

## DENCLUE

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### DENCLUE: using density functions

- ❖ DENsity-based CLUstEring: by Hinneburg & Keim (KDD'98)
- ❖ Major features
  - ▶ Solid mathematical foundation
  - ▶ Good for data sets with large amounts of noise
  - ▶ Allows a compact mathematical description of arbitrarily shaped clusters in high-dimensional data sets
  - ▶ Significant faster than existing algorithm (faster than DBSCAN by a factor of up to 45)
  - ▶ But needs a large number of parameters

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## Denclue: Technical Essence

- ❖ Uses grid cells but only keeps information about grid cells that do actually contain data points and manages these cells in a tree-based access structure.
- ❖ DENCLUE is based on the following concepts:
  - ▶ Influence function
  - ▶ Overall density of the data space
  - ▶ Density attractors

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## Definitions

- ❖ The **influence function**  $f^y(x)$  for a point  $y \in D$  (data space) at point  $x$  is a positive function that decays to zero as  $x$  “moves away” from  $y$  ( $d(x,y) \rightarrow \infty$ ).
- ❖ Influence function describes the impact of a data point within its neighborhood.
- ❖ Typical examples are:

$$f^y(x) = \begin{cases} 1, & \text{if } d(x,y) < \sigma \\ 0, & \text{otherwise} \end{cases}$$

and

$$f^y(x) = e^{-\frac{d(x,y)^2}{2\sigma^2}}$$

where  $\sigma$  is a user-defined function/parameter.

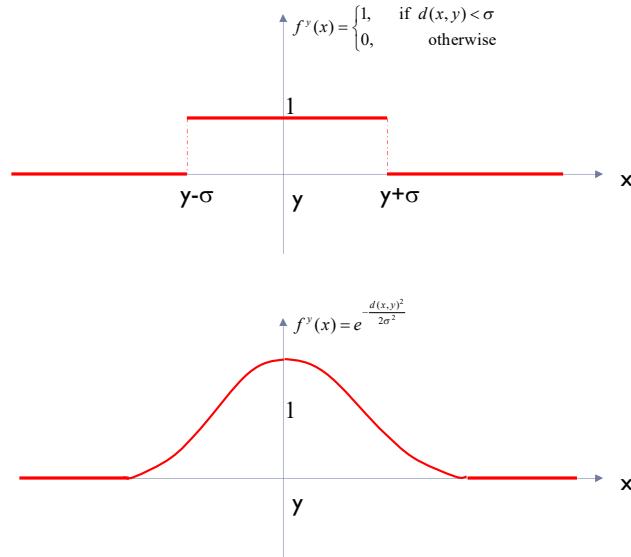
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## Definitions



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## Definitions

- ❖ The **density function** at  $x$  based on a *data space* of  $N$  points; i.e.  $D = \{x_1, \dots, x_N\}$ ; is defined as the sum of the influence function of all data points at  $\underline{x}$ :

$$f^D(x) = \sum_{i=1}^N f^{x_i}(x)$$

**The goal of the definition:**

- i. Identify all “**significant**” local maxima,  $x_j^*, j=1, \dots, m$  of  $f^D(x)$
- ii. Create a cluster  $C_j$  for each  $x_j^*$  and assign to  $C_j$  all points of  $D$  that lie within the “**region of attraction**” of  $x_j^*$ .

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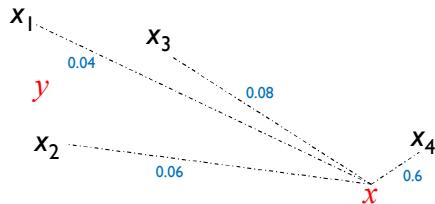
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## Definitions

### Example: Density Computation

$$D = \{x_1, x_2, x_3, x_4\}$$

$$\begin{aligned} f^D_{Gaussian}(x) &= \text{influence}(x_1) + \text{influence}(x_2) + \text{influence}(x_3) + \text{influence}(x_4) \\ &= 0.04 + 0.06 + 0.08 + 0.6 = 0.78 \end{aligned}$$



**Remark:** the density value of  $y$  would be larger than the one for  $x$

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## Definitions

### ❖ For a Gaussian influence function:

$$f^y_{Gaussian}(x) = e^{-\frac{d(x,y)^2}{2\sigma^2}}$$

Density function is:

$$f^D_{Gaussian}(x) = \sum_{i=1}^N e^{-\frac{d(x,x_i)^2}{2\sigma^2}}$$

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## Definitions

- ❖ **Gradient (The steepness of a slope):**

The gradient of function  $f^D(x)$  is defined as:

$$\nabla f^D(x, x_i) = \sum_{i=1}^N (x_i - x) \cdot f^{x_i}(x)$$

- ❖ Why is gradient defined in this way?

- ❖ Example:

$$f_{Gaussian}(x, y) = e^{-\frac{d(x, y)^2}{2\sigma^2}}$$

$$f_{Gaussian}^D(x) = \sum_{i=1}^N e^{-\frac{d(x, x_i)^2}{2\sigma^2}}$$

$$\nabla f_{Gaussian}^D(x, x_i) = \sum_{i=1}^N (x_i - x) \cdot e^{-\frac{d(x, x_i)^2}{2\sigma^2}}$$

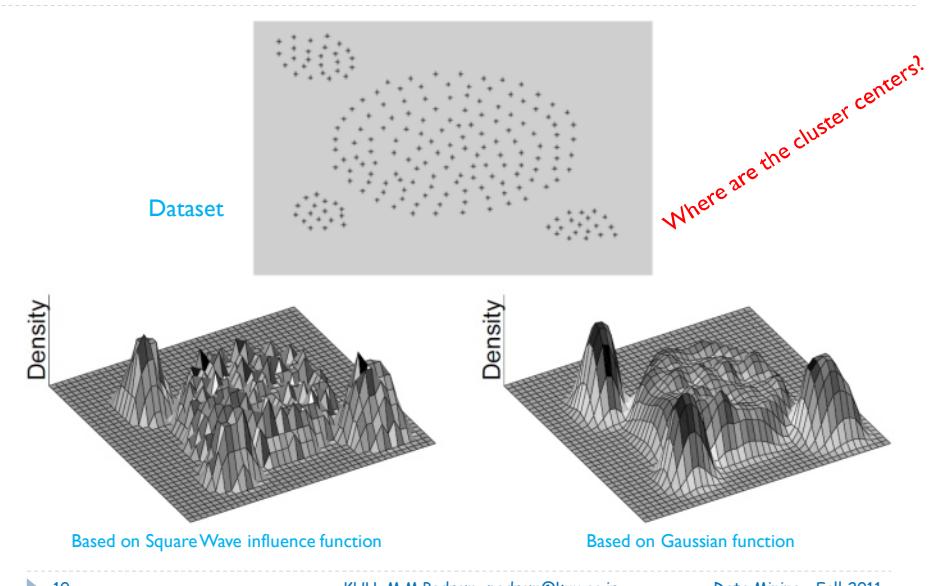
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## Definitions



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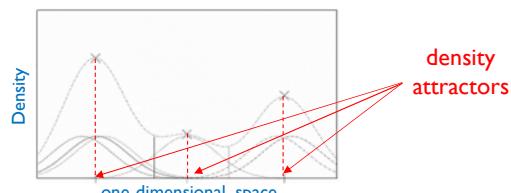
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## Definitions

- ❖ **Density attractors** are local maxima of the overall density function  $f^D(x)$ .
- ❖ Clusters can then be determined mathematically by identifying density attractors.
- ❖ A hill-climbing algorithm guided by the gradient can be used to determine the density attractor of a set of data points.



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## Definitions

- ❖ A point  $x$  is **density-attracted** to a density attractor  $x^*$ , if there exists a set of points  $x_0, x_1, \dots, x_k$  such that  $x_0 = x, x_k = x^*$  and the gradient of  $x_{i-1}$  is in the direction of  $x_i$  for  $0 < i < k$ .  
or iff  $\exists k \in \mathbb{N} : d(x^k, x^*) \leq \varepsilon$  with

$$x^0 = x, x^i = x^{i-1} + \delta \cdot \frac{\nabla f_B^D(x^{i-1})}{\|\nabla f_B^D(x^{i-1})\|}$$

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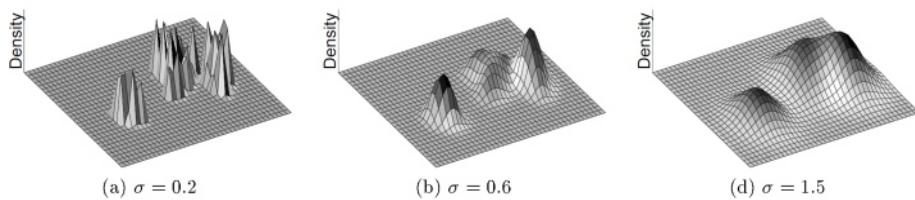
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## Definitions

### Center-Defined Cluster

- ❖ A center-defined cluster (w.r.t. to  $\sigma, \xi$ ) for a density attractor  $x^*$  is a subset  $C \subseteq D$ , with  $x \in C$  being density-attracted by  $x^*$  and  $f^D(x) \geq \xi$ .
- ❖ **Outlier:** Point  $x \in D$  is called outlier if it is density-attracted by a local maximum  $x_o^*$  with  $f^D(x_o^*) < \xi$ .



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کوهها و سطیغها



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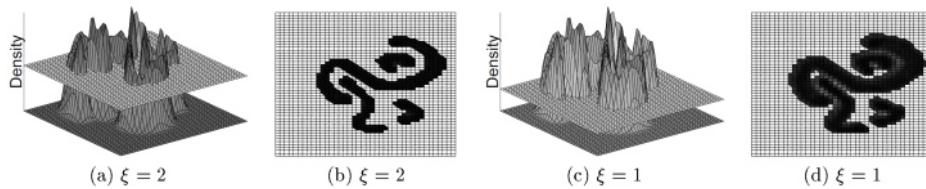
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## Definitions

### Arbitrary-Shape Cluster

- ❖ An arbitrary-shape cluster (w.r.t. to  $\sigma, \xi$ ) for a set of density attractors  $X$  is a subset  $C \subseteq D$ , where
  1.  $\forall x \in C \quad \exists x^* \in X : f^D(x^*) \geq \xi$ ,  $x$  is density-attracted to  $x^*$ , and
  2.  $\forall x^*_1, x^*_2 \in X : \exists$  a path  $P$  from  $x^*_1$  to  $x^*_2$  with  $\forall p \in P : f^D(p) \geq \xi$ .



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## Note 1

- ❖ Note that the number of clusters found by DENCLUE varies depending on  $\sigma, \xi$ .

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## Two clarifications

1. The **region of attraction** of  $x_j^*$  is defined as the set of points in  $x \in \mathbb{R}^l$  such that if a “hill-climbing” (such as the steepest ascent) method is applied, initialized by  $x$ , it will terminate arbitrarily close to  $x_j^*$ .
  2. A **local maximum** is considered as **significant** if  $f^D(x_j^*) \geq \zeta$  ( $\zeta$  is a user-defined parameter).
- ❖ Only points of the data set which are close to  $x$  actually contribute to the density. This leads to **approximation of  $f^D(x)$** , i.e. **local density function**

$$\hat{f}^D(x) = \sum_{x_i \in \text{Near}(x)} f^{x_i}(x)$$

where  $\text{Near}(x)$  is the set of points in  $D$  that lie “close” to  $x$ .

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## DENCLUE algorithm

- ❖ **Preclustering phase**
- ❖ **Main phase**

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## DENCLUE algorithm

### ❖ Preclustering phase (identification of regions dense in points of $D$ )

- A map of the relevant portion of the data space is constructed. The map is used to speed up the calculation of the density function which requires to efficiently access neighboring portions of the data space.

### ❖ Main phase (clustering)

- The second step is the actual clustering step, in which the algorithm identifies the density-attractors and the corresponding density attracted points.

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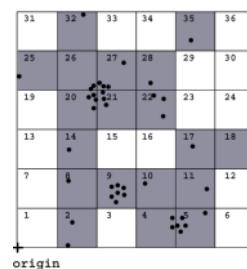
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## DENCLUE algorithm

### ❖ Preclustering phase (identification of regions dense in points of $D$ )

- Apply a  $d$ -dimensional grid of edge-length  $2\sigma$  in the  $\mathbb{R}^d$  space.
  - The hyper-cubes are numbered depending on their relative position from a given origin. In this way, the populated hyper-cubes (containing  $d$ -dimensional data points) can be mapped to one-dimensional keys and stored in tree. The keys of the populated cubes can be efficiently stored in a randomized search-tree or a B\*-tree.
- Determine the set  $C_p$  of the hyper-cubes that contain at least one point of  $D$ ; ( $C_p = \text{populated cube}$ )
- Connect neighboring populated cubes :
  - Two cubes  $c_1, c_2 \in C_{sp}$  are connected if  $d(\text{mean}(c_1), \text{mean}(c_2)) \leq 4\sigma$
  - this normally take  $O(C_p^2)$  time for all cubes.
  - To speed up, do as follow:
    - Determine the set  $C_{sp} (\subset C_p)$  that contains the "highly populated" cubes of  $C_p$ , i.e., cubes that contain at least  $\xi_c$  (outlier bound) points of  $D$ ; ( $\xi_c$  = a second outlier-bound to reduce the time needed for connecting the cubes):
 
$$C_{sp} = \{c \in C_p \mid N_c > \xi_c\}$$



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## DENCLUE algorithm

- In general, the number of highly populated cubes  $C_{sp}$  is much smaller than  $C_p$ , especially in high-dimensional space.
- The time needed for connecting the highly populated cubes with their neighbors is then  $O(|C_{sp}| \cdot |C_p|)$  with  $|C_{sp}| \ll |C_p|$ . The cardinality of  $|C_{sp}|$  depends on  $\zeta_c$ .
  - A good choice for  $\zeta_c$  is  $\zeta_c = \zeta/2d$ , since in high-dimensional spaces the clusters are usually located on lower-dimensional hyperplanes.

**Note:**

- ❖ The data structure generated in *Preclustering phase* has the following properties:
  1. The time to access the cubes for an arbitrary point is  $O(\log(C_p))$ .
  2. The time to access the relevant portion around a given cube (the connected neighboring cubes) is  $O(1)$ .

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## DENCLUE algorithm

❖ *Main phase*

- Determine the set  $C_r$  that contains:
  - the highly populated cubes, and
  - the cubes that have at least one connection with a highly populated cube.
$$C_r = C_{sp} \cup \{c \in C_p \mid \exists c_s \in C_{sp} \text{ and } \exists \text{connection}(c_s, c)\}$$
- For each point  $x$  in a cube  $c \in C_r$ , determine  $Near(x)$  as the set of points that belong to cubes  $c_j$  in  $C_r$  such that the mean values of  $c_j$ 's lie at distance less than  $\lambda\sigma$  from  $x$  (typically  $\lambda=4$ ).
- Determine local density-function for each point in the cubes of  $C_r$  based on the following approximation. Thus, local gradient can be computed:
 
$$\hat{f}^D(x) = \sum_{x_i \in Near(x)} e^{-\frac{d(x, y)^2}{2\sigma^2}}$$
- Determine the density-attractors for each point in the cubes of  $C_r$ , by a hill-climbing procedure based on the local density function and its gradient.
  - Note that after determining the density-attractor  $x^*$  for a point  $x$  and  $\hat{f}^D(x) \geq \xi$ , the point  $x$  is classified and attached to the cluster belonging to  $x^*$ .

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## DENCLUE algorithm

For each point  $x$  in a cube  $c \in C_r$

    Apply a hill climbing method starting from  $x$  and let  $x^*$  be the local maximum to which the method converges.

    If  $x^*$  is a significant local maximum ( $f^D(x^*) \geq \xi$ ) then

        If a cluster  $C$  associated with  $x^*$  has already been created, then

$x$  is assigned to  $C$

        Else

            Create a cluster  $C$  associated with  $x^*$

            Assign  $x$  to  $C$

        End if

    End if

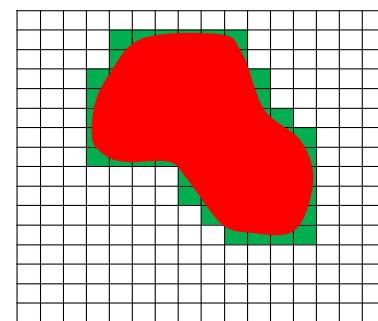
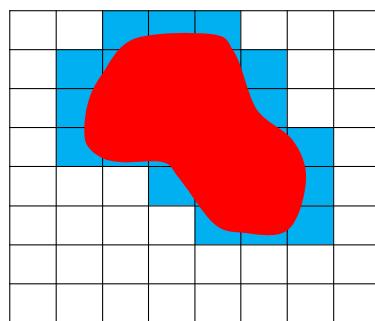
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## Remarks

- ❖ Shortcuts allow the assignment of points to clusters, without having to apply the hill-climbing procedure.
- ❖ DENCLUE is able to detect **arbitrarily** shaped clusters.
- ❖ The algorithm deals with noise very satisfactory.
- ❖ The **worst-case time complexity** of DENCLUE is  $O(N \log_2 N)$ .
- ❖ Experimental results indicate that the **average time complexity** is  $O(\log_2 N)$ .
- ❖ It works efficiently with high-dimensional data.
- ❖ DENCLUE needs at least 3 parameters to be determined, i.e.  $\sigma$ ,  $\xi$ ,  $\xi_c$ .