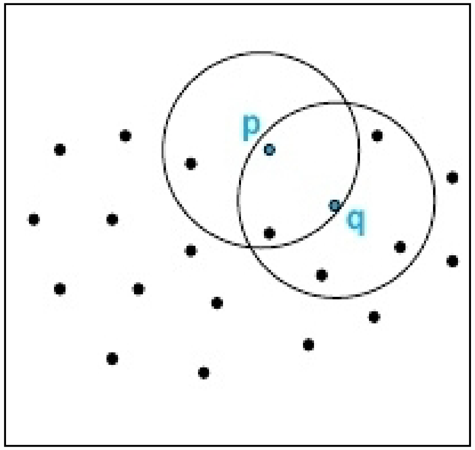
DBSCAN (Density Based Spatial Clustering of Applications with Noise)



Reachable point

p is **directly reachable** from q (given Eps and M), if $p \in N_{eps}(q)$ and $|N_{eps}(q)| \geq M$.

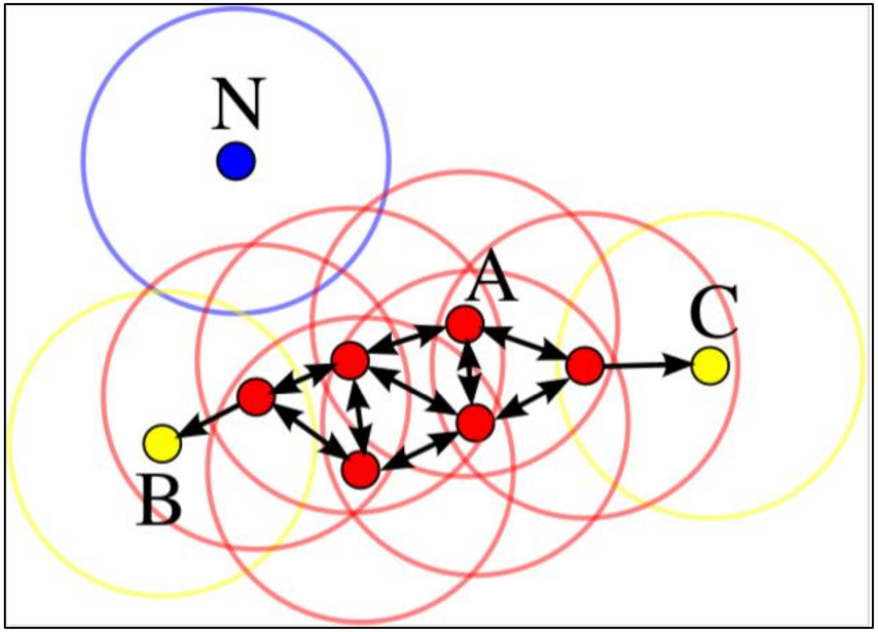




p is **reachable** from q (given Eps and M), if $\exists \{a_i\}, a_i$ is directly reachable from a_{i-1}.

Connected points

B is **connected** with C (given Eps and M), if $\exists A$, so that B and C are reachable from A (given Eps and M).



Cluster definition

Cluster C_j (given Eps and M) is non-empty set of points:

- $\forall p, q : p \in C_j$, q is reachable $p \Rightarrow q \in C_j$
- $\forall p, q \in C_j$: p connected with q.

DBSCAN algorithm

Input: $D -$ data, Eps, M $-$ parameters.

foreach $d_i \in D$: $V[d_i] =$ false, $j = 0$, $Noise = \emptyset$

for all $d_i \in D$:

    if $V[d_i] ==$ false **then**

        $V[d_i] =$ true, $N_i = N_{eps}(d_i)$

        if $|N_i| < M$ **then**

            $Noise = Noise + \{d_i\}$

        else

            $j = j + 1$, $\boldsymbol{Expand}(d_i, N_i, C_j, Eps, M)$

return $C = \{C_j\}$

Expand function

Input: d_i – current point, N_i – sphere, C_j – current cluster, Eps, M.

$C_j = C_j + \{d_i\}$

for all $d_k \in N_i$:

    if $V[d_k] ==$ false **then**

        $V[d_k] =$ true, $N_{ik} = N_{eps}(d_k)$

        if $|N_{ik}| \geq M$ **then**

            $N_i = N_i + N_{ik}$

    if $\nexists p : d_k \in C_p$ **then**

        $C_j = C_j + \{d_k\}$

return $C = \{C_j\}$

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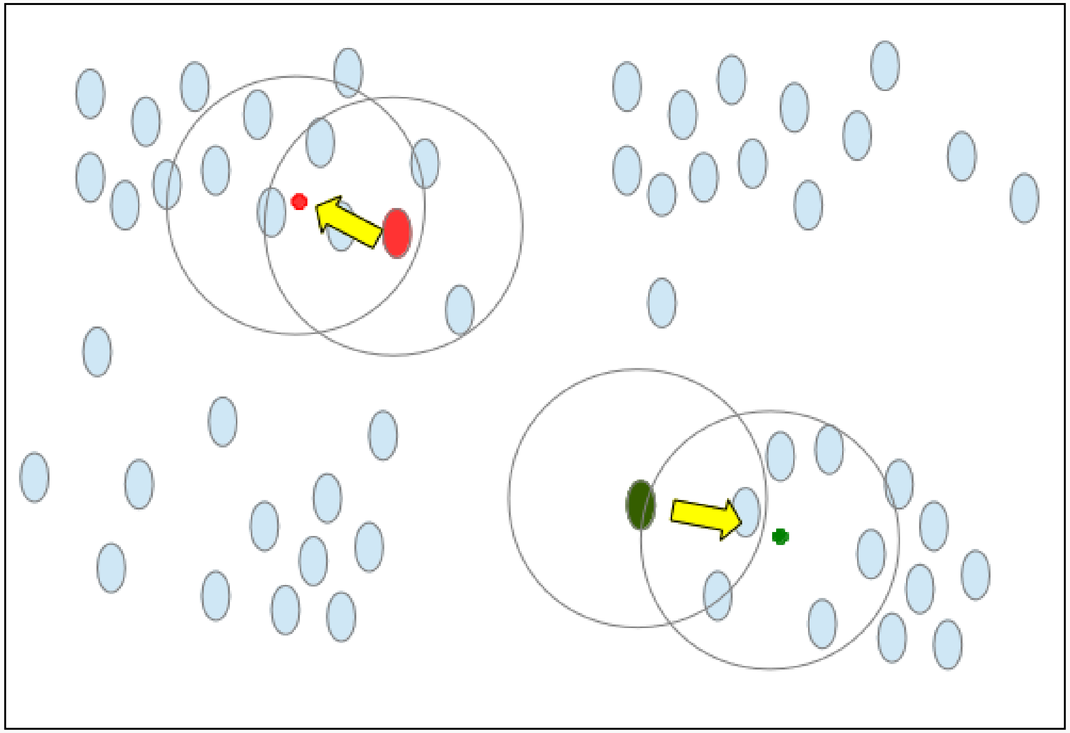
Main idea

Find mass center, with maximum point density, make it a centroid

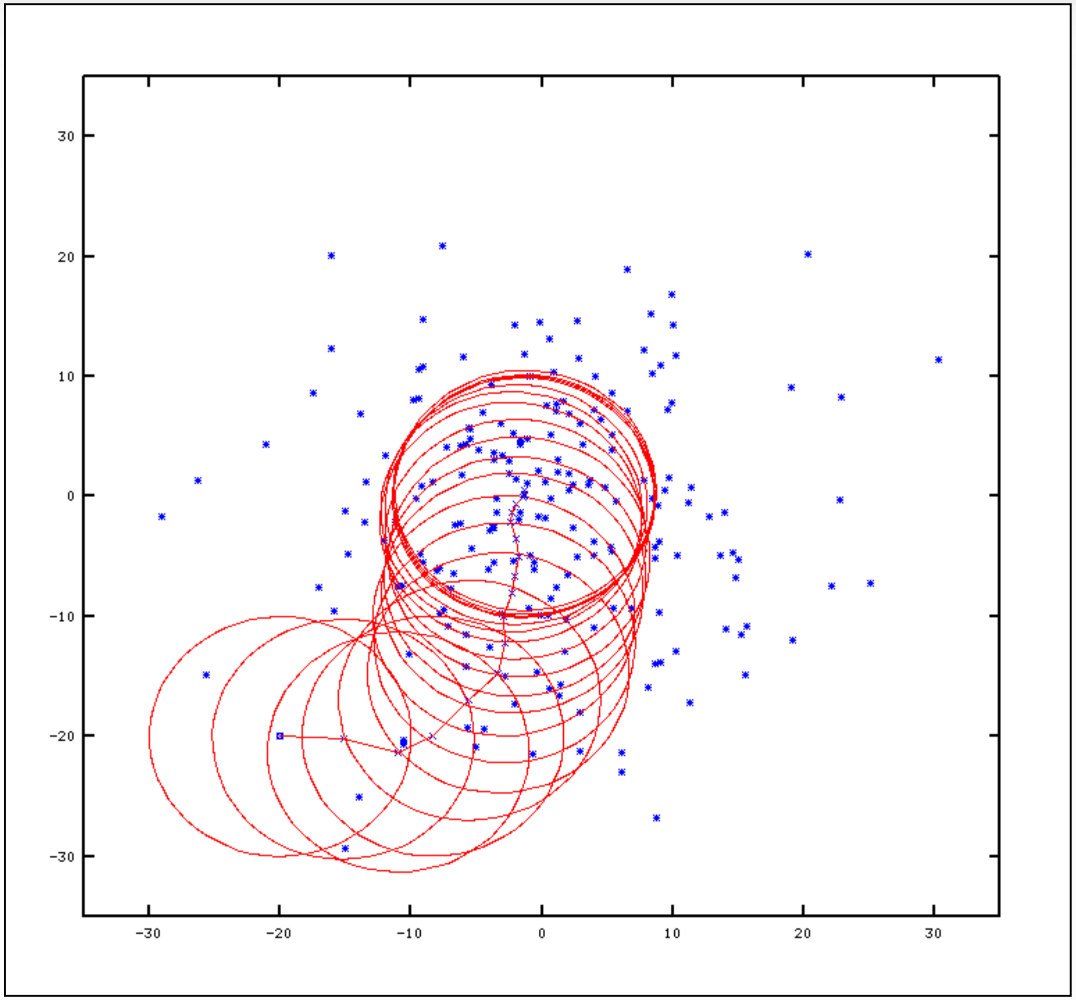


Mean-shift approach

- Set sphere around every point
- Find centroid of every sphere
- Move the center of the sphere to centroid

After each iteration centroids move to more «densed» spheres till convergence to **density modes**.

Mean-shift approach



Density modes

Mean-Shift uses gradient ascent:

$$\nabla \hat{f}(\mathbf{x}) = 1\frac{1}{nh^d}\sum_{i=1}^{n}\frac{\partial}{\partial \mathbf{x}}K(\frac{\mathbf{x} - \mathbf{x_i}}{h})$$

$$\nabla \hat{f}(\mathbf{x}) = 0$$

Gaussian kernel

$$\frac{\partial}{\partial \mathbf{x}} K\left(\frac{\mathbf{x} - \mathbf{x_i}}{h}\right) = K\left(\frac{\mathbf{x} - \mathbf{x_i}}{h}\right)\frac{\mathbf{x} - \mathbf{x_i}}{h}\frac{1}{h}$$

$$\Rightarrow \sum_{i=1}^{n} K\left(\frac{\mathbf{x} - \mathbf{x_i}}{h}\right)\mathbf{x} = \sum_{i=1}^{n} K\left(\frac{\mathbf{x} - \mathbf{x_i}}{h}\right)\mathbf{x_i}$$

«Ascending» direction

Vector of ascending kernel function

$$\mathrm{m}(\mathbf{x}) = \frac{\sum_{i=1}^{n} K(\frac{\mathbf{x} - \mathbf{x_i}}{h})\mathbf{x_i}}{\sum_{i=1}^{n} K(\frac{\mathbf{x} - \mathbf{x_i}}{h})}$$

Mean shift

$$\mathrm{m}(\mathbf{x}) - \mathbf{x} = \frac{\sum_{i=1}^{n} K\left(\frac{\mathbf{x} - \mathbf{x_i}}{h}\right)\mathbf{x_i}}{\sum_{i=1}^{n} K\left(\frac{\mathbf{x} - \mathbf{x_i}}{h}\right)} - \mathbf{x}$$

Mean-shift algorithm

Input: $D -$ data.

do

foreach $\mathbf{x}_i \in D$: count $\mathbf{m}(\mathbf{x_i})$

$\nabla \hat{f}(\mathbf{x}) \rightarrow \nabla \hat{f}(\mathbf{m}(\mathbf{x}) - \mathbf{x})$

while $\nabla \hat{f}(\mathbf{x}) \neq 0$

return $C = \{C_j\}$

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Problem formulation

A training sample is given, which is

$$\{(x_1, y_1), \dots, (x_\ell, y_\ell), x_{\ell+1}, \dots, x_{\ell+m}\} = T^\ell \cup X^m,$$

where $\ell \ll m$.

Solve as supervised problem (on T^ℓ, "forgetting" about X^m)

Solve as unsupervised problem (on $X^\ell \cup X^m$, "forgetting" about Y^m).

Semi-supervised learning

Three approaches:

- Solve with native methods
- Solve with supervised algorithms without estimating error on unlabeled objects
- Solve with unsupervised algorithm achieving clusters which contains at least one object and all objects belonging to a cluster have the same label

Why is it important to solve this problem?

Usually it's chip to get objects and it is expensive to label objects.

Object mining is automated and object-labeling is expert-based.

Typical example: data from Internet (posts, pictures, articles) or generic data.

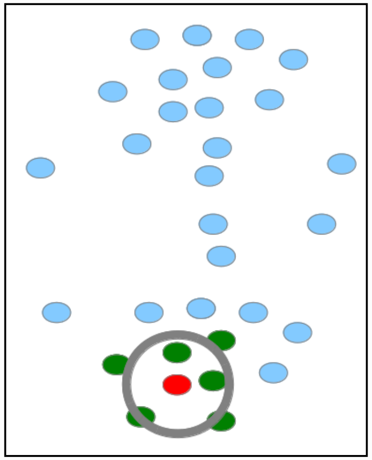
Method adaptation

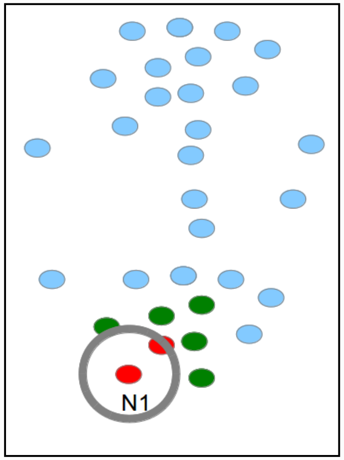
It's much simpler to adopt unsupervised methods.

Each method can be modified just by including a certain constrain, which should not allow to get clusters with differently labeled object.

DBSCAN. Пример

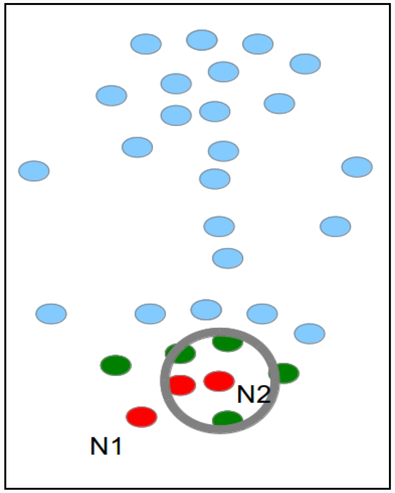
Начальные параметры: $M = 4, Eps > 0$. Берем наугад первую точку. У нее 6 соседей из N_{eps} (рис. слева) ⇒ создаем первый кластер (красный) и начинаем расширение. Первый из соседей N1 оказался граничным – добавляем его в кластер (рис. справа).

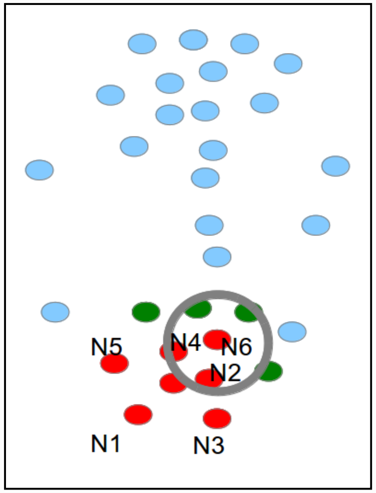




DBSCAN. Пример

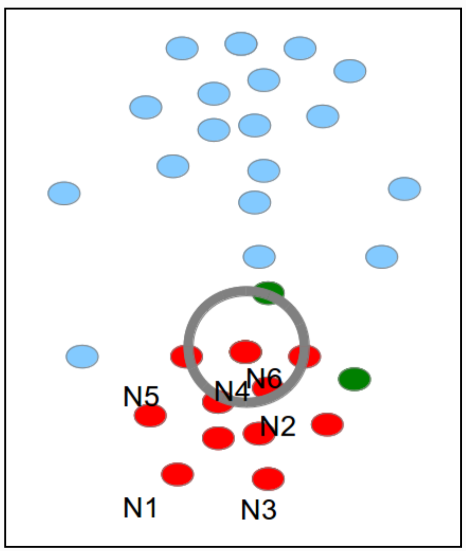
Переходим к следующему соседу N2. У него 5 своих соседей из N_{ik}. (рис. слева) ⇒ Добавляем новых соседей к старым (появился еще один зеленый сосед). И так далее. Когда обошли всех исходных соседей N1 – N6 (рис. справа), продолжаем с новыми, «зелеными».

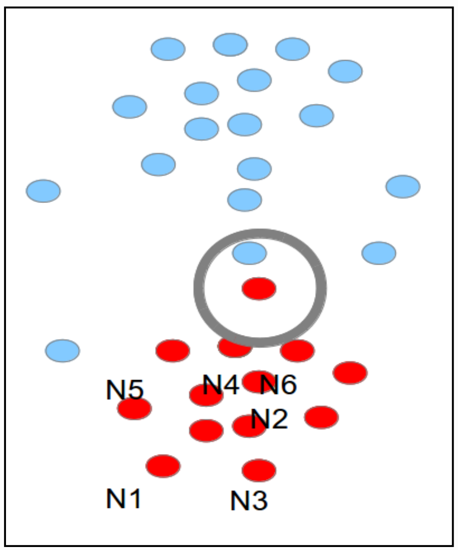




DBSCAN. Пример

После обхода соседей точек N1 – N6 остаются всего две «зеленые» точки (рис. слева), после обработки которых формируется первый кластер (рис. справа) и далее снова наугад берется точка из исходного массива.





DBSCAN. Пример

Когда выбор пал на «одинокую точку», у которой число соседей меньше $M = 4$ (рис. слева), она добавляется в массив шумов $Noise$, и далее опять наугад выбирается следующая непосещенная точка. В итоге в данном примере формируются 2 кластера, а 6 точек классифицируются как шумы (рис. справа). Заметим, что в число шумов попали и две точки между кластерами («перешеек»).