Clustering algorithms

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Unit 10

– Valley seeking clust. algorithms
– Branch & bound clust. Algorithms
– Simulated annealing-based clustering
– Deterministic annealing-based clustering(*)
– Genetic clustering algorithms
– Density-based clust. Algs. For large data sets (DBSCAN, DENCLUE(*))
– Spectral clustering

(*) These sections will **not** be examined

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Valley seeking clustering algorithms

Let $p(\boldsymbol{x})$ be the density function describing the distribution of the vectors in X.

- Clusters may be **viewed** as peaks of $p(\boldsymbol{x})$ **separated** by valleys.

Thus one may

- **Identify** these valleys and
- Try to **move** the borders of the clusters in these valleys.

A simple method in this spirit.

Preliminaries

- Let the distance $d(\boldsymbol{x}, \boldsymbol{y})$ be defined as

$$d(\boldsymbol{x}, \boldsymbol{y}) = (\boldsymbol{y} - \boldsymbol{x})^T A(\boldsymbol{y} - \boldsymbol{x})$$

where A is a positive definite matrix

- Let the local region of $\boldsymbol{x}$, $V(\boldsymbol{x})$, be defined as

$$V(\boldsymbol{x}) = \{\boldsymbol{y} \in X - \{\boldsymbol{x}\}: d(\boldsymbol{x}, \boldsymbol{y}) \leq a\}$$

where a is a user-defined parameter

- k_j^i be the number of vectors of the j cluster that belong to $V(\boldsymbol{x}_i) - \{\boldsymbol{x}_i\}$.
- $c_i \in \{1, \ldots, m\}$ denote the cluster to which $\boldsymbol{x}_i$ will be assigned.

Valley seeking clustering algorithms

Valley-Seeking algorithm

- **Fix** a.
- **Fix** the number of clusters m.
- **Define** an initial clustering X.
- **Repeat**
  - For $i = 1$ to N
    - **Find** j: $k_j^i = \max_{q=1,\ldots,m} k_q^i$
    - **Set** $c_i = j$
  - End For
  - For $i = 1$ to N
    - **Assign** $\boldsymbol{x}_i$ **to** cluster C_{c_i}.
  - End For
- **Until** no reclustering of vectors occurs.

Valley seeking clustering algorithms

The algorithm

- **Centers** a window defined by $d(\boldsymbol{x}, \boldsymbol{y}) \leq a$ at $\boldsymbol{x}$ and **counts** the points from different clusters in it.
- **Assigns** $\boldsymbol{x}$ to the *cluster with the larger number of points* in the window (the cluster that **corresponds** to the highest local pdf).

In other words:

- The boundary is **moved away** from the "winning" cluster.

Remarks:

- The algorithm is sensitive to a. It is suggested to perform several runs, for different values of a.
- The algorithm is of a mode-seeking nature (*if more than enough clusters are initially appointed, some of them will become empty*).

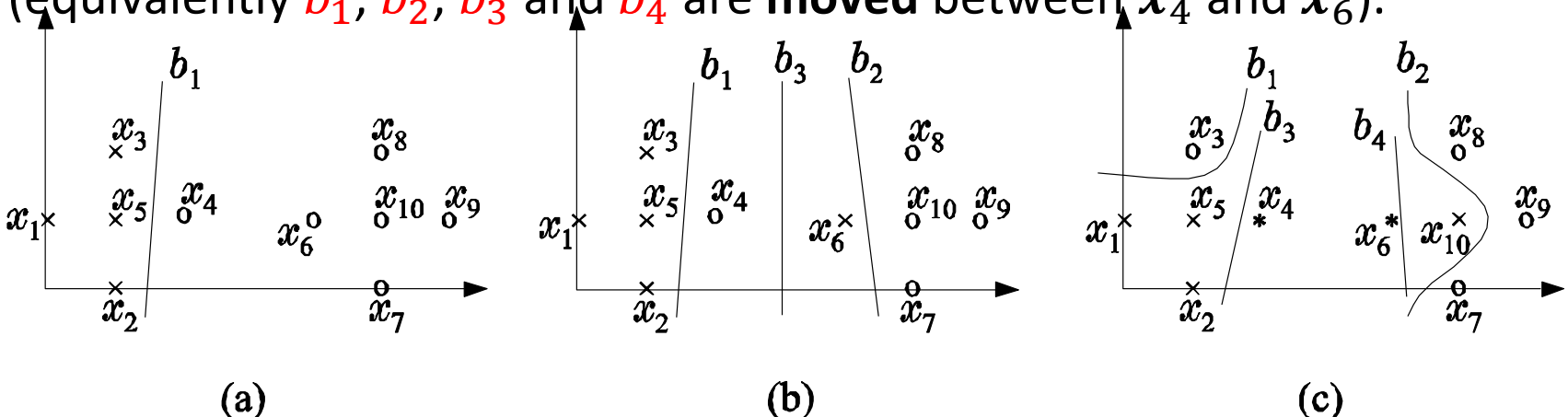
Valley seeking clustering algorithms

Example: Let $X = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{10}\}$ and $a = 1.1415\ (> \sqrt{2})$. X contains two physical clusters: $C_1 = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_5\}$, $C_2 = \{\boldsymbol{x}_6, \ldots, \boldsymbol{x}_{10}\}$.

(a) **Initially** two clusters are considered separated by b_1. After the convergence of the algorithm, C_1 and C_2 are identified (equivalently, b_1 is **moved** between $\boldsymbol{x}_4$ and $\boldsymbol{x}_6$).

(b) **Initially** two clusters are considered separated by b_1, b_2 and b_3. After the convergence of the algorithm, C_1 and C_2 are identified (equivalently b_1 and b_2 are **moved** to the area where b_3 lies).

(c) **Initially** three clusters are considered separated by b_1, b_2, b_3, b_4. After the convergence of the algorithm, only two clusters are identified, C_1 and C_2 (equivalently b_1, b_2, b_3 and b_4 are **moved** between $\boldsymbol{x}_4$ and $\boldsymbol{x}_6$).



Branch and Bound Clustering algorithms

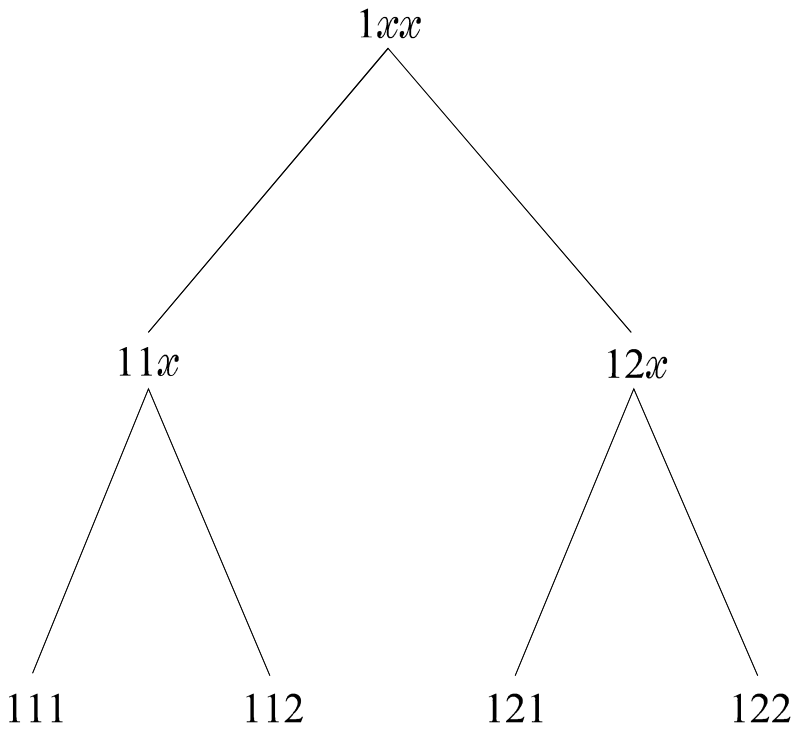
- They compute the globally optimal solution to combinatorial problems.
- They *avoid exhaustive search* via the employment of a monotonic criterion J.

Monotonic criterion J: *if* k *vectors of* X *have been assigned to clusters, the assignment of an extra vector to a cluster* ***does not decrease*** *the value of* J.

Consider the following 3-vectors, 2-class case:

121: 1st, 3rd vectors belong to class 1
2nd vector belongs to class 2.
(leaf of the tree)

$12x$: 1st vector belongs to class 1
2nd vector belongs to class 2
3rd vector is unassigned
(Partial clustering- node of the tree).



Branch and Bound Clustering algorithms

How exhaustive search is avoided

- Let B be the best value for criterion J computed so far.
- **If** at a node of the tree, the corresponding value of J is greater than B, **no further search** is **performed** for all subsequent descendants springing from this node.
- Let $\boldsymbol{C}_r = [c_1, \ldots, c_r]$, $1 \leq r \leq N$, denotes a partial clustering where $c_i \in \{1,2, \ldots, m\}$, $c_i = j$ if the vector $\boldsymbol{x}_i$ belongs to cluster C_j and $\boldsymbol{x}_{r+1}, \ldots, \boldsymbol{x}_N$ are yet unassigned.
- For compact clusters and fixed number of clusters, m, a suitable cost function is

$$J(\boldsymbol{C}_r) = \sum_{i=1}^{r} \left|\left|\boldsymbol{x}_i - \boldsymbol{m}_{c_i}(\boldsymbol{C}_r)\right|\right|^2$$

where $\boldsymbol{m}_{c_i}$ is the mean vector of the cluster C_{c_i}

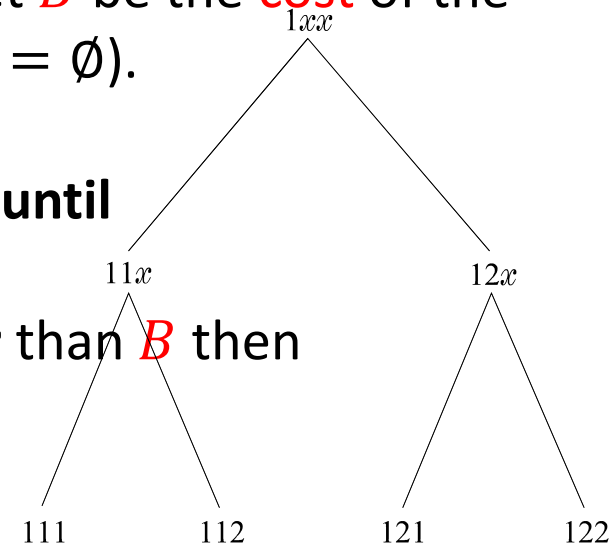
$$\boldsymbol{m}_j(\boldsymbol{C}_r) = \frac{1}{n_j(\boldsymbol{C}_r)} \sum_{\{q=1,\ldots,r, c_q=j\}} \boldsymbol{x}_q\,, \qquad j = 1, \ldots, m$$

with $n_j(\boldsymbol{C}_r)$ being the number of vectors $\boldsymbol{x} \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_r\}$ that belong to cluster C_j.

Branch and Bound Clustering algorithms

Initialization

- **Start** from the initial node and go down to a leaf. Let B be the cost of the corresponding clustering $\boldsymbol{C}$ (initially set $B = +\infty$, $\boldsymbol{C} = \emptyset$).



Main stage

- **Start** from the initial node of the tree and go down **until**
  - **Either** (i) A leaf is encountered.
    - If the cost B' of the corr. clustering $\boldsymbol{C}'$ is **smaller** than B then
      - $B = B'$
      - $\boldsymbol{C} = \boldsymbol{C}'$ is the best clustering found so far
    - End if
  - **Or** (ii) a node q with value of J **greater** than B is encountered. Then
    - No subsequent clustering branching from q is considered.
    - **Backtrack** to the parent of q, q^{par}, in order to **span** a different path.
    - **If** all paths branching from q^{par} have been considered then
      - **Move** to the grandparent of q.
    - End if
  - **End if**

Terminate when all possible paths have been considered explicitly or implicitly.

Branch and Bound Clustering algorithms

Remarks

- Variations of the above algorithm, where much tighter bounds of B are used (that is, many more clusterings are rejected without explicit consideration) have also been proposed.

- A disadvantage of the algorithm is the excessive (and unpredictable) amount of required computational time.

Simulated Annealing

- It **guarantees** (under certain conditions) in probability, the determination of the globally optimal solution of the problem at hand via the minimization of a cost function J.
- It **may escape** from local minima since it **allows** moves that temporarily may increase the value of J.

Definitions

- An important parameter of the algorithm is the "temperature" T, which **starts** at a high value and **reduces** gradually.
- A sweep is the time the algorithm spends at a given temperature so that the system can enter the "thermal equilibrium" in this temperature.

Notation

- T_{max} is the initial value of the temperature T.
- $\boldsymbol{C}_{init}$ is the initial clustering.
- $\boldsymbol{C}$ is the current clustering.
- t is the current sweep.

Simulated Annealing

The algorithm:

- **Set** $T = T_{max}$ and $\boldsymbol{C} = \boldsymbol{C}_{init}$.
- $t = 0$
- **Repeat**
  - $t = t + 1$
  - *Repeat*
    - **Compute** $J(\boldsymbol{C})$
    - **Produce** a new clustering, $\boldsymbol{C}'$, by **assigning** a randomly chosen vector from X to a different cluster.
    - **Compute** $J(\boldsymbol{C}')$
    - **If** $\Delta J = J(\boldsymbol{C}') - J(\boldsymbol{C}) < 0$ then
      - (A) $\boldsymbol{C} = \boldsymbol{C}'$
    - Else
      - (B) $\boldsymbol{C} = \boldsymbol{C}'$, with probability $P(\Delta J) = e^{-\Delta J/T}$.
    - End if
  - *Until* an equilibrium state is **reached** at this temperature.
  - $T = f(T_{max}, t)$
- **Until** a predetermined value T_{min} for T is reached

Simulated Annealing

Remarks:

- For $T \to \infty$, it is $p(\Delta J) \approx 1$. Thus almost all movements of vectors between clusters are allowed.
- For lower values of T fewer moves of type (B) (from lower to higher cost clusterings) are allowed.
- As $T \to 0$ the probability of moves of type (B) tends to zero.
- Thus as T decreases, it becomes more probable to reach clusterings that correspond to lower values of J.
- Keeping T positive, we **ensure** a nonzero probability for escaping from a local minimum.
- We assume that the equilibrium state has been reached

  "If for k successive random reassignments of vectors, $\boldsymbol{C}$ remains unchanged."
- A schedule for lowering T that guarantees convergence to the global minimum with probability 1, is

$$T = \frac{T_{max}}{\ln(1+t)}$$

- The method is computationally demanding.

Deterministic Annealing (DA) (*)

- It is inspired by the phase transition phenomenon observed when the temperature of a material changes. It **involves** the parameter $\beta = 1/T$, where T is defined as in simulated annealing.

- **The Goal of DA**: **Locate** a set of representatives $\boldsymbol{w}_j$, $j = 1, \ldots, m$ (m is fixed) in appropriate positions so that a distortion function J is minimized.

  J is defined as

$$J = -\frac{1}{\beta}\sum_{i=1}^{N} ln\left(\sum_{j=1}^{m} e^{-\beta d(\boldsymbol{x}_i, \boldsymbol{w}_j)}\right)$$

Assumption: $d(\boldsymbol{x}, \boldsymbol{w})$ is a *convex function* of $\boldsymbol{w}$ for **fixed** $\boldsymbol{x}$.

- Then, the optimal value of a specific $\boldsymbol{w}_r$ satisfies the following condition:

$$\frac{\partial J}{\partial \boldsymbol{w}_r} = \sum_{i=1}^{N} P_{ir} \frac{\partial d(\boldsymbol{x}_i, \boldsymbol{w}_r)}{\partial \boldsymbol{w}_r} = 0$$

where

$$P_{ir} = \frac{e^{-\beta d(\boldsymbol{x}_i, \boldsymbol{w}_r)}}{\sum_{j=1}^{m} e^{-\beta d(\boldsymbol{x}_i, \boldsymbol{w}_j)}}$$

- P_{ir} may be **interpreted** as the probability that $\boldsymbol{x}_i$ **belongs** to C_r, $r = 1, \ldots, m$.

Deterministic Annealing (*)

Assumption: $d(\boldsymbol{x}, \boldsymbol{w})$ is a convex function of $\boldsymbol{w}$ for **fixed** $\boldsymbol{x}$.

Stages of the algorithm

- For $\beta \longrightarrow 0$, **all** P_{ij}'s are almost equal to $\frac{1}{m}$, for all $\boldsymbol{x}_i$'s, $i = 1, \ldots, N$. Thus

$$\sum_{i=1}^{N} \frac{\partial d(\boldsymbol{x}_i, \boldsymbol{w}_r)}{\partial \boldsymbol{w}_r} = 0$$

Since $d(\boldsymbol{x}, \boldsymbol{w})$ is a convex function, $d(\boldsymbol{x}_1, \boldsymbol{w}_r) + \cdots + d(\boldsymbol{x}_N, \boldsymbol{w}_r)$ is a convex function. All representatives coincide with its unique global minimum (all the data belong to a single cluster).

- As β increases, it **reaches** a critical value where P_{ir}'s "depart sufficiently" from the uniform model. Then the representatives split up in order to provide an optimal presentation of the data set at the new phase.

- The increase of β **continues** *until* P_{ij} **approach** the hard clustering model (for all $\boldsymbol{x}_i$, $P_{ir} \approx 1$ for a specific r, and $P_{ij} \approx 0$, for $j \neq r$).

Deterministic Annealing (*)

Application: For the squared Euclidean distance $d(\boldsymbol{x}, \boldsymbol{w}) = (\boldsymbol{x} - \boldsymbol{w})^T(\boldsymbol{x} - \boldsymbol{w})$ it is

$$\frac{\partial J}{\partial \boldsymbol{w}_r} = \sum_{i=1}^{N} P_{ir} \frac{\partial d(\boldsymbol{x}_i, \boldsymbol{w}_r)}{\partial \boldsymbol{w}_r} = 2\sum_{i=1}^{N} P_{ir}(\boldsymbol{x}_i - \boldsymbol{w}_r) = 0 \Leftrightarrow \boldsymbol{w}_r = \frac{\sum_{i=1}^{N} P_{ir}\boldsymbol{x}_i}{\sum_{i=1}^{N} P_{ir}}$$

This is **coupled** wrt $\boldsymbol{w}_r$

Remarks:

- It is not guaranteed that it **reaches** the globally optimum clustering.
- If m is chosen **greater than** the "actual" number of clusters, the algorithm has the ability to represent the data properly.

Clustering using genetic algorithms (GA)

A few hints concerning genetic algorithms

- They have been **inspired** by the natural selection mechanism (Darwin).
- They consider a population of solutions of the problem at hand and they **perform** certain operators on this, so that the new population **of the same size** is improved compared to the previous one (wrt a *criterion function* F).
- The solutions are coded and the operators are applied on the coded versions of the solutions.

The most well-known operators are:

Reproduction:

- It ensures that, in probability, the better (worse) a solution in the current population is, the more (less) replicates it has in the next population.
- A simple implementation:
  - For each solution s_i, out of the population of the p solutions, compute the associated criterion function value $F(s_i)$.
    (it is assumed that the **higher** the value of F, the **better** the solution)
  - Assign to each s_i a probability $p_i = F(s_i) / \sum_{j=1}^{p} F(s_j)$.
  - Perform sampling with replacement to produce the next solution population.

Clustering using genetic algorithms (GA)

Crossover:

- It applies to the temporary population produced after the application of the reproduction operator.
- It **selects** pairs of solutions *randomly*, **splits** them at a *random position* and **exchanges** their second parts.

Mutation:

- It applies to the temporary population produced after the application of the crossover operator.
- It **selects** *randomly* an element of a solution and **alters** it with some probability.
- It may be viewed as a way out of getting stuck in local minima.

Aspects/Parameters that affect the performance of the algorithm

The coding of the solutions.

The number of solutions in a population, p.

The probability with which two solutions are **selected** for crossover.

The probability with which an element of a solution is **mutated**.

Clustering using genetic algorithms (GA)

GA Algorithmic scheme

$t = 0$

Choose an initial population $\wp_t$ of solutions.

Repeat

- **Apply** reproduction on $\wp_t$ and let $\wp'_t$ be the resulting temporary population.
- **Apply** crossover on $\wp'_t$ and let $\wp''_t$ be the resulting temporary population.
- **Apply** mutation on $\wp''_t$ and let $\wp_{t+1}$ be the resulting population.
- $t = t + 1$

Until a termination condition is met.

Return

- **either** the best solution of the last population,
- **or** the best solution found during the evolution of the algorithm.

Clustering using genetic algorithms (GA)

Genetic Algorithms in Clustering

The characteristics of a simple GA hard clustering algorithm suitable for compact clusters, whose number m is fixed, is discussed next.

A (not unique) way to **code** a solution is via the cluster representatives.

$$[\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m]$$

The cost function in use is

$$J = \sum_{i=1}^{N} u_{ij} d(\boldsymbol{x}_i, \boldsymbol{w}_j)$$

The *criterion function* can be defined e.g., as $F(s_i) = e^{-J(s_i)}$

where

$$u_{ij} = \begin{cases} 1, & if\, d(\boldsymbol{x}_i, \boldsymbol{w}_j) = min_{k=1,\ldots,m} d(\boldsymbol{x}_i, \boldsymbol{w}_k) \\ 0, & otherwise \end{cases}, i = 1, \ldots, N$$

The allowable cut points for the crossover operator **are** between different representatives.

The mutation operator ***selects*** randomly a coordinate and **decides** randomly to add a small random number to it.

Clustering using genetic algorithms (GA)

Remark:

- An alternative to the above scheme results if prior to the application of the reproduction operator, the hard clustering algorithm (GHAS), described in a previous lecture, **runs** p times, each time **using** a different solution of the current population as the initial state. The p resulting solutions constitute the population on which the reproduction operator will be applied.

Density-based algorithms for large data sets

These algorithms:

- Consider clusters as regions in the l-dimensional space that are "dense" in points of X.

- Have, in principle, the ability to **recover** arbitrarily shaped clusters (however, difficulties may arise in the case where the clusters differ in terms of their density).

- **Handle** efficiently outliers.

- Have time complexity **less** than $O(N^2)$.

Typical density-based algorithms are:

- The DBSCAN algorithm.
- The DBCLASD algorithm.
- The DENCLUE algorithm.

Density-based algorithms for large data sets

Density-Based Spatial Clustering of Applications with Noise (DBSCAN)

Algorithm

The "density" around a point $\boldsymbol{x}$ is **estimated** as the number of points in X that fall inside a specific region of the l-dimensional space surrounding $\boldsymbol{x}$.

Notation

- $V_\varepsilon(\boldsymbol{x})$ is the hypersphere of radius ε (user-defined parameter) **centered** at $\boldsymbol{x}$.
- $N_\varepsilon(\boldsymbol{x})$ the number of points of X **lying** in $V_\varepsilon(\boldsymbol{x})$.
- q is the **minimum number** of points of X that must be contained in $V_\varepsilon(\boldsymbol{x})$, in order for $\boldsymbol{x}$ to be considered an "interior" point of a cluster.

Definitions

1. A point $\boldsymbol{y}$ is directly density reachable from a point $\boldsymbol{x} \in X$ if
   (i) $\boldsymbol{y} \in V_\varepsilon(\boldsymbol{x})$
   (ii) $N_\varepsilon(\boldsymbol{x}) \geq q$ (fig. (a)).
2. A point $\boldsymbol{y}$ is density reachable from a point $\boldsymbol{x} \in X$ if there is a sequence of points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_p \in X$, with $\boldsymbol{x}_1 = \boldsymbol{x}$, $\boldsymbol{x}_p = \boldsymbol{y}$, such that $\boldsymbol{x}_{i+1}$ is **directly** density reachable from $\boldsymbol{x}_i$ (fig. (b)).

Density-based algorithms for large data sets

DBSCAN Algorithm (cont.)

3. A point $\boldsymbol{x}$ is density connected to a point $\boldsymbol{y} \in X$ if there exists $\boldsymbol{z} \in X$ such that *both* $\boldsymbol{x}$ and $\boldsymbol{y}$ are **density reachable** from $\boldsymbol{z}$ (fig. (c)).

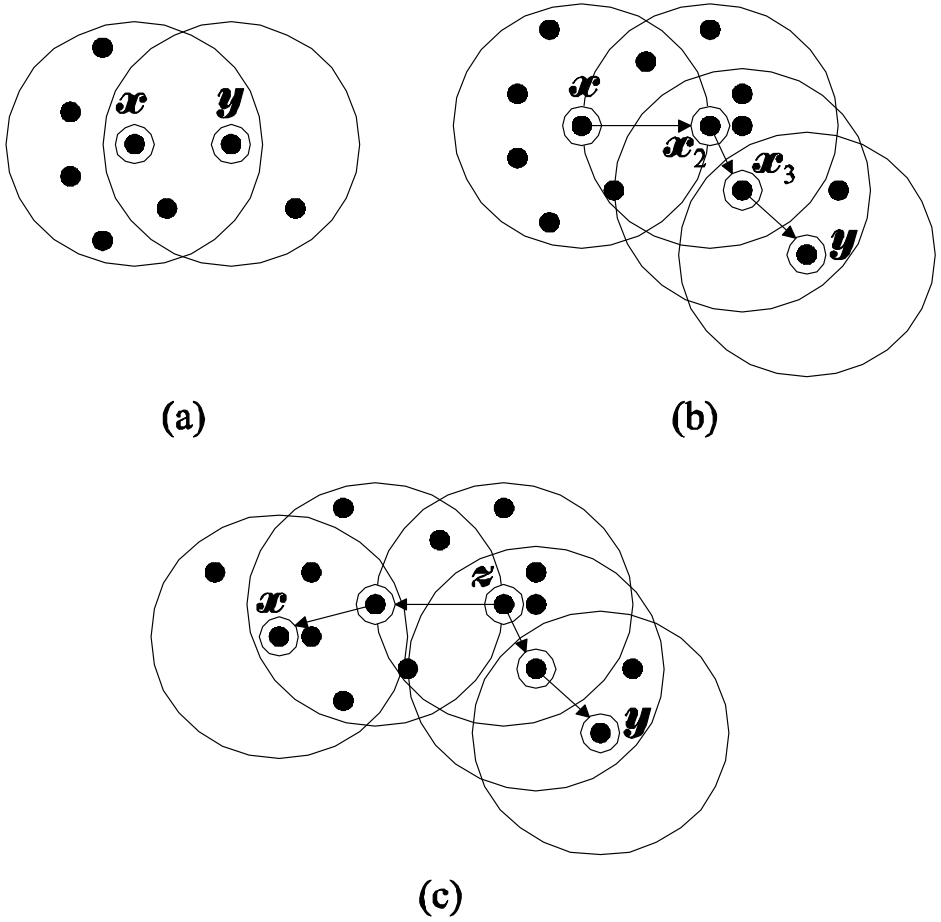
Example:

Assuming that $q = 5$,

(a) $\boldsymbol{y}$ is directly density reachable from x, but not vice versa,

(b) $\boldsymbol{y}$ is density reachable from x, but not vice versa, and

(c) $\boldsymbol{x}$ and $\boldsymbol{y}$ are density connected (in addition, $\boldsymbol{y}$ is density reachable from $\boldsymbol{x}$, but not vice versa).



(a) (b)

(c)

Density-based algorithms for large data sets

DBSCAN Algorithm (cont.)

4. A cluster C in DBSCAN is defined as a nonempty subset of X satisfying the following conditions:
   - *If* $\boldsymbol{x}$ **belongs** to C and $\boldsymbol{y} \in X$ is density reachable from $\boldsymbol{x}$, *then* $\boldsymbol{y} \in C$.
   - For each pair $(\boldsymbol{x}, \boldsymbol{y}) \in C$, $\boldsymbol{x}$ and $\boldsymbol{y}$ are density connected.

5. Let $C_1, \ldots, C_m$ be the clusters in X. The set of points that are not connected in any of the $C_1, \ldots, C_m$ is known as noise.

6. A point $\boldsymbol{x}$ is called a core (noncore) point if it has at least (less than) q points in its neighborhood.
   A noncore point may be either
   - a border point of a cluster (that is, density reachable from a core point) or
   - a noisy point (that is, not density reachable from other points in X).

Density-based algorithms for large data sets

DBSCAN Algorithm (cont.)

Proposition 1: *If* $\boldsymbol{x}$ is a core point and D is the set of points in X that are density reachable from $\boldsymbol{x}$, *then* D is a cluster.

Proposition 2: *If* C is a cluster and $\boldsymbol{x}$ is a core point in C, *then* C **equals** to the set of the points $\boldsymbol{y} \in X$ that are density reachable from $\boldsymbol{x}$.

Therefore: A cluster is **uniquely determined** by any of its core points.

Notation

- X_{un} is the set of points in X that have **not** been **considered yet**.
- m denotes the number of clusters.

Density-based algorithms for large data sets

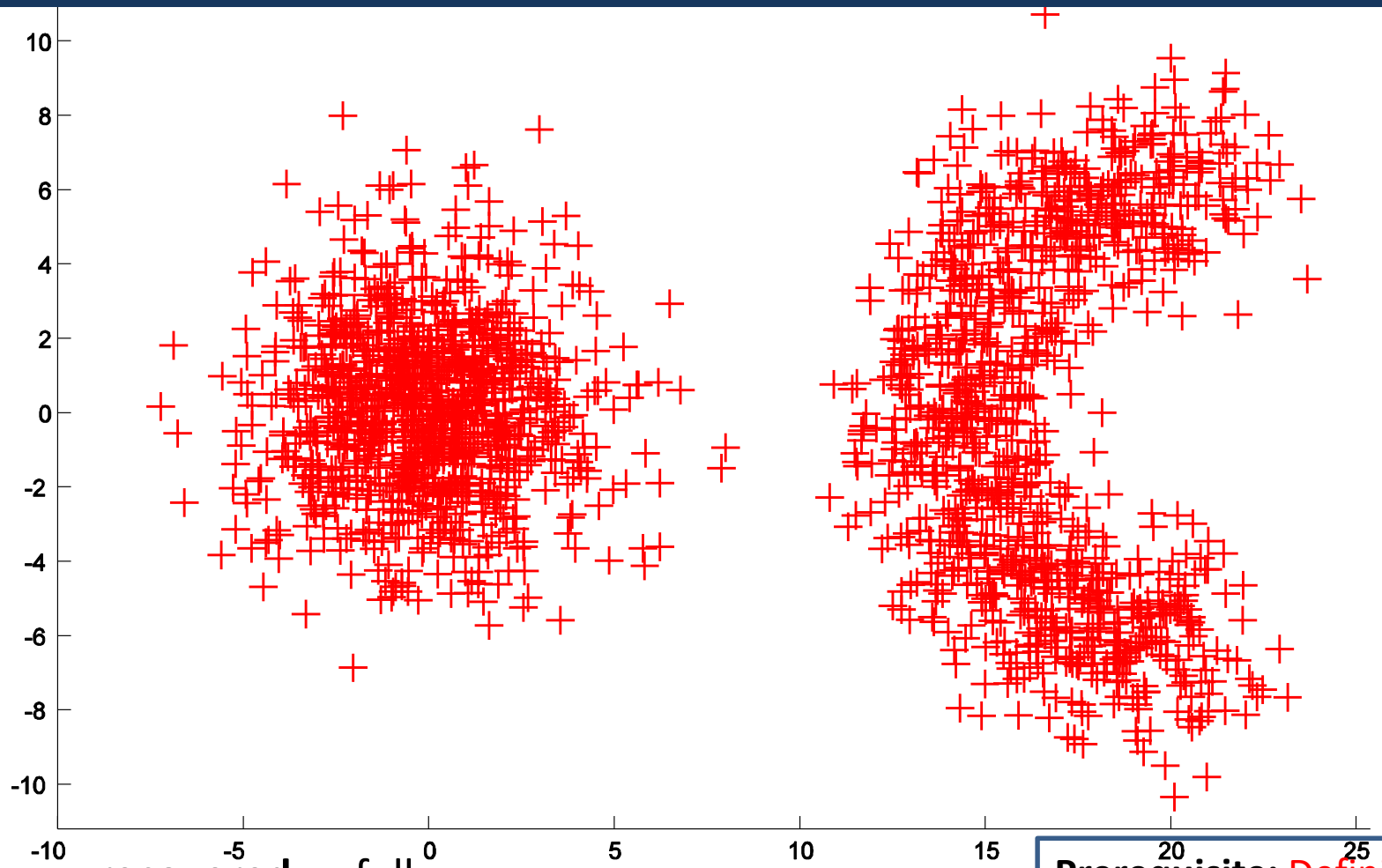
DBSCAN Algorithm (cont.)

DBSCAN Algorithm

- **Set** $X_{un} = X$
- **Set** $m = 0$
- **While** $X_{un} \neq \emptyset$ do
  - Arbitrarily **select** a $\boldsymbol{x} \in X_{un}$
  - *If* $\boldsymbol{x}$ is a noncore point then
    - **Mark** $\boldsymbol{x}$ as noise point
    - $X_{un} = X_{un} - \{\boldsymbol{x}\}$
  - *End if*

  - *If* $\boldsymbol{x}$ is a core point *then*
    - $m = m + 1$
    - **Determine all** density-reachable points $\boldsymbol{y} \in X$ from $\boldsymbol{x}$.
    - **Assign** $\boldsymbol{x}$ and the previous points to the cluster C_m. The border points among them that may have been **marked** as "noise" are also **assigned** to C_m.
    - $X_{un} = X_{un} - C_m$
  - End {if}
- **End** {while}

Clustering – Density-based algorithms

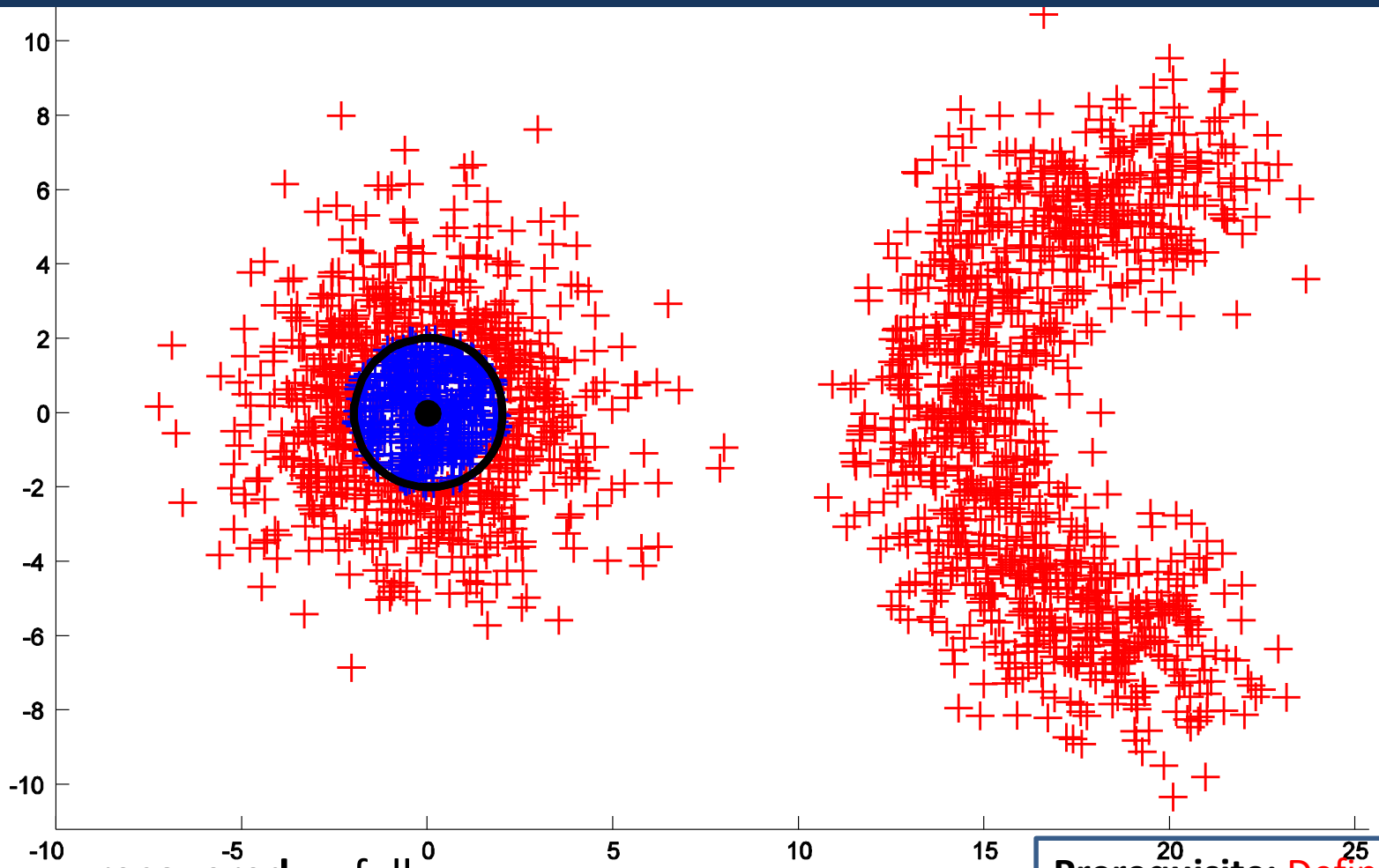


Clusters are **recovered** as follows:

- **Start** a new cluster C by **choosing** a data point $\boldsymbol{x}$.
- **Assign** all the data points that lie in the neighborhood of $\boldsymbol{x}$ to the same cluster.
- **Repeat** recursively the previous step **until** all neighboring points of ALL $\boldsymbol{x} \in C$ are **assigned** to C.

Prerequisite: Definition of the neighborhood size

Clustering – Density-based algorithms



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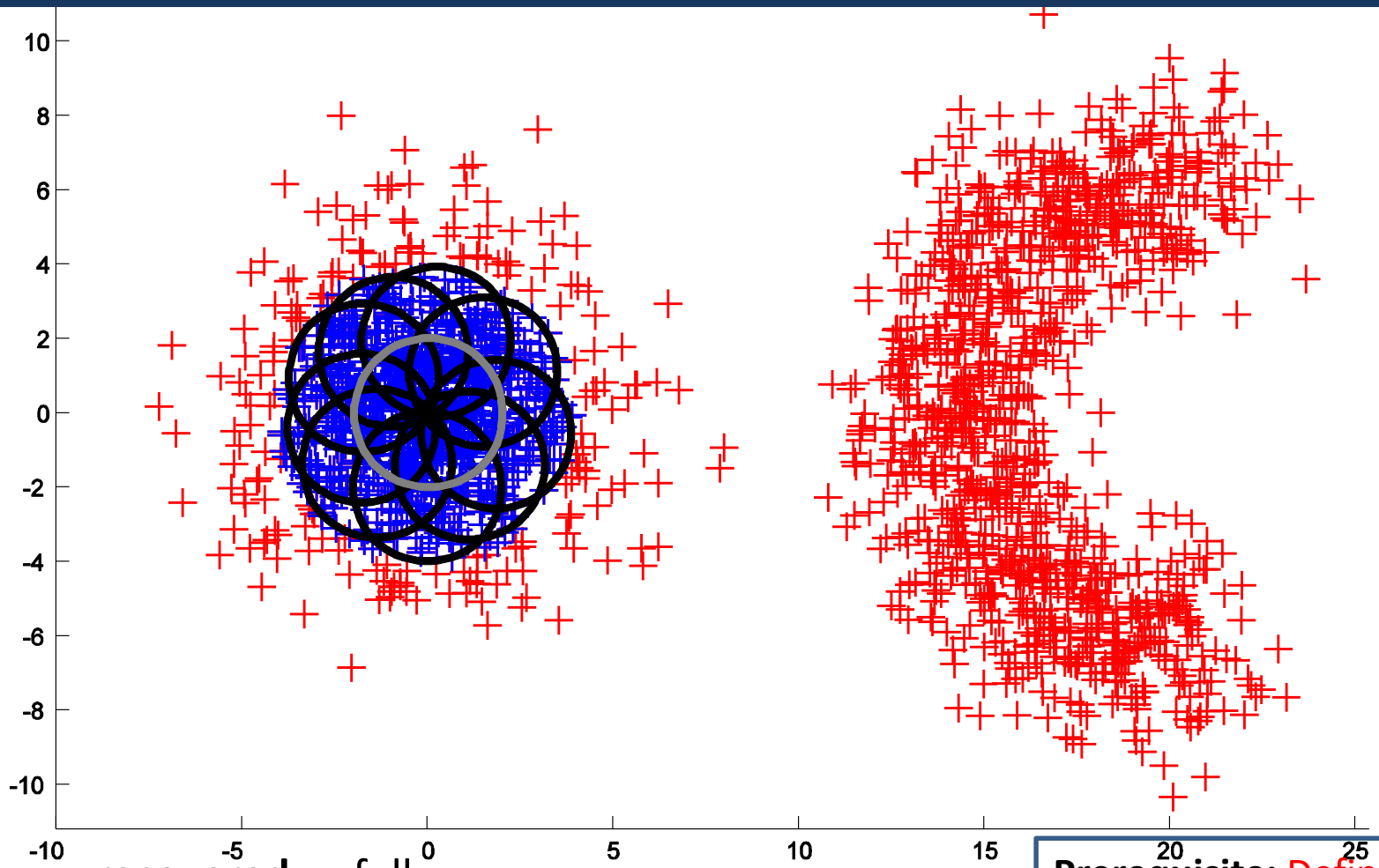

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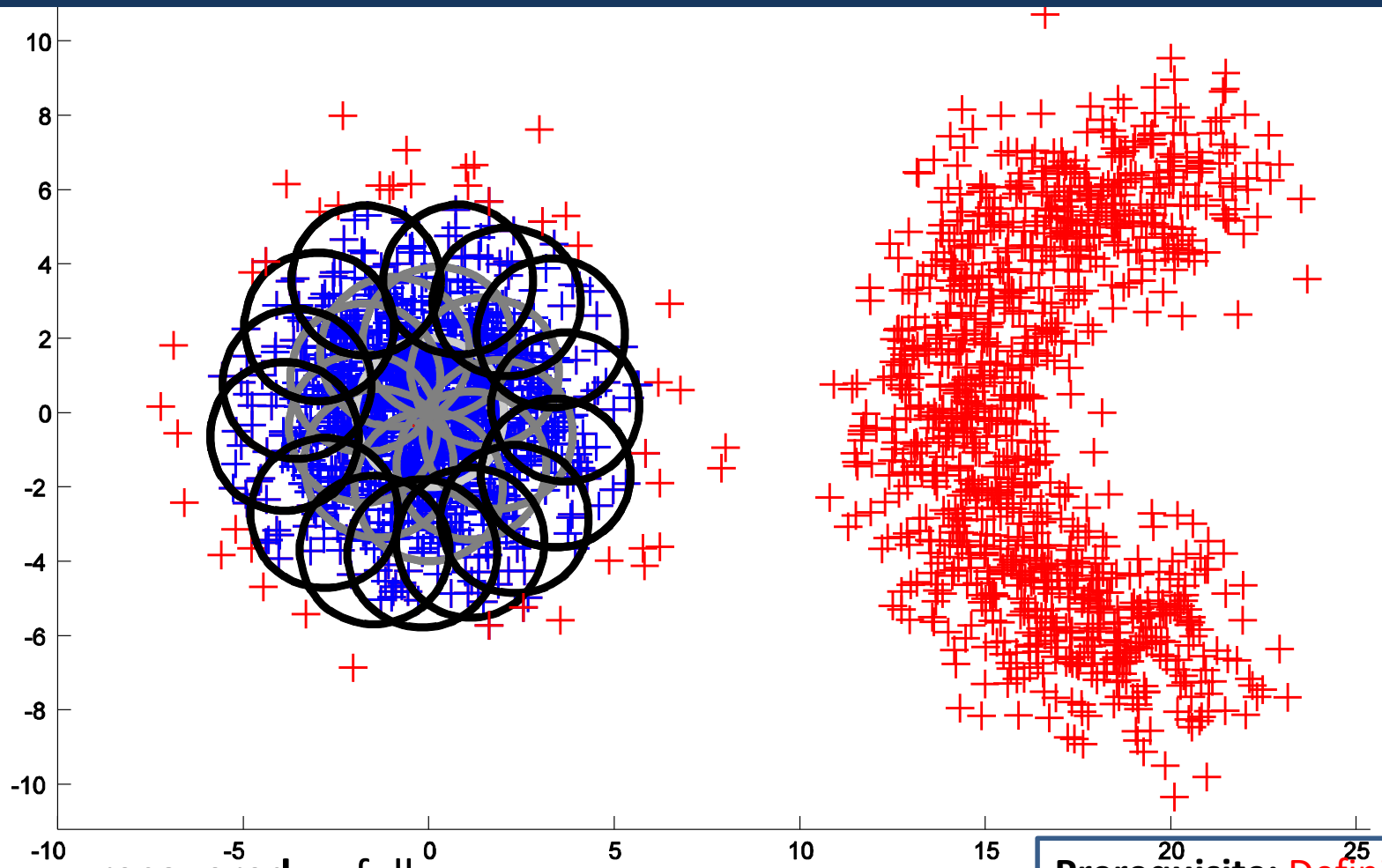

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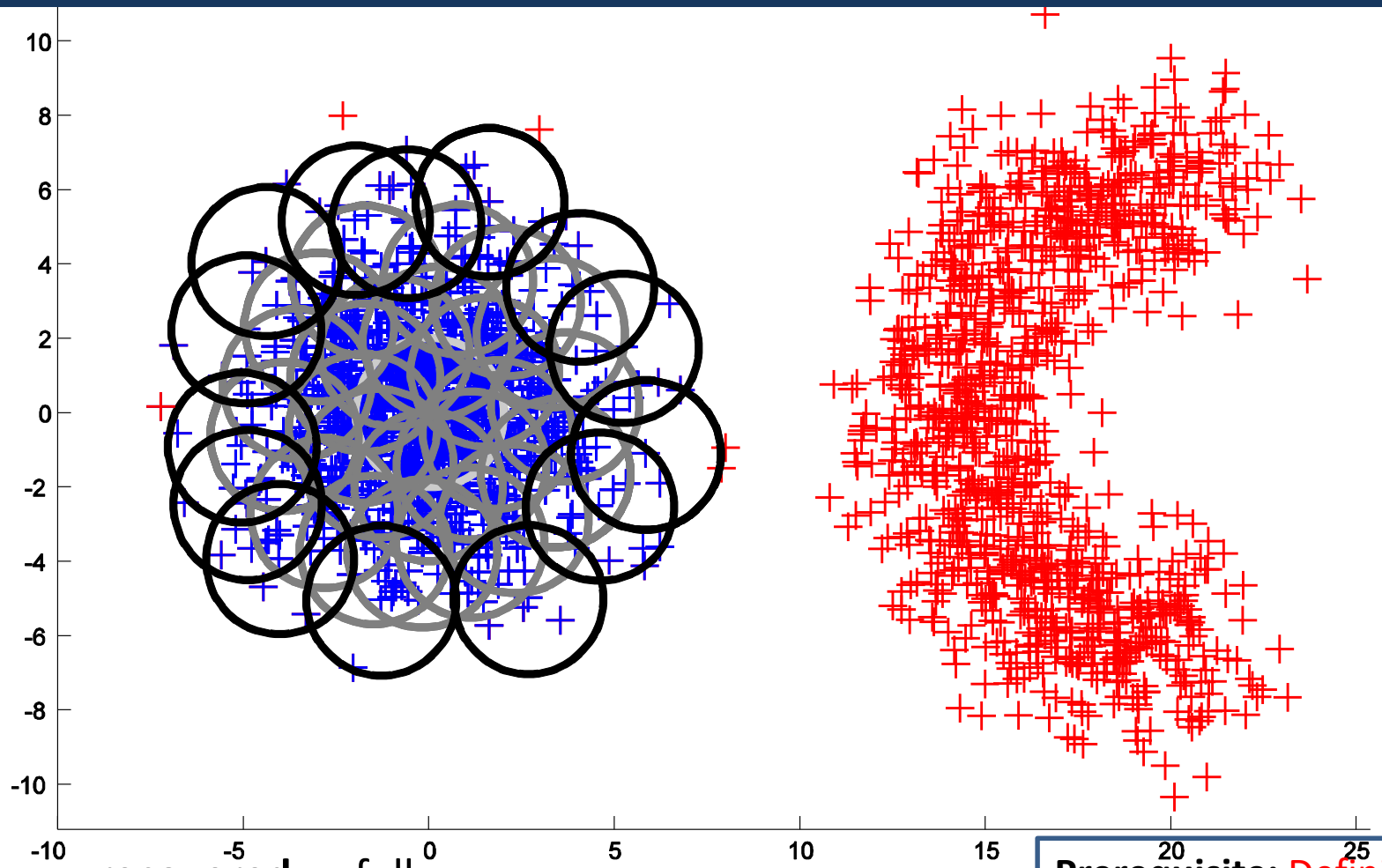

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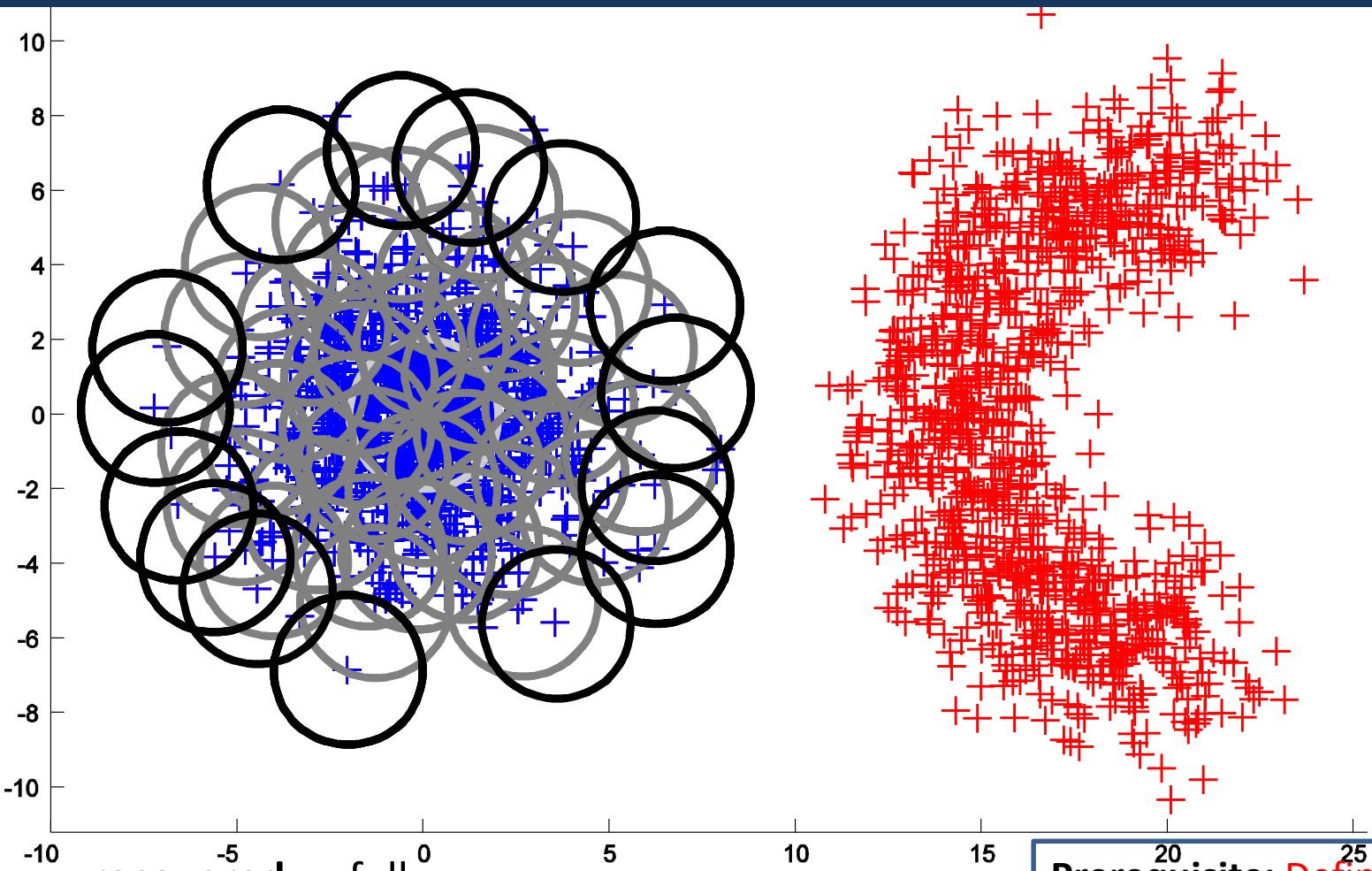

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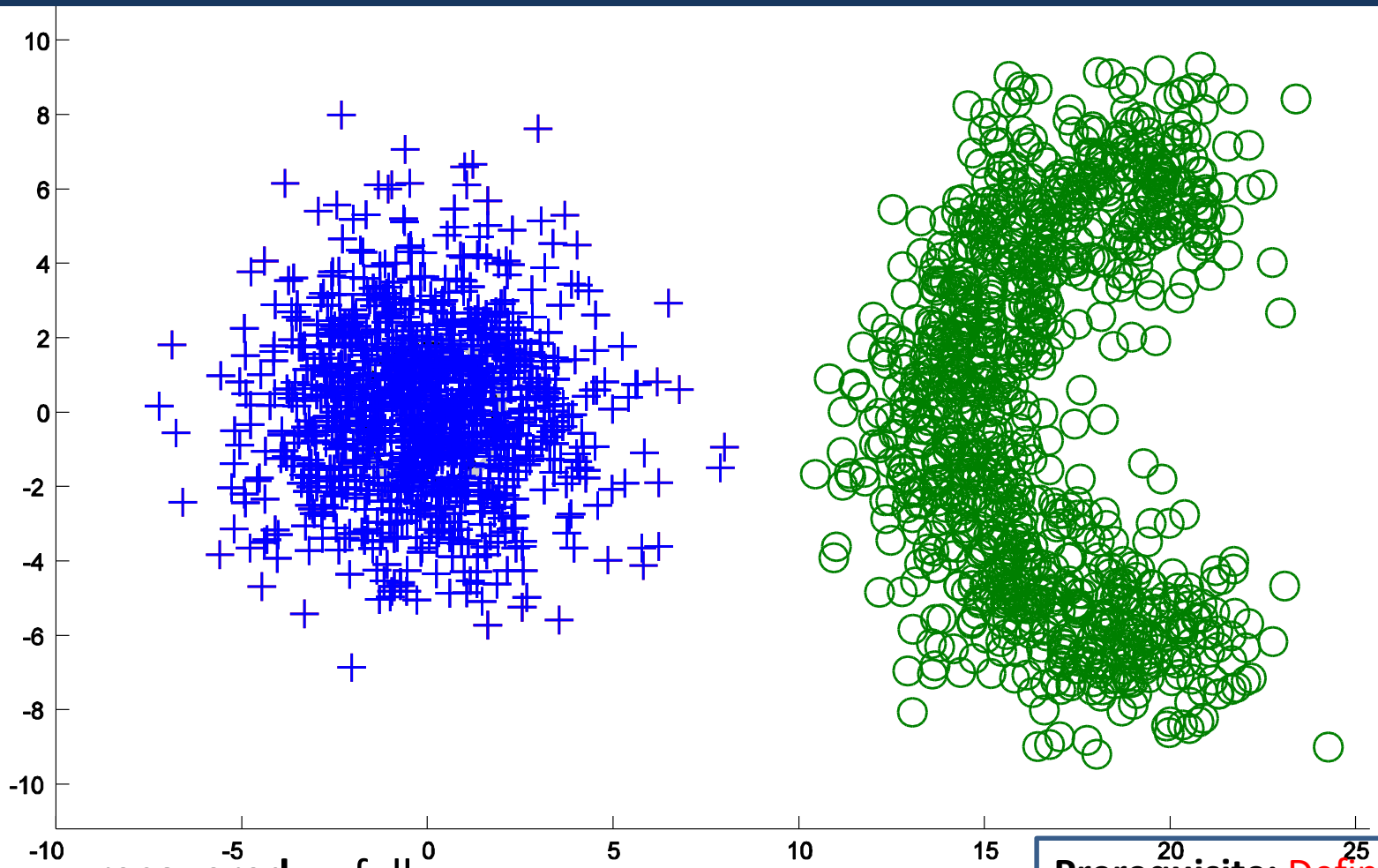
- **Start** a new cluster C by **choosing** a data point $\boldsymbol{x}$.
- **Assign** all the data points that lie in the neighborhood of $\boldsymbol{x}$ to the same cluster.
- **Repeat** recursively the previous step **until** all neighboring points of ALL $\boldsymbol{x} \in C$ are **assigned** to C.

Prerequisite: Definition of the neighborhood size

Clustering – Density-based algorithms



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Prerequisite: Definition of the neighborhood size

Density-based algorithms for large data sets

DBSCAN Algorithm (cont.)

Important notes:

- If a border point $\boldsymbol{y}$ of a cluster C is selected, it will be **marked initially** as a noise point. However, ***when*** **(a)** a core point $\boldsymbol{x}$ in C is selected later on, and **(b)** $\boldsymbol{y}$ is identified as a density-reachable point from $\boldsymbol{x}$ ***then*** $\boldsymbol{y}$ will assigned to C.
- If an actual noise point $\boldsymbol{y}$ is selected, it will be marked as such and since it is not density reachable by any of the core points in X, its "noise" label will remain unaltered.

Remarks:

- The parameters ε and q influence significantly the performance of DBSCAN. These should be **selected** such that the algorithm is able to detect the least "dense" cluster (experimentation with several values for ε and q should be carried out).
- Implementation of DBSCAN using R^*-tree data structure can achieve time complexity of $O(N \log_2 N)$ for low-dimensional data sets.
- DBSCAN is **not well suited** for cases where clusters exhibit significant differences in density as well as for applications of high-dimensional data.

Density-based algorithms for large data sets (*)

DENsity-based CLUstEring (DENCLUE) Algorithm

Definitions

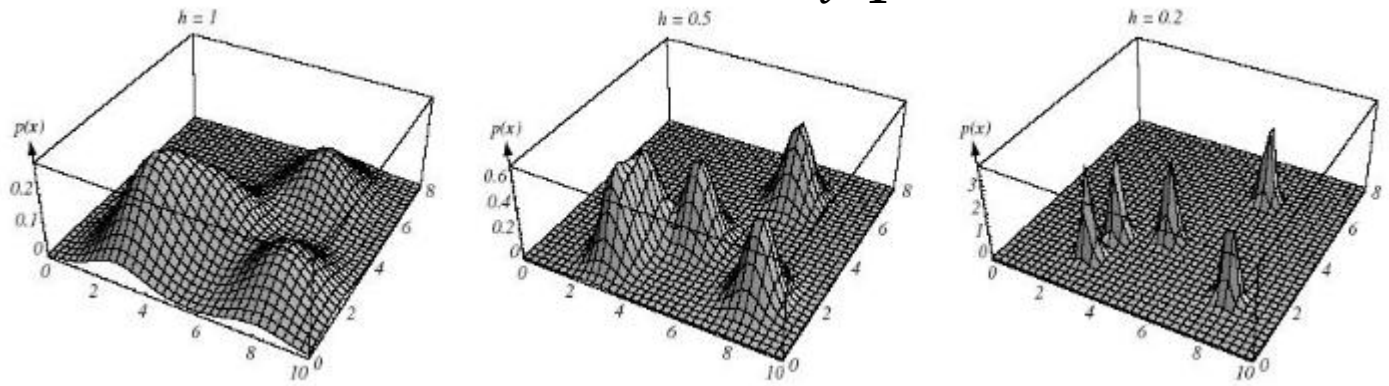
The influence function $f^{\boldsymbol{y}}(\boldsymbol{x})$ for a point $\boldsymbol{y} \in X$ is a positive function that decays to zero as $\boldsymbol{x}$ "moves away" from $\boldsymbol{y}$ ($d(\boldsymbol{x}, \boldsymbol{y}) \to \infty$). Typical examples are:

$$f^{\boldsymbol{y}}(\boldsymbol{x}) = \begin{cases} 1, & if\ d(\boldsymbol{x}, \boldsymbol{y}) < \sigma \\ 0, & otherwise \end{cases}, \qquad f^{\boldsymbol{y}}(\boldsymbol{x}) = e^{-\frac{d(\boldsymbol{x},\boldsymbol{y})^2}{2\sigma^2}}$$

where σ is a user-defined function.

The density function based on X is defined as (Recall the Parzen windows):

$$f^{X}(\boldsymbol{x}) = \sum_{i=1}^{N} f^{\boldsymbol{x}_i}(\boldsymbol{x})$$



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The Goal:

(a) **Identify** all "significant" local maxima, $\boldsymbol{x}_j^*, j = 1, \ldots, m$, of $f^X(\boldsymbol{x})$

(b) **Create** a cluster C_j for each $\boldsymbol{x}_j^*$ and **assign** to C_j all points $\boldsymbol{x}$ of X that lie within the "region of attraction" of $\boldsymbol{x}_j^*$.

Density-based algorithms for large data sets (*)

The DENCLUE Algorithm (cont.)

Two clarifications

- The region of attraction of $\boldsymbol{x}_j^*$ is defined as the set of points $\boldsymbol{x} \in R^l$ such that if a "hill-climbing" (such as the steepest ascent) method is **applied** on $f^X(\boldsymbol{x})$, initialized by $\boldsymbol{x}$, it will **terminate** arbitrarily close to $\boldsymbol{x}_j^*$.

- A local maximum is considered as significant if $f^X(\boldsymbol{x}_j^*) \geq \xi$ (ξ is a user-defined parameter).

Approximation of $f^X(\boldsymbol{x})$

$$f^X(\boldsymbol{x}) = \sum_{i=1}^{N} f^{\boldsymbol{x}_i}(\boldsymbol{x}) \approx \sum_{\boldsymbol{x}_i \in Y(\boldsymbol{x})} f^{\boldsymbol{x}_i}(\boldsymbol{x})$$

where $Y(\boldsymbol{x})$ is the set of points in X that lie "close" to $\boldsymbol{x}$.

The above framework is used by the DENCLUE algorithm.

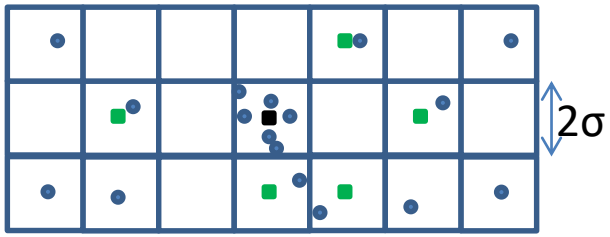
Density-based algorithms for large data sets (*)

The DENCLUE Algorithm (cont.)

DENCLUE algorithm

- *Preclustering stage* (identification of regions dense in points of X)
  - **Apply** an l-dimensional grid of *edge-length* 2σ in the R^l space.
  - **Determine** the set D_p of the hypercubes that **contain** at least one point of X.
  - **Determine** the set $D_{sp} (\subset D_p)$ that contains the "highly populated" cubes of D_p (that is, cubes that contain at least $\xi_c (> 1)$ points of X).
  - For each $c \in D_{sp}$ **define** a connection with all neighboring cubes c_j in D_p for which $d(\boldsymbol{m}_c, \boldsymbol{m}_{c_j}) \leq 4\sigma$, where $\boldsymbol{m}_c, \boldsymbol{m}_{c_j}$ are the means of c and c_j, respectively.

- *Main stage*
  - **Determine** the set D_r that contains:
    –the highly populated cubes and
    –the cubes that have at least **one connection** with a highly populated cube.

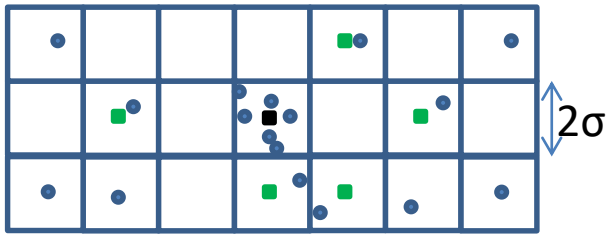


Density-based algorithms for large data sets (*)

DENCLUE algorithm (cont.)

- *Main stage (cont.)*

- **For** each point $\boldsymbol{x}$ in a cube $c \in D_r$
  - **Determine** $Y(\boldsymbol{x})$ as the set of points of X that belong to cubes c_j in D_r such that the mean values of c_j's lie at distance less than $\lambda \cdot \sigma$ from $\boldsymbol{x}$ (typically $\lambda = 4$).
  - **Apply** a hill climbing method on $f^X(\boldsymbol{x}) = \sum_{\boldsymbol{x}_i \in Y(\boldsymbol{x})} f^{\boldsymbol{x}_i}(\boldsymbol{x})$ **starting** from $\boldsymbol{x}$ and let $\boldsymbol{x}^*$ be the local maximum to which the method converges.
  - **If** $\boldsymbol{x}^*$ is a **significant** local maximum ($f^X(\boldsymbol{x}^*) \geq \xi$) then
    - *If* a cluster C **associated** with $\boldsymbol{x}^*$ *has already been created* then
      - $\boldsymbol{x}$ is **assigned** to C
    - *Else*
      - **Create** a cluster C **associated** with $\boldsymbol{x}^*$
      - **Assign** $\boldsymbol{x}$ to C
    - *End if*
  - **End if**
- **End for**



Density-based algorithms for large data sets (*)

The DENCLUE Algorithm (cont.)

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.

Spectral clustering

Spectral clustering is **based** on graph theory concepts.

Rationale: It actually maps the data from their original space, where they may form arbitrarily-shaped clusters, to a new space, where (their images) form compact clusters.

Main stages:

- **Definition** of a similarity graph G based on the given data set X.
- **Utilization** of the Laplacian matrix L associated with G.
- **Mapping** of the data set **to** a space spanned by **some** eigenvectors of L.
- **Performing** clustering on the images of the data in the transformed space.

In principle, spectral clustering is able to **recover** arbitrarily shaped clusters (see discussion later).

Spectral clustering

Similarity graph

- Data set $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$
- Similarity graph $G = (V, E)$

We consider **only** undirected graphs.

$X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$

$V = \{v_1, v_2, \dots, v_N\}$

Definition of a similarity graph

About V

- The set V consists of N vertices/nodes, $v_1, v_2, \dots, v_N$
- Each vertex $v_i \in V$ corresponds to a $\boldsymbol{x}_i \in X, i = 1, \dots, N$.

About E

By convention, $w_{ij} = 0$, **implies** absence of e_{ij}.

Various scenarios lead to various graphs:

(a) The ε-neighborhood graph:

- An edge e_{ij} is **added** between vertices v_i and v_j, **if** $d(\boldsymbol{x}_i, \boldsymbol{x}_j) < \varepsilon$.
- Usually it is **considered** as an unweighted graph (it is $w_{ij} = 1$, for all e_{ij}'s).

Spectral clustering

Similarity graph

Definition of a similarity graph

About E

(b) The k-nearest neighbor graph:

- An edge e_{ij} is **added** between vertices v_i and v_j, **if** v_i is among the k-nearest neighbors of v_j **OR** vice versa.
- Each e_{ij} is **weighted** by the similarity between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$.

(c) The mutual k-nearest neighbor graph:

- An edge e_{ij} is **added** between vertices v_i and v_j, **if** v_i is among the k-nearest neighbors of v_j **AND** vice versa.
- Each e_{ij} is **weighted** by the similarity between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$.

(d) The fully connected graph:

- All possible edges e_{ij} are added in the graph.
- Each e_{ij} is **weighted** by the similarity between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$, e.g.,

$$s(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp\left(-\frac{\left||x_i - x_j|\right|^2}{2\sigma^2}\right)$$

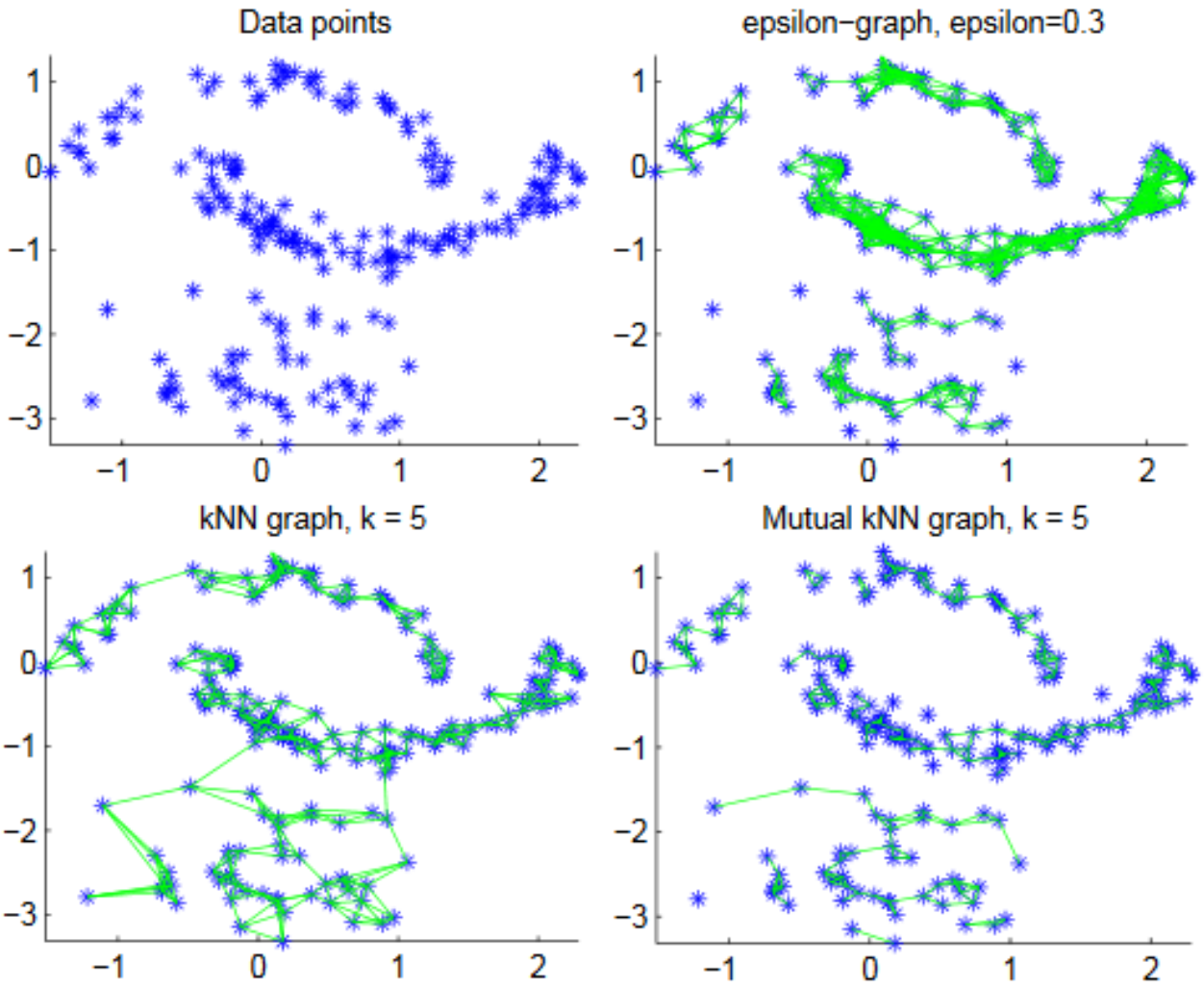
Spectral clustering

Similarity graph

Example:

The data set consists of
(i) two “half moon” clusters and
(ii) a compact cluster of different density from the previous ones.

The resulting graphs are shown in the figure.



Spectral clustering

Graph Laplacians

- There are various definitions for graph Laplacian matrix.
- All such matrices share some properties that allow their exploitation in the frame of clustering.

Some definitions:

w_{ij} is the **weight** of the edge connecting v_i and v_j.

- *Weighted adjacency matrix*:

$$W = [w_{ij}]_{N\times N}$$

- Degree of a vertex v_i:

$$d_i = \sum_{j=1}^{N} w_{ij},\ i = 1, \dots, N$$

- Degree matrix:

$$D_{N\times N} = diag(d_1, d_2, \dots, d_N) = \begin{bmatrix} d_1 & \cdots & 0 \\ 0 & \ddots & 0 \\ 0 & \cdots & d_N \end{bmatrix}_{N\times N}$$

- (Unnormalized) graph Laplacian matrix:

$$L_{N\times N} = D - W$$

Spectral clustering

Graph Laplacians

Some results for the unnormalized graph Laplacian L:

1. $\forall \boldsymbol{x} = [x_1, \dots, x_N]^T \in R^N$ it is

$$\boldsymbol{x}^T L \boldsymbol{x} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij} (x_i - x_j)^2$$

2. L is symmetric and positive semidefinite.
3. The smallest eigenvalue of L is 0.
4. L has N non-negative real-valued eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$.

5. Let G be an undirected graph with nonnegative weights. Then the multiplicity k of the zero eigenvalue **equals** to the number of the connected components $A_1, \dots, A_k$, of the graph. In addition, the eigenspace of the zero eigenvalues is **spanned** by the (N-dimensional) *indicator vectors* of those components, $\mathbf{1}_{A_1}, \dots, \mathbf{1}_{A_k}$.

The indicator vector $\mathbf{1}_{A_i}$ has all of its components equal 0 **except** those corresponding to the points that **belong** to the k-th connected component., which are equal to 1.

Spectral clustering

Graph Laplacians: *Some results for the unnormalized graph Laplacian L:*

5. Let G be an undirected graph with nonnegative weights ($w_{ij} \geq 0$). Then the multiplicity k of the zero eigenvalue **equals** to the number of the connected components $A_1, \dots, A_k$, of the graph. In addition, the eigenspace of the zero eigenvalue is **spanned** by the (N-dimensional) indicator vectors of those components, $\mathbf{1}_{A_1}, \dots, \mathbf{1}_{A_k}$.

$d_i = \sum_{j=1}^{N} w_{ij}$, $w_{ii} = 0$

- The $k = 1$ case (connected graph): It is $0 = |L - \lambda \mathrm{I}| =$

$$\begin{vmatrix} d_1 - \lambda & -w_{12} & \cdots & -w_{1N} \\ -w_{12} & d_2 - \lambda & \cdots & -w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ -w_{1N} & -w_{2N} & \cdots & d_N - \lambda \end{vmatrix} = \begin{vmatrix} -\lambda & -w_{12} & \cdots & -w_{1N} \\ -\lambda & d_2 - \lambda & \cdots & -w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ -\lambda & -w_{2N} & \cdots & d_N - \lambda \end{vmatrix} =$$

$$-\lambda \begin{vmatrix} 1 & -w_{12} & \cdots & -w_{1N} \\ 1 & d_2 - \lambda & \cdots & -w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & -w_{2N} & \cdots & d_N - \lambda \end{vmatrix} = -\lambda \begin{vmatrix} 1 & -w_{12} & \cdots & -w_{1N} \\ 0 & d_2 + w_{12} - \lambda & \cdots & -w_{2N} + w_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & -w_{2N} + w_{12} & \cdots & d_N + w_{1N} - \lambda \end{vmatrix}$$

$$= -\lambda \begin{vmatrix} d_2 + w_{12} - \lambda & \cdots & -w_{2N} + w_{1N} \\ \vdots & \ddots & \vdots \\ -w_{2N} + w_{12} & \cdots & d_N + w_{1N} - \lambda \end{vmatrix} \Leftrightarrow \lambda_1 = 0, (\lambda_2, \dots \lambda_N > 0)$$

Thus, multiplicity of the zero eigenvalue is 1.

The *associated* eigenvector is the $\mathbf{1}$,since $\mathbf{0} = 0 \cdot \mathbf{1} = L \cdot \mathbf{1}$

$d_i = \sum_{i=1}^{N} w_{ij}$

Spectral clustering

Graph Laplacians: *Some results for the unnormalized graph Laplacian L:*

5. Let G be an undirected graph with nonnegative weights ($w_{ij} \geq 0$). Then the multiplicity k of the zero eigenvalue **equals** to the number of the connected components $A_1, \dots, A_k$, of the graph. In addition, the eigenspace of the zero eigenvalue is **spanned** by the (N-dimensional) indicator vectors of those components, $\mathbf{1}_{A_1}, \dots, \mathbf{1}_{A_k}$.

- The $k = 1$ case (connected graph):
- The *associated* eigenvector is the $\mathbf{1}$,since $\mathbf{0} = 0 \cdot \mathbf{1} = L \cdot \mathbf{1}$

$$\mathbf{0} = 0 \cdot \mathbf{1} = 0 \cdot \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} d_1 & -w_{12} & \cdots & -w_{1N} \\ -w_{12} & d_2 & \cdots & -w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ -w_{1N} & -w_{2N} & \cdots & d_N \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = L \cdot \mathbf{1}$$

$d_i = \sum_{j=1}^{N} w_{ij}$, $w_{ii} = 0$

Spectral clustering

Graph Laplacians: *Some results for the unnormalized graph Laplacian L:*

5. Let G be an undirected graph with nonnegative weights ($w_{ij} \geq 0$). Then the multiplicity k of the zero eigenvalue **equals** to the number of the connected components $A_1, \dots, A_k$, of the graph. In addition, the eigenspace of the zero eigenvalue is **spanned** by the (N-dimensional) indicator vectors of those components, $\mathbf{1}_{A_1}, \dots, \mathbf{1}_{A_k}$.

- The $k > 1$ case (k connected components):
  - Considering each connected component individually, the i-th component has its own associated Laplacian L_i
  - Then the Laplacian for the whole graph can be written as

$$L = \begin{bmatrix} L_1 & & \\ & \ddots & \\ & & L_k \end{bmatrix}$$

The spectrum of L is given by the **union** of the spectra of L_i's.

  - Since, the multiplicity of the zero eigenvalue is 1 for each $L_i \Longrightarrow$ the multiplicity of the zero eigenvalue is k for L.
  - Denoting $|A_1| = n_1$, $\mathbf{1}_{A_1}$ has its first n_1 (resp. remaining) components equal to 1(resp. 0), $\mathbf{1}_{A_1} = [1,1, \dots, 1,0,0, \dots, 0]^T$. Then,

$$\mathbf{0}_{n_1 \times 1} = 0 \cdot \mathbf{1}_{n_1 \times 1} = L_1 \cdot \mathbf{1}_{n_1 \times 1} \Rightarrow \mathbf{0}_{N \times 1} = 0 \cdot \mathbf{1}_{\boldsymbol{A_1}, N \times 1} = L \cdot \mathbf{1}_{N \times 1}$$

Spectral clustering

Unnormalized spectral clustering algorithm

Input: (a) Similarity matrix $S \in R^{N \times N}$, **(b)** the number of clusters m

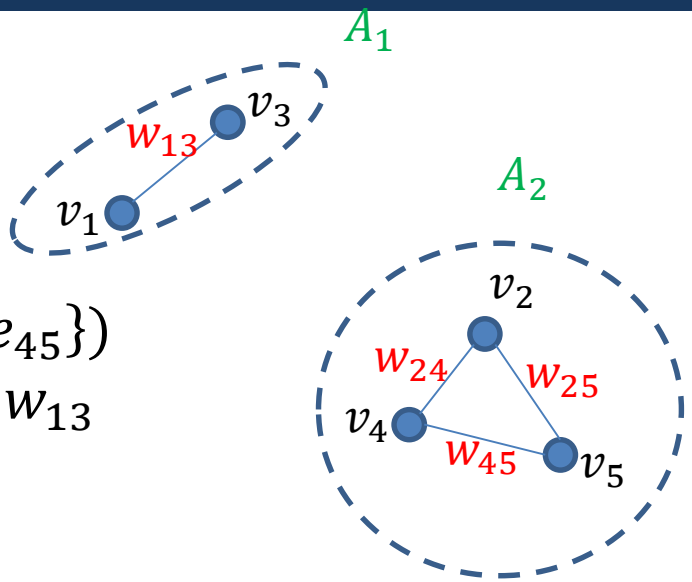
- **Construct** a similarity graph with weighed adjacency matrix W.
- **Compute** the unnormalized Laplacian L.
- **Compute** the *first* m (column) eigenvectors of L, $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m$.
- **Stack** $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m$ on an $N \times m$ matrix U.
- **Represent** each data vector $\boldsymbol{x}_i$ by the i-th row $\boldsymbol{y}_i$ of U.
- **Cluster** the points $\boldsymbol{y}_i \in R^m$, $i = 1, \ldots, N$, using e.g., the k-means algorithm, into clusters $C_1', C_2', \ldots, C_m'$.

Output: Clusters $C_1, C_2, \ldots, C_m$, with $C_i = \{\boldsymbol{x}_j : \boldsymbol{y}_j \in C_i'\}$

Spectral clustering

Unnormalized spectral clustering algorithm

Example:



Data set $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5\}$

Similarity graph:

$G = (V, E) = (\{v_1, v_2, v_3, v_4, v_5\}, \{e_{13}, e_{24}, e_{25}, e_{45}\})$

Nodes degree: $d_1 = w_{13}, d_2 = w_{24} + w_{25}, d_3 = w_{13}$

$d_4 = w_{24} + w_{45}, \; d_5 = w_{25} + w_{45}$

***Laplacian** of the whole graph*:

$$L = D - W$$

$$= \begin{bmatrix} w_{13} & 0 & -w_{13} & 0 & 0 \\ 0 & w_{24} + w_{25} & 0 & -w_{24} & -w_{25} \\ -w_{13} & 0 & w_{13} & 0 & 0 \\ 0 & -w_{24} & 0 & w_{24} + w_{45} & -w_{45} \\ 0 & -w_{25} & 0 & -w_{45} & w_{25} + w_{45} \end{bmatrix}$$

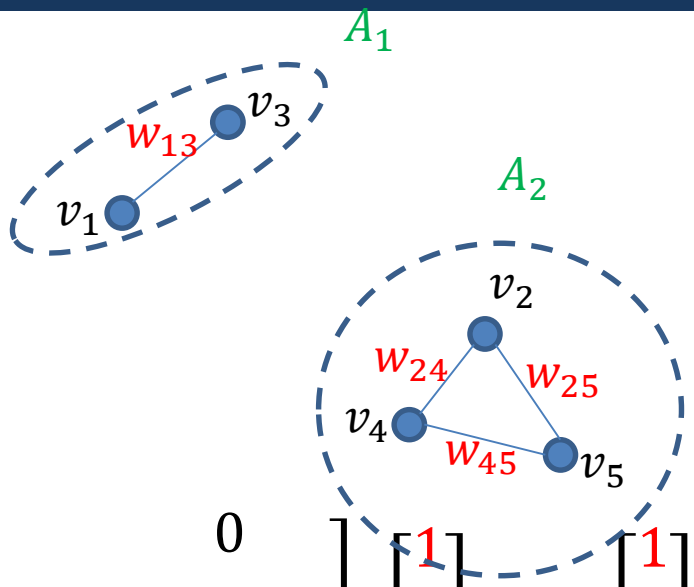
$$|L - \lambda I| = \cdots = \lambda^2 \begin{vmatrix} 2w_{13} - \lambda & 0 & 0 \\ 0 & 2w_{24} + w_{45} - \lambda & w_{25} - w_{45} \\ 0 & w_{24} - w_{45} & 2w_{25} + w_{45} - \lambda \end{vmatrix} = 0 \Leftrightarrow$$

$\lambda = 0$ double root

Spectral clustering

Unnormalized spectral clustering algorithm

Example:



Data set $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5\}$

Corresponding eigenvectors $\boldsymbol{e}$ ($L \cdot \boldsymbol{e} = 0 \cdot \boldsymbol{e}$):

$\boldsymbol{u}_1 = [1,0,1,0,0]^T$ and $\boldsymbol{u}_2 = [0,1,0,1,1]^T$ since

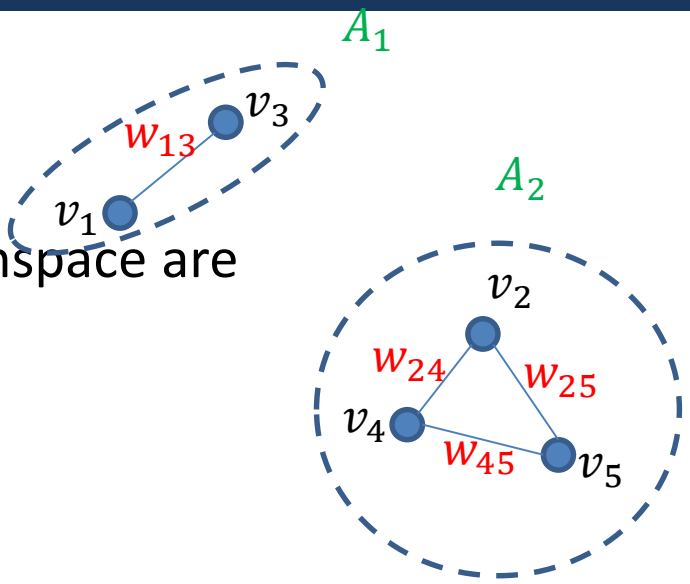
$$\begin{bmatrix} w_{13} & 0 & -w_{13} & 0 & 0 \\ 0 & w_{24}+w_{25} & 0 & -w_{24} & -w_{25} \\ -w_{13} & 0 & w_{13} & 0 & 0 \\ 0 & -w_{24} & 0 & w_{24}+w_{45} & -w_{45} \\ 0 & -w_{25} & 0 & -w_{45} & w_{25}+w_{45} \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = 0 \cdot \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} w_{13} & 0 & -w_{13} & 0 & 0 \\ 0 & w_{24}+w_{25} & 0 & -w_{24} & -w_{25} \\ -w_{13} & 0 & w_{13} & 0 & 0 \\ 0 & -w_{24} & 0 & w_{24}+w_{45} & -w_{45} \\ 0 & -w_{25} & 0 & -w_{45} & w_{25}+w_{45} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} = 0 \cdot \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

Spectral clustering

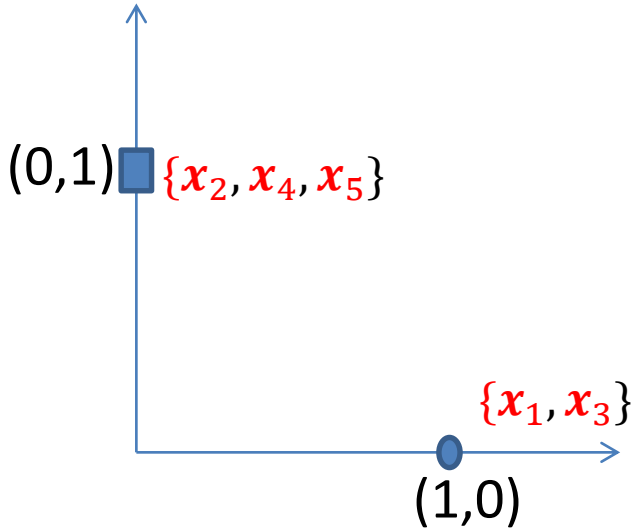
Unnormalized spectral clustering algorithm

Example:



The eigenvectors corresponding to the zero eigenspace are $\boldsymbol{u}_1 = [1,0,1,0,0]^T$ and $\boldsymbol{u}_2 = [0,1,0,1,1]^T$

The matrix $U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \equiv \begin{matrix} \boldsymbol{y}_1 \rightarrow \boldsymbol{x}_1 \\ \boldsymbol{y}_2 \rightarrow \boldsymbol{x}_2 \\ \boldsymbol{y}_3 \rightarrow \boldsymbol{x}_3 \\ \boldsymbol{y}_4 \rightarrow \boldsymbol{x}_4 \\ \boldsymbol{y}_5 \rightarrow \boldsymbol{x}_5 \end{matrix}$



Spectral clustering

Other Laplacian matrices

- Symmetric Laplacian matrix: $L_{sym} = D^{-1/2} \cdot L \cdot D^{-1/2}$
- Random walk Laplacian matrix: $L_{rw} = D^{-1} \cdot L$

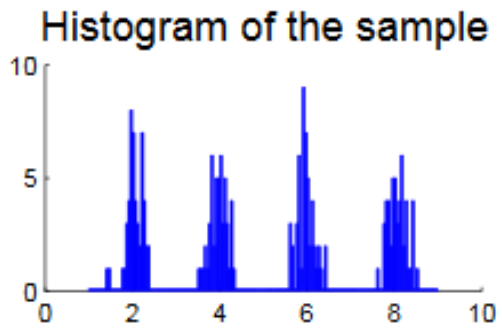
All Laplacians share similar properties concerning the zero eigenvalue.
In (von Luxburg, 2007), it is suggested to use L_{rw}.

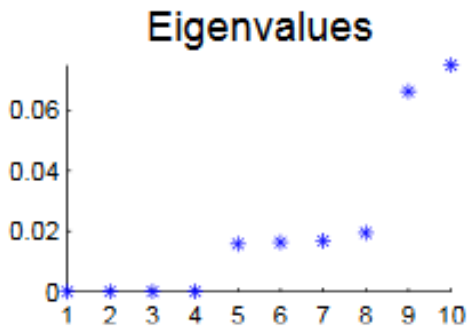
Spectral clustering

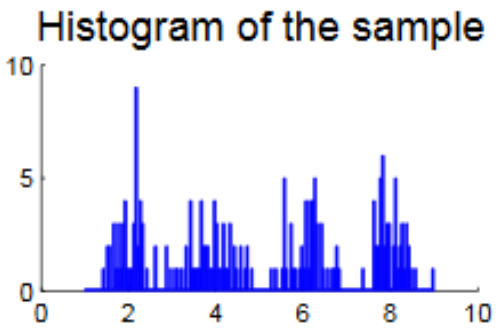
Choice of the number of clusters

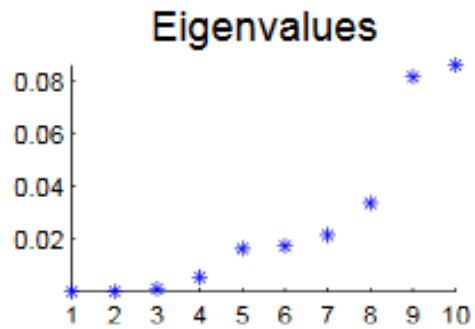
Example:

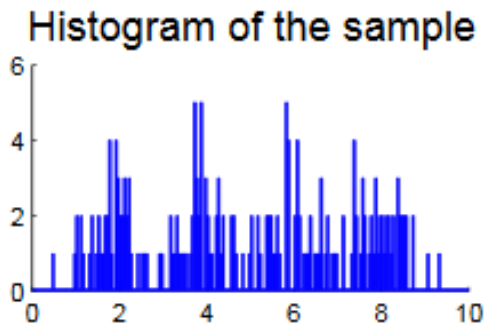
The ten smallest eigenvalues of L_{rw} for a 1-dim. four-clusters problem.

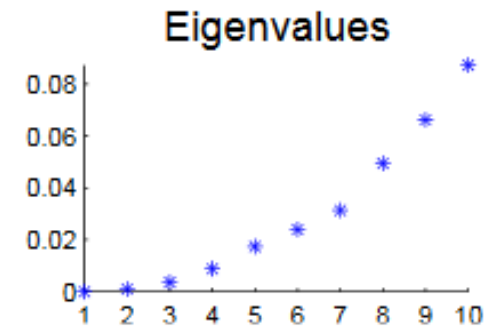












In the case where m is not apriori known, it can be estimated by **sorting** the Laplacian eigenvalues and **determining** the number of the first m eigenvalues that **(a)** are sufficiently close to 0 and **(b)** the $m+1$ differs significantly from them.