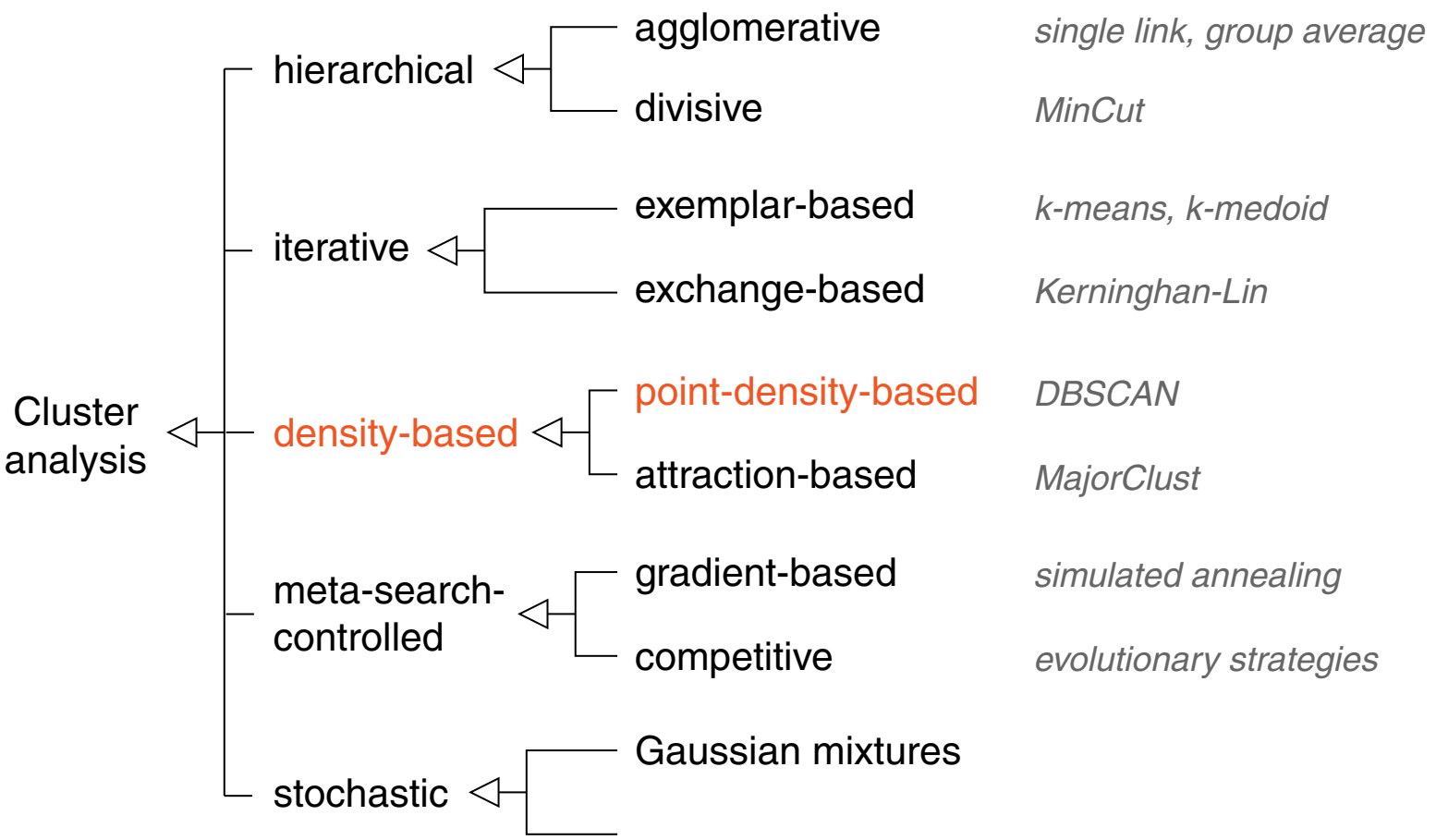
# Chapter DM:II (continued)

## II. Cluster Analysis

- Cluster Analysis Basics
- Hierarchical Cluster Analysis
- Iterative Cluster Analysis
- Density-Based Cluster Analysis
- Cluster Evaluation
- Constrained Cluster Analysis

# Density-Based Cluster Analysis

## Merging Principles



# Density-Based Cluster Analysis

Density-based algorithms strive to partition the graph $G = \langle V, E, w \rangle$, better: the set of points $V$, into regions of similar density.

Approaches to density estimation:

- parameter-based: the type of the underlying data distribution is known
- parameterless: construction of histograms, superposition of kernel density estimators

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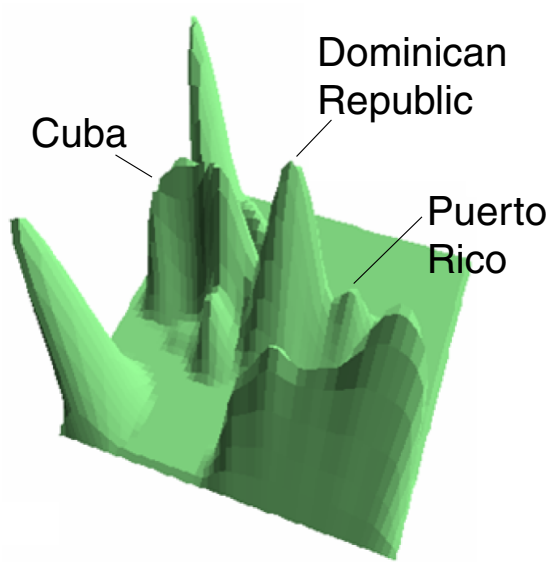
Example (Caribbean Islands) :

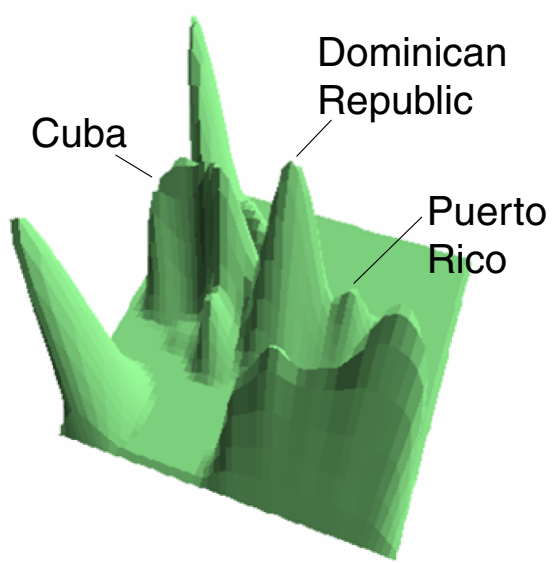

# Density-Based Cluster Analysis

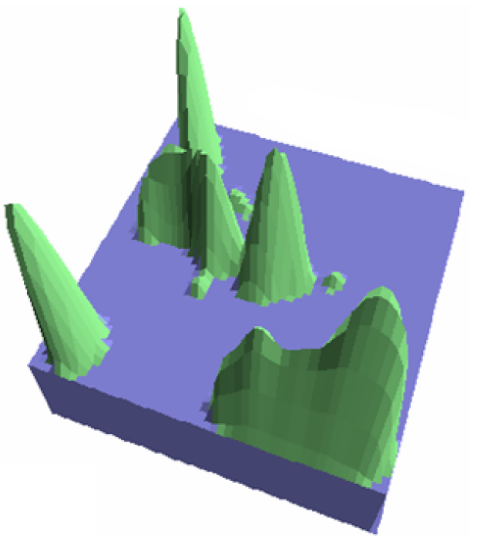
## Density Estimation with Gaussian Kernel for the Example



# Density-Based Cluster Analysis

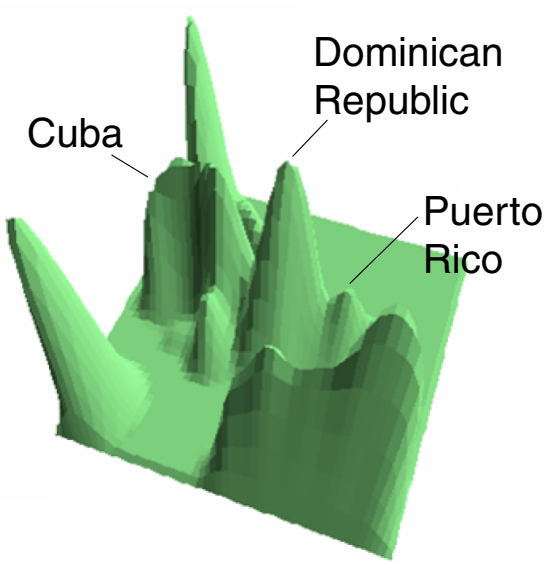
## Density Estimation with Gaussian Kernel for the Example

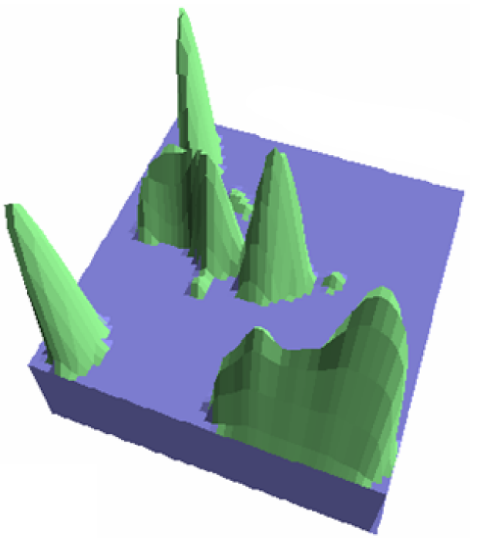


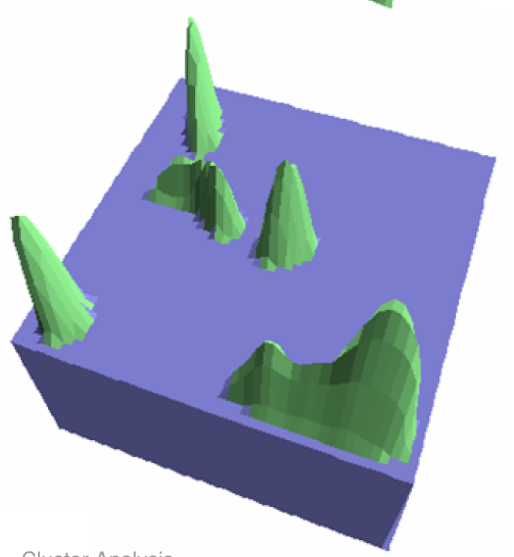



# Density-Based Cluster Analysis

## Density Estimation with Gaussian Kernel for the Example

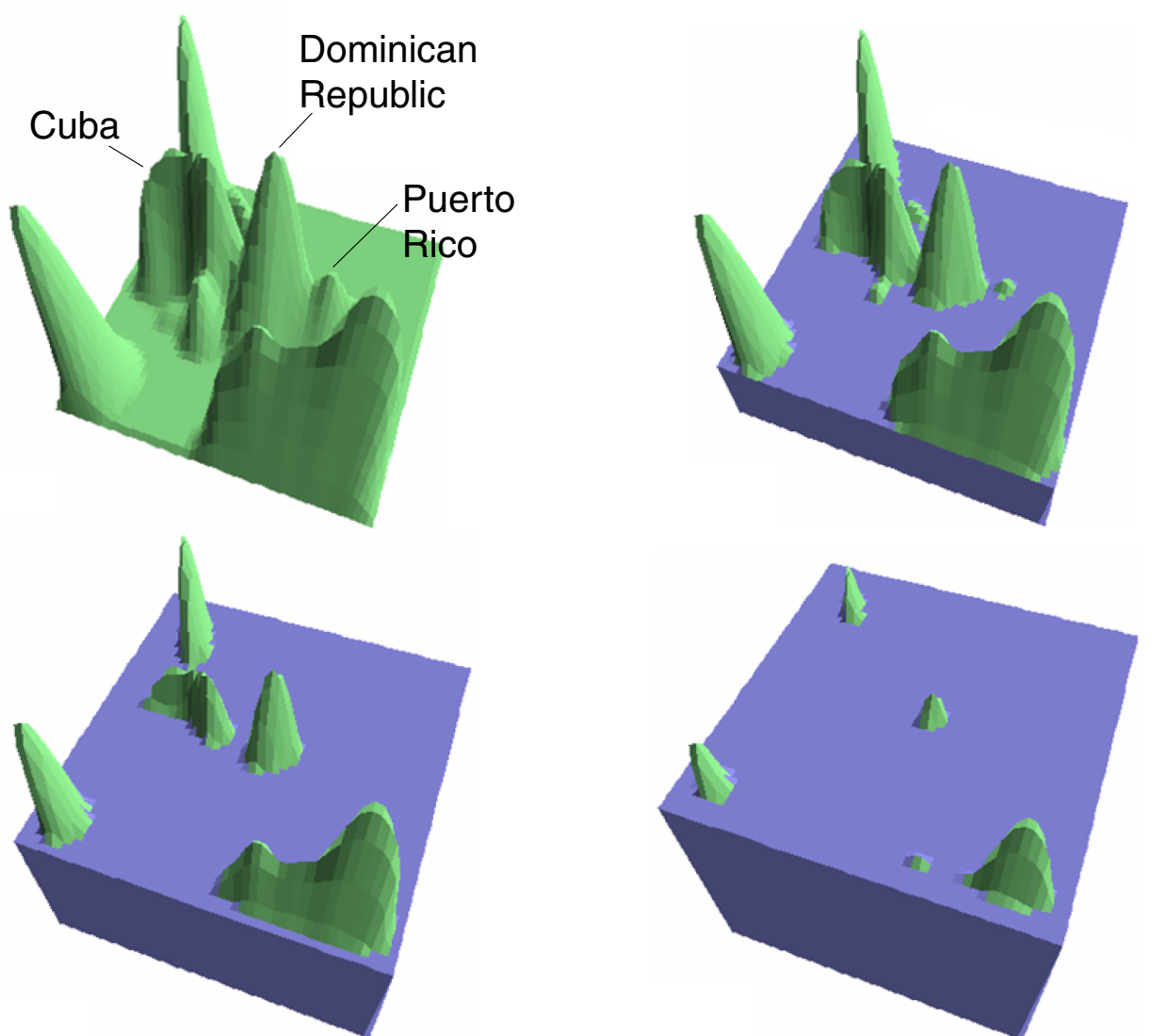




# Density-Based Cluster Analysis

## Density Estimation with Gaussian Kernel for the Example



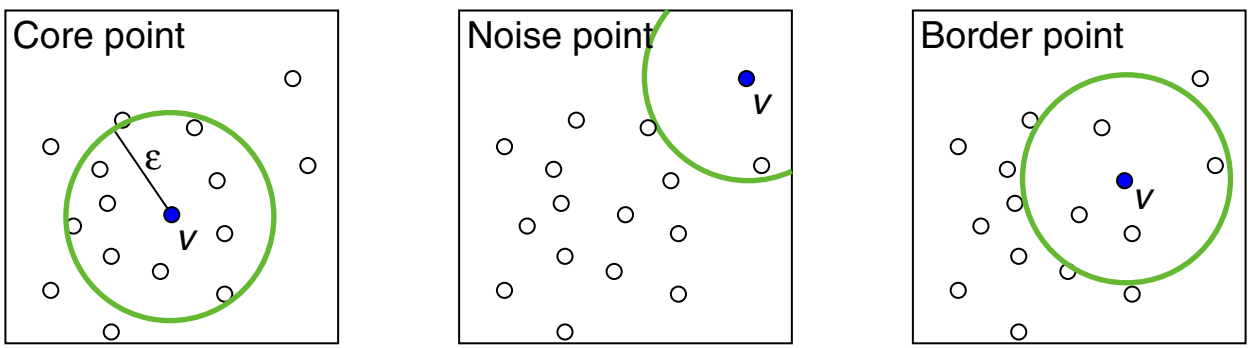
Remarks:

- The green three-dimensional landscape is the result of associating each point of the rasterized map (right-hand side) with a three-dimensional Gaussian kernel and superimposing them.
- Raising the “water level” in the three-dimensional landscape ($\sim$ clipping at a certain contour line) coressponds to splitting the dendrogram and reveals possible clusters. Observe that no single water level (contour line) can be chosen such that all clusters can be identified.

# Density-Based Cluster Analysis

## DBSCAN: Density Estimation Principle [Ester et al. 1996]

Let $N_\varepsilon(v)$ denote the $\varepsilon$-neighborhood of some point $v \in V$. Distinguish between three kinds of points:




1. $v$ is a core point $\Leftrightarrow$ $|N_\varepsilon(v)| \geq$ *MinPts*

2. $v$ is a noise point $\Leftrightarrow$
   $v$ is not density-reachable from any core point

3. $v$ is a border point otherwise

# Density-Based Cluster Analysis

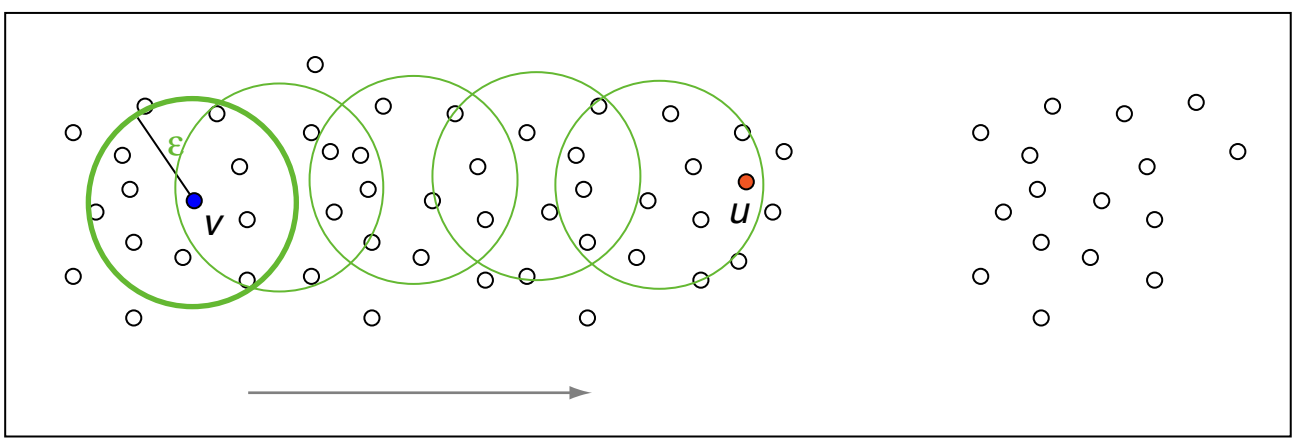
## DBSCAN: Density Estimation Principle

A point $u$ is density-reachable from a point $v$, if either of the following conditions hold:

(a) $u \in N_\varepsilon(v)$, where $v$ is a core point.

(b) There exists a set of points $\{v_1, \ldots, v_l\}$, where

$v_{i+1} \in N_\varepsilon(v_i)$ and $v_i$ is core point, $i = 1, \ldots, l-1$, with $v_1 = v$, $v_l = u$.



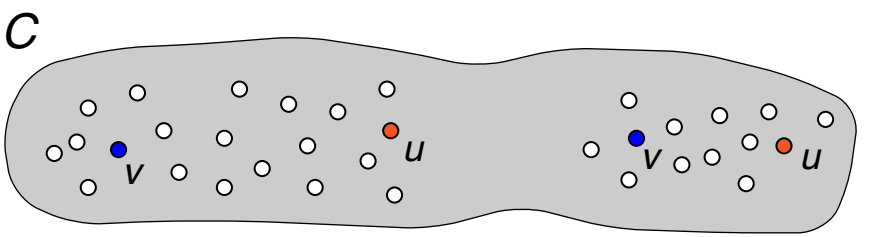

Condition (b) can be considered as the transitive application of Condition (a).

# Density-Based Cluster Analysis

## DBSCAN: Cluster Interpretation

A cluster $C \subseteq V$ fulfills the following two conditions:

1. $\forall u, v$ : If $v \in C$ and $u$ is density-reachable from $v$, then $u \in C$.




Maximality condition

# Density-Based Cluster Analysis

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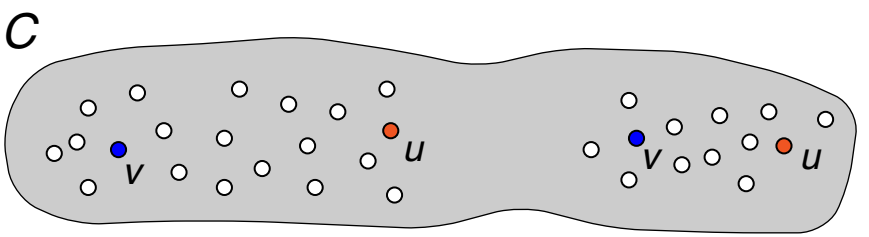
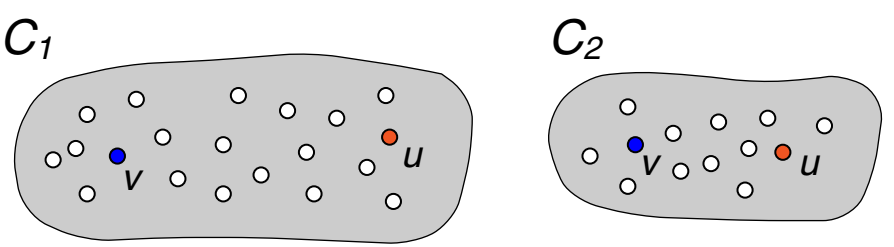



Maximality condition

2. $\forall u, v \in C$ : $u$ is density-connected with $v$, which is defined as follows:

   There exists a point $t$ wherefrom $u$ and $v$ are density-reachable.




Connectivity condition

Remarks:

- Condition 1 (maximality) states a constraint between any two points.
  Condition 2 (connectivity) states an additional constraint with respect to a third point.
- The maximality condition is problematic if a border point lies in the $\varepsilon$-neighborhoods of two core points that belong to two different clusters. Such a border point would then belong to both clusters; however, the algorithm breaks this tie by assigning this point to the first cluster found.

# Density-Based Cluster Analysis

## DBSCAN: Algorithm

Input: $G = \langle V, E, w \rangle$. Weighted graph.
$d$. Distance measure for two nodes in $V$.
$\varepsilon$. Neighborhood radius.
*MinPts*. Lower bound for point number in $\varepsilon$-neighborhood.

Output: $\gamma : V \to \mathbf{Z}$. Cluster assignment function.

```
1.
2.
3.    v = choose_unclassified_point(V)
4.    N_ε(v) = neighborhood(G, d, v, ε)
5.    IF |N_ε(v)| ≥ MinPts THEN // v is core point
6.
7.      C_i = density_reachable_hull(G, d, N_ε(v)) // identify dense region
8.      FOREACH v ∈ C_i DO γ(v) = i // assign points in region to cluster i
9.    ELSE γ(v) = −1 // classify v _tentatively_ as noise (-1)
10.
11.
```

# Density-Based Cluster Analysis

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*MinPts*. Lower bound for point number in $\varepsilon$-neighborhood.

Output: $\gamma : V \to \mathbf{Z}$. Cluster assignment function.

```
1.  i = 0
2.  WHILE ∃v : (v ∈ V AND γ(v) = ⊥) DO // check for unclassified (⊥) points
3.    v = choose_unclassified_point(V)

4.    N_ε(v) = neighborhood(G, d, v, ε)
5.    IF |N_ε(v)| ≥ MinPts THEN // v is core point
6.      i = i + 1
7.      C_i = density_reachable_hull(G, d, N_ε(v)) // identify dense region
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10. ENDDO
11. RETURN(γ)
```
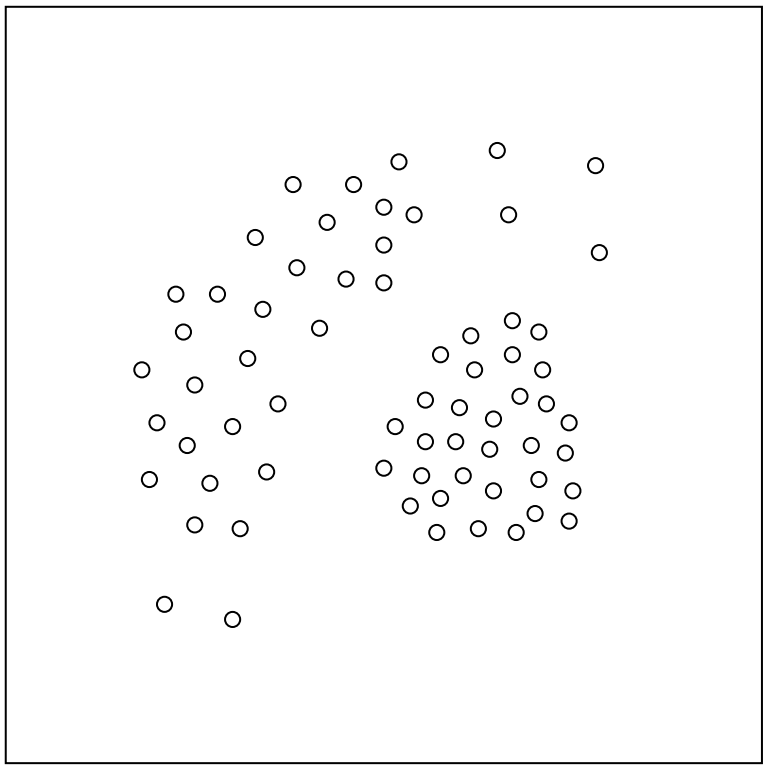

# Density-Based Cluster Analysis

## DBSCAN



# Density-Based Cluster Analysis

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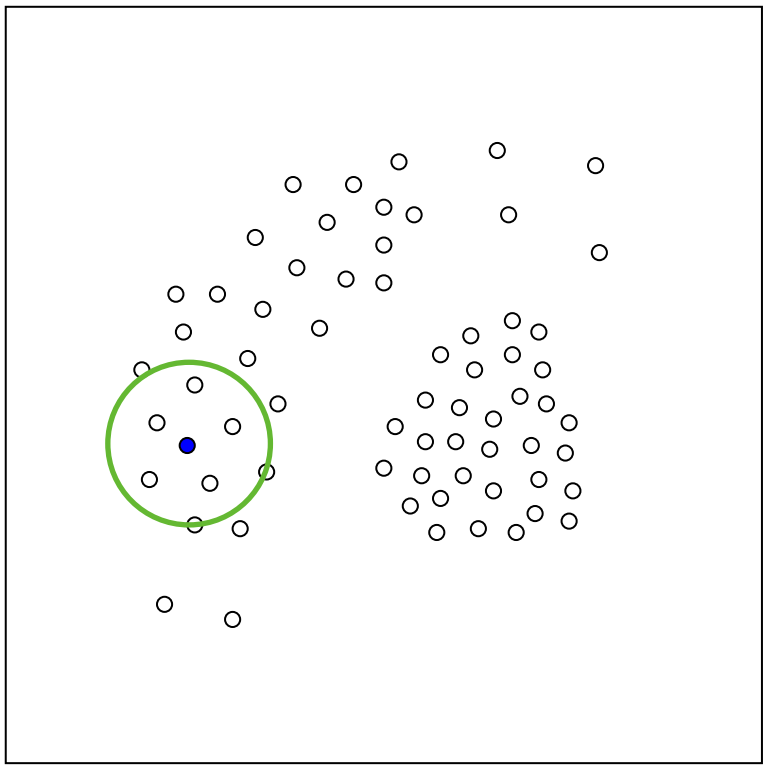

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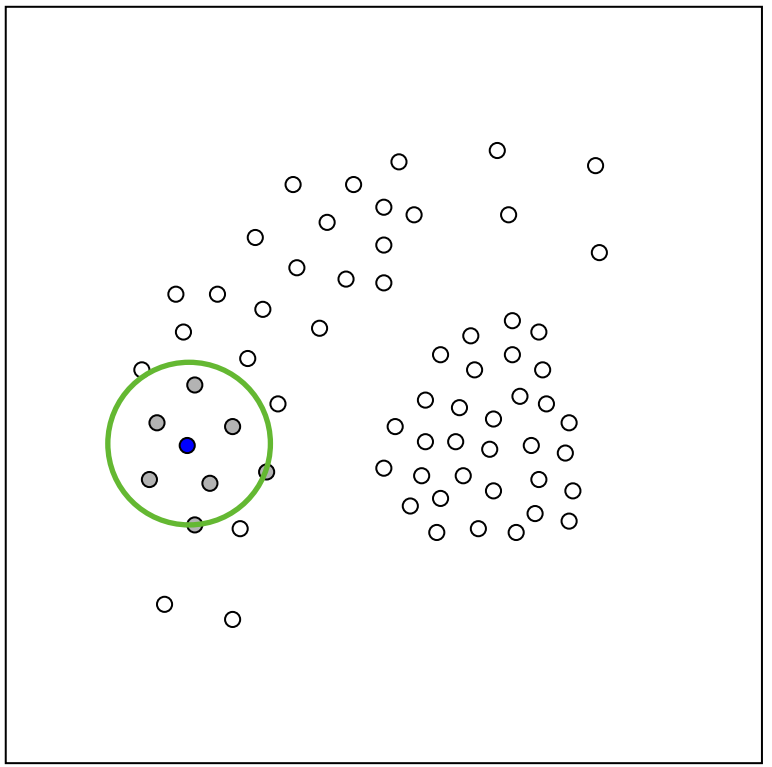
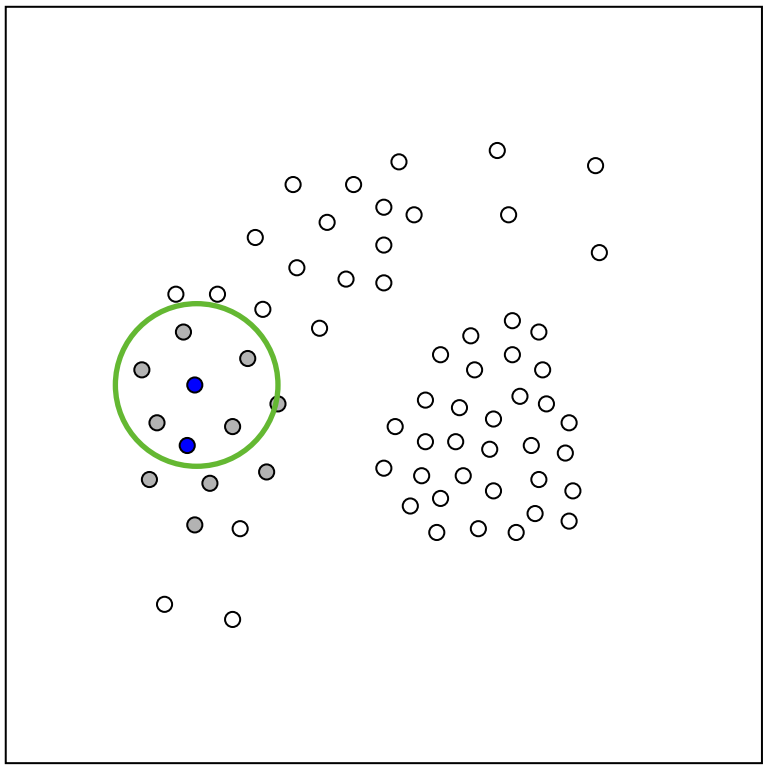


# Density-Based Cluster Analysis

## DBSCAN



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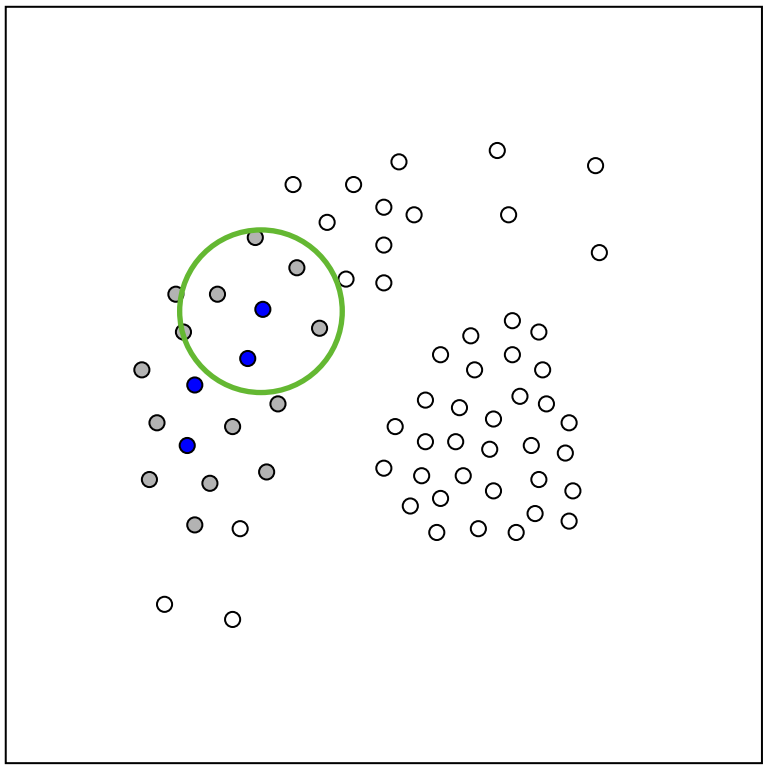

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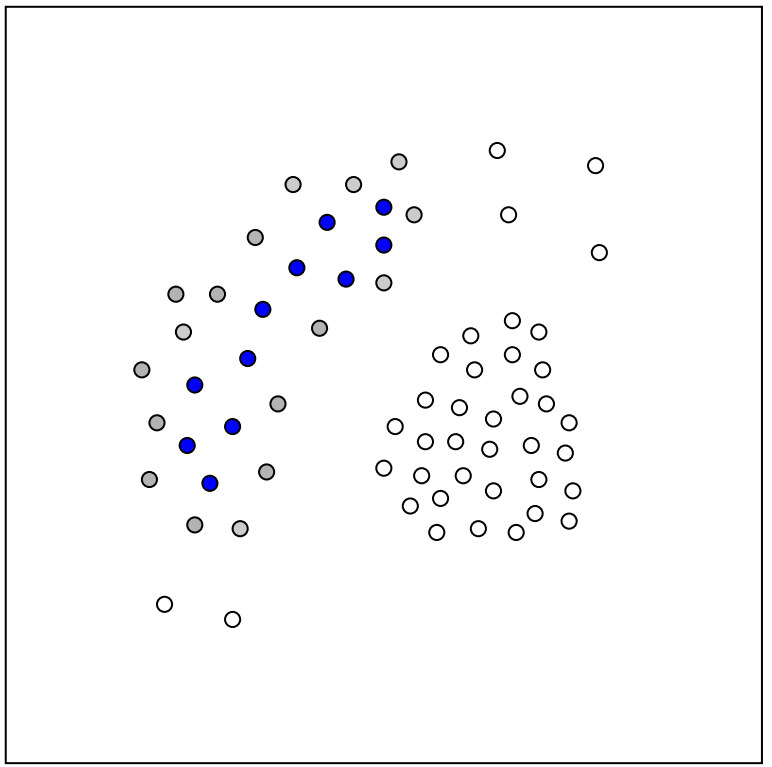
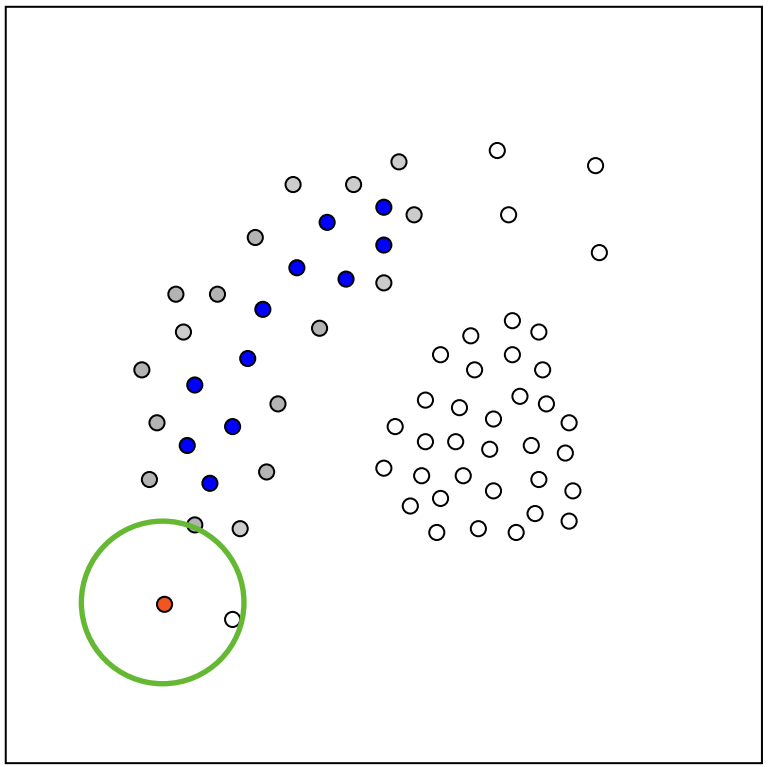


Core point
Border point

# Density-Based Cluster Analysis

## DBSCAN



- Core point
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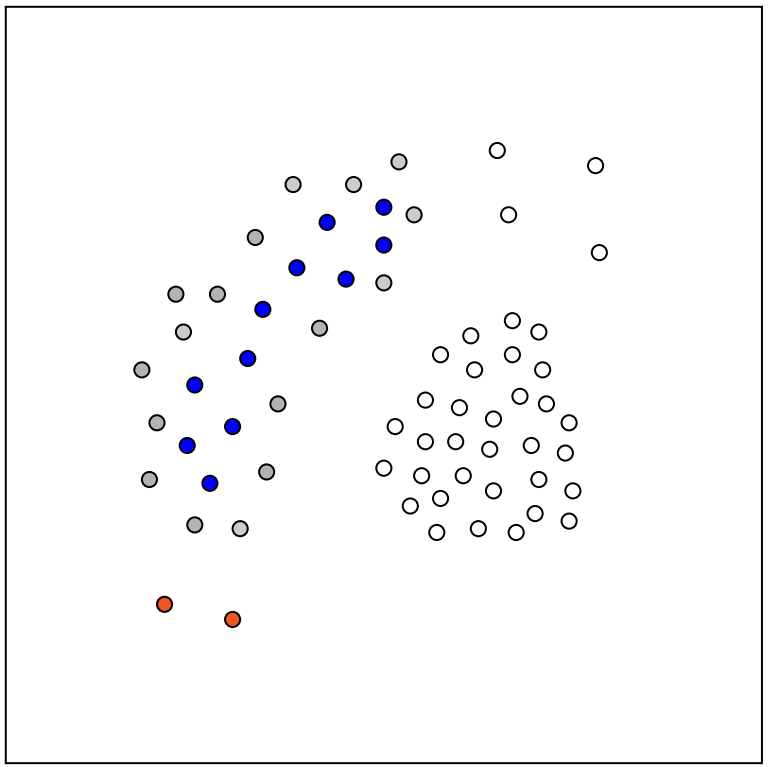
# Density-Based Cluster Analysis

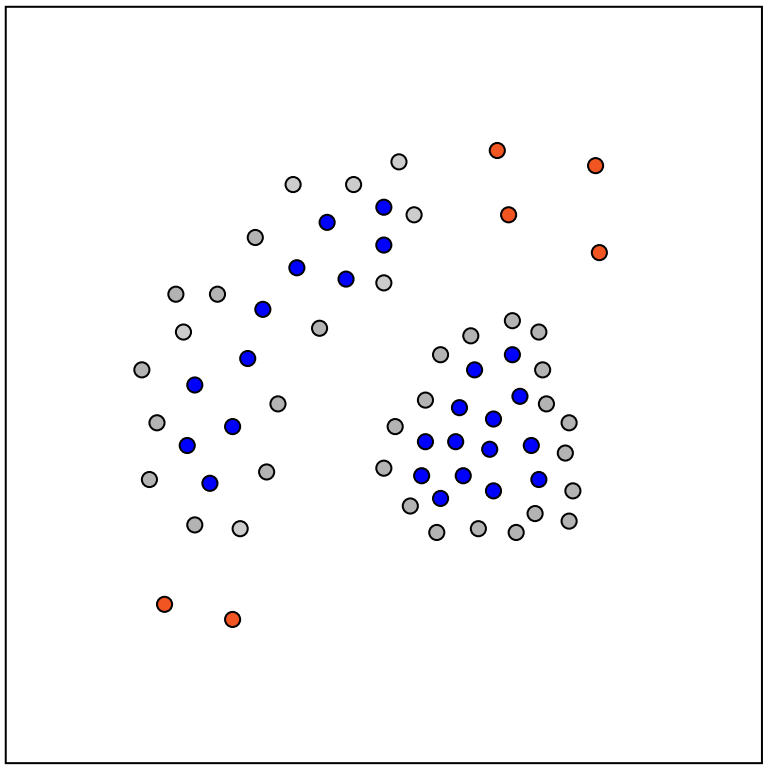
## DBSCAN



- Core point
- Border point
- Noise point

# Density-Based Cluster Analysis

## DBSCAN



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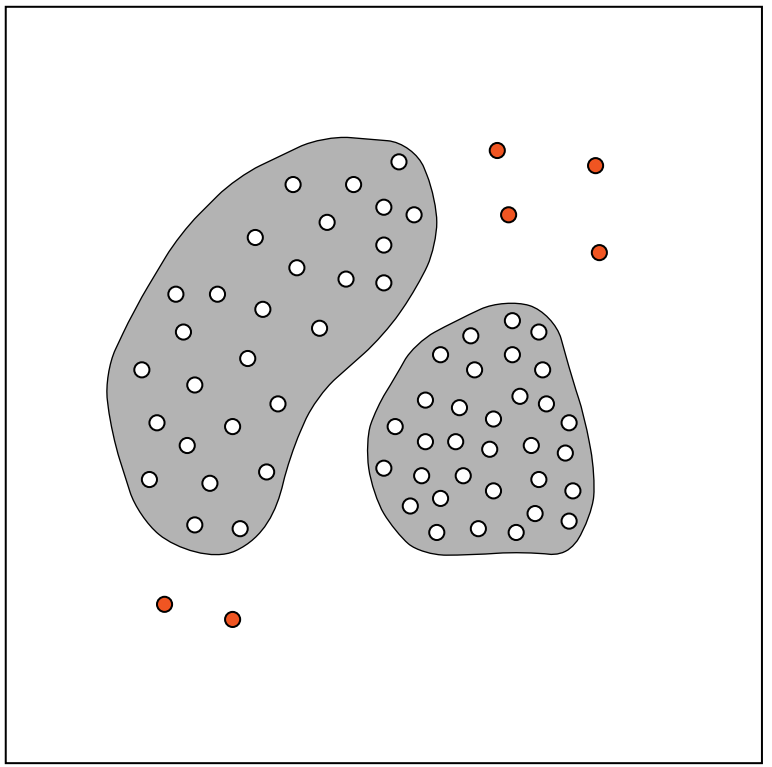
# Density-Based Cluster Analysis

## DBSCAN



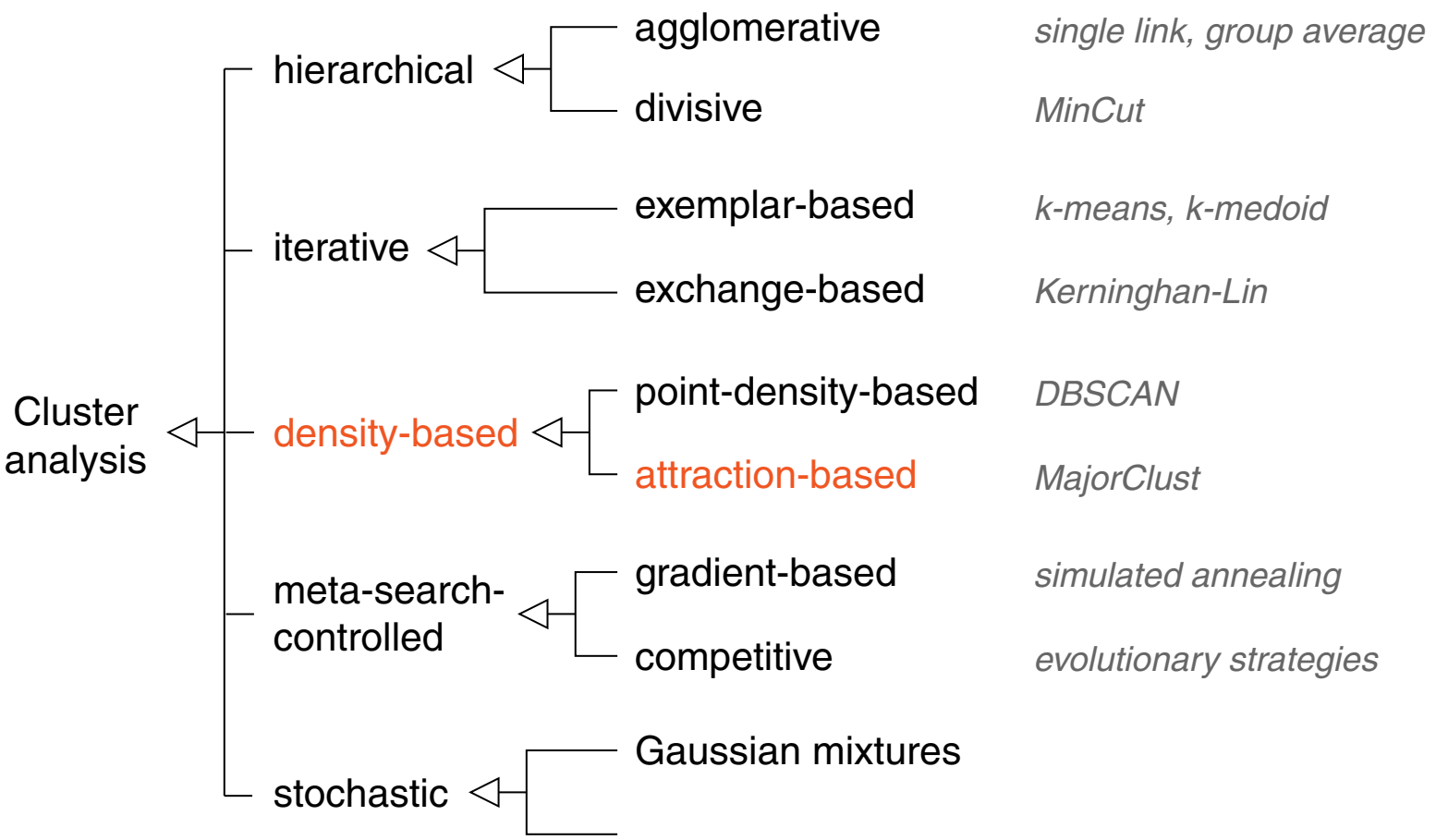
- Noise point

Remarks:

- Note that points that are labeled as noise can be re-labeled with a cluster number exactly once. I.e., a point will retain its tentative noise label only if it is not density-reachable from any other point.
- The construction of $C_i$ as the density-reachable hull of $N_\varepsilon(v)$ (Line 7) corresponds to a recursive analysis of the points in $N_\varepsilon(v)$ with regard to their density reachability.
- A slightly different and compact formulation of the algorithm is given in [Tan/Steinbach/Kumar 2005, p. 528].

# Density-Based Cluster Analysis

## Merging Principles



# Density-Based Cluster Analysis

## MajorClust: Density Estimation Principle [Stein/Niggemann 1999]

The weighted edges in a graph $G = \langle V, E, w \rangle$ are interpreted as attracting forces, where members of the same cluster combine their forces.

Unique membership situation, leading to a merge of two clusters:

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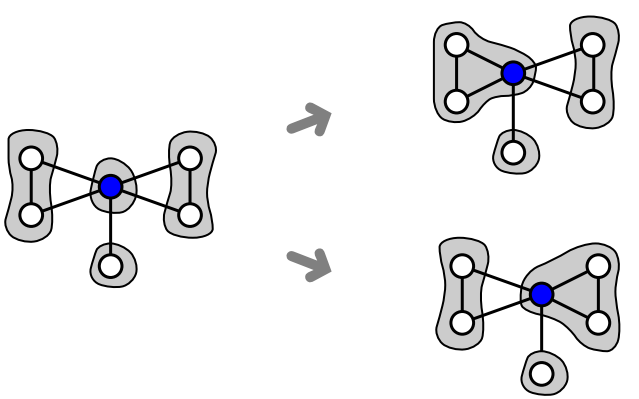
Unique membership situation, leading to a merge of two clusters:

Unique membership situation, leading to a change of cluster membership:

Ambiguous membership situation:



# Density-Based Cluster Analysis

## MajorClust: Algorithm

Input: $G = \langle V, E, w \rangle$. Weighted graph.
$d$. Distance measure for two nodes in $V$.

Output: $\gamma : V \to \mathbf{N}$. Cluster assignment function.

1.
2.
3.
4.
5. **FOREACH** $v \in V$ **DO**
6. $\gamma^* = \underset{i:\, i \in \{1,\ldots,|V|\}}{\text{argmax}} \sum_{\{u,v\}:\, \{u,v\} \in E \wedge \gamma(u) = i} w(u,v)$ `// find strongest cluster for` $v$
7. **IF** $\gamma(v) \neq \gamma^*$ **THEN** $\gamma(v) = \gamma^*$, $t = \mathit{False}$ **ENDIF** `// reassign` $v$
8. **ENDDO**
9.
10.

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$d$. Distance measure for two nodes in $V$.

Output: $\gamma : V \to \mathbf{N}$. Cluster assignment function.

1. $i = 0$, $t =$ *False*
2. **FOREACH** $v \in V$ **DO** $i = i + 1$, $\gamma(v) = i$ **ENDDO** // initial clustering
3. **UNLESS** $t$ **DO**
4. $t =$ *True*
5. **FOREACH** $v \in V$ **DO**
6. $\gamma^* = \underset{i:\, i \in \{1,\ldots,|V|\}}{\operatorname{argmax}} \sum_{\{u,v\}:\, \{u,v\} \in E \wedge \gamma(u) = i} w(u,v)$ // find strongest cluster for $v$
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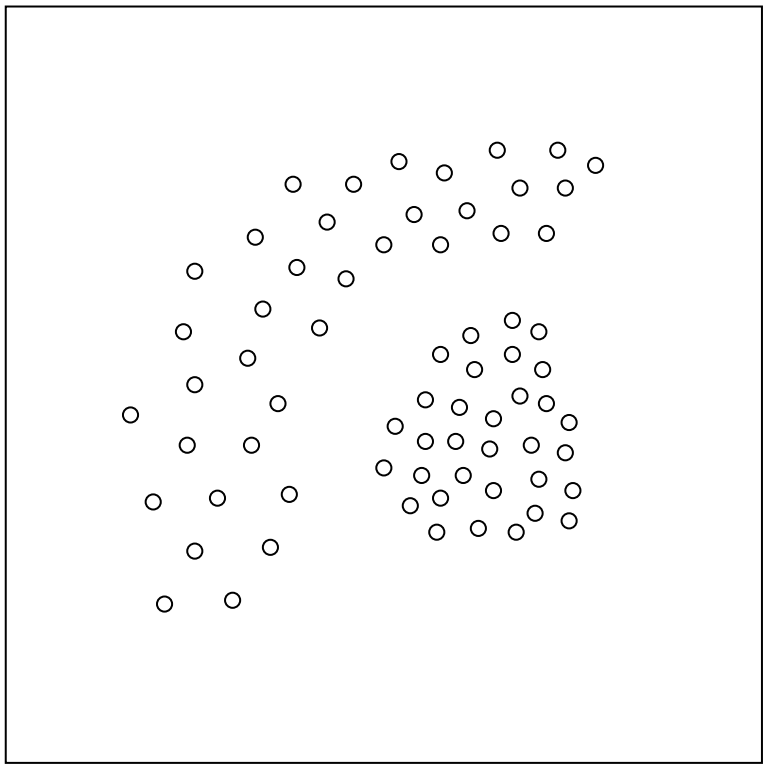
8. **ENDDO**
9. **ENDDO**
10. **RETURN**$(\gamma)$

# Density-Based Cluster Analysis

## MajorClust



# Density-Based Cluster Analysis

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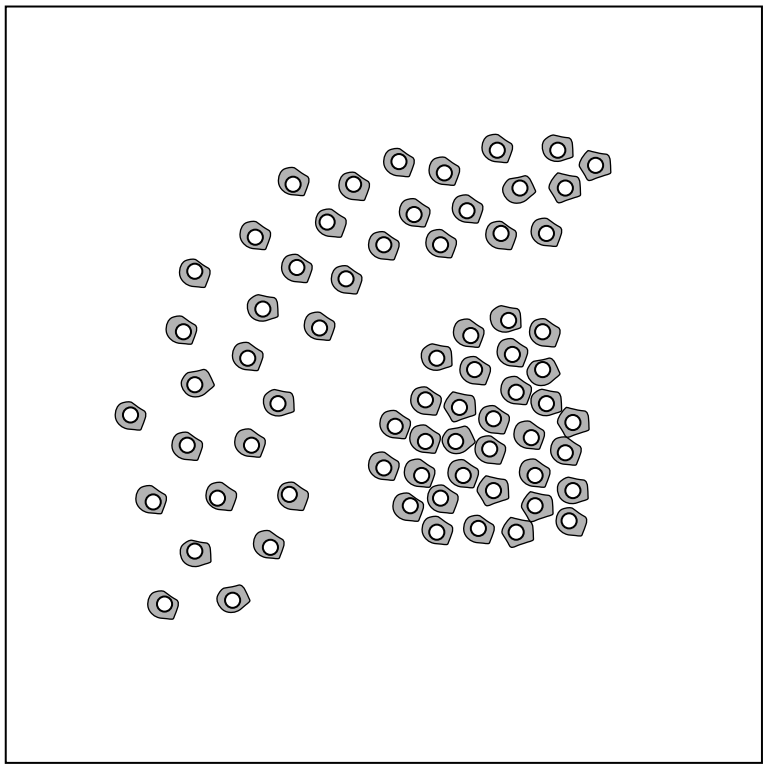

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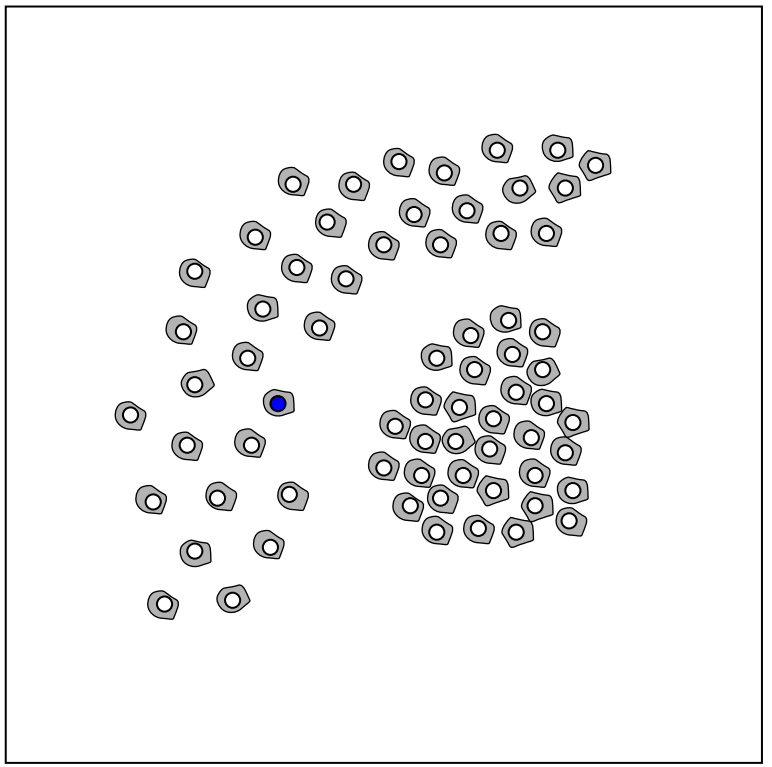

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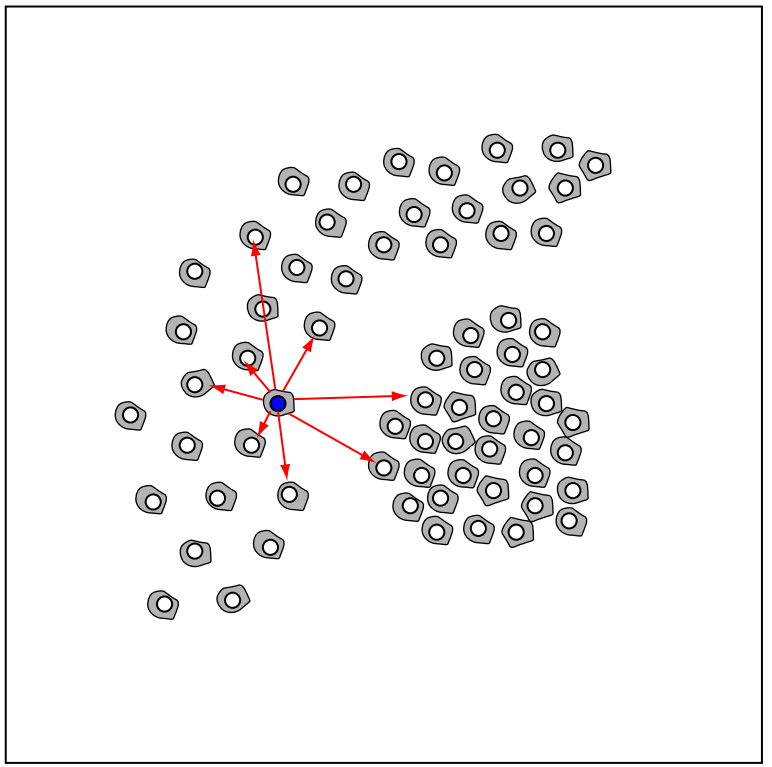

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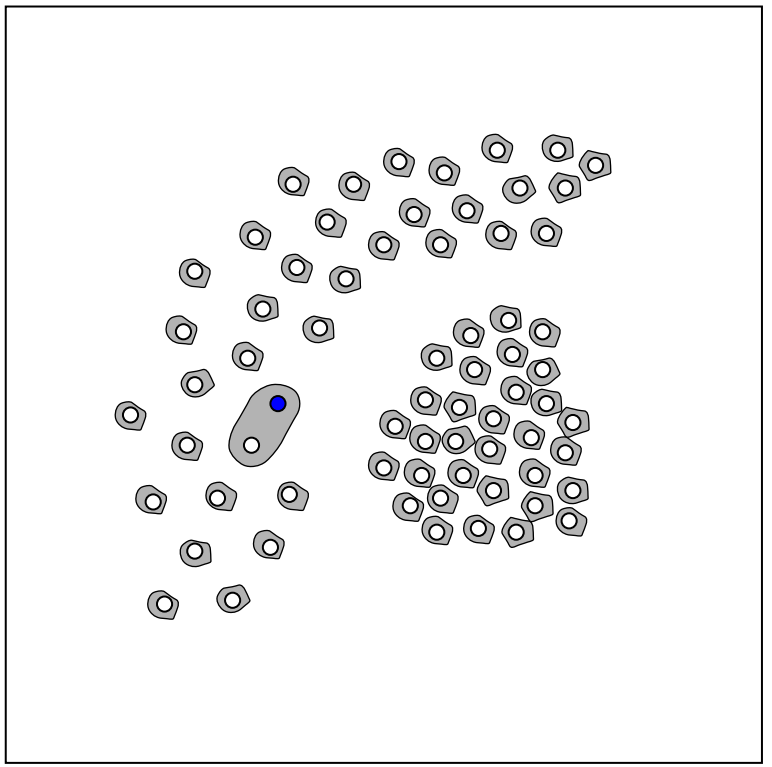

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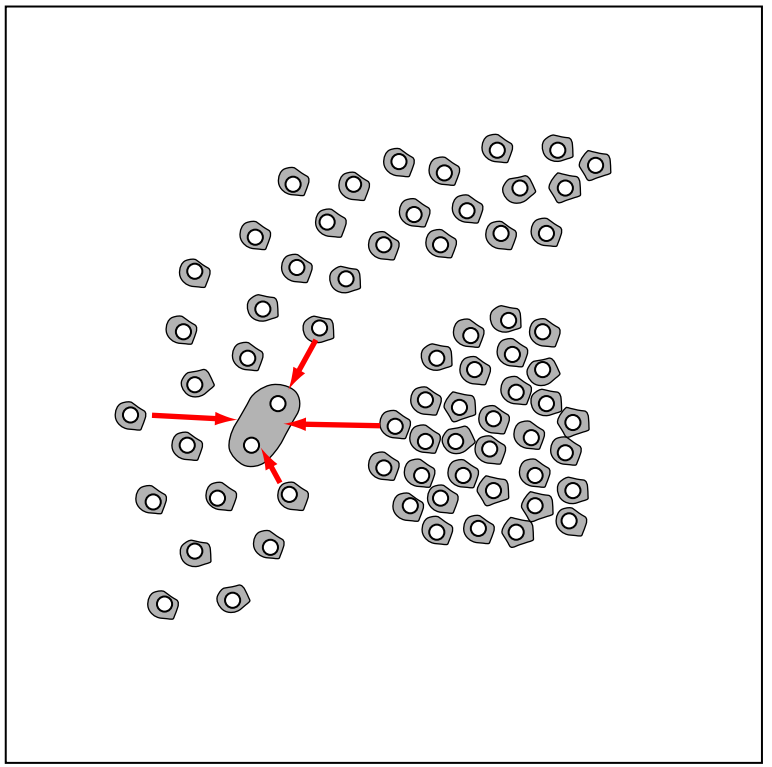

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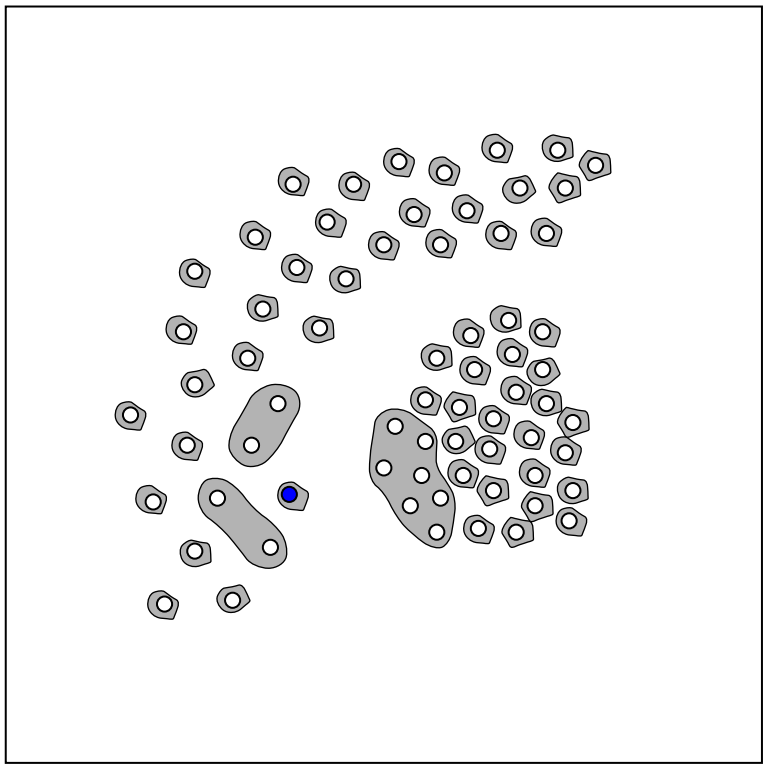
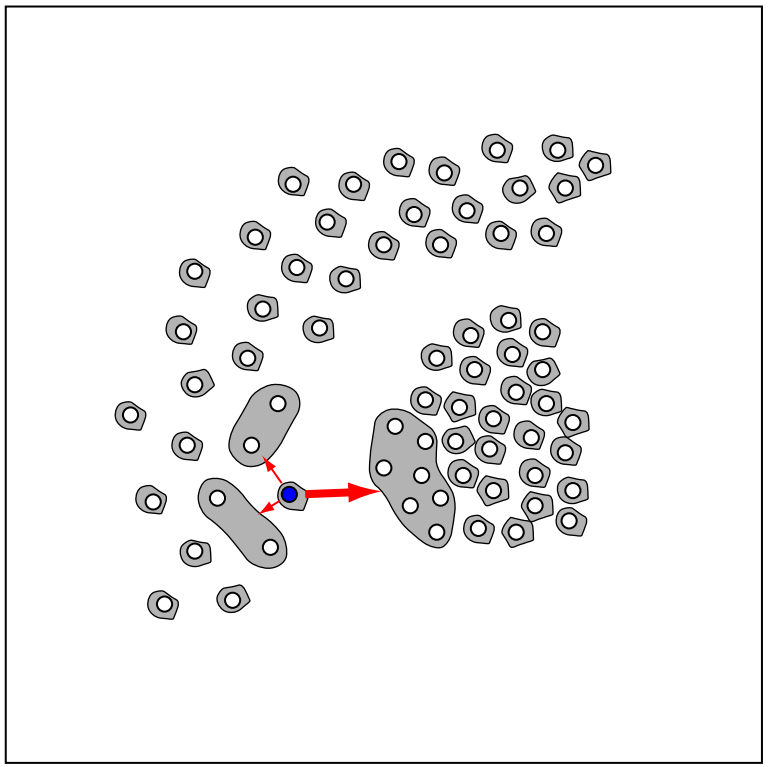


# Density-Based Cluster Analysis

## MajorClust



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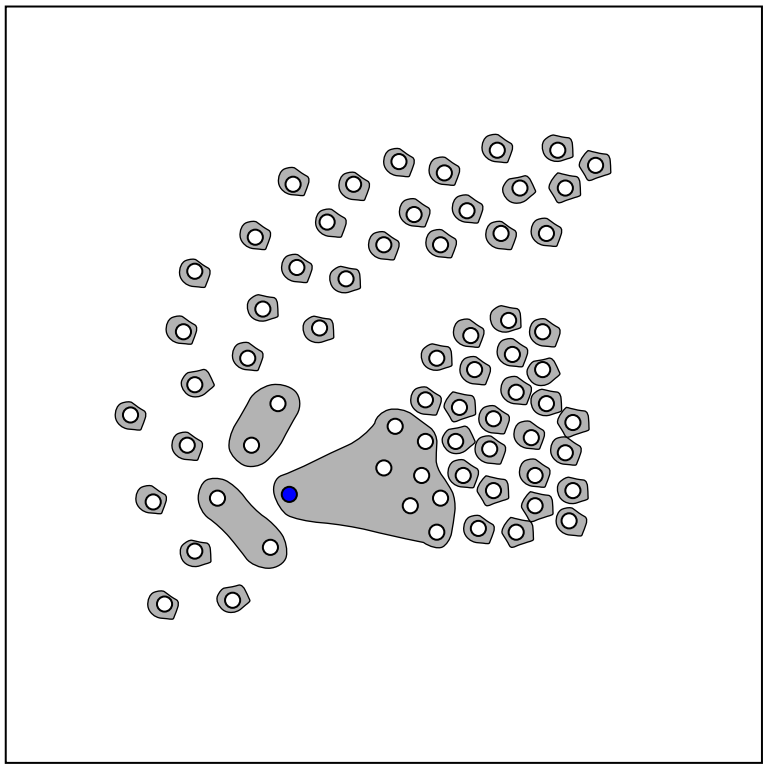

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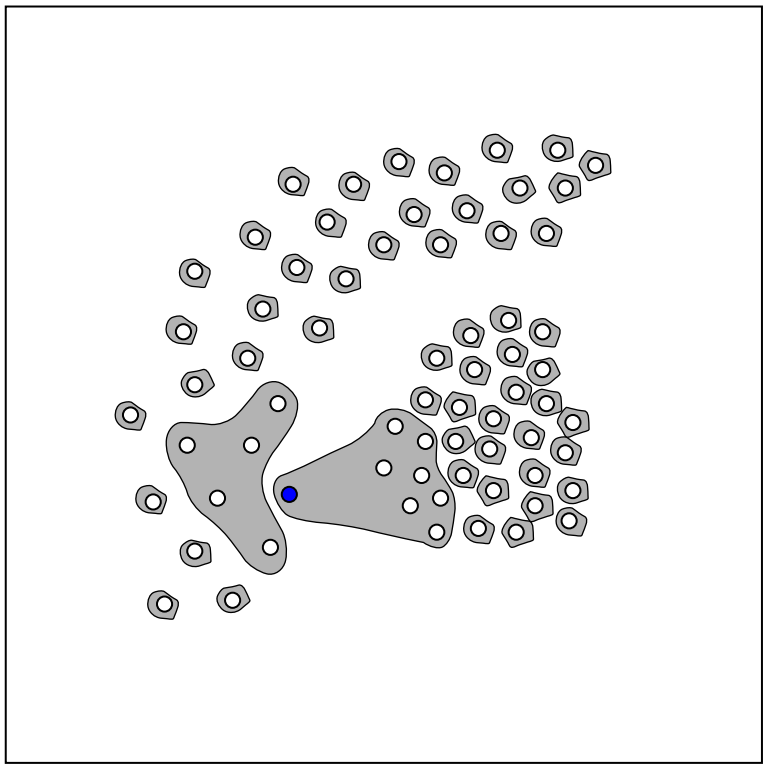

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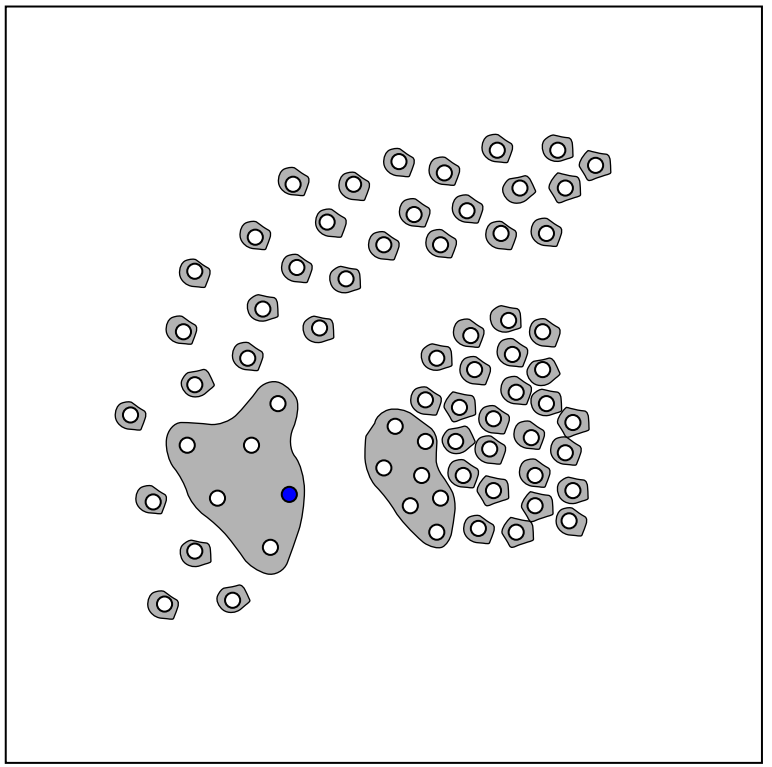
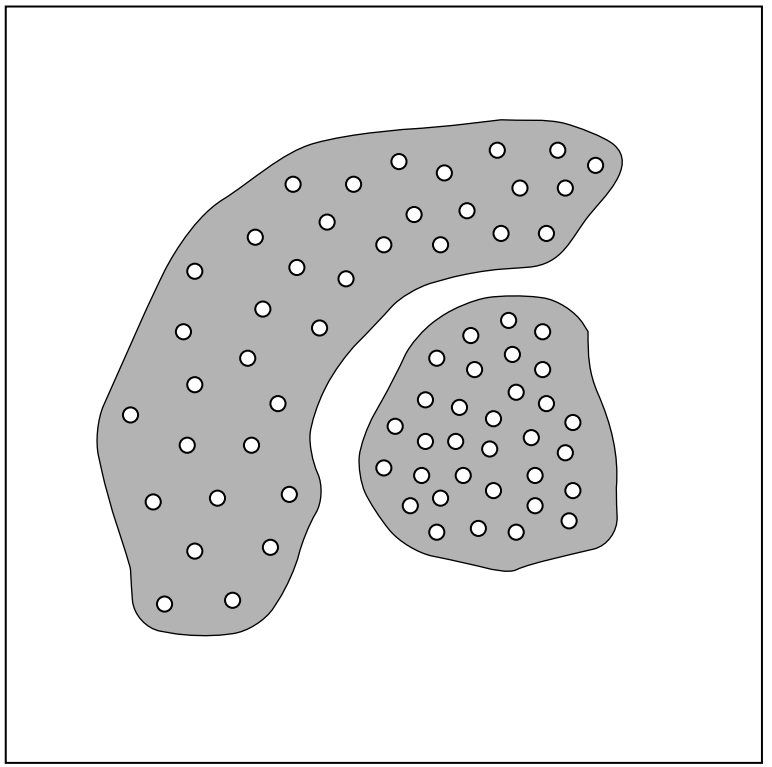


# Density-Based Cluster Analysis

## MajorClust



Remarks:

- MajorClust combines properties from other paradigms:
  - distance-depending analysis (hierarchical paradigm, iterative paradigm)
  - reversible merging decisions (iterative paradigm)
  - distribution-dependent analysis (density paradigm)

# Density-Based Cluster Analysis

## MajorClust: Density Estimation Principle (continued)

Each clustering $\mathcal{C} = \{C_1, \ldots, C_k\}$ induces $k$ subgraphs within $G = \langle V, E, w \rangle$.
MajorClust is a heuristic to maximize the *weighted partial edge connectivity*, $\Lambda(\mathcal{C})$.

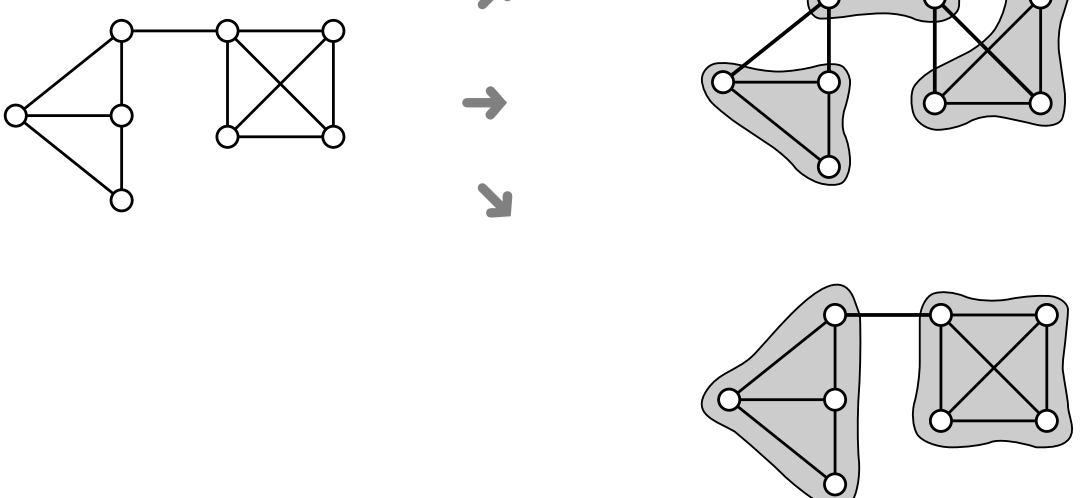
$$\Lambda(\mathcal{C}) = \sum_{i=1}^{k} |C_i| \cdot \lambda_i$$

# Density-Based Cluster Analysis

## MajorClust: Density Estimation Principle (continued)

Each clustering $\mathcal{C} = \{C_1, \ldots, C_k\}$ induces $k$ subgraphs within $G = \langle V, E, w \rangle$.
MajorClust is a heuristic to maximize the *weighted partial edge connectivity*, $\Lambda(\mathcal{C})$.

$$\Lambda(\mathcal{C}) = \sum_{i=1}^{k} |C_i| \cdot \lambda_i$$



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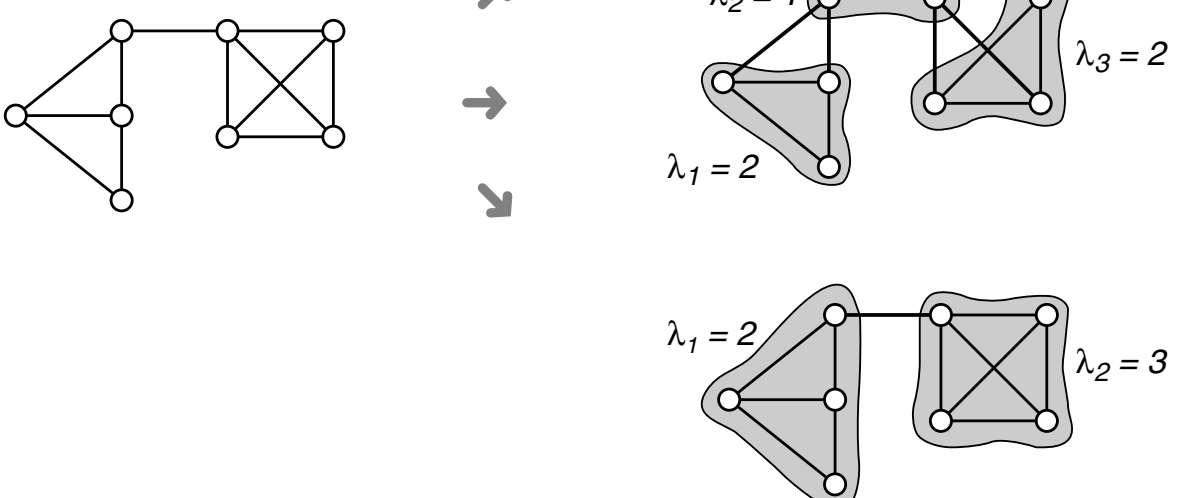

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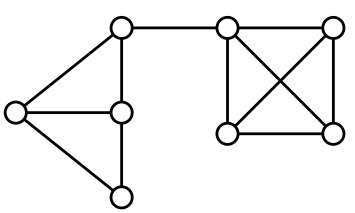

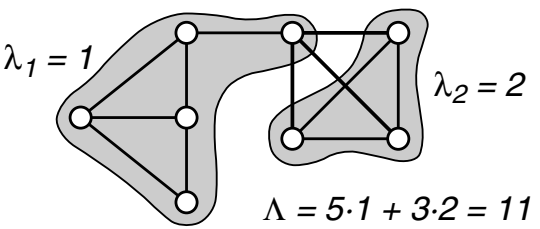


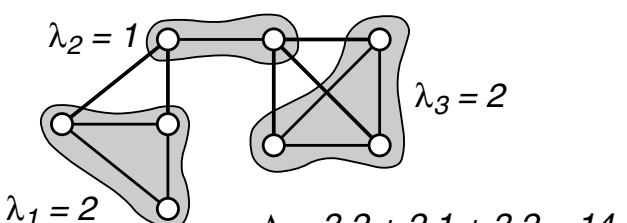


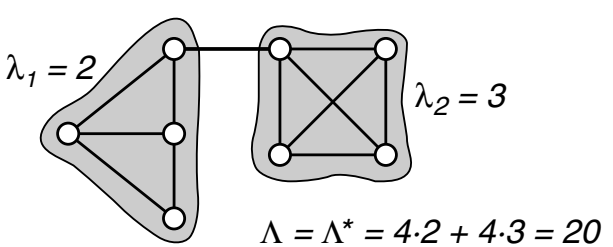

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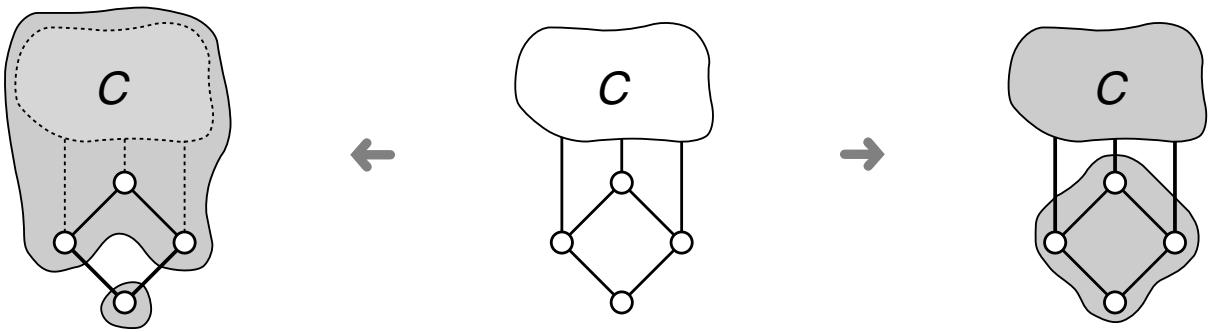
## MajorClust: Density Estimation Principle (continued)

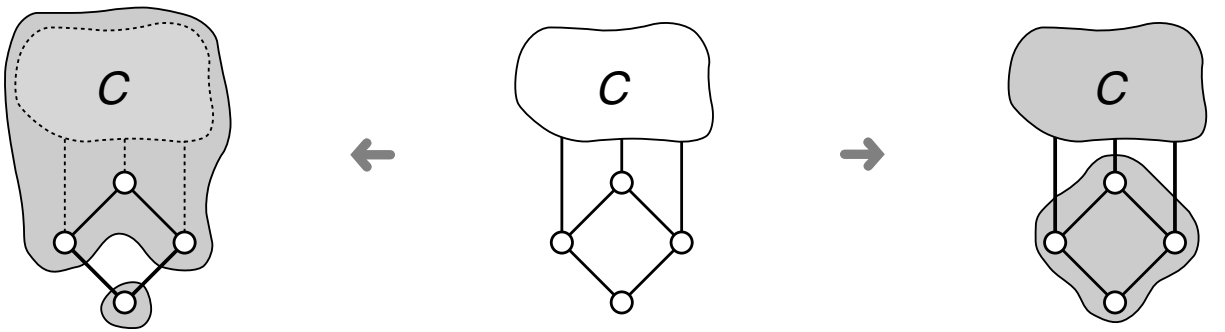



minimization of cut weight

$\Lambda$ maximization

# Density-Based Cluster Analysis

## MajorClust: Density Estimation Principle (continued)




minimization of cut weight

$\Lambda$ maximization

**Theorem 5 (Strong Splitting Condition** [Stein/Niggemann 1999]**)**

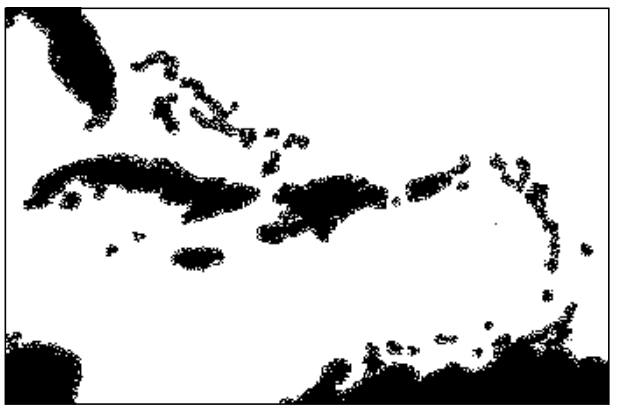
Let $\mathcal{C} = \{C_1, \ldots, C_k\}$ be a partitioning of a graph $G = \langle V, E, w \rangle$. Moreover, let $\lambda(G)$ denote the edge connectivity of $G$, and let $\lambda_1, \ldots, \lambda_k$ denote the edge connectivity values of the $k$ subgraphs that are induced by $C_1, \ldots, C_k$.

If the inequality $\lambda(G) < \min\{\lambda_1, \ldots, \lambda_k\}$ holds, then the partitioning defined by $\Lambda$-maximization corresponds to the minimum cut splitting of $G$. The inequality is denoted as “Strong Splitting Condition”.

# Density-Based Cluster Analysis

## DBSCAN versus MajorClust: Low-Dimensional Data

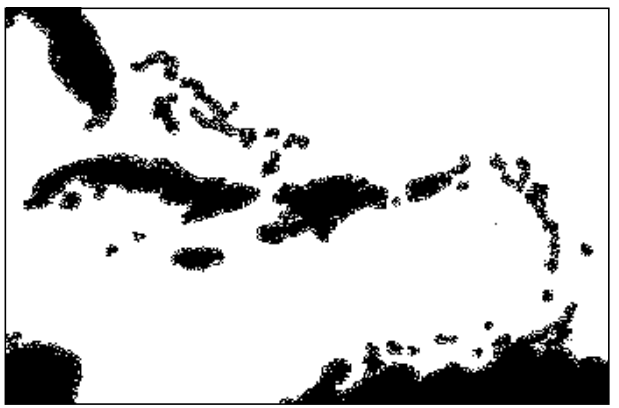
Caribbean Islands, about 20.000 points:

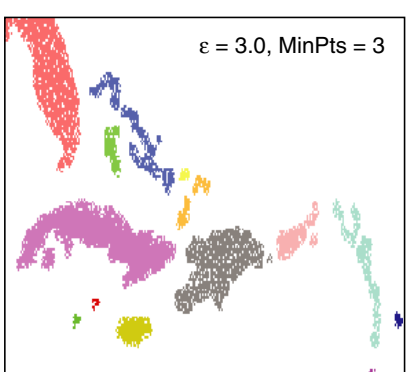
# Density-Based Cluster Analysis

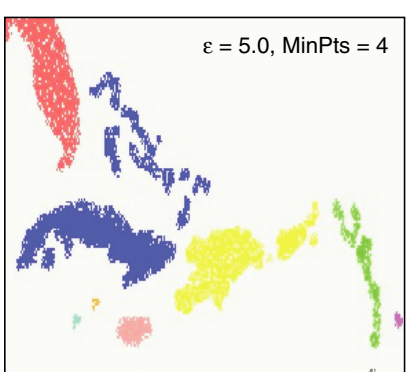
## DBSCAN versus MajorClust: Low-Dimensional Data (continued)

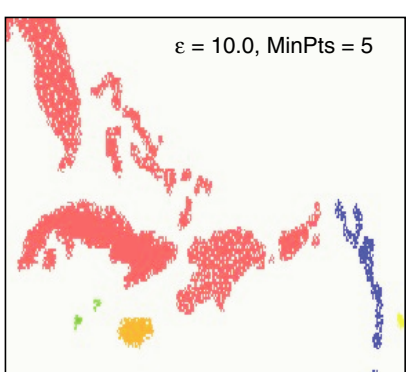
Caribbean Islands, about 20.000 points:

Cluster analysis by DBSCAN:



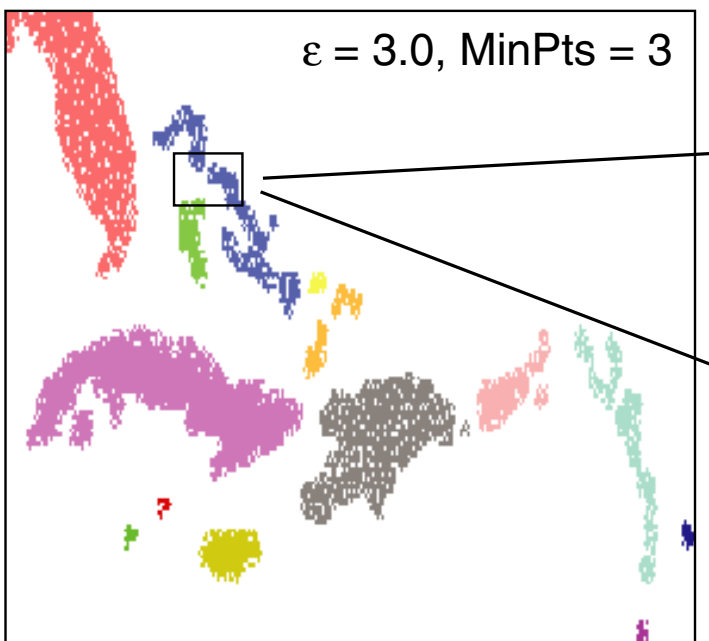



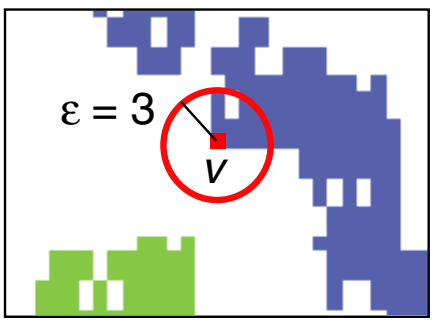



# Density-Based Cluster Analysis

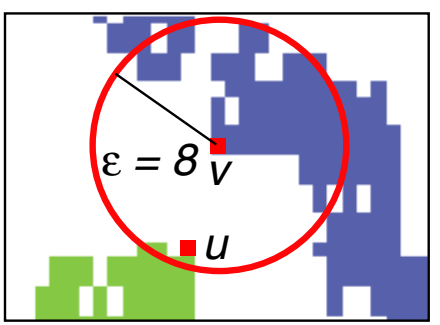
## DBSCAN versus MajorClust: Low-Dimensional Data (continued)

The problem of finding useful $\varepsilon$-values for DBSCAN:




Two separate clusters will be detected.

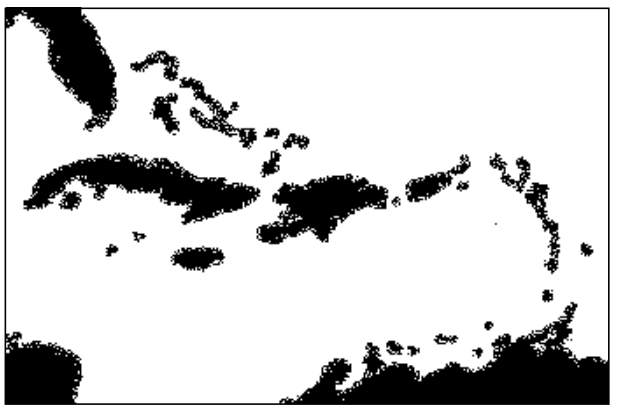



The clusters will be merged.

# Density-Based Cluster Analysis

## DBSCAN versus MajorClust: Low-Dimensional Data (continued)

Caribbean Islands, about 20.000 points:

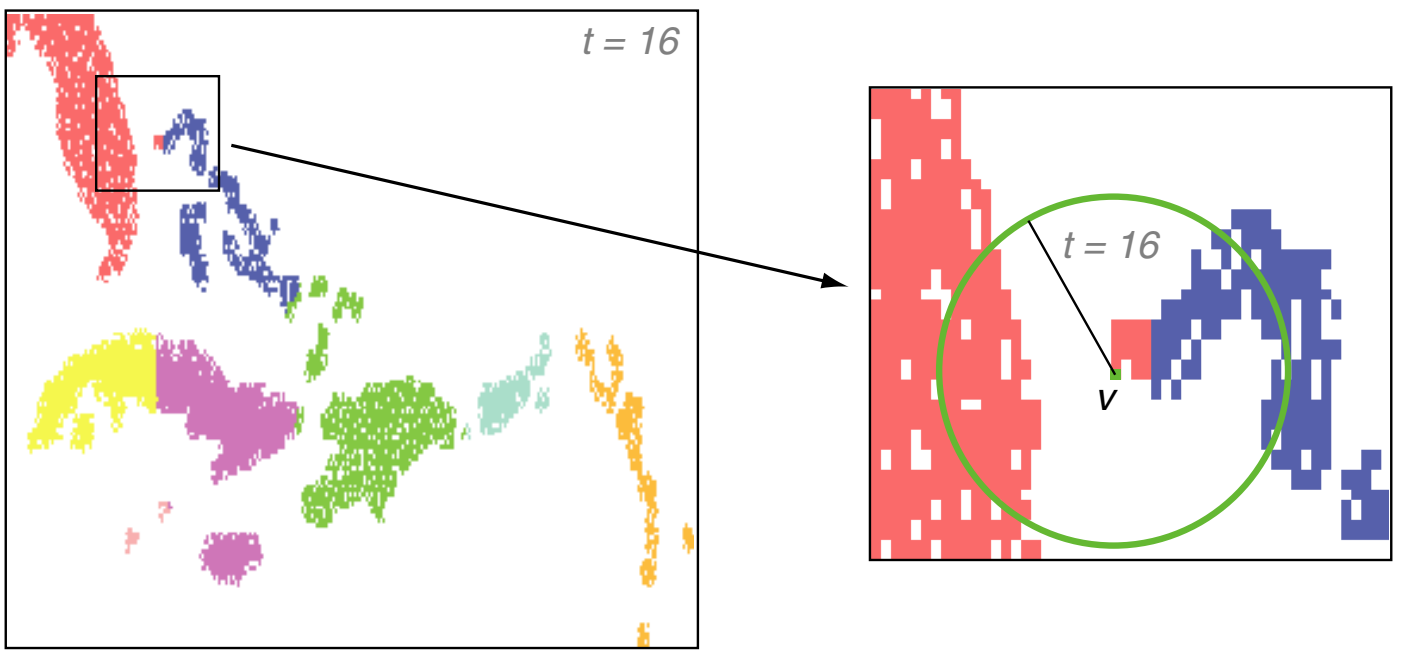



Cluster analysis by MajorClust:

# Density-Based Cluster Analysis

## DBSCAN versus MajorClust: Low-Dimensional Data (continued)

The problem of the global analysis approach (no restriction by means of an $\varepsilon$-neighborhood) in MajorClust:



Remarks:

- MajorClust is superior to DBSCAN with regard to the identification of differently dense clusters within the same clustering. DBSCAN is more flexible (= can be better adapted) than MajorClust with regard to point densities in different clusterings.
- MajorClust considers always all points of $V$, while DBSCAN works locally, i.e., on small subsets of $V$.

# Density-Based Cluster Analysis

## DBSCAN versus MajorClust: High-Dimensional Data

Typical document categorization setting:

- $10^4$ - $10^5$ documents
- 10 - 100 categories: politics, culture, economics, etc.
- documents belong to one category
- dimension of the feature space $> 10\,000$

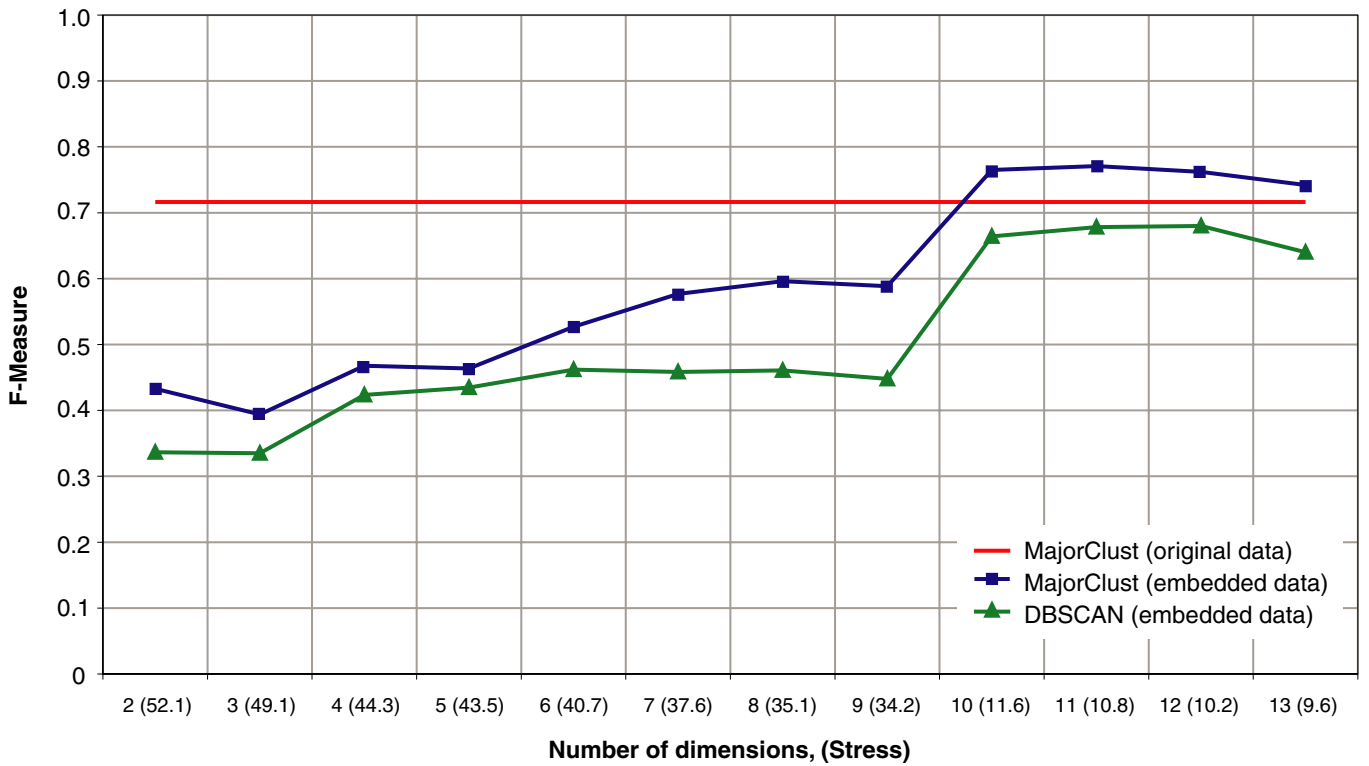
DBSCAN:

- degenerates with increasing number of dimensions
- the degeneration is rooted in the computation of the $\varepsilon$-neighborhood
- dimension reduction provides a way out, e.g. by embedding the data with multi-dimensional scaling, MDS

# Density-Based Cluster Analysis

## DBSCAN versus MajorClust: High-Dimensional Data (continued)

Classification effectiveness ($F$ measure) over dimension number:




[Stein/Busch 2005]

Remarks:

- Usually, the neighborhood search in high-dimensional spaces cannot be solved efficiently. Given $p$ dimensions with $p$ about 10 or larger, an exhaustive search, i.e., a linear scan of all feature vectors will be more efficient than the application of a space partitioning data structure (quad-tree, k-d tree, etc,) or a data partitioning data structure ($R$-tree, $Rf$-tree, $X$-tree, etc.).
- DBSCAN employs the $R$-tree data structure to compute $\varepsilon$-neighborhoods. This data structure accomplishes the major part of the DBSCAN cluster analysis approach and is ideally suited for treating low-dimensional data efficiently. The application of DBSCAN to high-dimensional data either requires an embedding into a low-dimensional space or to accept the runtime for a naive construction of $\varepsilon$-neighborhoods.
- Neighborhood search in high-dimensional spaces can be addressed with approximate methods such as locality sensitive hashing (LSH), or Fuzzy fingerprinting. [Weber 1999] [Gionis/Indyk/Motwani 1999-2004] [Stein 2005-2007] [Andoni 2009]