Cluster Discovery Methods for Large Data Bases

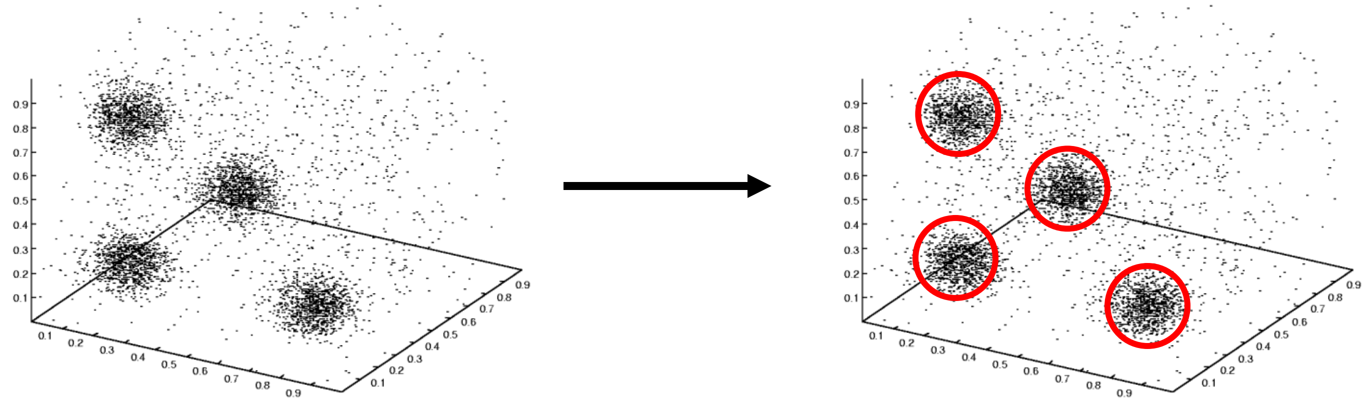
From the Past to the Future

Alexander Hinneburg, Daniel A. Keim

University of Halle

Introduction

- **Application Example:** Marketing
  - Given:
    - Large data base of customer data containing their properties and past buying records
  - Goal:
    - Find groups of customers with similar behavior
    - Find customers with unusual behavior



Introduction

- **Application Example:**
  Class Finding in CAD-Databases
  - Given:
    - Large data base of CAD data containing abstract feature vectors (Fourier, Wavelet, ...)
  - Goal:
    - Find homogeneous groups of similar CAD parts
    - Determine standard parts for each group
    - Use standard parts instead of special parts
      ($\rightarrow$ reduction of the number of parts to be produced)

Introduction

Problem Description

- Given:

  A data set with *N* *d*-dimensional data items.

- Task:

  Determine a (good/natural) partitioning of the data set into a number of clusters (k) and noise.

Introduction

From the Past ...

- Clustering is a well-known problem in statistics [Sch 64, Wis 69]
- more recent research in
  - machine learning [Roj 96],
  - databases [CHY 96], and
  - visualization [Kei 96] ...

Introduction

... to the Future

- *Effective* and *efficient* clustering algorithms for *large high-dimensional* data sets with *high noise level*
- Requires ***Scalability*** with respect to
  - the *number of data points (**N**)*
  - the *number of dimensions (**d**)*
  - the *noise level*

Overview

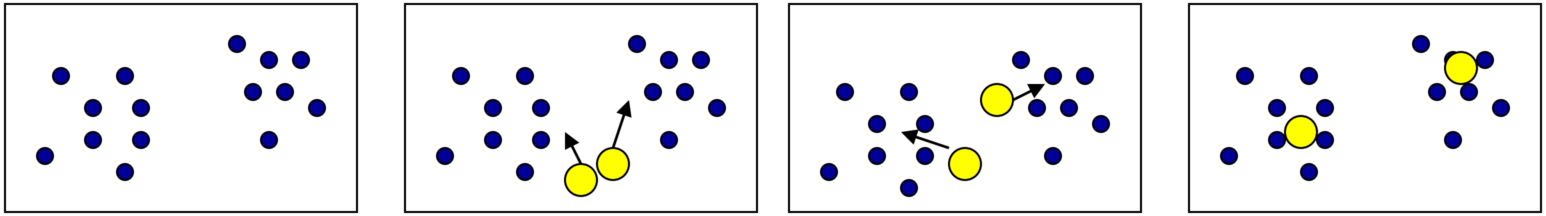
1. Introduction
2. Clustering Methods
    2.1 Model- and Optimization-based Approaches
    2.2 Density-based Approaches
    2.3 Hybrid Approaches
3. Techniques for Improving the Effectiveness and Efficiency
    4.1 Hierarchical Variants
    4.2 Scaling Up Clustering Algorithms
4. Summary and Conclusions

Clustering Methods

- Model- and Optimization-Based Approaches
- Density-Based Approaches
- Hybrid Approaches

K-Means [Fuk 90]

- Determine k prototypes of a given data
- Optimize a distance criteria: $\sum_{i=1}^{k}\sum_{j=1}^{N} d(p_i, x_j^i) / N$
- Iterative Algorithm:
  - •Assign the data points to the nearest prototype
  - •Shift the prototypes towards the mean of their point set

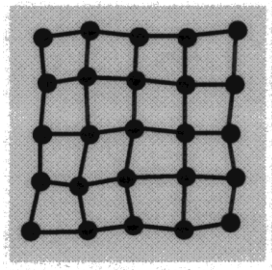


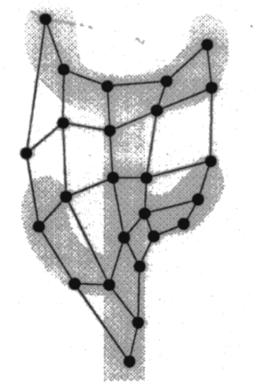
Expectation Maximization [Lau 95]

- Estimate parameters of k Gaussians
- Optimize the probability, that the mixture of parameterized Gaussians fits the data
- Iterative algorithm similar to k-Means

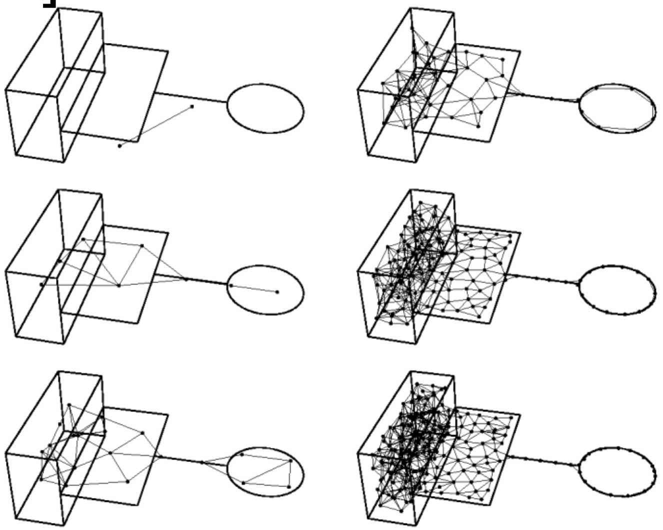
AI Methods [Fri 95, KMS+91]

- Self-Organizing Maps [Roj 96, KMS 91]
  - Fixed map topology (grid, line)



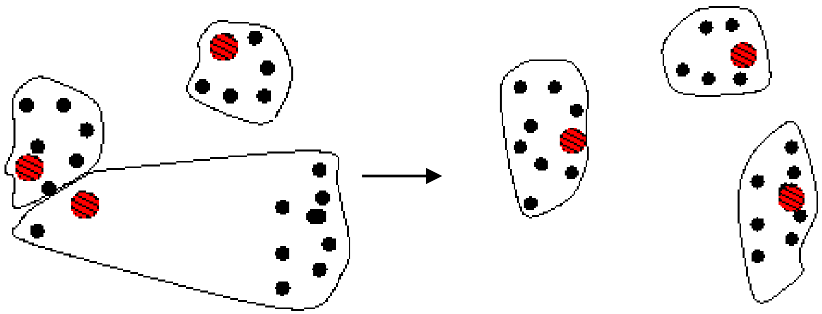


- Growing Networks [Fri 95]
  - Iterative insertion of nodes
  - Adaptive map topology



CLARANS [NH 94]

- Medoid Method:
  - Medoids are special data points
  - All data points are assigned to the nearest medoid



- Optimization Criterion:

$$average\_distance(c) = \sum_{m_i \in M} \sum_{o \in cluster(m_i)} dist(o, m_i) / n$$

CLARANS

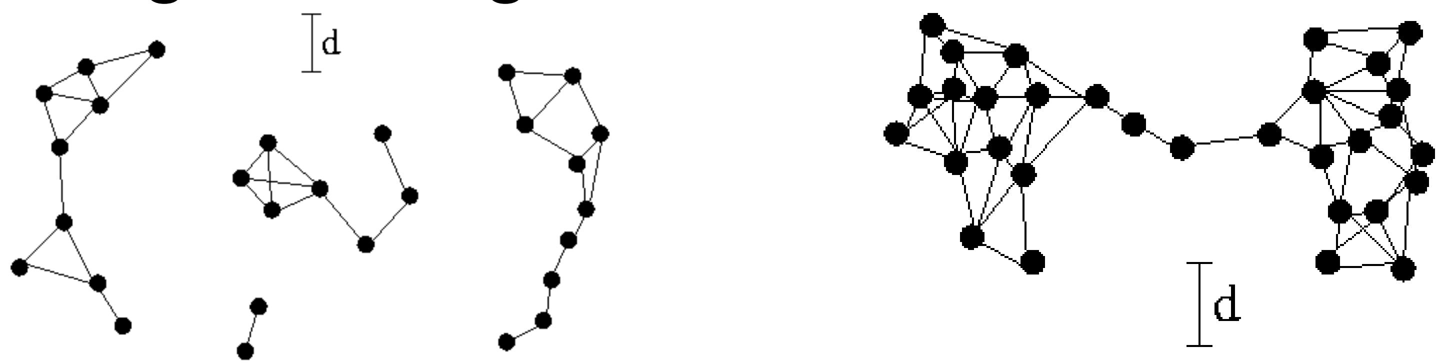
- Graph Interpretation:
  - Search process can be symbolized by a graph
  - Each node corresponds to a specific set of medoids
  - The change of one medoid corresponds to a jump to a neighboring node in the search graph
- Complexity Considerations:
  - The search graph has $\binom{N}{k}$ nodes and each node has *N*k* edges
  - The search is bound by a fixed number of jumps *(num_local)* in the search graph
  - Each jump is optimized by randomized search and costs *max_neighbor* scans over the data (to evaluate the cost function)

Density-based Methods

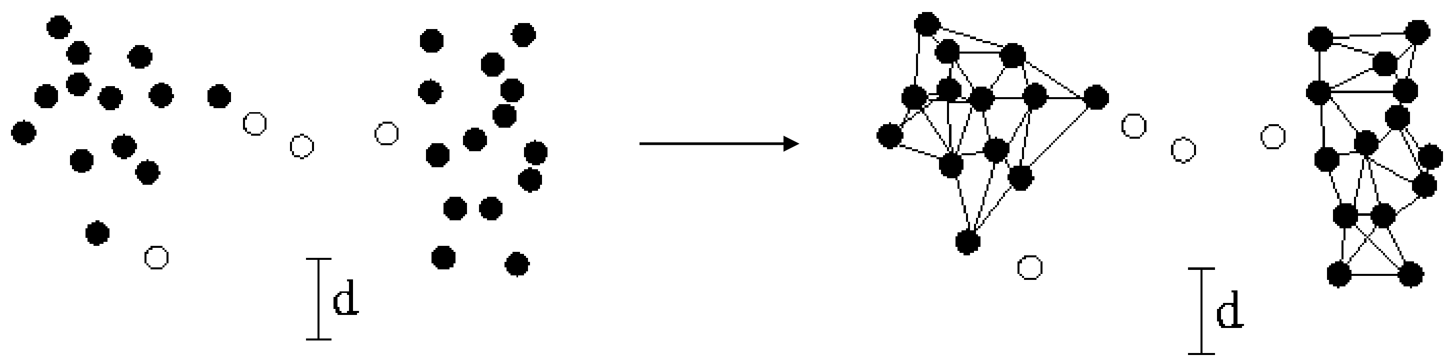
- Linkage -based Methods [Boc 74]
- DBSCAN [EKS+ 96]
- DBCLASD [XEK+ 98]
- STING [WYM 97]
- Hierarchical Grid Clustering [Sch 96]
- WaveCluster [SCZ 98]
- DENCLUE [HK 98]

Linkage -based Methods
(from Statistics) [Boc 74]

- Single Linkage (Connected components for distance d)



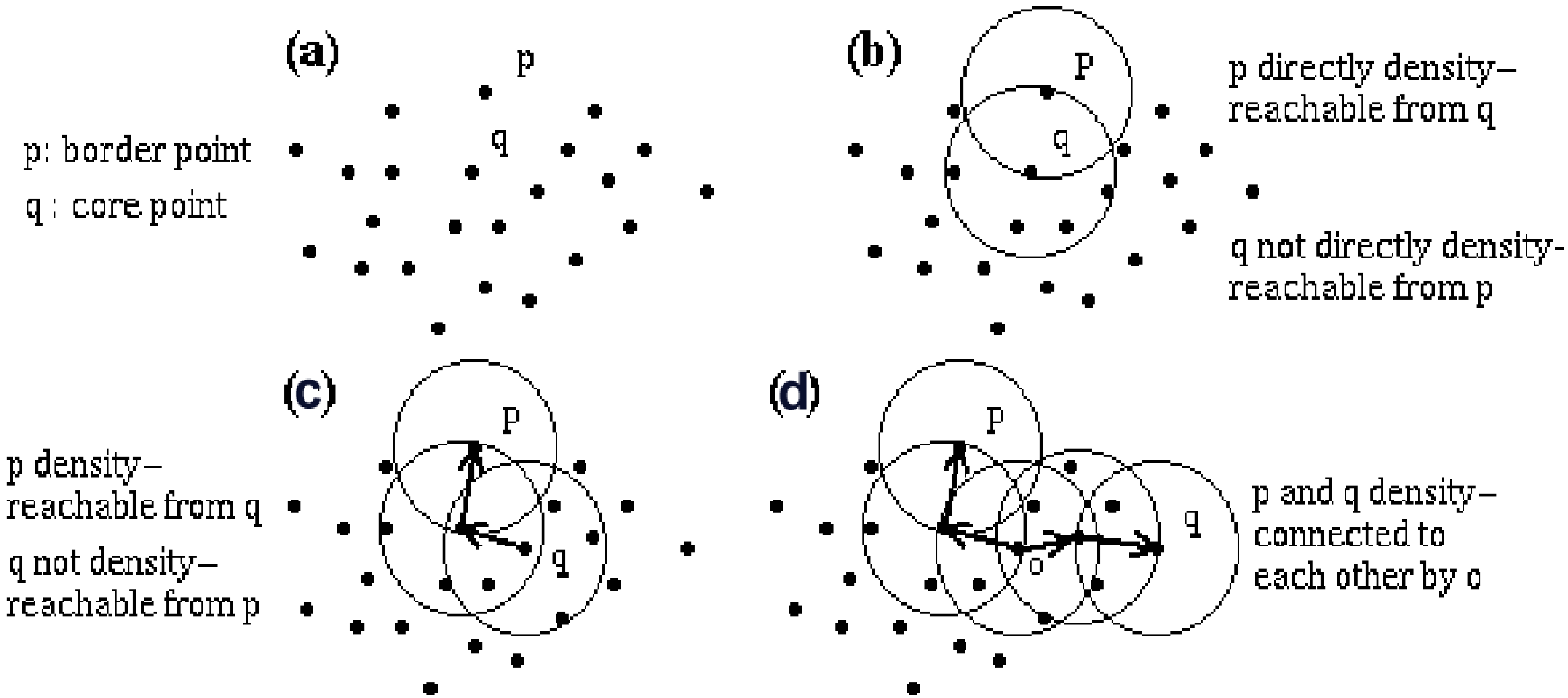
- Method of Wishart [Wis 69] (Min. no. of points: c=4)



Reduce data set   Apply Single Linkage

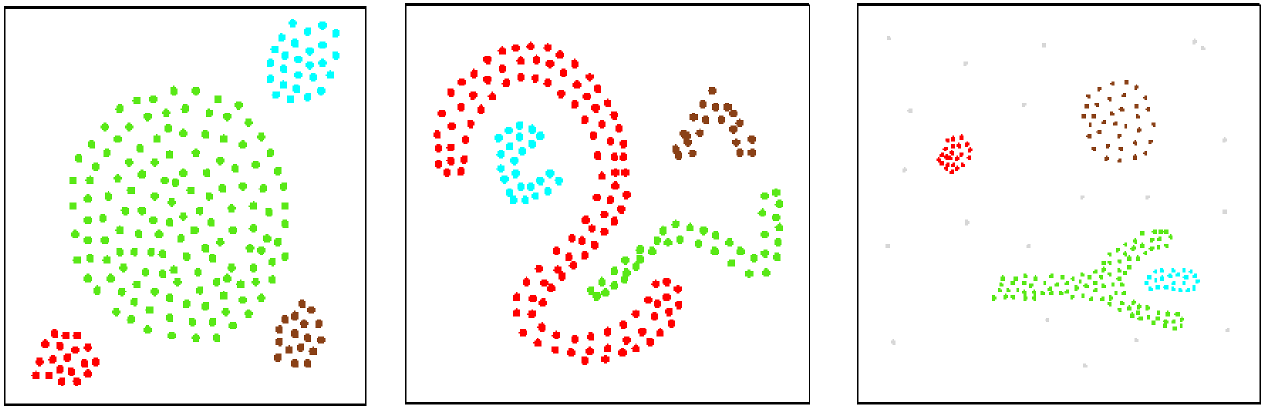
DBSCAN [EKS+ 96]

- Clusters are defined as Density-Connected Sets (wrt. MinPts, ε)



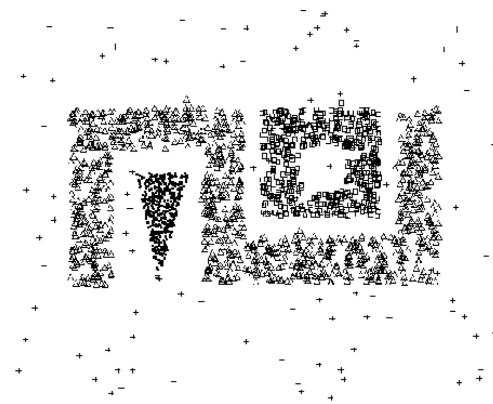
DBSCAN

- For each point, DBSCAN determines the ε-environment and checks, whether it contains more than MinPts data points
- DBSCAN uses index structures for determining the ε-environment
- Arbitrary shape clusters found by DBSCAN

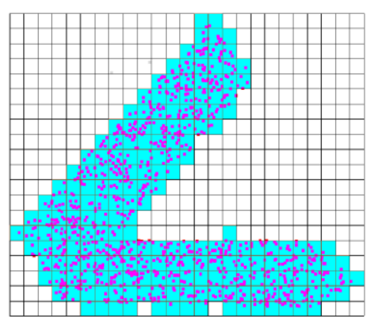


DBCLASD [XEK+ 98]

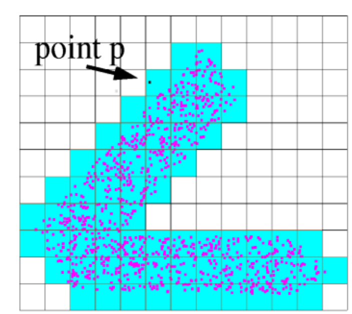
- Distribution-based method
- Assumes arbitrary-shape clusters of uniform distribution
- Requires no parameters
- Provides grid-based approximation of clusters



Before the insertion of point p



After the insertion of point p



DBCLASD

- Definition of a cluster *C* based on the distribution of the NN-distance *(NNDistSet)*:

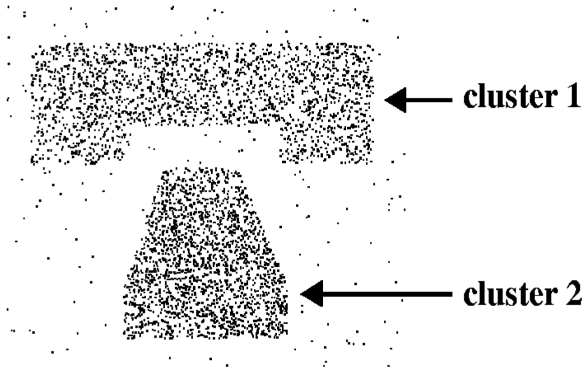
(1) *NNDistSet(C)* has the expected distribution with a required confidence level.

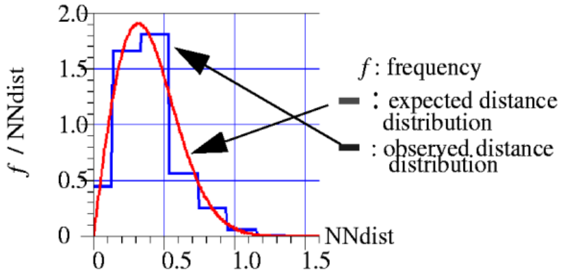
(2) *C* is *maximal*, i.e. each extension of C by neighboring points does not fulfill condition (1). (maximality).

(3) *C* is *connected*, i.e. for each pair of points (a,b) of the cluster there is a path of occupied grid cells connecting a and b (connectivity).

DBCLASD

- Step (1) uses the concept of the χ^2-test



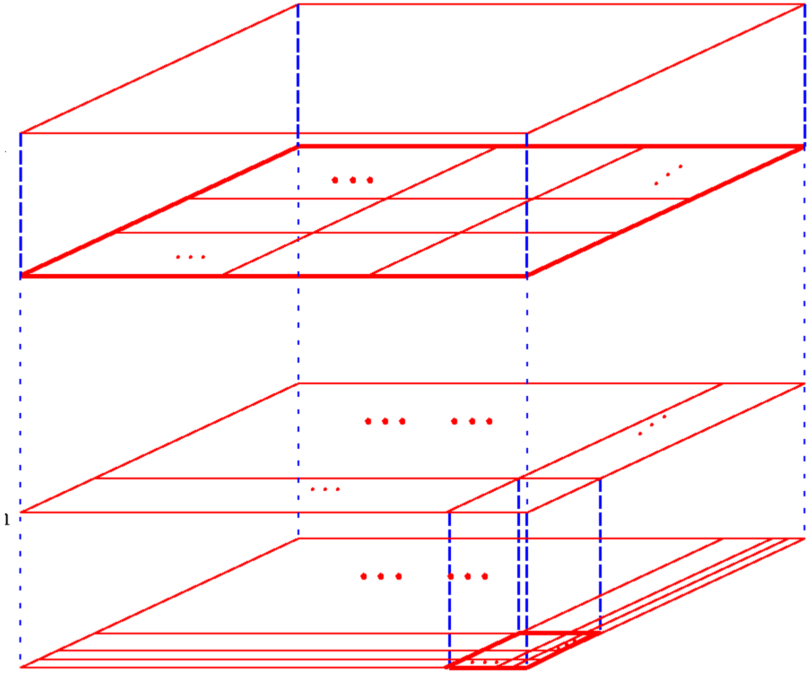


The expected and the observed distance distributions for cluster 1

- Incremental augmentation of clusters by neighboring points (order-depended)
  - unsuccessful candidates are tried again later
  - points already assigned to some cluster may switch to another cluster

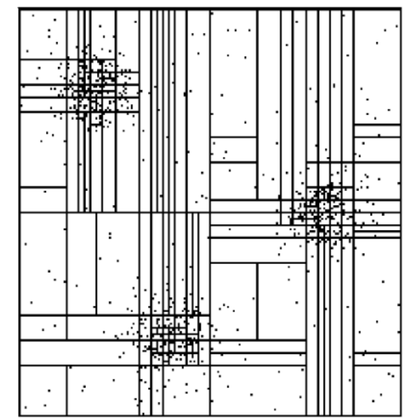
STING [WYM 97]

- Uses a quadtree-like structure for condensing the data into grid cells
- The nodes of the quadtree contain statistical information about the data in the corresponding cells
- STING determines clusters as the density-connected components of the grid
- STING approximates the clusters found by DBSCAN



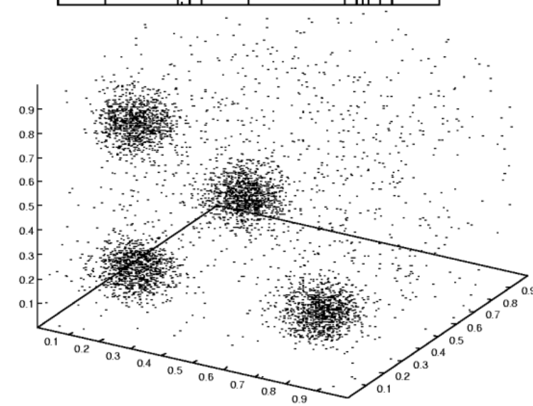
Hierarchical Grid Clustering

[Sch 96]

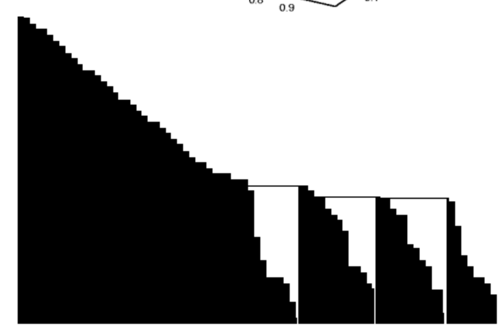


- Organize the data space as a grid-file
- Sort the blocks by their density

$$DB = \frac{p_B}{V_B} \longrightarrow \langle B_{1'}, B_{2'}, \ldots B_{b'} \rangle$$



- Scan the blocks iteratively and merge blocks, which are adjacent over a (d-1)-dim. hyperplane.
- The order of the merges forms a hierarchy



WaveCluster [SCZ 98]

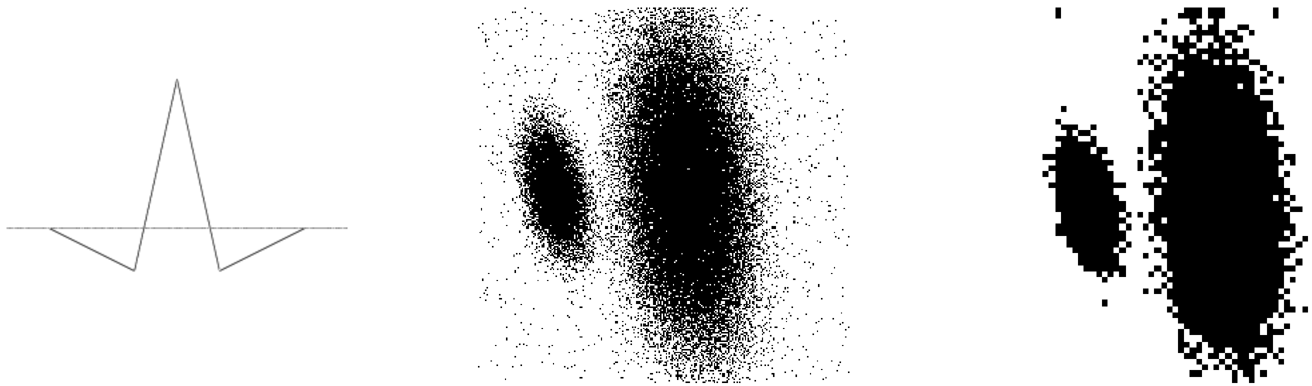
- Clustering from a signal processing perspective using wavelets

Input: Multidimensional data objects' feature vectors
Output: clustered objects

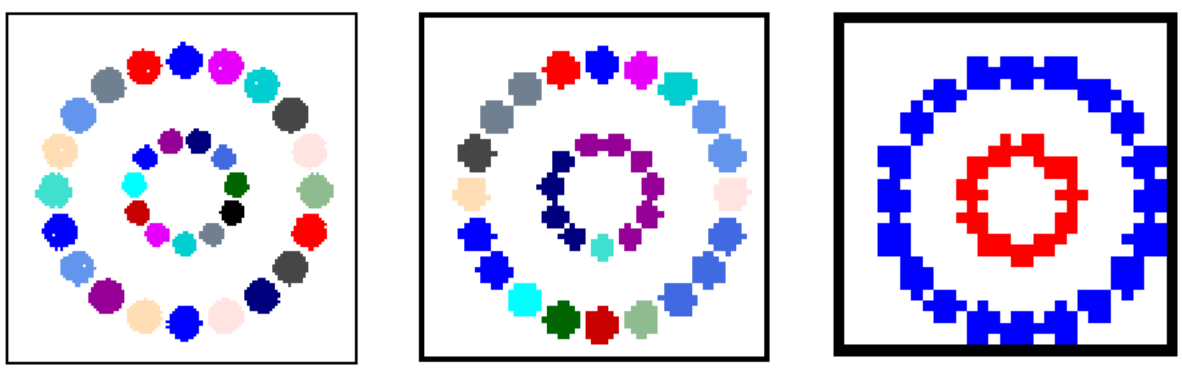
1. Quantize feature space, then assign objects to the units.
2. Apply wavelet transform on the feature space.
3. Find the connected components (clusters) in the subbands of transformed feature space, at different levels.
4. Assign label to the units.
5. Make the lookup table.
6. Map the objects to the clusters.

WaveCluster

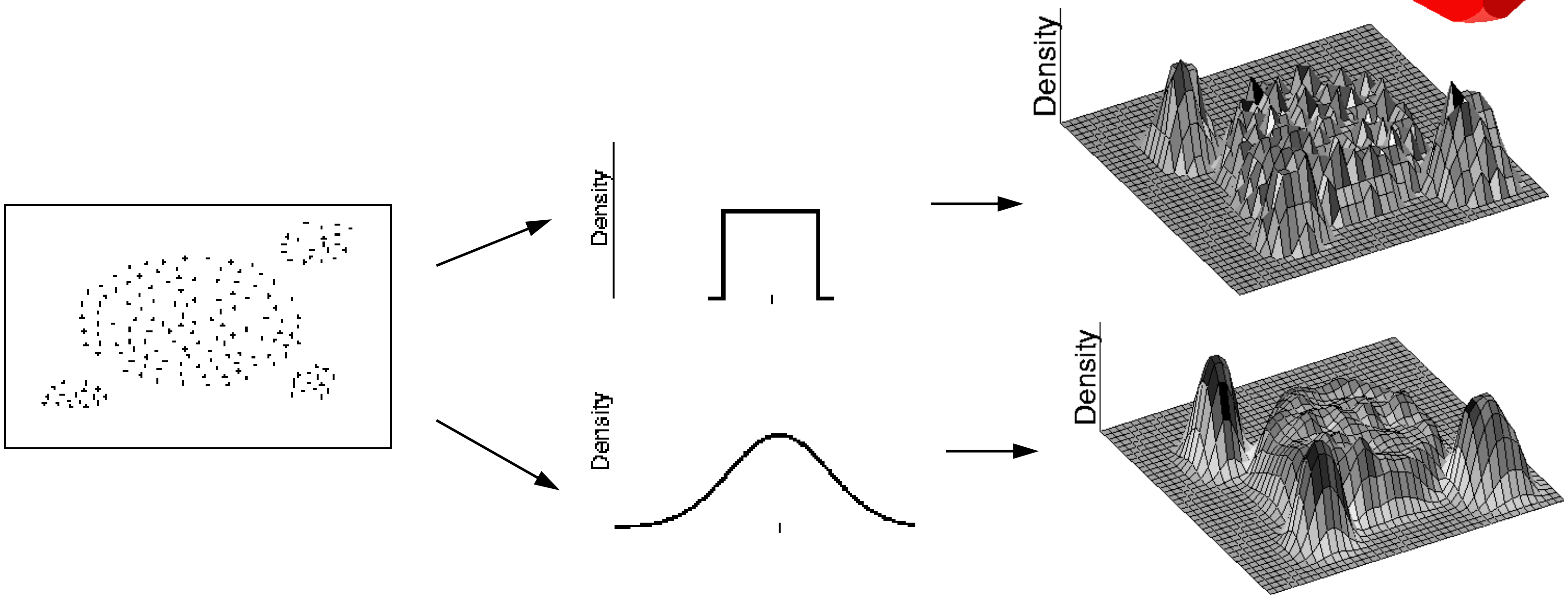
- Signal transformation using wavelets



- Arbitrary shape clusters found by WaveCluster at different resolutions



DENCLUE [HK 98]



Data Set ***Influence Function*** ***Density Function***

Influence Function: Influence of a data point in its neighborhood

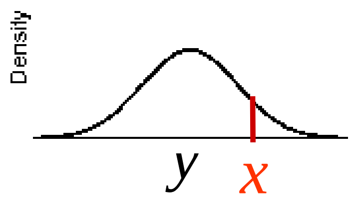
Density Function: Sum of the influences of all data points

DENCLUE

Influence Function

The influence of a data point *y* at a point *x* in the data space is modeled by a function $f_B^y : F^d \to \Re$,

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

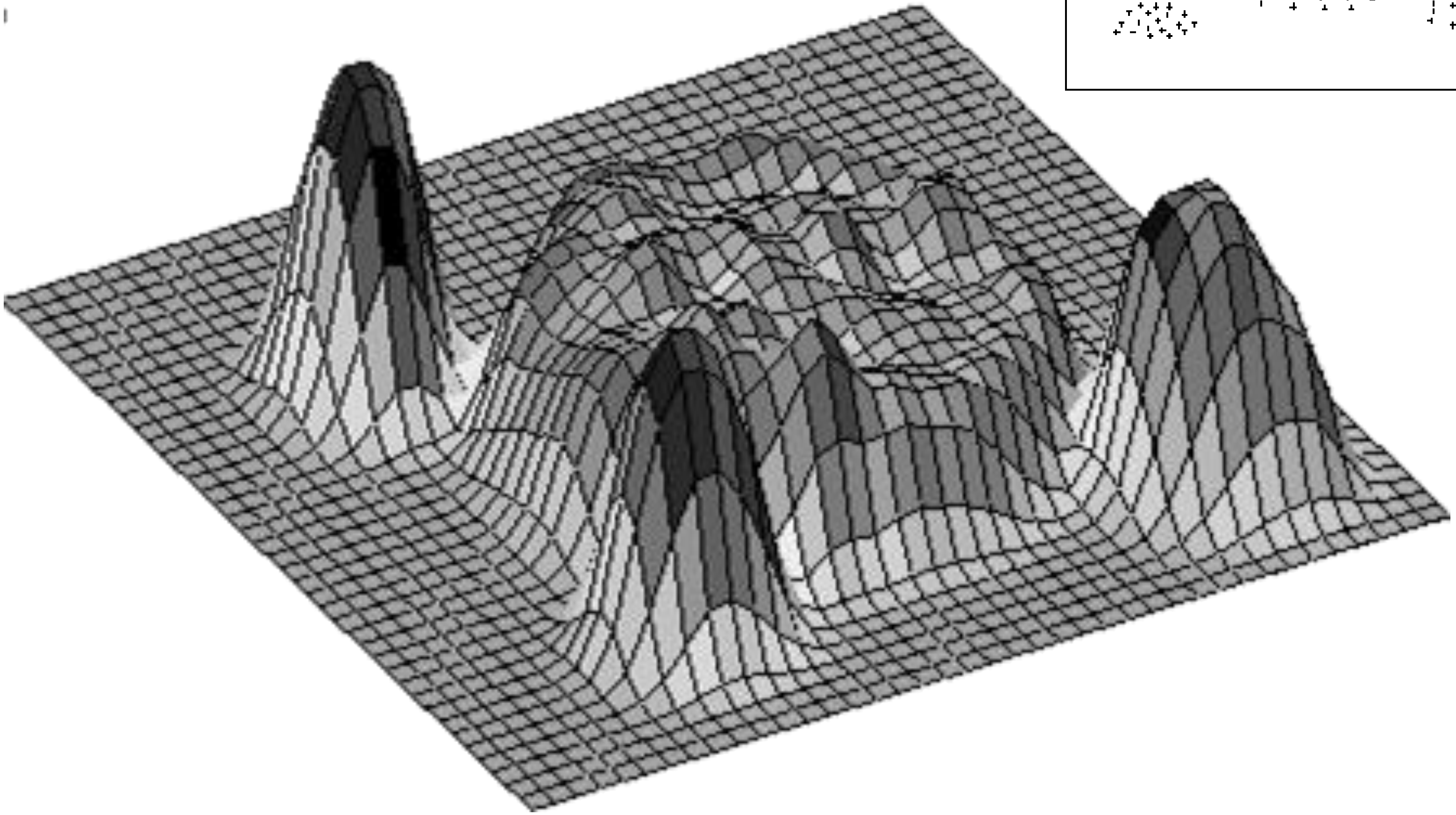


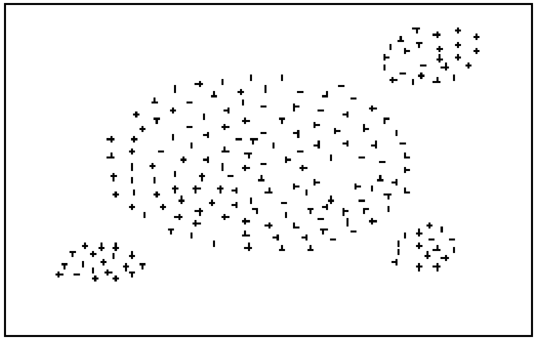
Density Function

The density at a point *x* in the data space is defined as the sum of influences of all data points x_i, i.e.

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

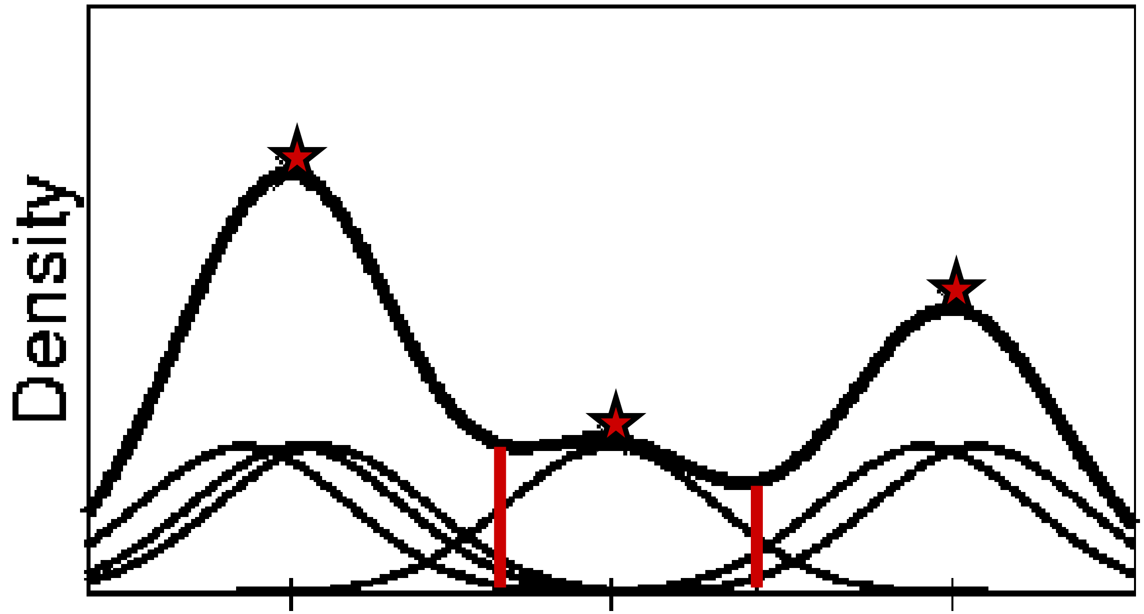
DENCLUE





DENCLUE

Definitions of Clusters



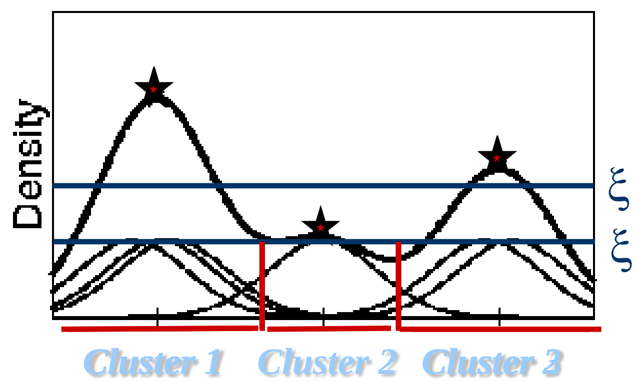
Density Attractor/Density-Attracted Points (★)

- local maximum of the density function
- density-attracted points are determined by a gradient-based hill-climbing method

DENCLUE

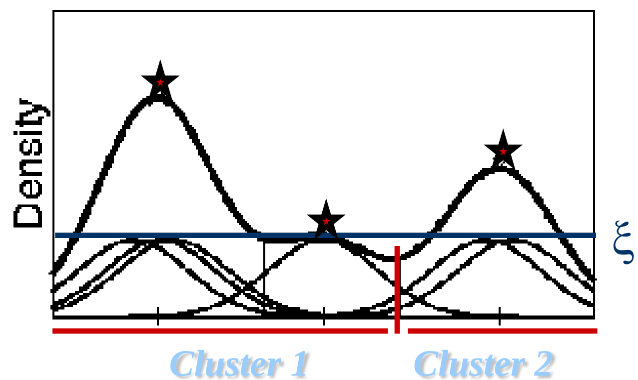
Center-Defined Cluster

A center-defined cluster with density-attractor x* ($f_B^D(x^*) > \xi$) is the subset of the database which is density-attracted by x*.



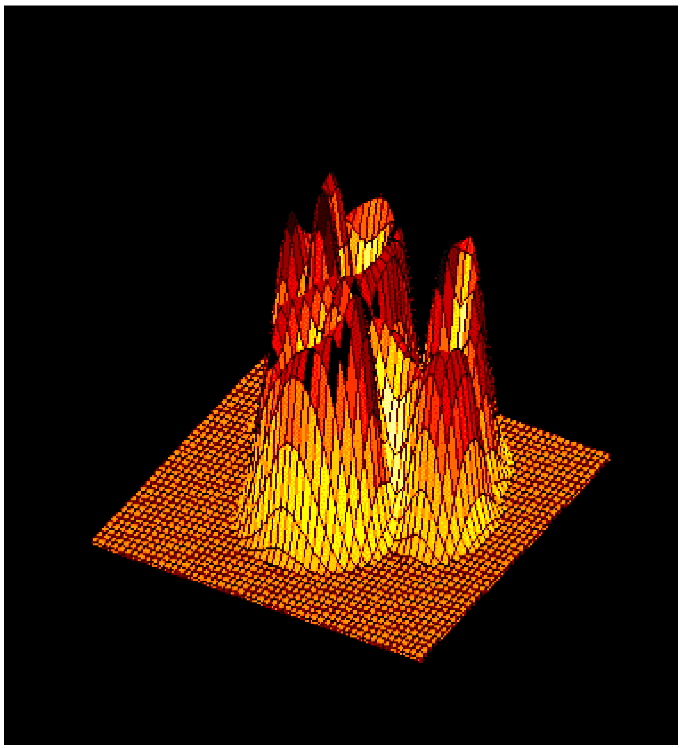
Multi-Center-Defined Cluster

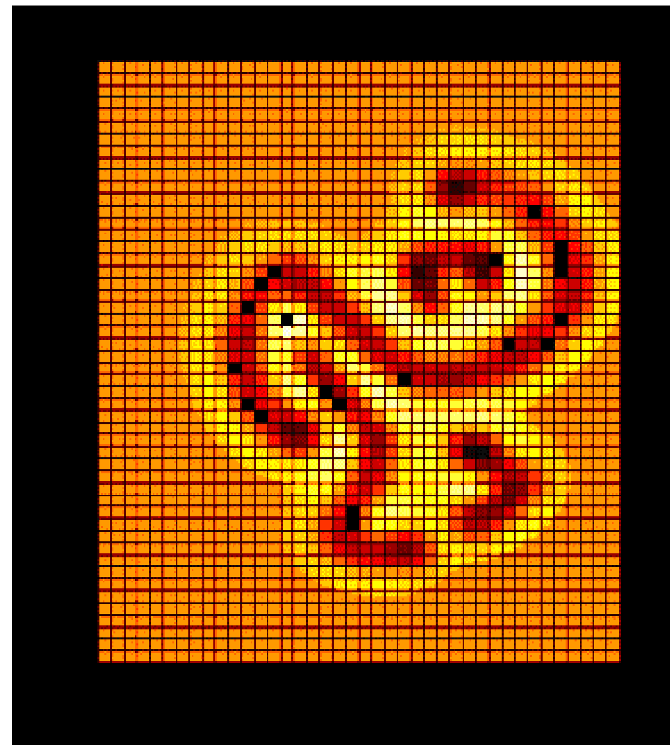
A multi-center-defined cluster consists of a set of center-defined clusters which are linked by a path with significance ξ.



DENCLUE

Impact of different Significance Levels (ξ)

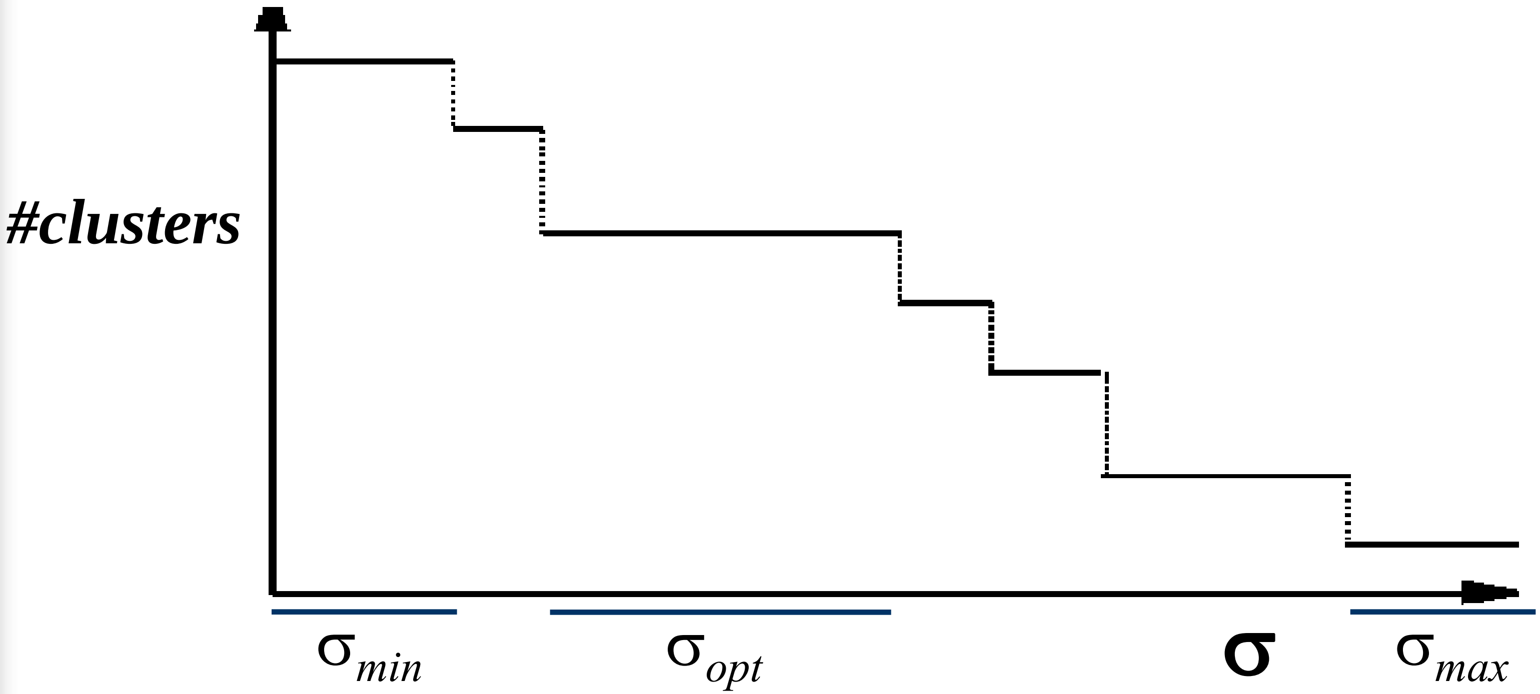




DENCLUE

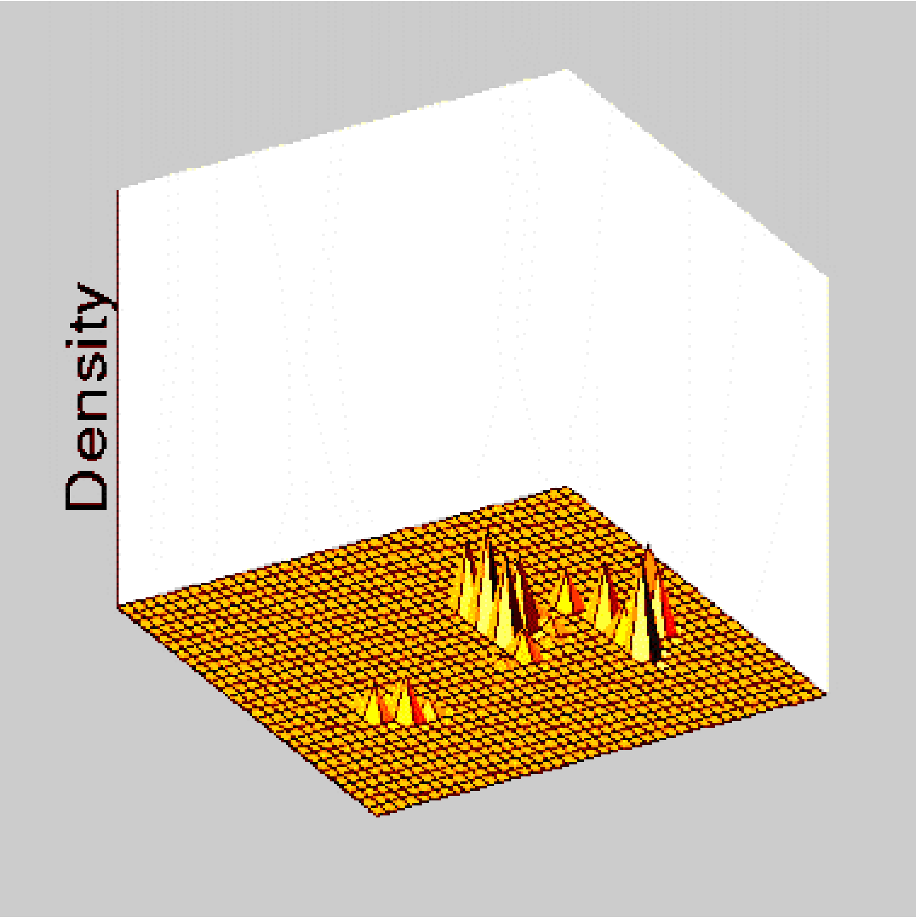
Choice of the Smoothness Level (σ)

Choose σ such that *number of density attractors* is constant for a long interval of σ!



DENCLUE

Variation of the Smoothness Level (σ)



DENCLUE

DENCLUE generalizes other clustering methods:

- ***density-based clustering***
  (e.g., *DBSCAN:* Square Wave influence function, multi-center-defined clusters, σ = EPS, ξ =MinPts)
- ***partition-based clustering***
  (e.g., *k-means Clustering:* Gaussian influence function, center-defined clusters, $\xi = 0$,
  determine σ such that *k* clusters)
- ***hierarchical clustering***
  (center-defined clusters for different values of σ form hierarchy)

DENCLUE

Noise Invariance

Assumption: Noise is uniformly distributed in the data space

Lemma:

The density-attractors do not change when increasing the noise level.

Idea of the Proof:

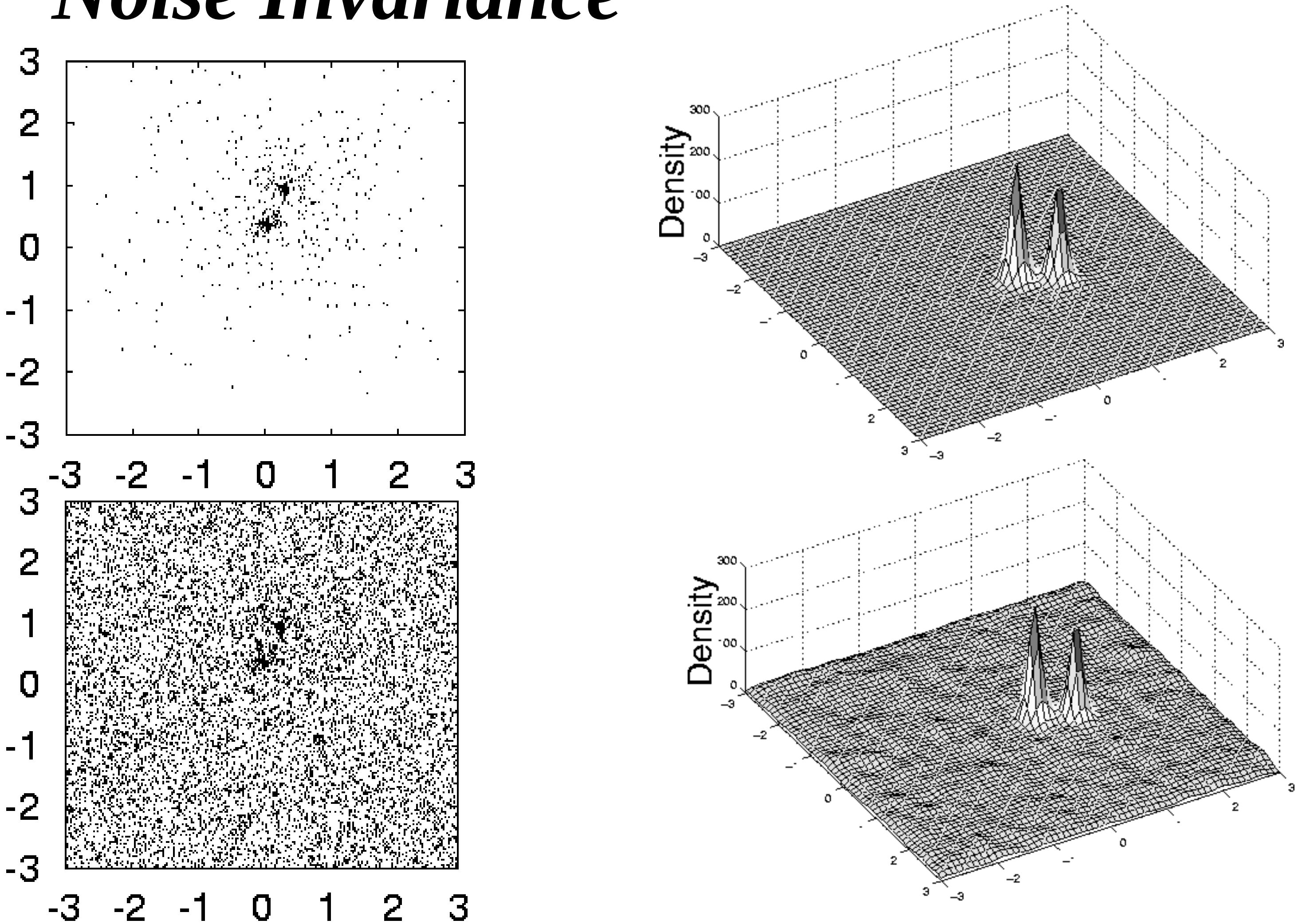
- partition density function into signal and noise

$$f^D(x) = f^{D_C}(x) + f^N(x)$$

- density function of noise approximates a constant $(f^N(x) \approx const.)$

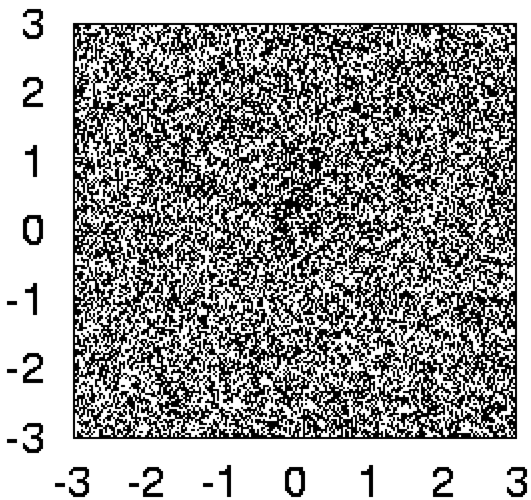
DENCLUE

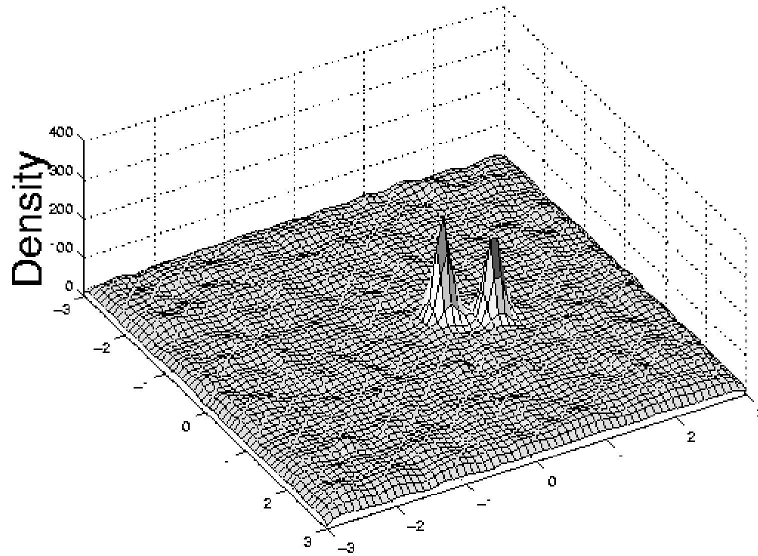
Noise Invariance

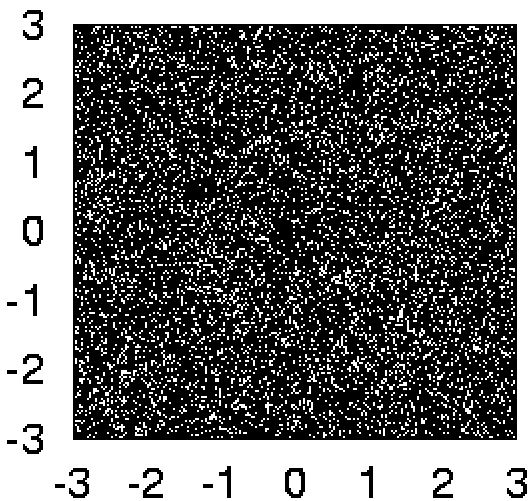


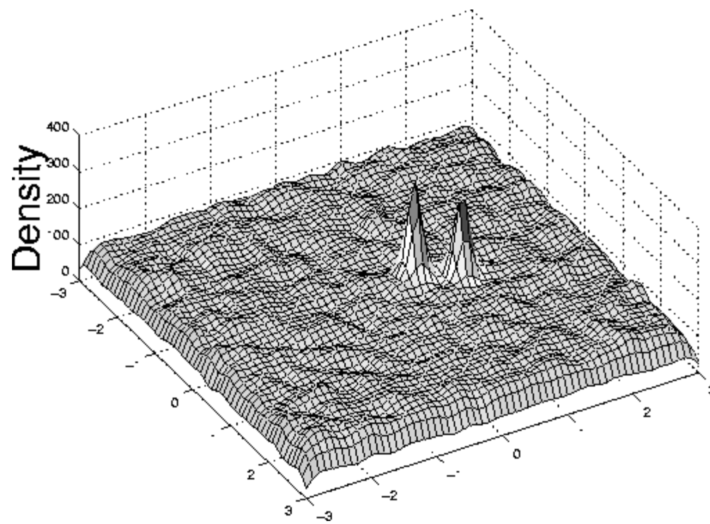
DENCLUE

Noise Invariance







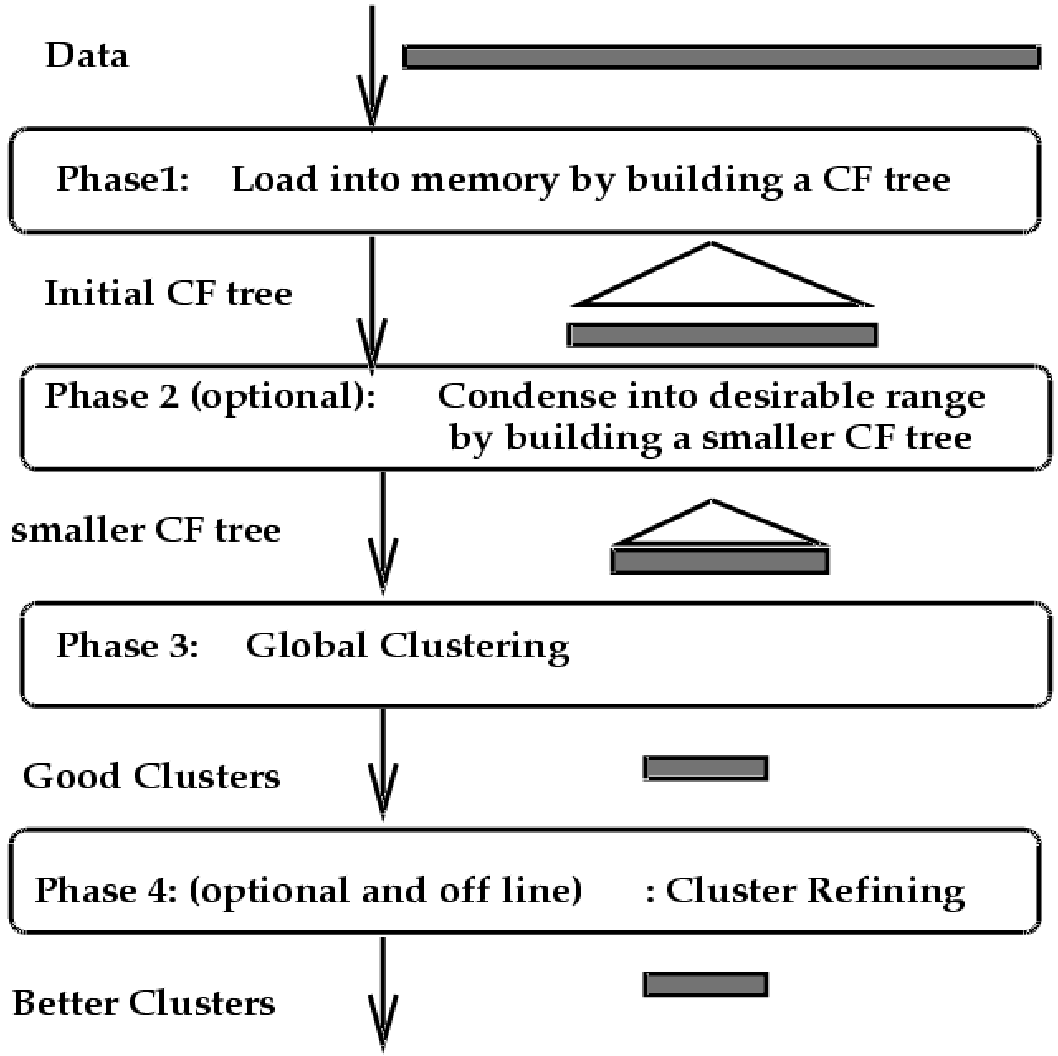


Hybrid Methods

- BIRCH [ZRL 96]
- CLIQUE [AGG+ 98]

BIRCH [ZRL 96]

Clustering in BIRCH



BIRCH

Basic Idea of the CF-Tree

- Condensation of the data $\{\vec{X}_i\}$ using CF-Vect $\mathbf{CF} = (N, \vec{LS}, SS)$

$$\vec{LS} = \sum_{i=1}^{N} \vec{X}_i \, , \; SS = \sum_{i=1}^{N} \vec{X}_i^{\,2}$$

- CF-tree uses sum of CF-vectors to build higher levels of the CF-tree

BIRCH

Insertion algorithm for a point x:

(1) Find the closest leaf b

(2) If x fits in b, insert x in b;

otherwise split b

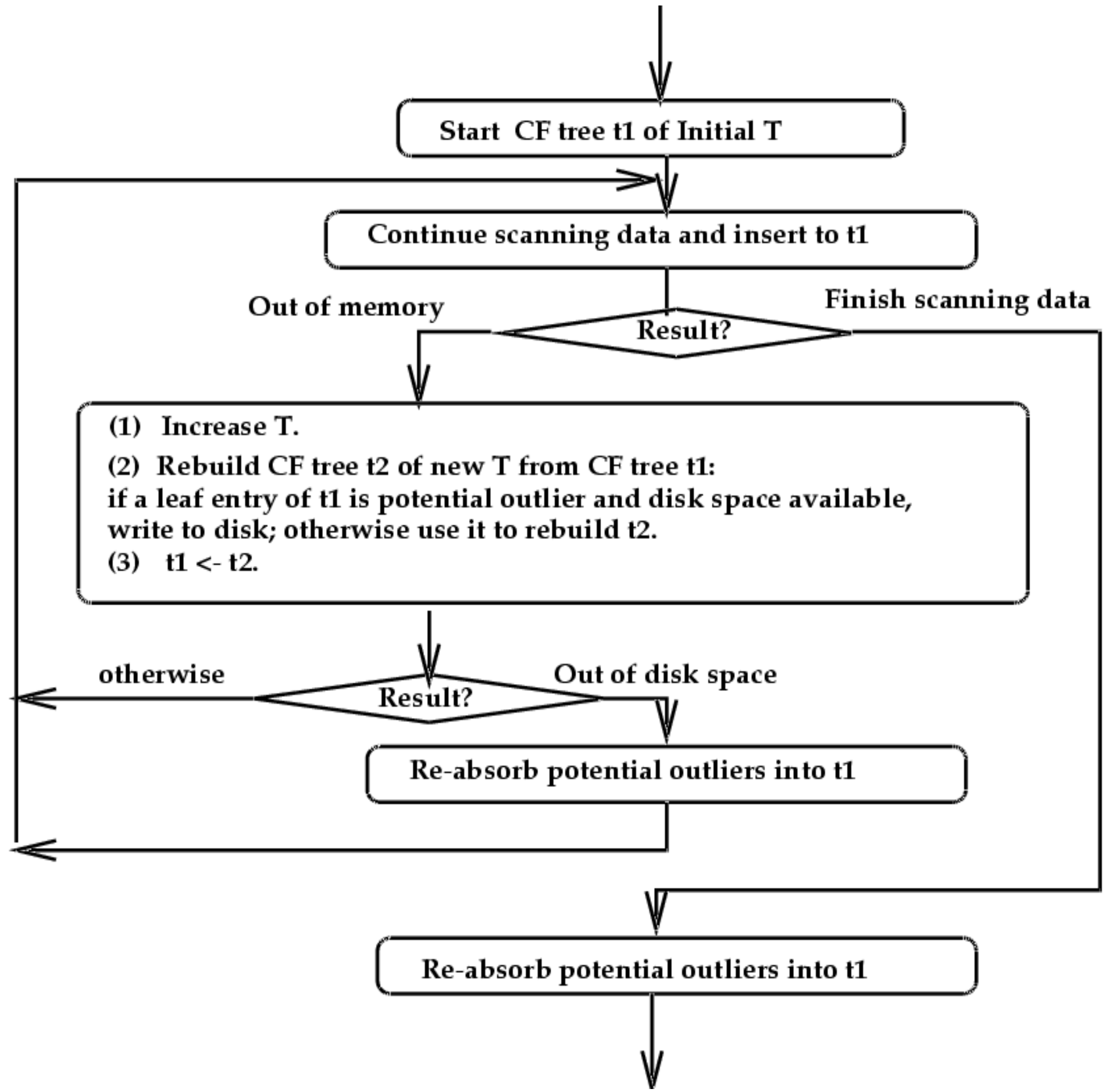
(3) Modify the path for b

(4) If tree is to large, condense the tree

by merging the closest leaves

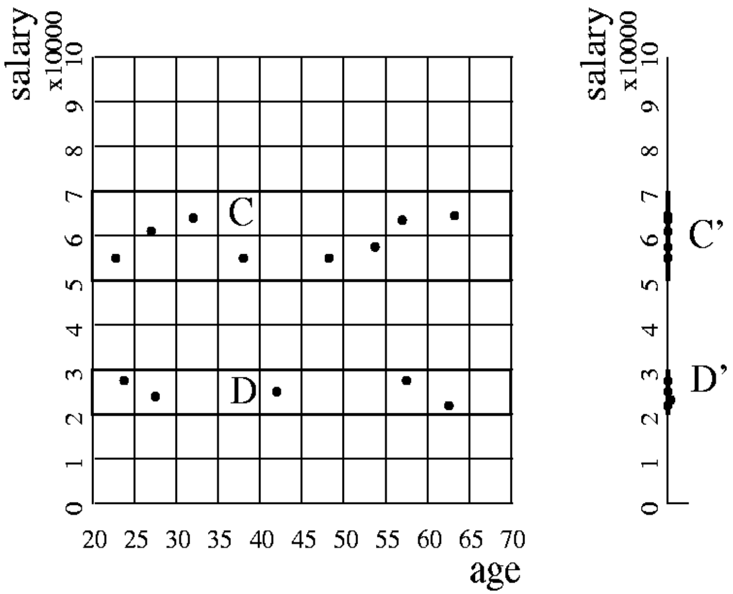
BIRCH

CF-Tree Construction



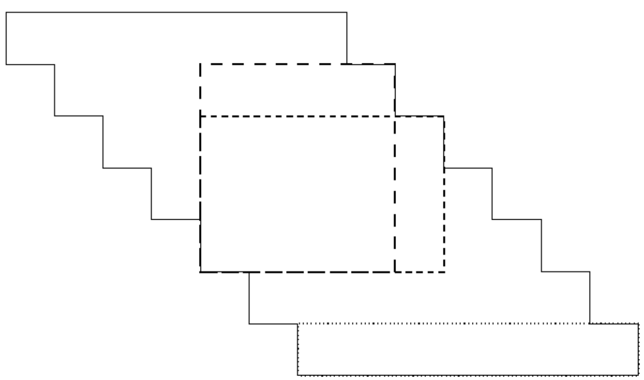
CLIQUE [AGG+ 98]

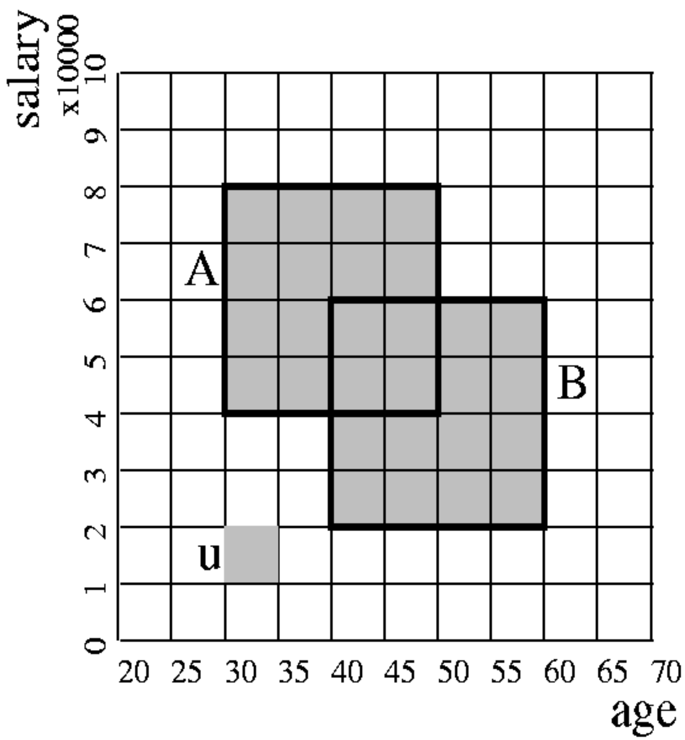
- Subspace Clustering
- Monotonicity Lemma:
  If a collection of points *S* is a cluster in a *k*-dimensional space, then S is also part of a cluster in any (k-1)-dimensional projection of this space.
- Bottom-up Algorithm for determining the projections



CLIQUE

- Cluster description in disjunctive normal Form





Techniques for Improving the Efficiency and Effectiveness

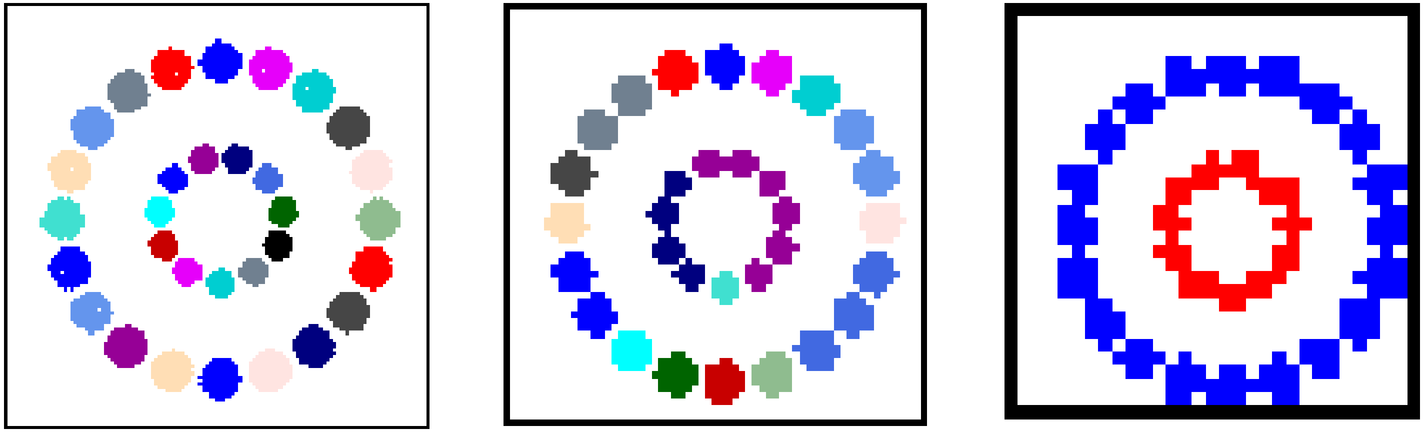
- Hierarchical Variants of Cluster Algorithms
  (for Improving the Effectiveness)
- Scaling Up of Cluster Algorithms
  (for Improving the Efficiency)
  – Sampling Techniques
  – Bounded Optimization Techniques
  – Indexing Techniques
  – Condensation Techniques
  – Grid-based Techniques

Scalability Problems

- Effectiveness degenerates
  - with dimensionality (d)
  - with noise level
- Efficiency degenerates
  - linearly with no of data points (N) and
  - exponentially with dimensionality (d)

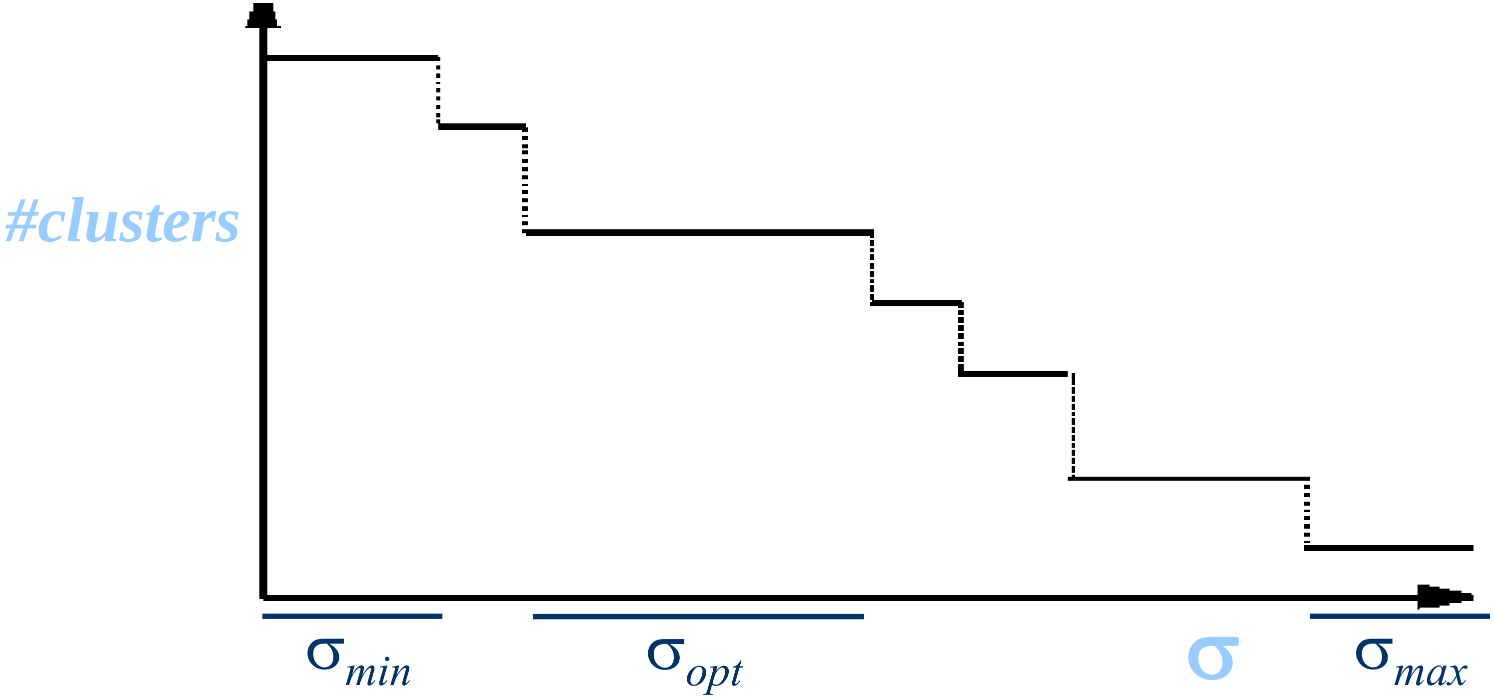
Hierarchical Variant of WaveCluster [SCZ 98]

- WaveCluster can be used to perform multiresolution clustering
- Using coarser grids, cluster start to merge

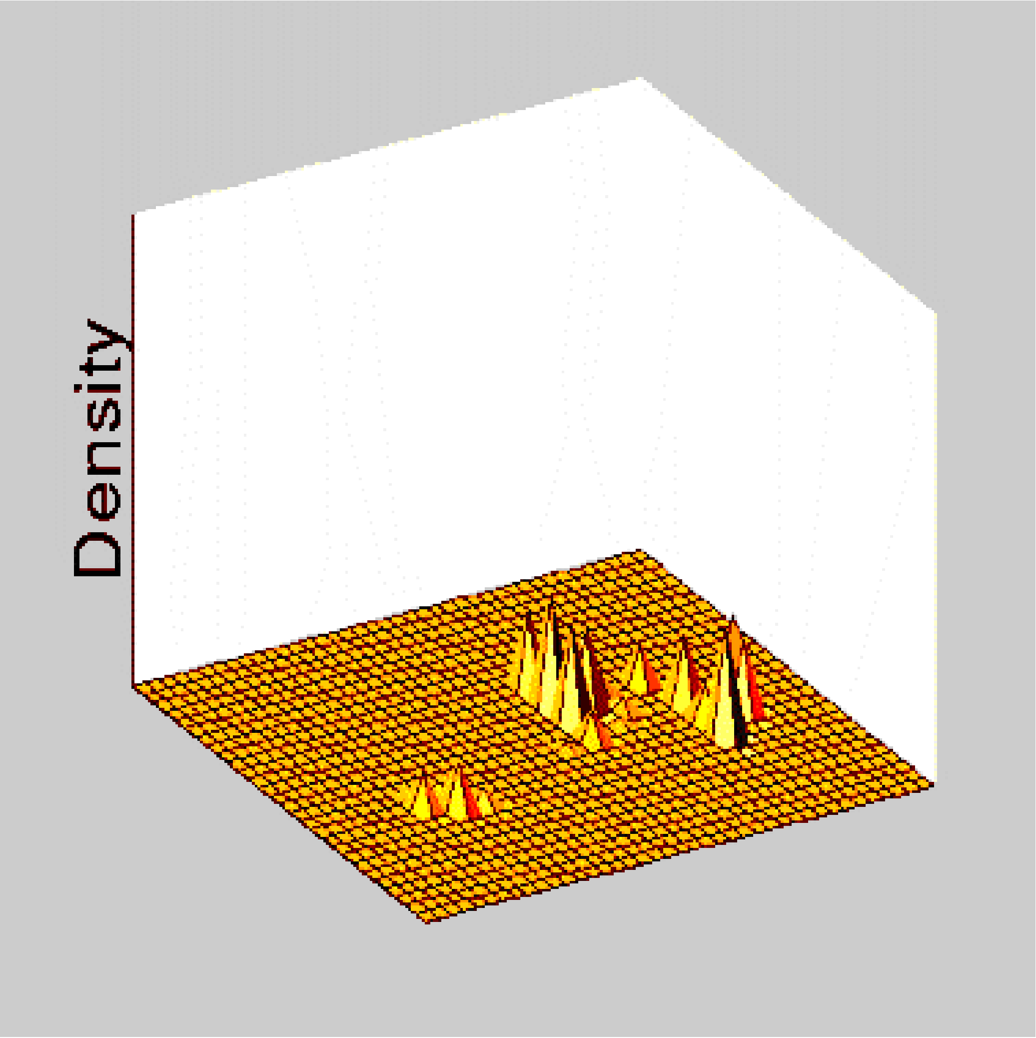


Hierarchical Variant of DENCLUE [HK 98]

- DENCLUE is able to determine a hierarchy of cluster using smoother kernels ($\sigma_{\min} \leq \sigma \leq \sigma_{\max}$)



Building Hierarchies (σ)

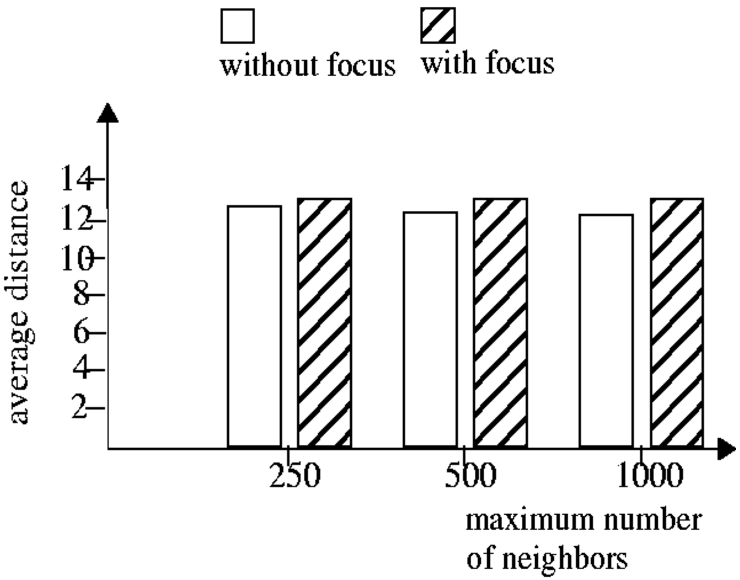


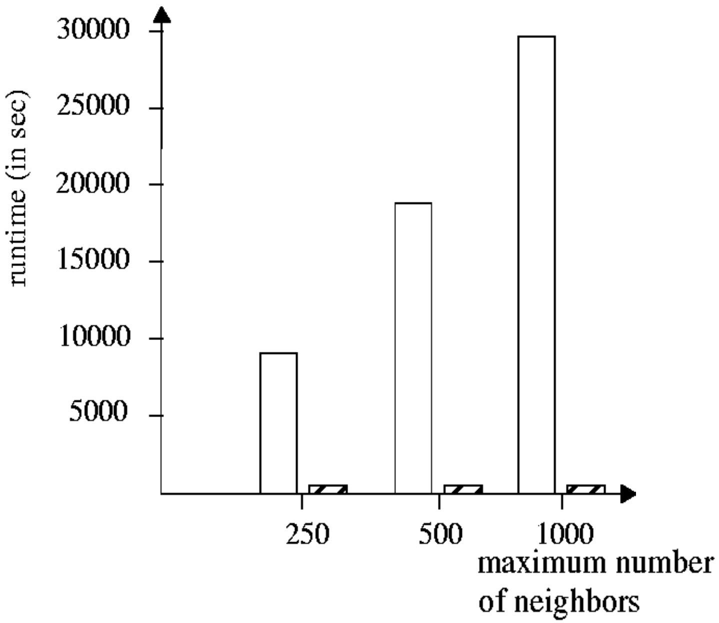
Scaling Up of Cluster Algorithms

- Sampling Techniques [EKX 95]
- Bounded Optimization Techniques [NH 94]
- Indexing Techniques [BK 98]
- Condensation Techniques [ZRL 96]
- Grid-based Techniques [SCZ 98, HK 98]

Sampling [EKX 95]

- R*-Tree Sampling
- Comparison of Effectiveness versus Efficiency (example CLARANS)





Bounded Optimization [NH 94]

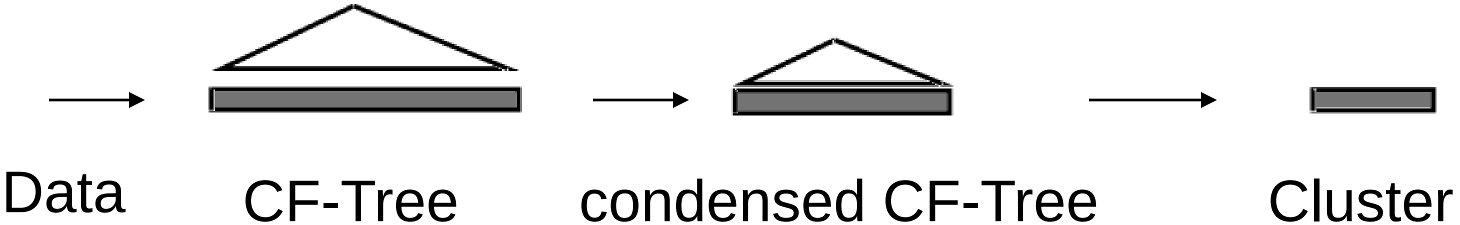
- CLARANS uses two bounds to restricts the optimization: *num_local, max_neighbor*
- Impact of the Parameter:
  - *num_local* $\longrightarrow$ Number of iterations
  - *max_neighbors* $\longrightarrow$ Number of tested neighbors per iteration

Indexing [BK 98]

- Cluster algorithms and their index structures
  - BIRCH: CF-Tree [ZRL 96]
  - DBSCAN: R*-Tree [Gut 84]
    X-Tree [BKK 96] (range queries)
  - WaveCluster: Grid / Array [SCZ 98]
  - DENCLUE: B^+-Tree, Grid / Array [HK 98]

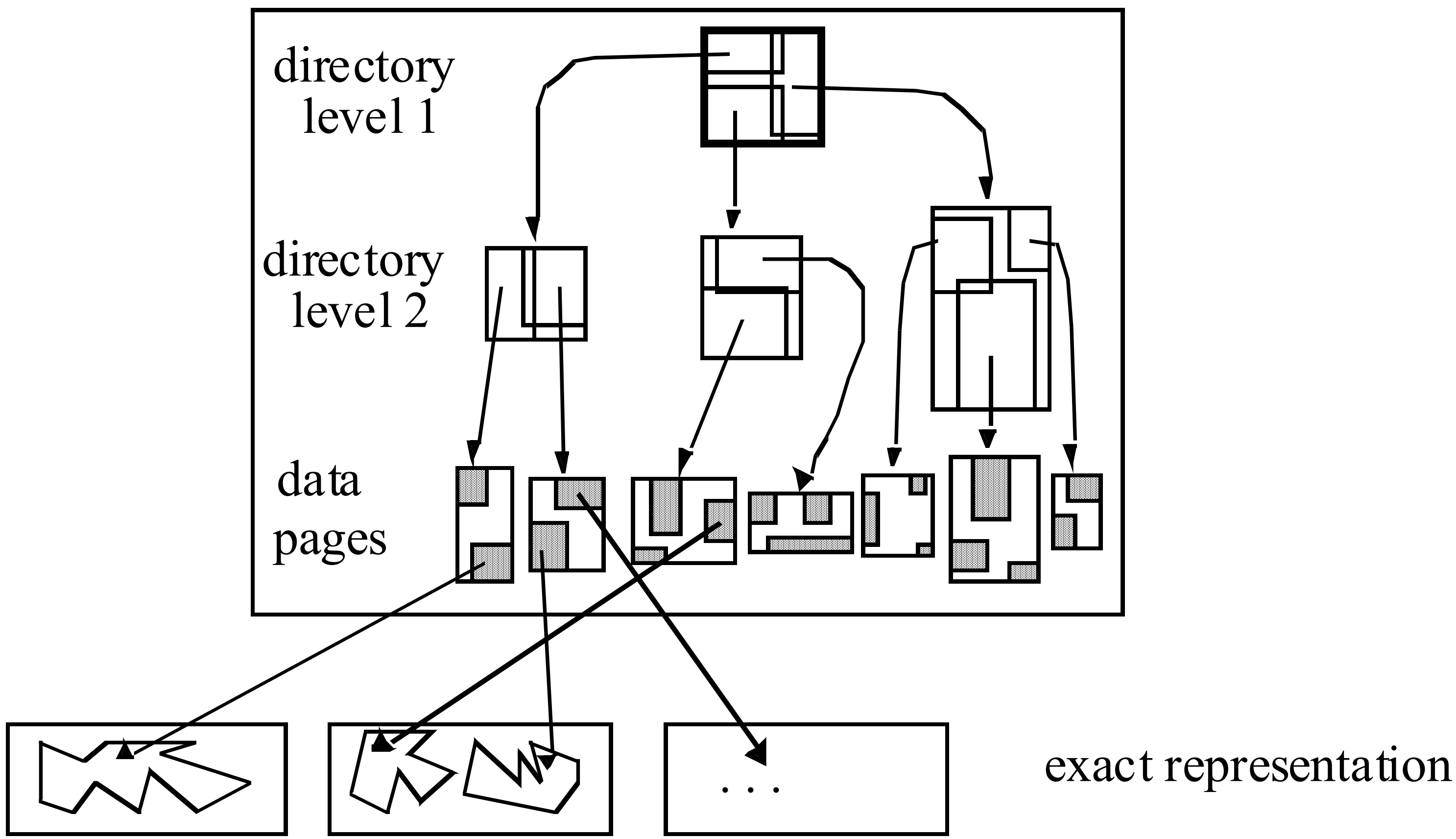
Condensing Data

- BIRCH [ZRL 96]:
  - Phase 1-2 makes a condensed representation of the data (CF-tree)
  - Phase 3-4 applies a separate cluster algorithm to the leafs of the CF-tree
- Condensing data is crucial for efficiency



R-Tree: [Gut 84]

The Concept of Overlapping Regions



Variants of the R-Tree

Low-dimensional

- R^+-Tree [SRF 87]
- R^*-Tree [BKSS 90]
- Hilbert R-Tree [KF94]

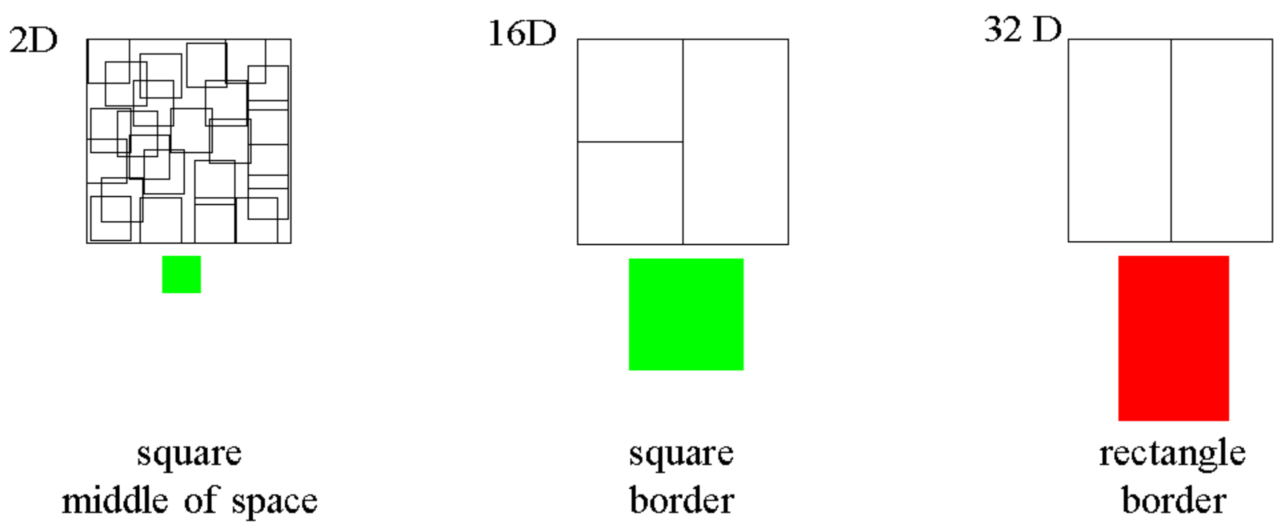
High-dimensional

- TV-Tree [LJF 94]
- X-Tree [BKK 96]
- SS-Tree [WJ 96]
- SR-Tree [KS 97]

Effects of High Dimensionality

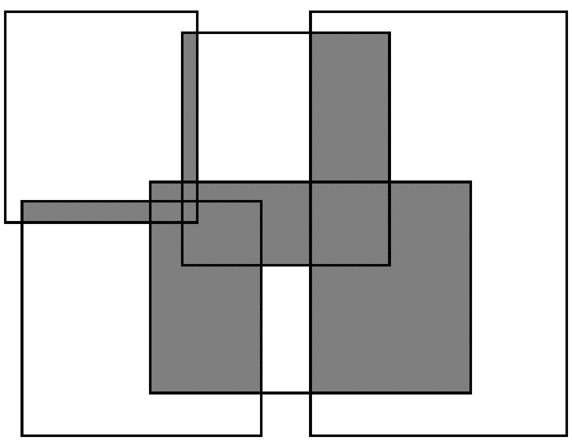
Location and Shape of Data Pages

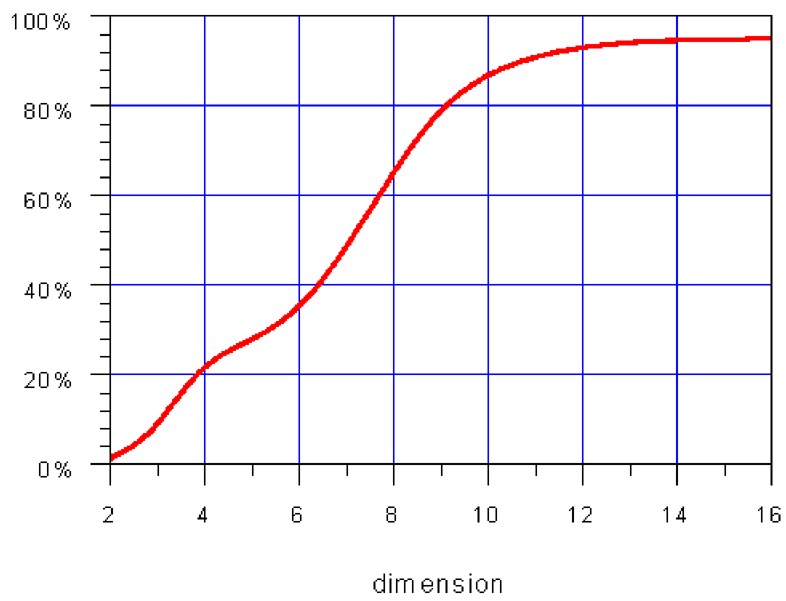
- Data pages have large extensions
- Most data pages touch the surface of the data space on most sides



The X-Tree [BKK 96]
(eXtended-Node Tree)

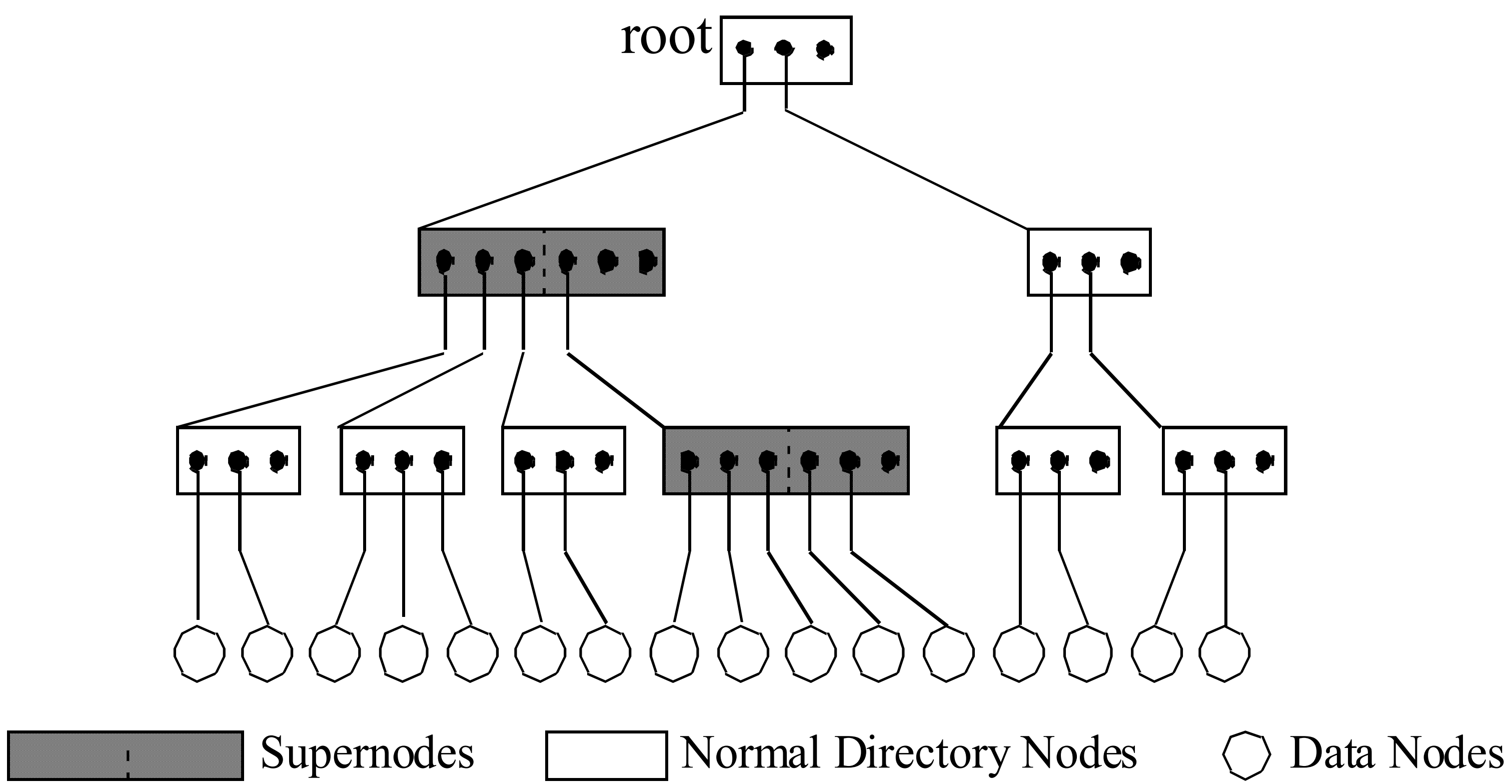
- Motivation:
  Performance of the R-Tree degenerates in high dimensions
- Reason: overlap in the directory



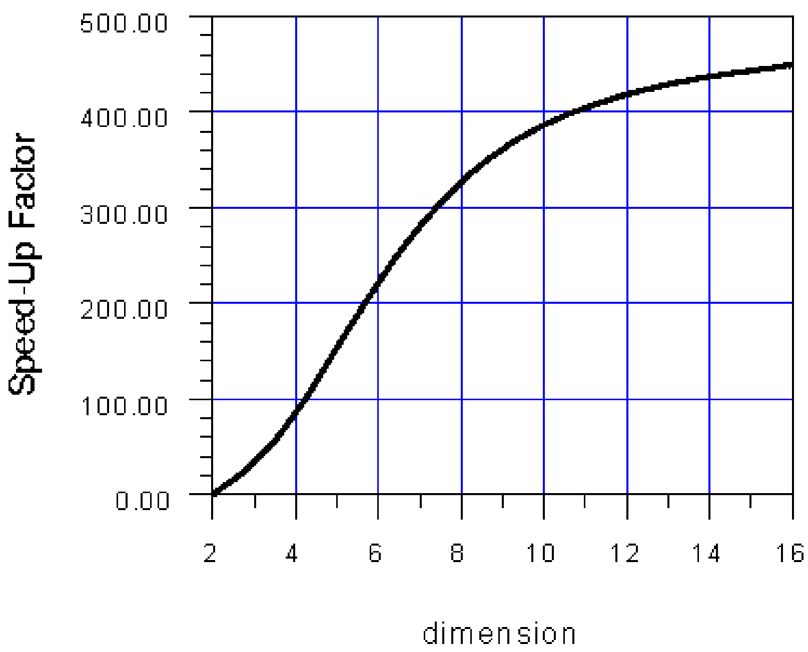


The X-Tree

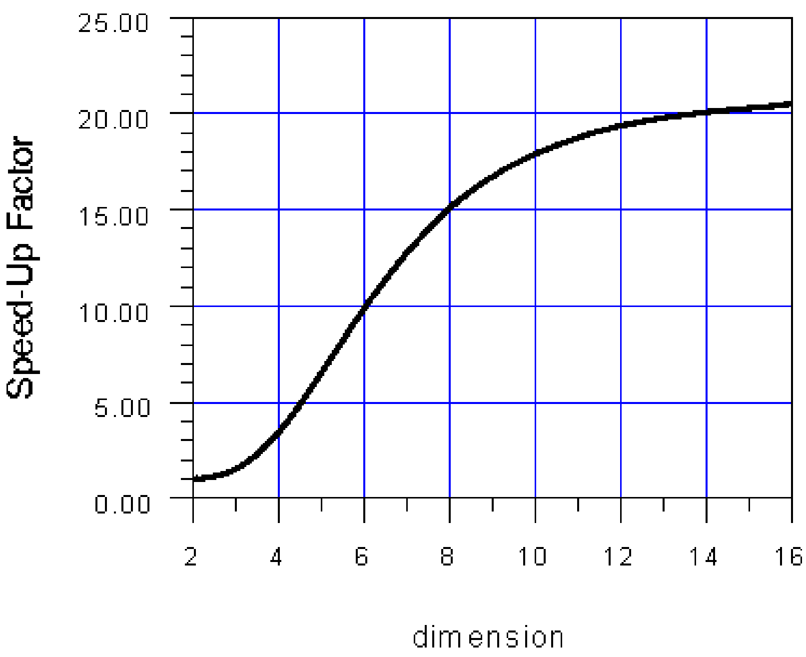
- X-tree avoids overlap in the directory by using
  - an overlap-free split
  - the concept of supernodes



Speed-Up of X-Tree over the R*-Tree



Point Query



10 NN Query

Grid Approaches WaveCluster

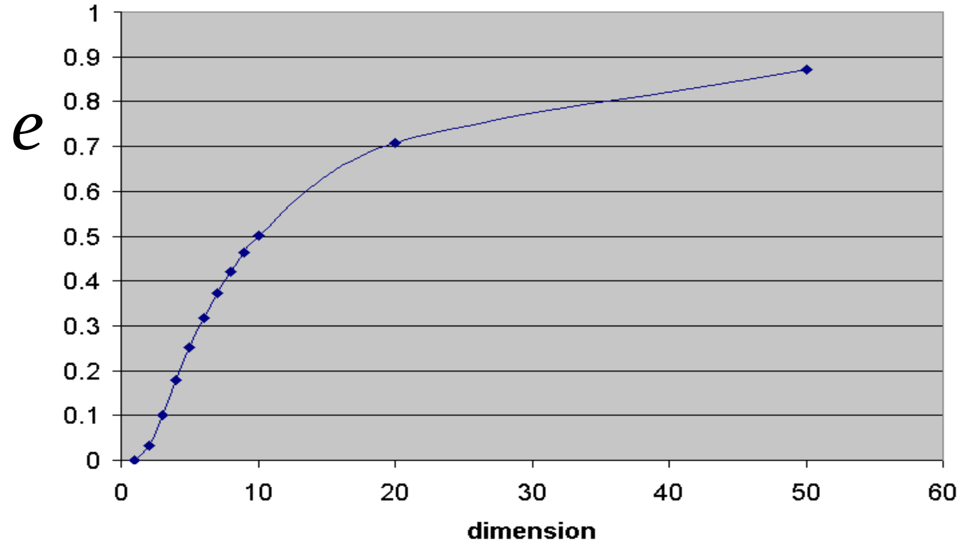
- WaveCluster [SCZ 98]
  - Partition the data space by a grid → reduce the number of data objects by making a small error
  - Apply the wavelet-transformation to the reduced feature space
  - Find the connected components as clusters
- Compression of the grid is crucial for the efficiency
- Does not work in high dimensional space!

Effects of High Dimensionality

Selectivity of Range Queries

- The selectivity depends on the volume of the query

$$e = \sqrt[d]{Vol_{cube}}$$



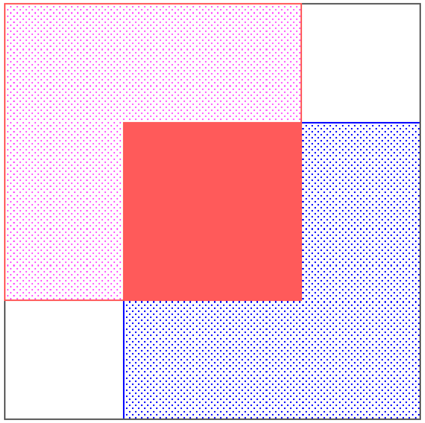
selectivity = 0.1 %

$\Rightarrow$ **no fixed ε-environment (as in DBSCAN)**

Effects of High Dimensionality

Selectivity of Range Queries

- In high-dimensional data spaces, there exists a region in the data space which is affected by ANY range query (assuming uniformly distributed data)



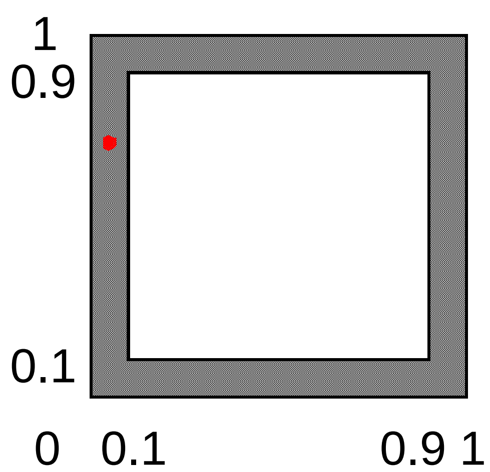
⇒ **difficult to build an efficient index structure**

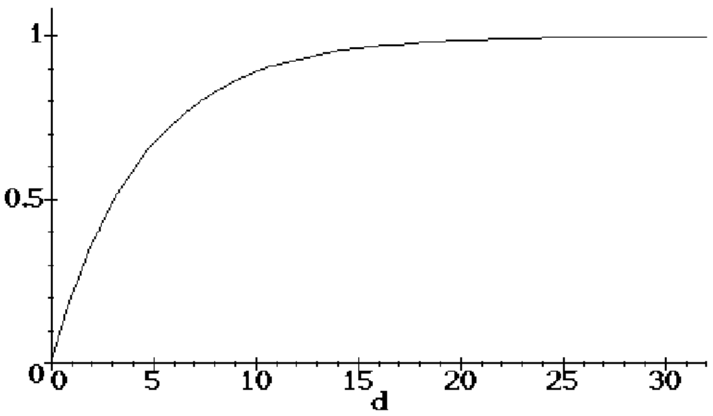
⇒ **no efficient support of range queries (as in DBCLASD)**

Effects of High Dimensionality

The Surface is Everything

- Probability that a point is closer than 0.1 to a (*d*-1)-dimensional surface





$\Rightarrow$ **no of directions (from center) increases exponentially**

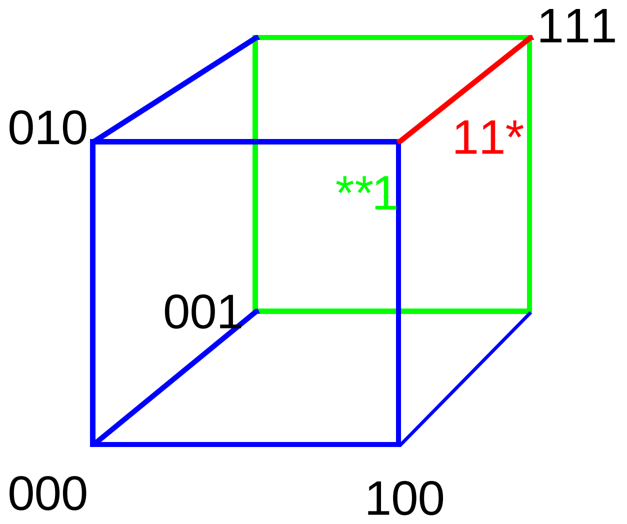
Effects of High Dimensionality

Number of Surfaces and Grid Cells

- Number of *k*-dimensional surfaces in a *d*-dimensional hypercube?

$$\binom{d}{k} \cdot 2^{(d-k)}$$

***



- Number of grid cells resulting from a binary partitioning?

$$2^d$$

$\Rightarrow$ **grid cells can not be stored explicitly**

$\Rightarrow$ **most grid cells do not contain any data points**

DENCLUE Algorithm [HK 98]

Basic Idea

- Use ***Local Density Function*** which approximates the Global Density Function
- Use ***CubeMap Data Structure*** for efficiently locating the relevant points

DENCLUE

Local Density Function

__Definition__

The local density $\hat{f}_B^D(x)$ is defined as

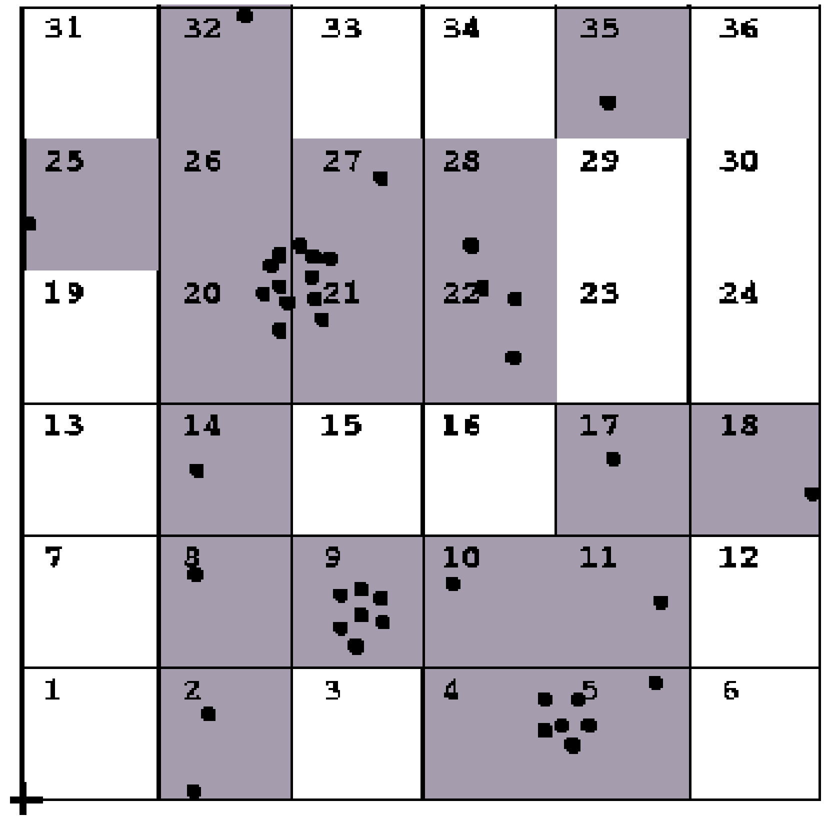
$$\hat{f}_B^D(x) = \sum_{x_i \in near(x)} f_B^{x_i}(x) \, .$$

__Lemma (Error Bound)__

If $near(x) = \{x_i \in D \mid d(x, x_i) \leq k\sigma\}$, the error is bound by:

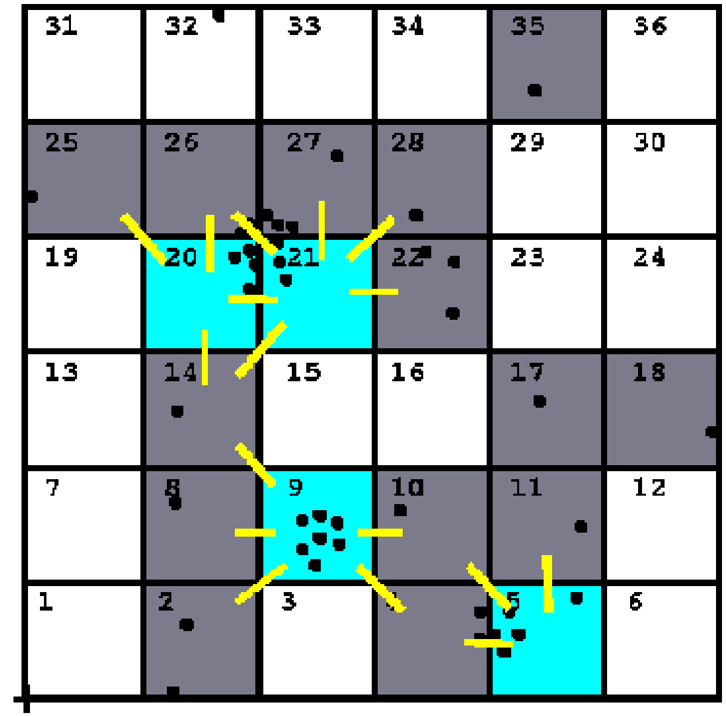
$$Error = \sum_{x_i \in D,\, d(x_i, x) > k\sigma} e^{-\frac{d(x, x_i)^2}{2\sigma^2}} \leq \| \{x_i \in D \mid d(x, x_i) > k\sigma\} \| \cdot e^{-\frac{k^2}{2}}$$

CubeMap



Data Structure based on regular cubes for storing the data and efficiently determining the density function

DENCLUE Algorithm



DENCLUE (D, σ, ξ)

(a) $MBR \leftarrow DetermineMBR(D)$

(b) $C_p \leftarrow DetPopCubes(D, MBR, \sigma)$

$C_{sp} \leftarrow DetHighlyPopCubes(C_p, \xi_c)$

(c) $map, C_r \leftarrow ConnectMap(C_p, C_{sp}, \sigma)$

(d) $clusters \leftarrow DetDensAttractors(map, C_r, \sigma, \xi)$

Summary and Conclusions

- A number of *effective* and *efficient* Clustering Algorithms is available for *small to medium size* data sets and *small dimensionality*
- **Efficiency** suffers severely for large dimensionality *(d)*
- **Effectiveness** suffers severely for large dimensionality (*d*), especially in combination with a high *noise level*

Open Research Issues

- *Efficient Data Structures* for large ***N*** and large ***d***
- *Clustering Algorithms* which work *effectively* for large ***N***, large ***d*** and large *Noise Levels*
- *Integrated Tools* for an Effective Clustering of High-Dimensional Data *(combination of automatic, visual and interactive clustering techniques)*

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