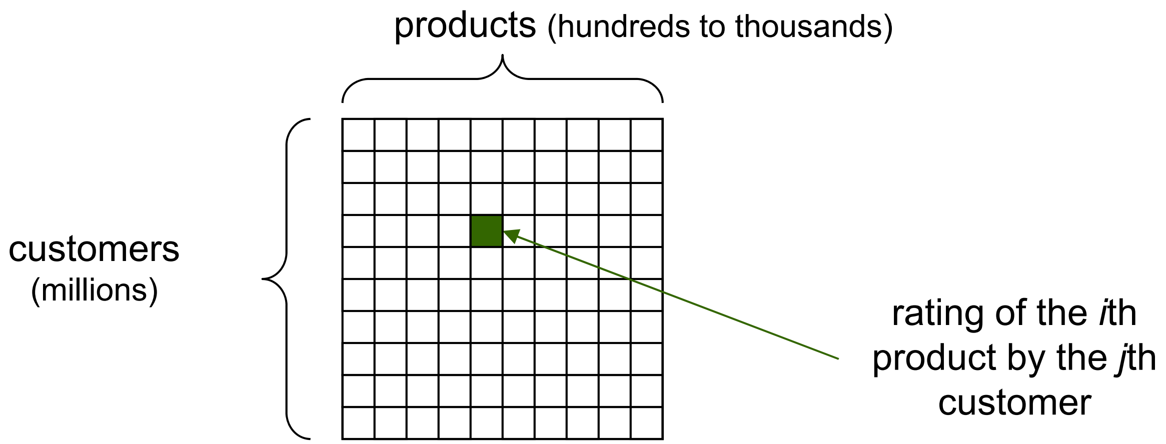
Outline

1. Introduction and challenges of high dimensionality
2. Feature Selection
3. Feature Reduction and Metric Learning
4. Clustering in High-Dimensional Data

Challenges for Clustering High-Dimensional Data

- Customer Recommendation / Target Marketing
  - Data
    - Customer ratings for given products
    - Data matrix:

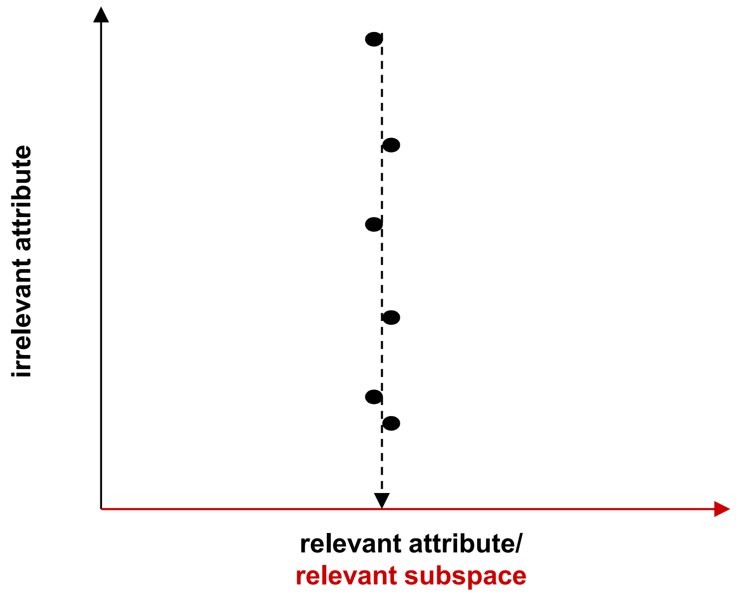


  - Task: Cluster customers to find groups of persons that share similar preferences or disfavor (e.g. to do personalized target marketing)
    - *Challenge*:

      customers may be grouped differently according to different preferences/disfavors, i.e. different subsets of products

Challenges for Clustering High-Dimensional Data

- *Relevant* and *irrelevant* attributes
  - Not all features, but a subset of the features may be relevant for clustering
  - Groups of similar ("dense") points may be identified when considering only these features

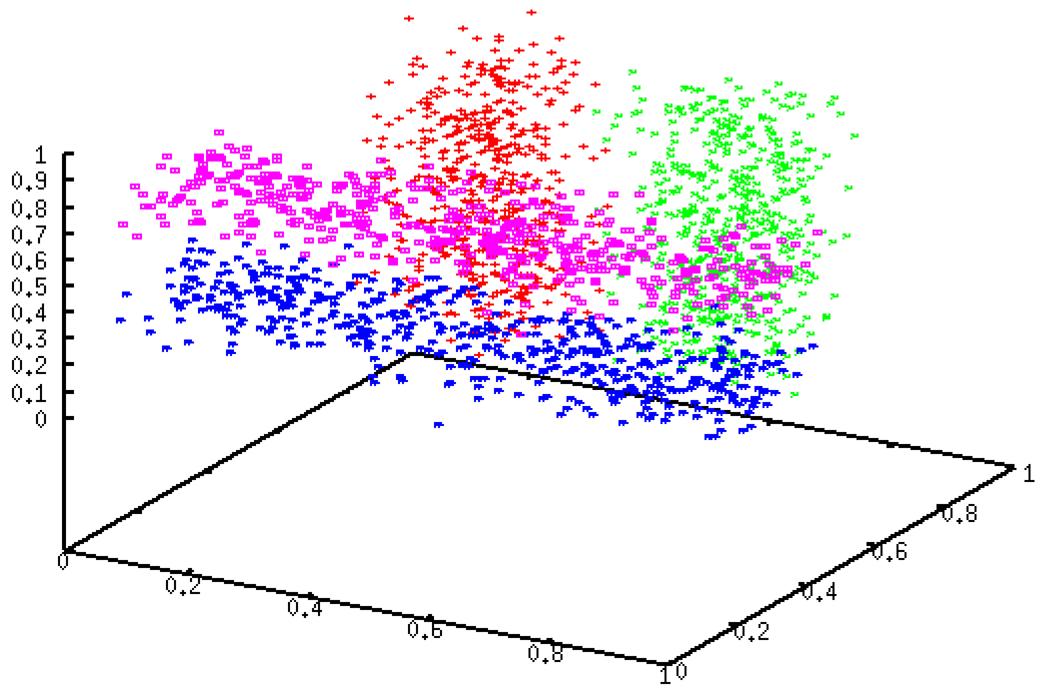


  - Different subsets of attributes may be relevant for different clusters

Challenges for Clustering High-Dimensional Data

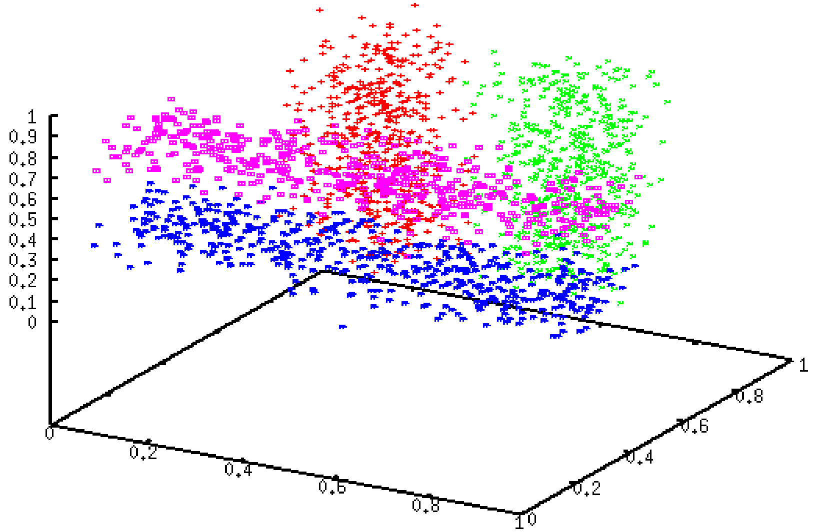
Effect on clustering:

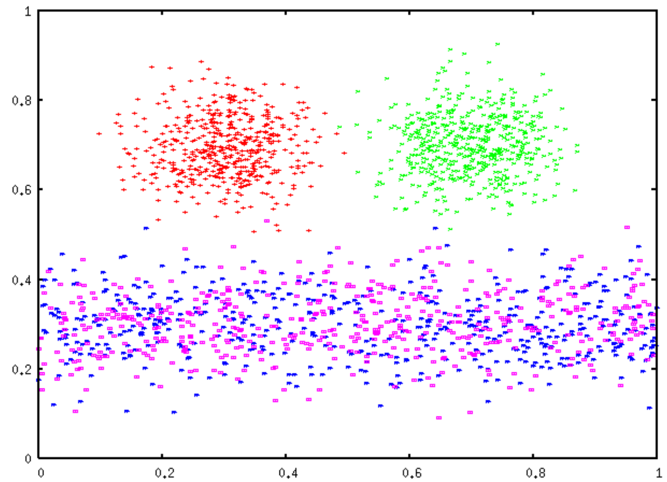
- Traditional distance functions give equal weight to all dimensions
- However, not all dimensions are of equal importance
- Adding irrelevant dimensions ruins any clustering based on a distance function that equally weights all dimensions

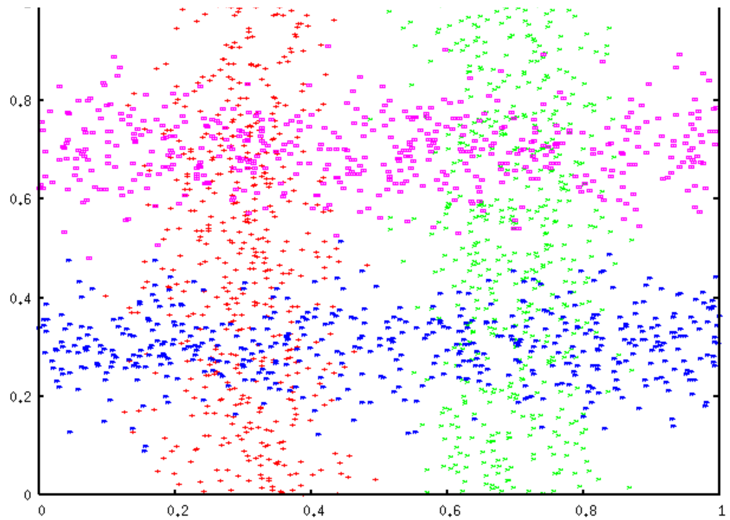


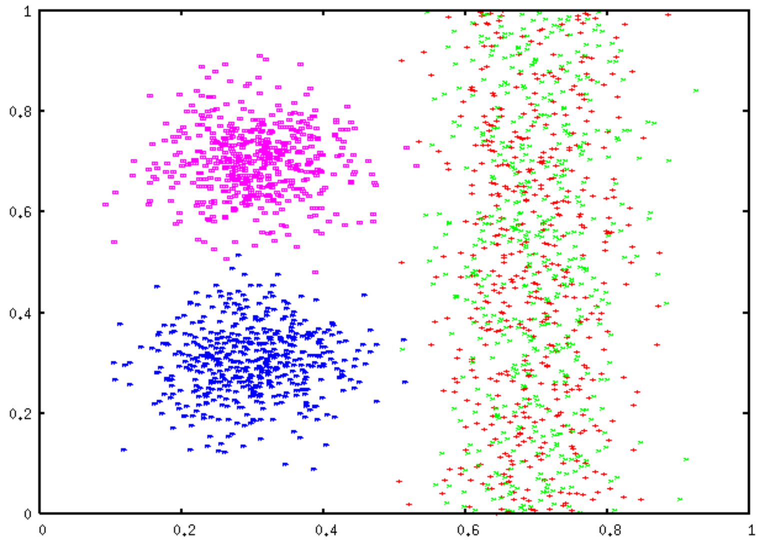
Challenges for Clustering High-Dimensional Data

again: different attributes are relevant for different clusters







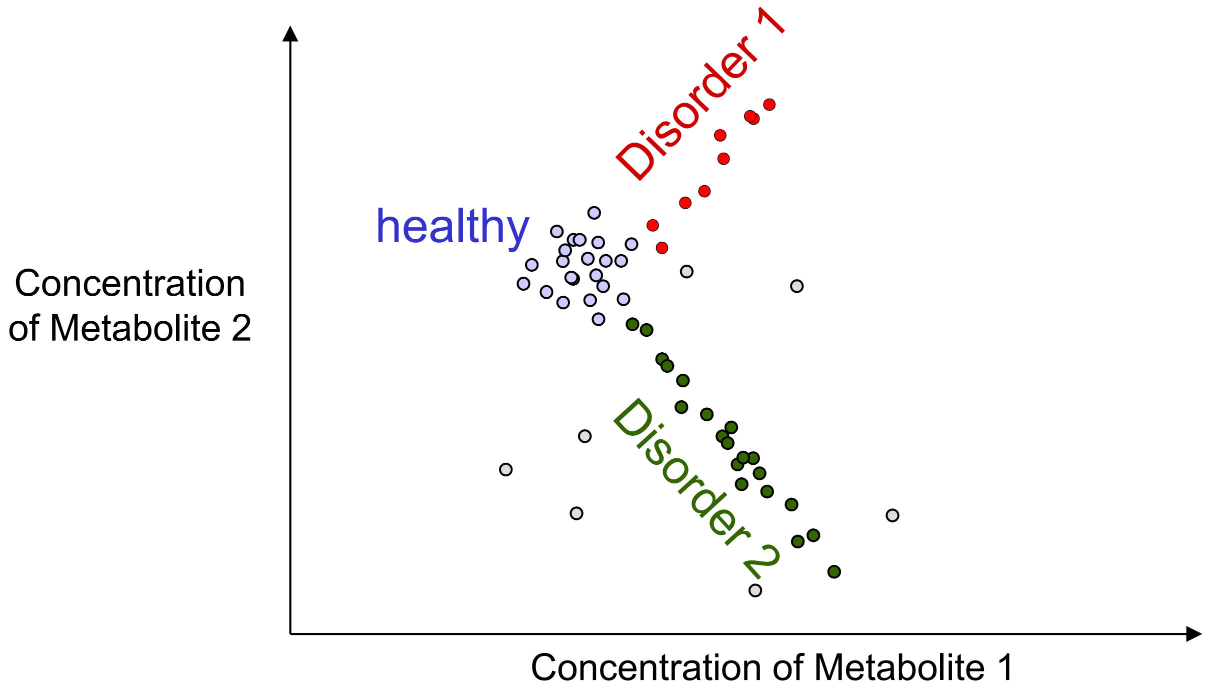


Challenges for Clustering High-Dimensional Data

Task: Cluster test persons to find groups of individuals with similar correlation among the concentrations of metabolites indicating homogeneous metabolic behavior (e.g. disorder)

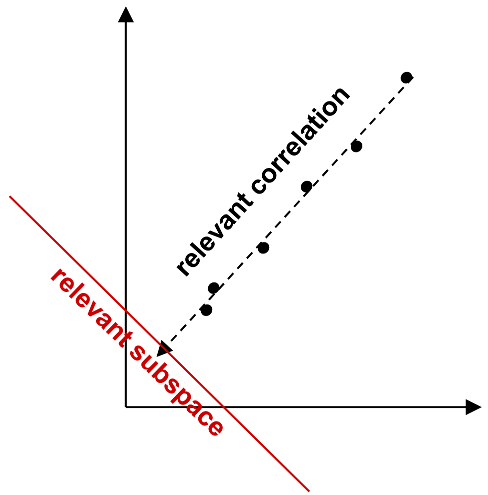
- *Challenge*:

  different metabolic disorders appear through different correlations of (subsets of) metabolites



Challenges for Clustering High-Dimensional Data

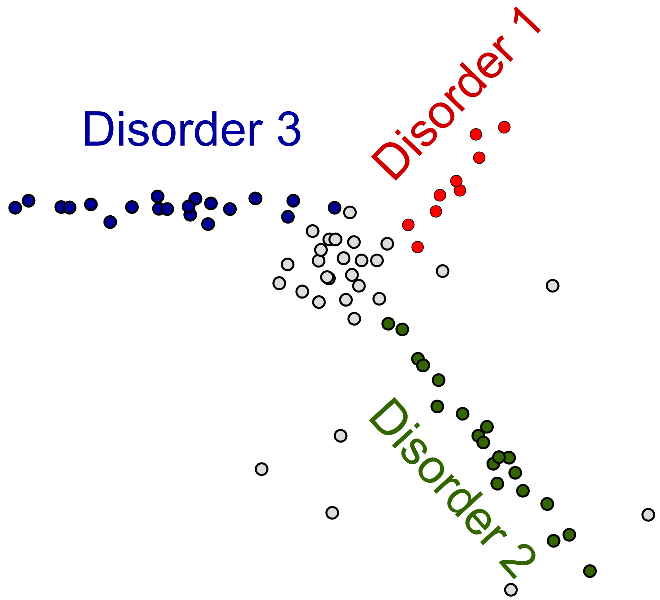
- *Correlation among attributes*
  - A subset of features may be correlated
  - Groups of similar ("dense") points may be identified when considering this correlation of features only



  - Different correlations of attributes may be relevant for different clusters

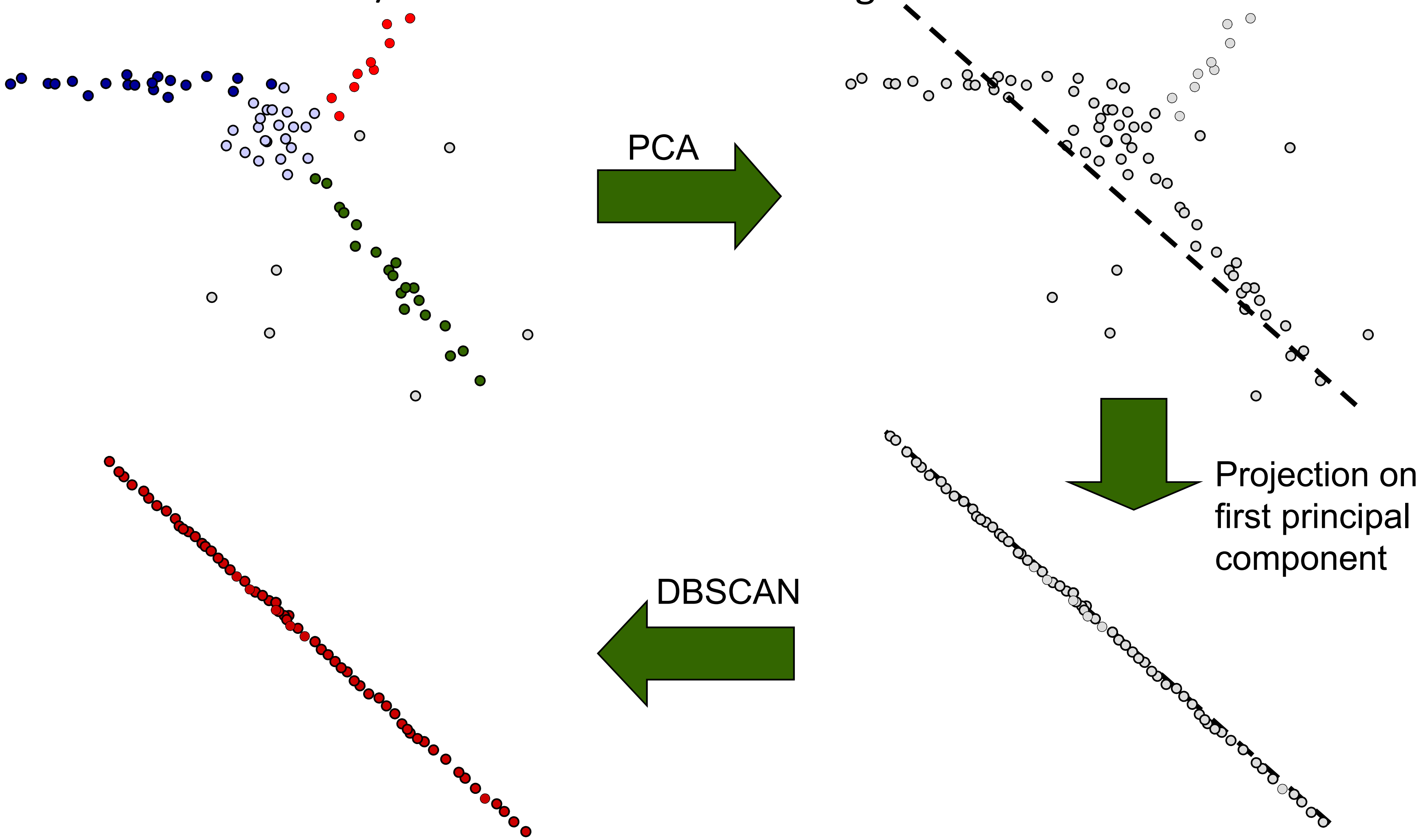
Why not feature selection/reduction?

– (Unsupervised) feature selection/reduction is *global* (e.g. PCA)
– We face a local feature relevance/correlation: some features (or combinations of them) may be relevant for one cluster, but may be irrelevant for a second one



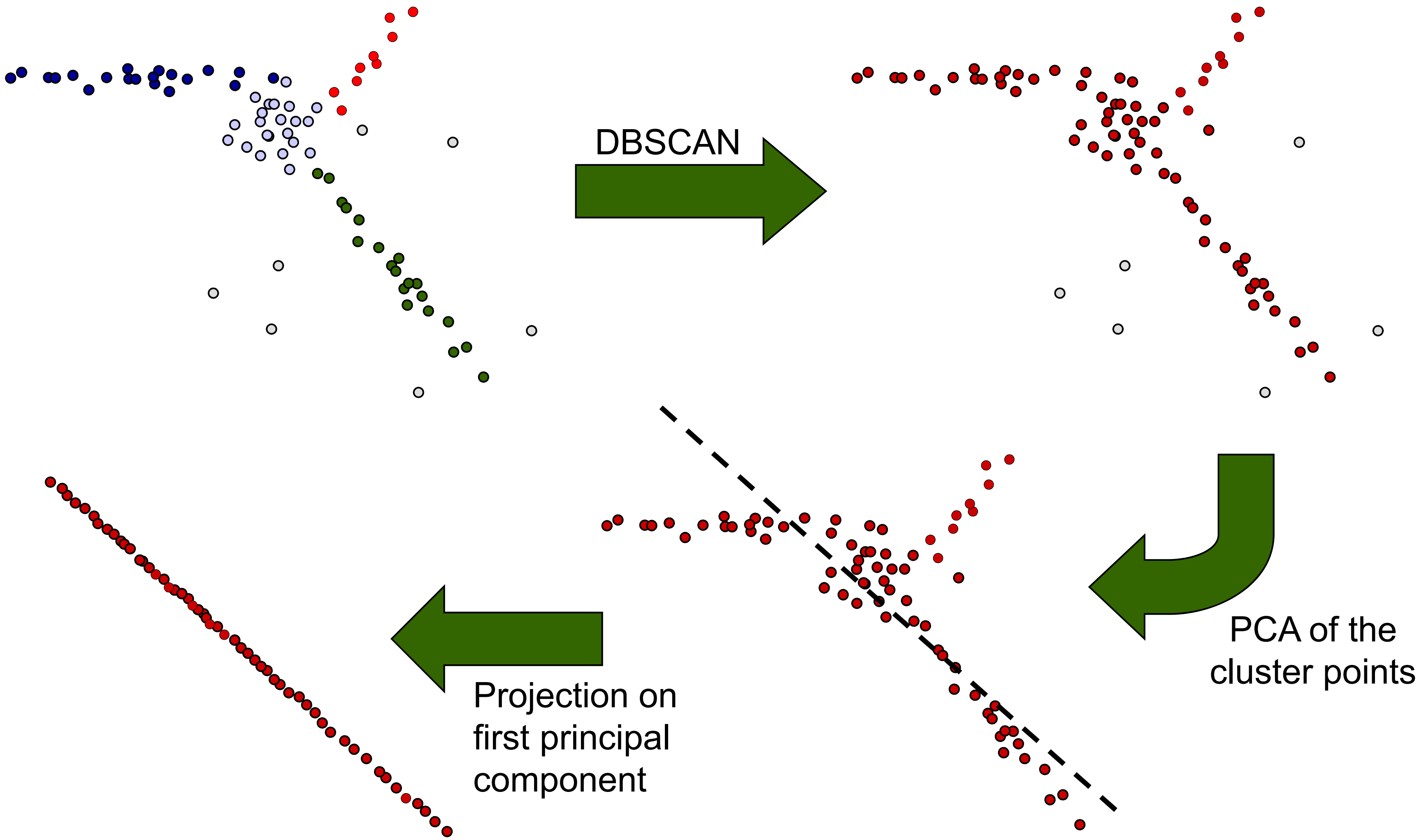
Challenges for Clustering High-Dimensional Data

Use feature selection/reduction before clustering



Challenges for Clustering High-Dimensional Data

Cluster first and then apply PCA



Problem Summary

- Feature relevance and correlation
  - Usually, no clusters in the full dimensional space
  - Often, clusters are hidden in subspaces of the data, i.e. only a subset of features is relevant for the clustering
  - E.g. a gene plays a certain role in a subset of experimental conditions
- Local feature relevance/correlation
  - For each cluster, a different subset of features or a different correlation of features may be relevant
  - E.g. different genes are responsible for different phenotypes
- Overlapping clusters
  - Clusters may overlap, i.e. an object may be clustered differently in varying subspaces
  - E.g. a gene plays different functional roles depending on the environment

Challenges for Clustering High-Dimensional Data

- General problem setting of clustering high dimensional data

Search for clusters in
(in general arbitrarily oriented) subspaces
of the original feature space

- Challenges:
  - Find the correct subspace of each cluster
    - Search space:
      - all possible arbitrarily oriented subspaces of a feature space
      - infinite
  - Find the correct cluster in each relevant subspace
    - Search space:
      - "Best" partitioning of points (see: minimal cut of the similarity graph)
      - NP-complete [SCH75]

Challenges for Clustering High-Dimensional Data

- Even worse: ***Circular Dependency***
  - Both challenges depend on each other:
    - In order to determine the correct subspace of a cluster, we need to know (at least some) cluster members
    - In order to determine the correct cluster memberships, we need to know the subspaces of all clusters

- How to solve the circular dependency problem?
  - Integrate subspace search into the clustering process
  - Thus, we need heuristics to solve
    - the subspace search problem
    - the clustering problem

    simultaneously

Overview of the discussed methods

- Bottom-Up approaches: Subspace Clustering
  - CLIQUE [AGGR98]
  - SUBCLU [KKK04]

Find all clusters in all subspaces.

Axis-parallel subspaces

- Top-Down Approaches: Projected Clustering
  - PROCLUS [APW+99]
  - PREDECON[BKKK04]

Each point is assigned to one subspace cluster or noise.

Axis-parallel subspaces

- Top-Down Approaches: Correlation Clustering
  - ORCLUS[AY00]
  - 4C [BKKZ04]

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Arbitrary oriented subspaces

- Pattern based clustering

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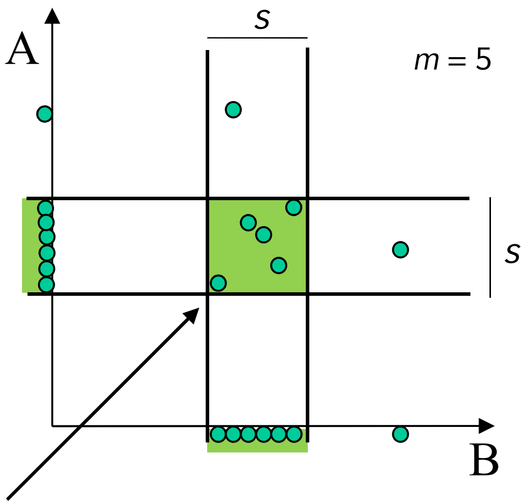
Bottom-up Algorithms

- Rational:
  - Similar to Branch-and-Bound feature selection: Start with 1-dimensional subspaces or subspace clusters and merge them to compute higher dimensional ones.
  - Most approaches transfer this problem into frequent item set mining.
    - The cluster criterion must implement the downward closure (monotonicity) property:
      - If the criterion holds for a *k*-dimensional subspace *S*, then it also holds for any (*k*–1)-dimensional projection of *S*
      - Use the reverse implication for pruning: If the criterion does not hold for a (*k*–1)-dimensional projection of *S*, then the criterion also does not hold for *S*
  - Some approaches use other search heuristics (especially if monotonicity does not hold) like best-first-search, greedy-search, etc.
    - Better average and worst-case performance
    - No guaranty on the completeness of results

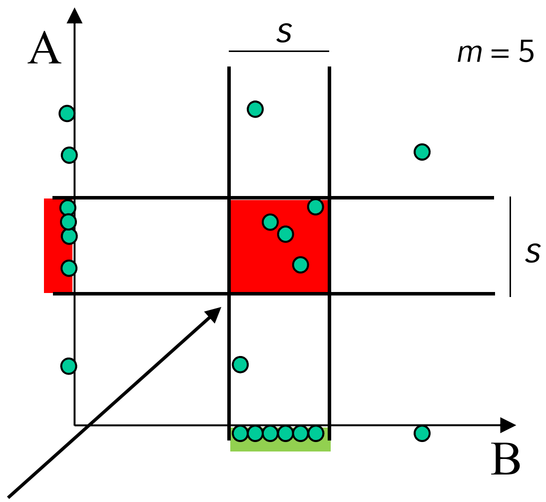
Bottom-up Algorithms

Downward-closure property: example

- Simple cluster criterion (density of grid cells):
  – If a cell *C* of side length *s* contains more than *m* points, it represents a cluster
- Monotonicity:
  – if *C* contains more than *m* points in subspace *S* then *C* also contains more than *m* points in any subspace $T \subset S$
  – Example: monotonicity (left) and reverse implication (right)



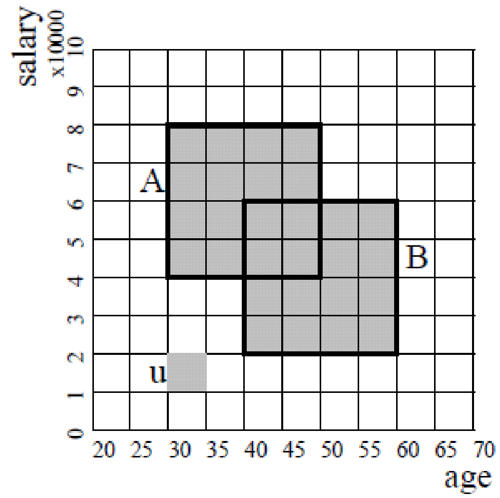
Cell *C* contains more than *m*=5 points in subspace „AB“
=> Also in subspaces „A“⊂ „AB“ and „B“⊂ „AB“



Cell *C* contains less than *m*=5 points in subspace „A“
=> Also in subspace „AB“

CLIQUE [AGGR98]

CLIQUE is probably the first bottom-up algorithm; it uses a density-grid-based cluster model.



Cluster Model

- Clusters are "dense regions" in the feature space
- Partition the feature space into ξ equal sized parts in dimension (implicitly fixing side length *s*).
- A *unit* is the intersection of one interval from each dimension
- *Dense* unit: If unit *u* contains more than τ objects, τ = density threshold

  => monotonicity of dense units holds (see previous slide)
- *Clusters* are maximal sets of connected dense units (e.g., *A U B*)

2-step Approach:

1. Find subspaces (with dense units)
2. Find subspace clusters (union of connected dense units in the same subspace)

CLIQUE: 1. Identify subspaces containing clusters

1. Task: Find subspaces with dense units

- Greedy approach (Bottom-Up), comparable to APRIORI for finding frequent itemsets (Downward Closure):
  - Determine 1-dimensional dense units D_1
  - Candidate generation procedure:
    - Based on D_{k-1}, the set of (k-1) dimensional dense units, generate candidate set C_k by self joining D_{k-1}
      - Join condition: units share first k-2 dimensions
    - Discard those candidates which have a k-1 projection not included in D_{k-1}
    - For the remaining candidates: check density

CLIQUE: 2. Identify clusters

2. Task: Find maximal sets of connected dense units

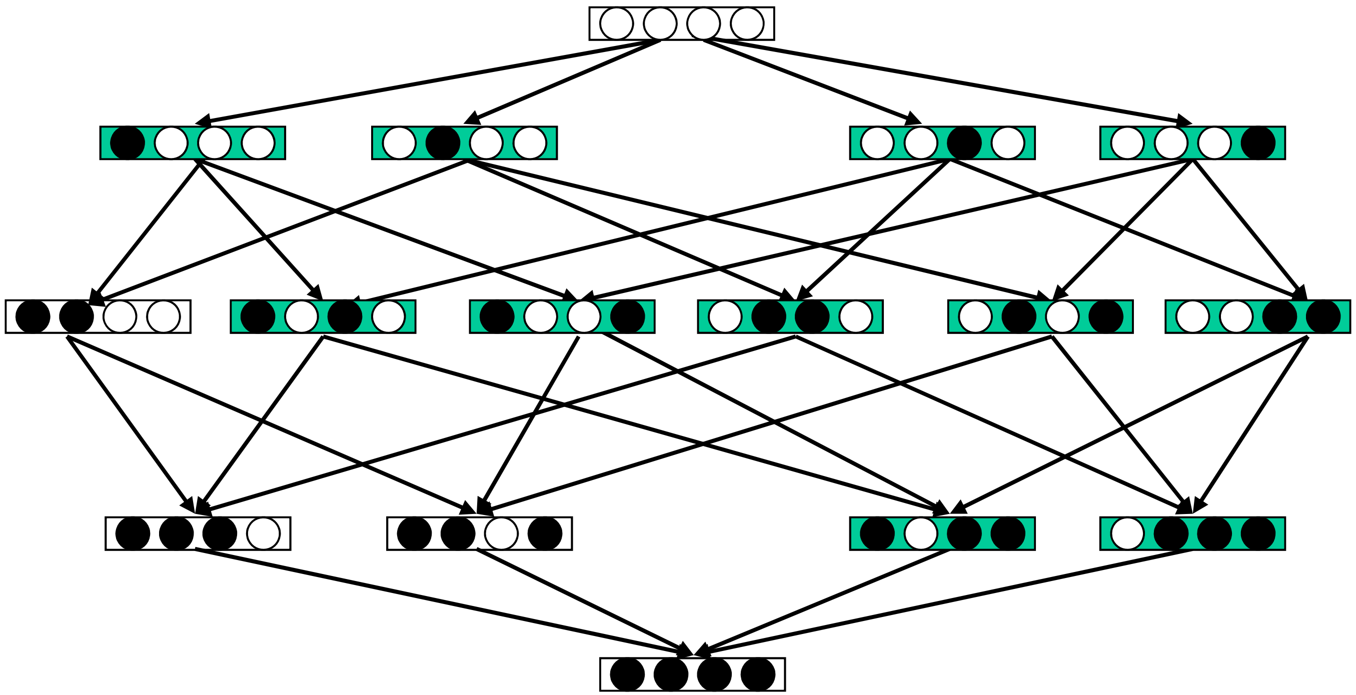
Given: a set of dense units *D* in the same *k*-dimensional subspace *S*

Output: A partition of *D* into clusters $D_1, \ldots, D_k$ of connected dense units

- The problem is equivalent to finding connected components in a graph
  - Nodes: dense units
  - Edge between two nodes if the corresponding dense units have a common face (neighboring units)
  - Depth-first search algorithm: Start with a unit *u* in *D*, assign it to a new cluster ID and find all the units it is connected to. Repeat if there are nodes not yet visited

CLIQUE: Discussion

- Inputparameters: ξ and τ specifying the density threshold
- Output: *all* clusters in *all* subspaces, clusters may overlap/be redundant
- Simple but efficient cluster model: Uses a fixed density threshold for all subspaces (in order to ensure the downward closure property) => to represent a cluster, a unit in 10D must contain as many points (or more) as in 2D …



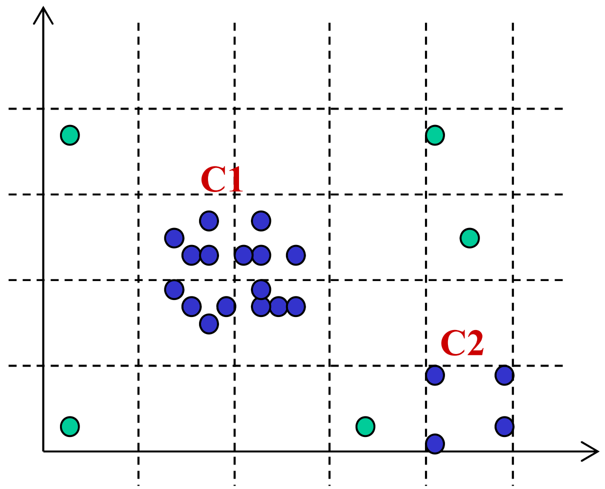
SUBCLU [KKK04] 1/6

Motivation:

Drawbacks of a grid-based clustering model:

- Positioning of the grid influences the clustering
- Only rectangular regions
- Selection of ξ and τ is very sensitive
  Example:

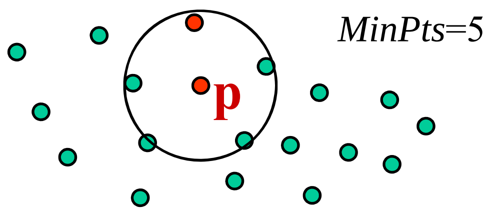
Cluster for $\tau = 4$
(is C_2 a cluster?)
for $\tau > 4$: no cluster
(C_1 is lost)



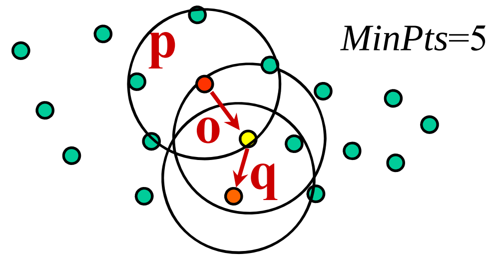
$\Rightarrow$ define regions based on the neighborhood of data points
$\Rightarrow$ use density-based clustering

SUBCLU: Cluster model 2/6

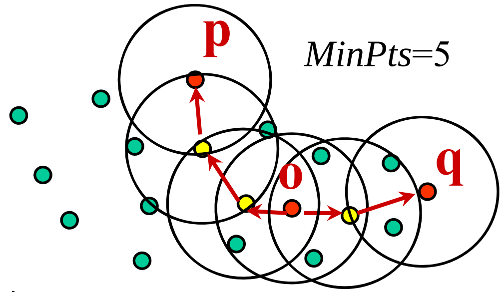
- Density-based cluster model of DBSCAN
- Clusters are *maximal* sets of *density-connected* points
- Density connectivity is defined based on *core points*
- Core points have at least *MinPts* points in their ε-neighborhood



p is core



p is core; o is directly density reachable from *p*; q is density reachable from o is o core?



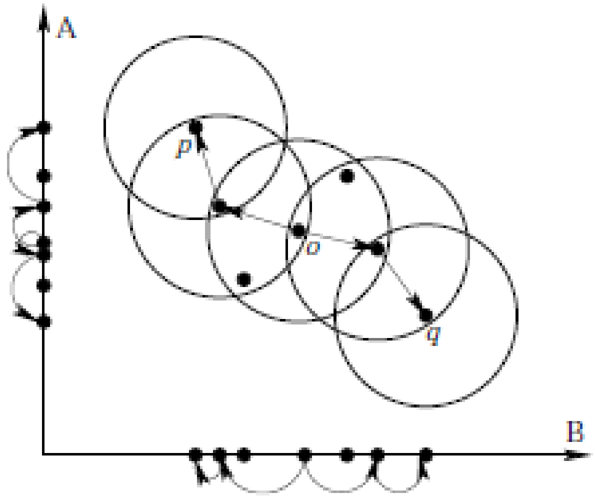
p and *q* are density connected

- Detects clusters of arbitrary shapes and positionings (in the corresponding subspaces)
- Naïve approach: Apply DBSCAN in all possible subspaces → exponential (2^d)
- Idea: Exploit clustering information from previous step (subspaces)
  - Density-connected clusters are not monotonic
  - But, density connected sets are monotonic!

SUBCLU: Downward closure of density connected sets 3/6

If C is a density connected set in subspace S then C is a density connected set in any subspace $T \subset S$.

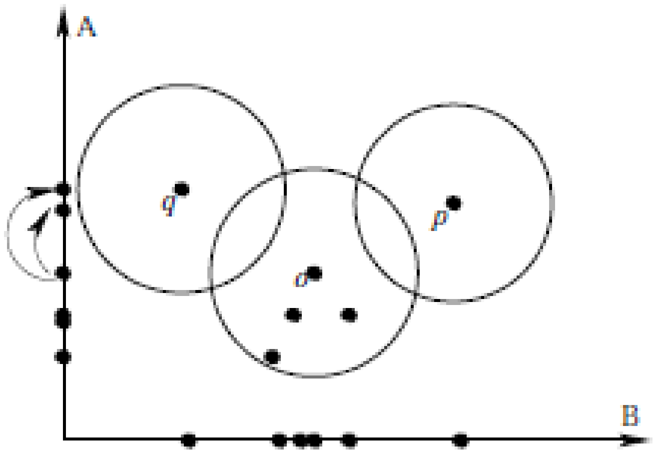
- But, if C is a cluster in S, it need not to be a cluster in $T \subset S$ – maximality might be violated
- All clusters in a higher-dimensional subspace will be subsets of the clusters detected in this first clustering.



(a) p and q are density-connected via o

ε: circles indicate

MinPts = 4



(b) p and q are not density-connected

p and *q* density connected in {A,B}.
Thus, they are also density connected in {A} and {B}

p and *q* not density connected in {B}.
Thus, they are not density connected in{A,B}, although they are density connected in {A}.

SUBCLU: Discussion 6/6

- Algorithm
  - All subspaces that contain any density-connected set are computed using the bottom-up approach (similar to CLIQUE/APRIORI)
  - Density-connected clusters are computed using a specialized DBSCAN run in the resulting subspace to generate the subspace clusters

- Discussion
  - Input: ε and *MinPts* specifying the density threshold
  - Output: all clusters in all subspaces, clusters may overlap
  - Uses a fixed density threshold for all subspaces
  - Advanced but costly cluster model

Bottom-up Algorithms: Discussion

The key limitation: *global density thresholds*

- Usually, the cluster criterion relies on density
- In order to ensure the downward closure property, the density threshold must be fixed
- Consequence: the points in an e.g. 20-dimensional subspace cluster must be as dense as in an e.g. 2-dimensional cluster
- This is a rather optimistic assumption since the data space grows exponentially with increasing dimensionality (see "curse" discussion)
- Consequences:
  - A strict threshold will most likely produce only lower dimensional clusters
  - A loose threshold will most likely produce higher dimensional clusters but also a huge amount of (potentially meaningless) low dimensional clusters

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Arbitrary oriented subspaces

- Pattern based clustering

Top-down Algorithms

Rational:

- Cluster-based approach:
  - Learn the subspace of a cluster in the *entire* d-dimensional feature space
  - Start with full-dimensional clusters
  - Iteratively refine the cluster memberships of points and the subspaces of the cluster
  - PROCLUS[APW+99], ORCLUS[AY00]
- Instance-based approach:
  - Learn for each *point* its subspace preference in the entire *d*-dimensional feature space
  - The subspace preference specifies the subspace in which each point “clusters best”
  - Merge points having similar subspace preferences to generate the clusters
  - PREDECON[BKKK04] 4C[BKKZ04]

Top-down Algorithms: The key problem

How should we learn the subspace preference of a cluster or a point?

- Most approaches rely on the so-called "locality assumption"
  - The subspace is usually learned from the local neighborhood of cluster representatives/cluster members in the entire feature space:
    - Cluster-based approach: the *local neighborhood* of each cluster representative is evaluated in the *d*-dimensional space to learn the "correct" subspace of the cluster
    - Instance-based approach: the *local neighborhood* of each point is evaluated in the *d*-dimensional space to learn the "correct" subspace preference of this point (i.e. the subspace in which the cluster exists that accommodates this point)
- *The locality assumption*: the subspace preference can be learned from the *local neighborhood* in the *d*-dimensional space
- Other approaches learn the subspace preference of a cluster or a point from *randomly sampled points*

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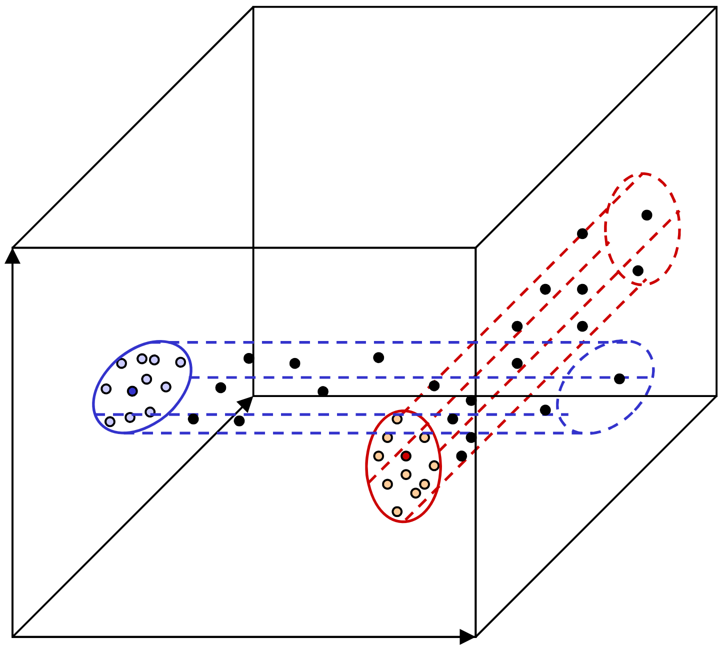
PROCLUS [APW+99] 1/6

- PROjected CLUStering
  - *Cluster-based* top-down approach: we learn the subspace for each cluster
  - *K*-medoid cluster model
    - Cluster is represented by its medoid
    - To each cluster a subspace (of relevant attributes) is assigned
    - Each point is assigned to the nearest medoid (where the distance to each medoid is based on the corresponding subspace of the medoid)
    - Points that have a large distance to their nearest medoids are classified as noise



PROCLUS: Algorithm –Initialization phase 2/6

- 3-phase algorithm: initialization, iterative phase, refinement
  - Input:
    - The set of data points
    - Number of clusters, denoted by k
    - Average number of dimensions for each clusters, denoted by L
  - Output:
    - The clusters found, and the their associated dimensions

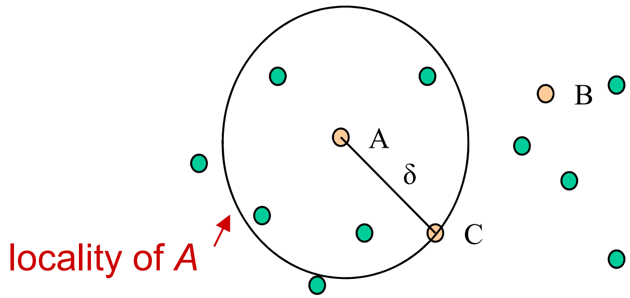
- [**Phase 1**] Initialization of cluster medoids
  - Ideally we want a set of centroids, where each centroid comes from a different cluster.
  - We don't know which are these *k* points though, so we choose a superset M of b*k medoids such that they are well separated.
    - Chose a random sample (S) of a*k data points
    - Out of S, select b*k points (M) by greedy selection : medoids are picked iteratively so that the current medoid is well separated from the medoids that have been chosen so far.
  - Input parameters *a* and *b* are introduced for performance reasons

PROCLUS: Algorithm –Iterative phase 3/6

- [**Phase 2**] Iterative phase (works similar to any *k*-medoid clustering)
  - *k* randomly chosen medoids from *M* are the initial cluster medoids
  - Idea: replace the “bad” medoids with other points in M if necessary → we should be able to evaluate the quality of the clustering by a given set of medoids.
  - Procedure:
    - Find dimensions related to the medoids
    - Assign data points to the medoids
    - Evaluate the clusters formed
    - Find the bad medoid, and try the result of replacing bad medoid

PROCLUS: Algorithm –Iterative phase – Find cluster dimensions 4/6

- For each medoid m_i, let δ be the nearest distance to its closest medoid
- All the data points within δ will be assigned to the medoid m_i (L_i, locality of m_i)



- Intuition: to each medoid we want to associate those dimensions where the points are closed to the medoid in that dimension
- Compute the average distance along each dimension from the points in L_i to m_i.
  - Let $X_{i,j}$ be the avg distance along dimension j
- Calculate for m_i the mean $Y_{i,j}$ and standard deviation $\sigma_{I,j}$ of $X_{i,j}$
- Calculate $Z_{i,j} = (X_{i,j} - Y_{i,j}) / \sigma_{I,j}$
- Choose $k \times l$ smallest values $Z_{i,j}$ with at least 2 chosen for each medoids
- Output: A set of k medoids and their associated dimensions

PROCLUS: Algorithm –Iterative phase – Assigning data points –evaluate clusters 5/6

- *Assign each data point* to its closest medoid using Manhattan segmental distance (only relevant dimensions count)
- Manhattan segmental distance (A variance of Manhattan distance): For any two points x1,x2 and any set of dimensions D, |D|≤ d:

$$d_D(x_1, x_2) = \frac{\sum_{i \in D} \left| x_{1,i} - x_{2,i} \right|}{|D|}$$

- How to *evaluate the clusters*?
  - Use average Manhattan segmental distance from the points in C_i to the *centroid* of C_i along dimension j

$$w_i = \frac{\sum_j Y_{i,j}}{|D_i|} \qquad E = \frac{\sum_{i=k}^{k} |C_i| \cdot w_i}{N}$$

- Replace bad medoids with random points from *M*
- Terminate if the clustering quality does not increase after a given number of current medoids have been exchanged with medoids from *M* (it is not clear, if there is another hidden parameter in that criterion)

PROCLUS: Algorithm –Iterative phase 6/6

- [**Phase 3**] Refinement
  - Reassign subspaces to medoids as above (but use only the points assigned to each cluster rather than the locality of each cluster, i.e., C_i not L_i)
  - Reassign points to medoids
  - Points that are not in the locality of any medoid are classified as noise

PREDECON[BKKK04] 1/3

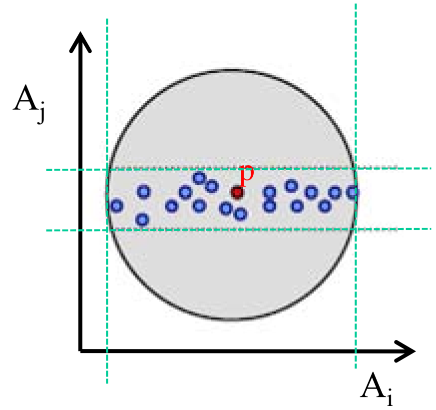
- Instance-based top-down approach: we learn the subspace for each instance
- Extends DBSCAN to high dimensional spaces by incorporating the notion of dimension preferences in the distance function

- For each point p, it defines its subspace preference vector:

$$\bar{\mathbf{w}}_p = (w_1, w_2, \ldots w_d) \qquad w_i = \begin{cases} 1 & \text{if} \quad \text{VAR}_i > \delta \\ \kappa & \text{if} \quad \text{VAR}_i \leq \delta \end{cases}$$

- VAR_i is the variance along dimension j in $N_\varepsilon(p)$:

$$\text{VAR}_{A_i}(\mathcal{N}_\varepsilon(p)) = \frac{\sum_{q \in \mathcal{N}_\varepsilon(p)} (dist(\pi_{A_i}(p), \pi_{A_i}(q)))^2}{|\mathcal{N}_\varepsilon(p)|}$$



δ, κ (κ>>1) are input parameters

PREDECON[BKKK04] 2/3

- Preference weighted distance function:

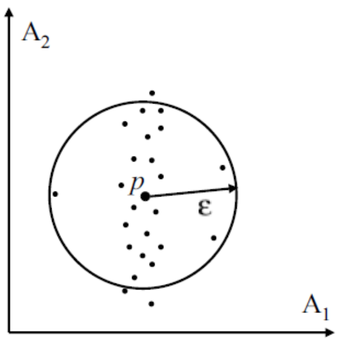
$$dist_p(p,q) = \sqrt{\sum_{i=1}^{d} \frac{1}{w_i} \cdot (\pi_{A_i}(p) - \pi_{A_i}(q))^2}$$

$$dist_{pref}(p,q) = \max\{dist_p(p,q), dist_q(q,p)\}$$

- Preference weighted ε-neighborhood:

$$\mathcal{N}_\varepsilon^{\bar{\mathbf{w}}_p}(p) = \{x \in \mathcal{D} \mid dist_{pref}(p,x) \le \varepsilon\}$$

simple
ε-neighborhood



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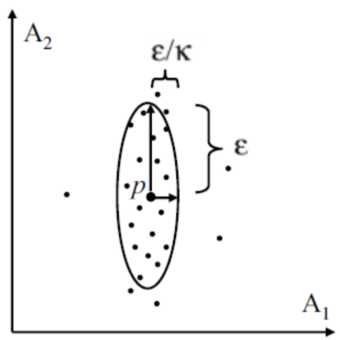
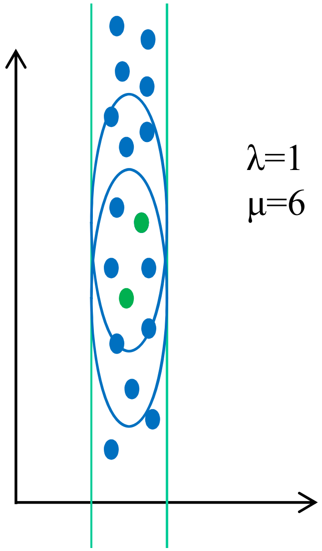


preference weighted
ε-neighborhood

PREDECON[BKKK04] 3/3

- Preference weighted core points:

$$\text{CORE}_{\text{den}}^{\text{pref}}(p) \Leftrightarrow \text{PDIM}(\mathcal{N}_\varepsilon(p)) \leq \lambda \wedge |\mathcal{N}_\varepsilon^{\bar{w}_o}(p)| \geq \mu$$



- Direct density reachability, reachability and connectivity are defined based on preference weighted core points

- A *subspace preference cluster* is a maximal density connected set of points associated with a certain subspace preference vector.

Overview of the discussed methods

- Bottom-Up approaches: Subspace Clustering
  - CLIQUE [AGGR98]
  - SUBCLU [KKK04]

Find all clusters in all subspaces.

Axis-parallel subspaces

- Top-Down Approaches: Projected Clustering
  - PROCLUS [APW+99]
  - PREDECON[BKKK04]

Each point is assigned to one subspace cluster or noise.

Axis-parallel subspaces

- Top-Down Approaches: Correlation Clustering
  - ORCLUS[AY00]
  - 4C [BKKZ04]

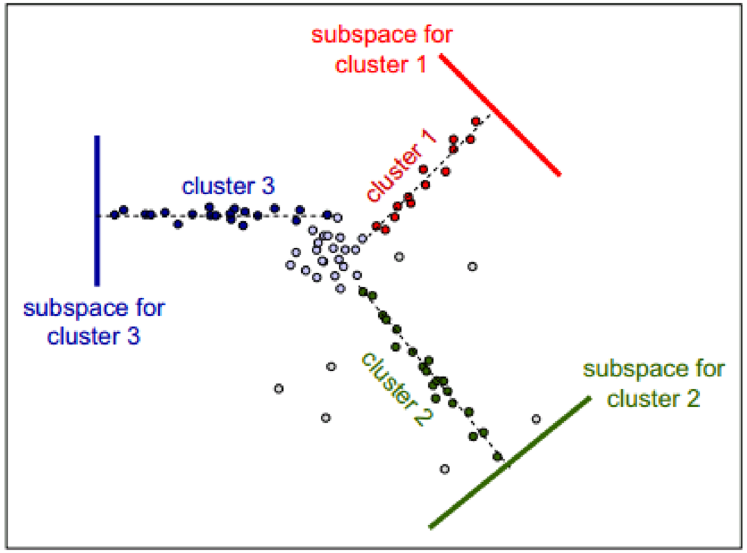
Each point is assigned to one subspace cluster or noise.

Arbitrary oriented subspaces

- Pattern based clustering

Correlation Clustering

- Motivating example:
  - Cluster 3 exists in an axis-parallel subspace
  - Clusters 1 and 2 exist in (different) arbitrarily oriented subspaces: if the cluster members are projected onto the depicted subspaces, the points are “densely packed”



- Subspace clustering and projected clustering algorithms find axis-parallel subspaces
- Correlation clustering for finding clusters in arbitrary oriented subspaces

ORCLUS[AY00] 1/3

- ORCLUS (arbitrarily ORiented projected CLUSter generation) first approach to generalized projected clustering
- A *generalized projected cluster* is a set of vectors E and a set of points C such that the points in C are closely clustered in the subspace defined by the vectors E.
  - E is a set of orthonormal vectors, $|E| \leq d$

Input:

- The number of clusters k
- The dimensionality of the subspace of the clusters, l (=|E|)

Output

- A set of k clusters and their associated subspaces of dimensionality l

Main idea

- To find the subspace of a cluster C_i, compute the dxd covariance matrix M_i for C_i and determine the eigenvectors. Pick the l_c eigenvectors with the smallest eigenvalues.

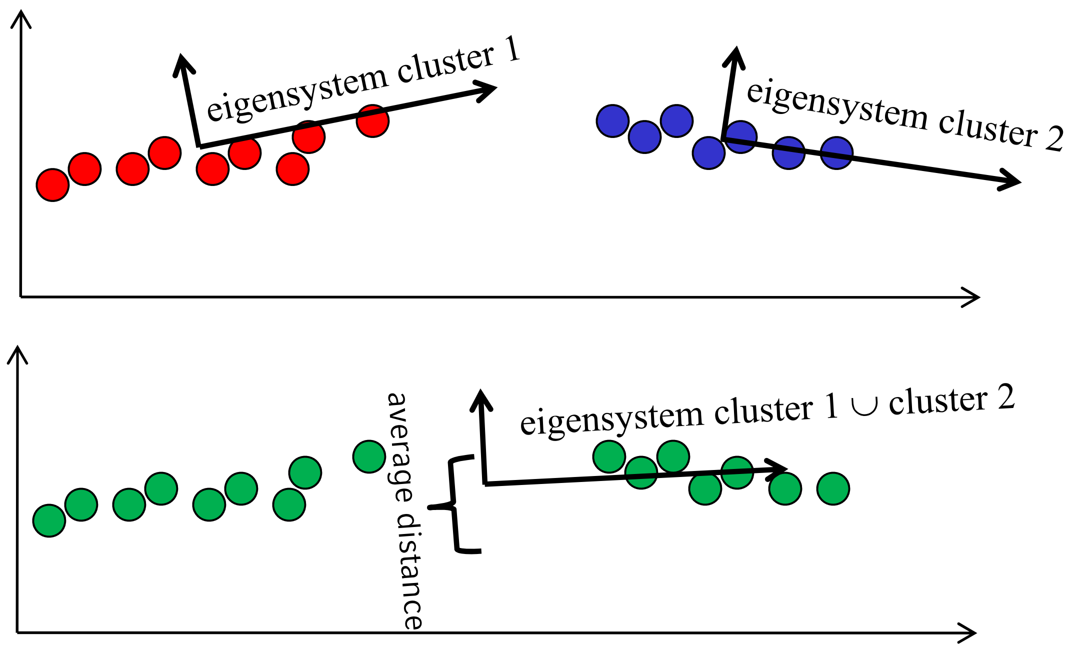
- Relies on cluster-based locality assumption: subspace of each cluster is learned from its members

ORCLUS: Algorithm 2/3

- similar ideas to PROCLUS [APW+99]
- *k*-means like approach
- start with $k_c > k$ seeds
- assign points to clusters according to distance function based on the eigensystem of the current cluster (starting with axes of data space, i.e. Euclidean distance)
- The eigensystem is iteratively adapted based on the updated cluster members
- Reduce the number of clusters k_c in each iteration by merging best-fitting cluster pairs

ORCLUS: Merging clusters 3/3

- Each cluster C_i exists in a possible different subspace S_i, how do we decide what to merge?
- Compute the subspace of their union $C_i \cup C_j$ (eigenvectors corresponding to the smallest l eigenvalues)
- Check the cluster energy of $C_i \cup C_j$ in this subspace (mean square distance of the points from the centroid in this subspace) – indicator of how well the points combine



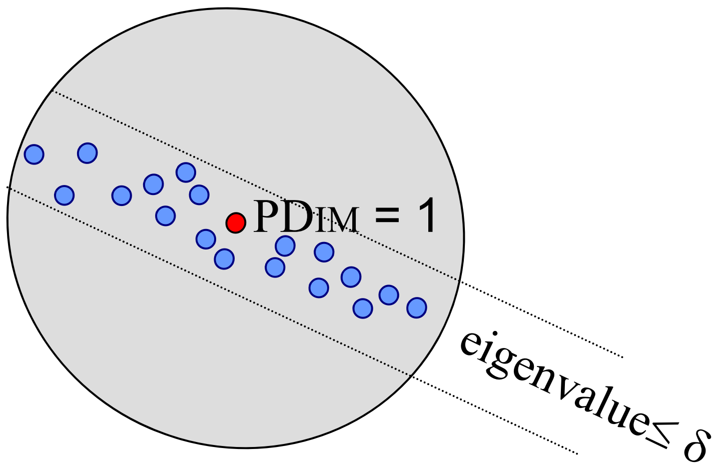
- Assess average distance in all merged pairs of clusters and finally merge the best fitting pair, that with the smallest cluster energy
- Continue until the desired number of clusters, k, is achieved.

4C [BKKZ04]

4C = Computing Correlation Connected Clusters
Idea: Integrate PCA into density-based clustering.

Approach**:**

- Check the core point property of a point p in the complete feature space
- Perform PCA on the local neighborhood S of p to find subspace correlations

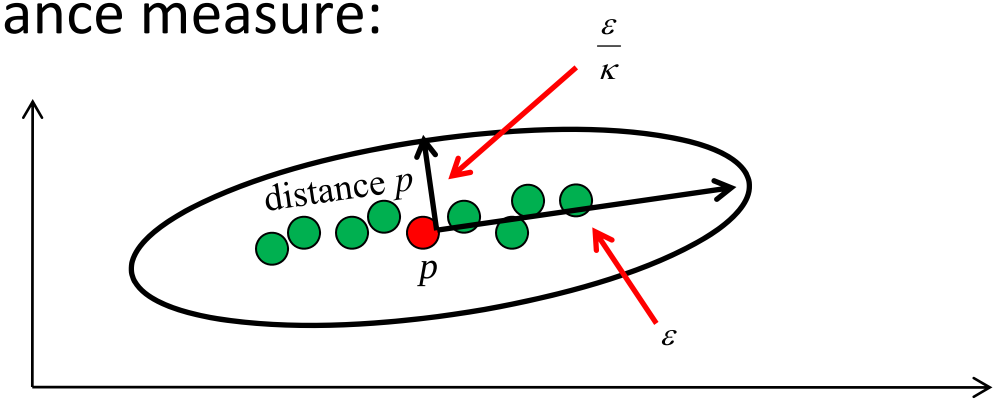


PCA factorizes M_P into $M_P = V\ E\ V^T$
V: eigenvectors
E: eigenvalues

- A parameter δ discerns large from small eigenvalues.
- CorDim(S)=#eigenvalues>δ
- In the eigenvalue matrix of p, large eigenvalues are replaced by 1, small eigenvalues by a value κ >>1 → adapted eigenvalue matrix E'_p

4C: Distance measure

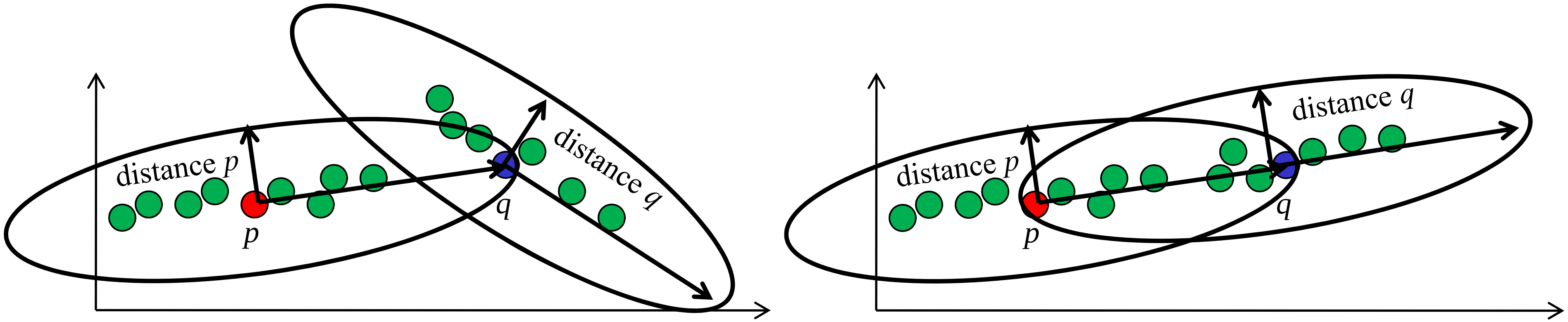
- effect on distance measure:



- distance of *p* and *q* w.r.t. *p*: $\sqrt{(p-q)\cdot V_p \cdot E'_p \cdot V_p^{\mathrm{T}} \cdot (p-q)^{\mathrm{T}}}$
- distance of *p* and *q* w.r.t. *q*: $\sqrt{(q-p)\cdot V_q \cdot E'_q \cdot V_q^{\mathrm{T}} \cdot (q-p)^{\mathrm{T}}}$

4C: correlation neighbors

- symmetry of distance measure by choosing the maximum:

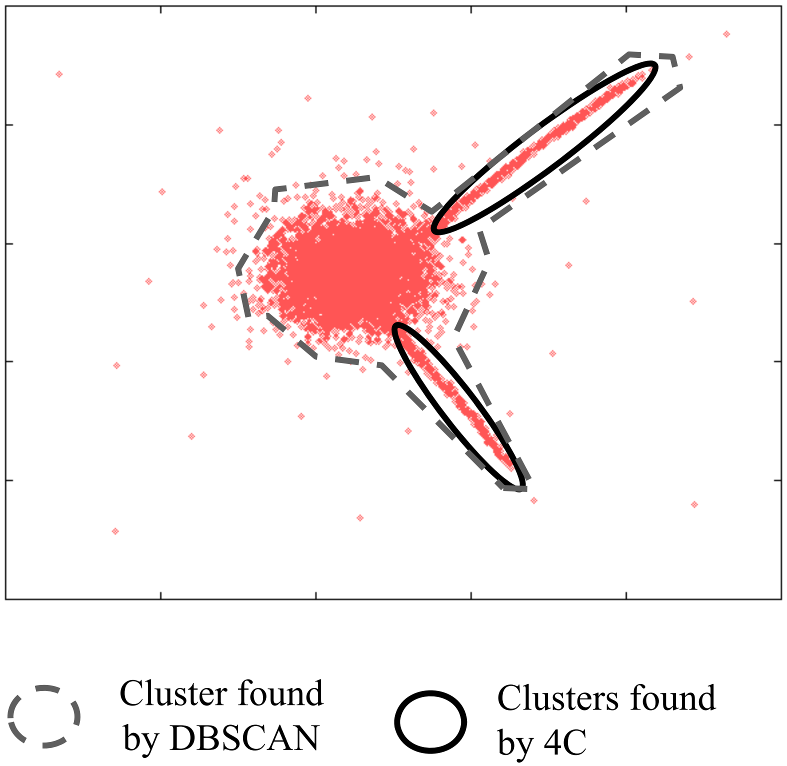


- *p* and *q* are correlation-neighbors if

$$\max\left\{\begin{array}{l}\sqrt{(p-q)\cdot V_p\cdot E'_p\cdot V_p^{\mathrm{T}}\cdot(p-q)^{\mathrm{T}}},\\ \sqrt{(q-p)\cdot V_q\cdot E'_q\cdot V_q^{\mathrm{T}}\cdot(q-p)^{\mathrm{T}}}\end{array}\right\}\leq\varepsilon$$

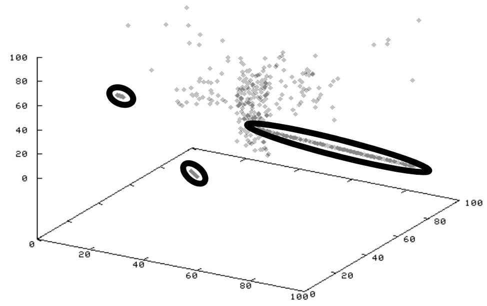
4C

4C vs. DBSCAN

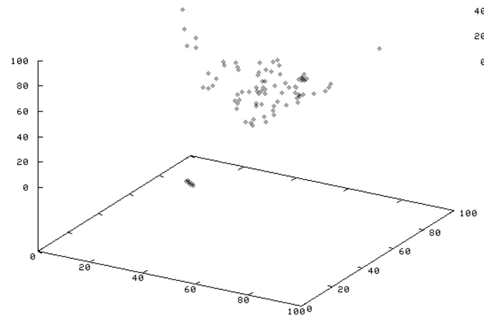


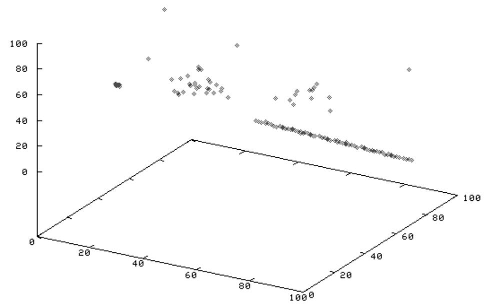
4C vs. ORCLUS

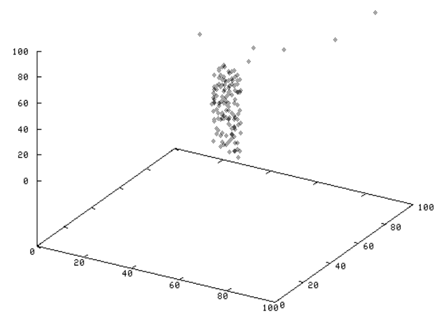
4C



ORCLUS







4C: discussion

- finds arbitrary number of clusters
- requires specification of density-thresholds
  - μ (minimum number of points): rather intuitive
  - ε (radius of neighborhood): hard to guess
- biased to maximal dimensionality λ of correlation clusters (user specified)
- instance-based locality assumption: correlation distance measure specifying the subspace is learned from local neighborhood of each point in the *d*-dimensional space

enhancements also based on PCA:

- COPAC [ABK+07c] and
- ERiC [ABK+07b]

Correlation clustering with PCA: Discussion

- PCA: mature technique, allows construction of a broad range of similarity measures for local correlation of attributes
- drawback: all approaches suffer from locality assumption
- successfully employing PCA in correlation clustering in "really" high-dimensional data requires more effort henceforth

- So how to overcome the locality assumption???

  => different method to determine correlation?

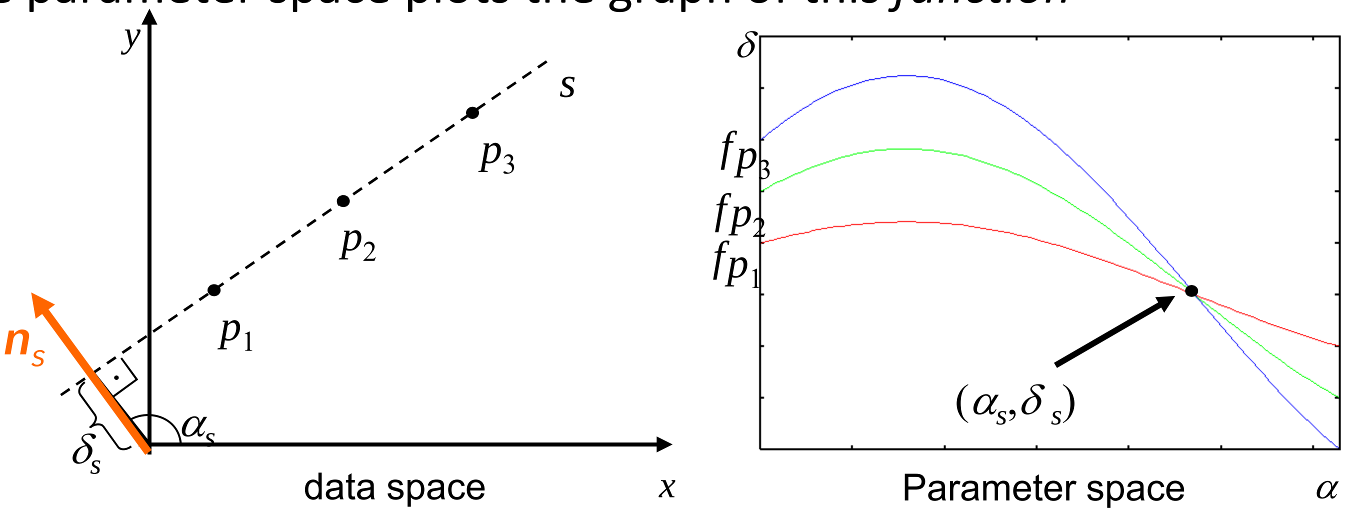
  => Hough transform (computer graphics)

  find structures (e.g. lines, circles) in images

CASH [ABKKZ 07]

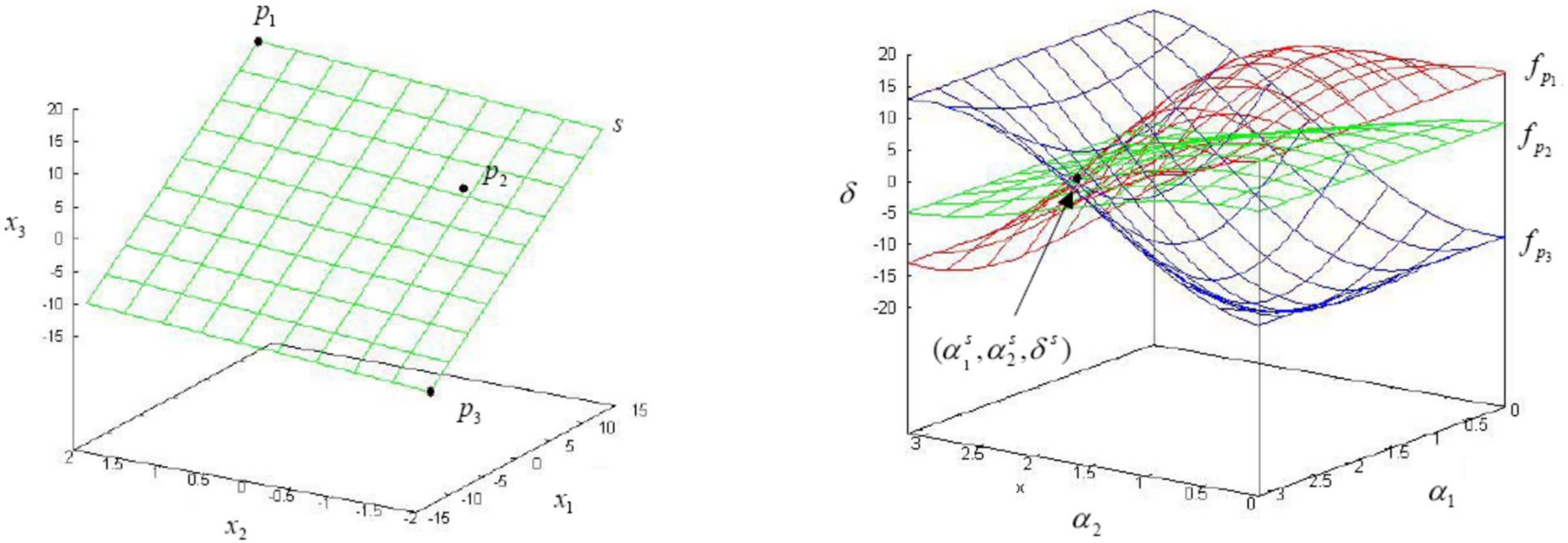
- Basic idea of CASH (= Clustering in Arbitrary Subspaces based on the Hough transform)
  - Transform each object into a so-called *parameter space* representing all possible subspaces accommodating this object (i.e. all hyper-planes through this object)
  - This parameter space is a *continuum* of all these subspaces
  - The subspaces are represented by a considerably small number of parameters
  - This transform is a generalization of the Hough Transform (which is designed to detect linear structures in 2D images) for arbitrary dimensions

- Transform
  - For each d-dimensional point p there is an infinite number of (d-1)-dimensional hyper-planes through p
  - Each of these hyper-planes s is defined by $(p,\alpha_1,\ldots,\alpha_{d-1})$, where $\alpha_1,\ldots,\alpha_{d-1}$ is the normal vector $\boldsymbol{n}_s$ of the hyper-plane s
  - The function $f_p(\alpha_1,\ldots,\alpha_{d-1}) = \delta_s = \langle p,\boldsymbol{n}_s\rangle$ maps p and $\alpha_1,\ldots,\alpha_{d-1}$ onto the distance δ_s of the hyper-plane s to the origin
  - The parameter space plots the graph of this *function*



CASH

- Properties of this transform
  - point in the data space = sinusoide curve in the parameter space
  - point in the parameter space = hyper-plane in the data space
  - points on a common hyper-plane in the data space (cluster)
    = sinusoide curves intersecting at ***one*** point in the parameter space
  - intersection of sinusoide curves in the parameter space
    = hyper-plane accommodating the corresponding points in data space



CASH

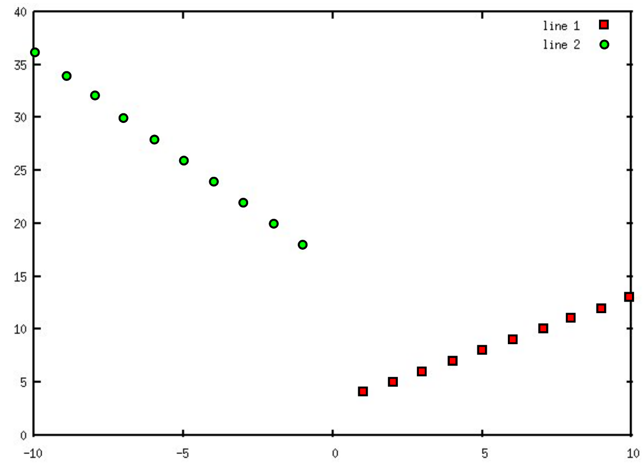
- Detecting clusters
  – determine all intersection points of at least *m* curves in the parameter space => (d-1)-dimensional cluster
  – Exact solution (check all pair-wise intersections) is too costly
  – Heuristics are employed
- Grid-based bisecting search

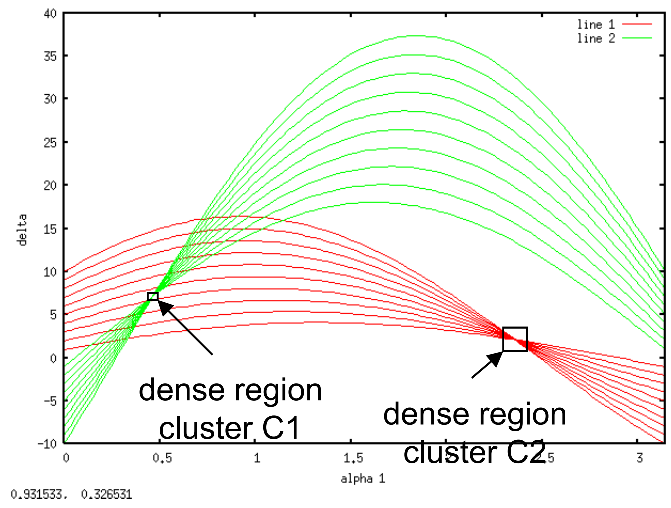
  => Find cells with at least *m* curves

  ☺ determining the curves that are within a given cell is in O(d^3)

  ☹ Number of cells O($\boldsymbol{r}^d$), where *r* is the resolution of the grid

  ☹ high value for ***r*** necessary

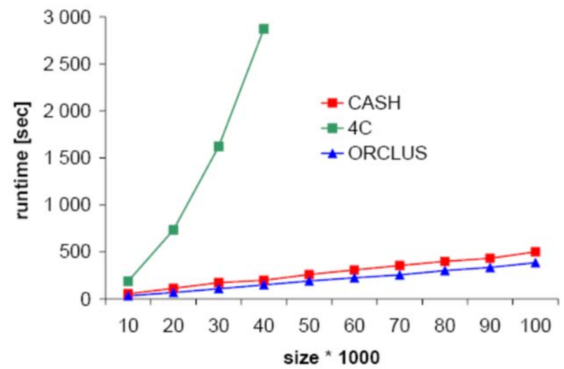


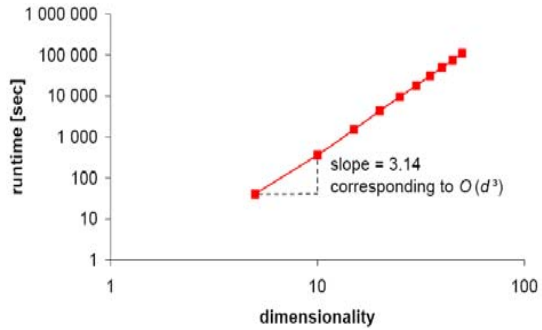


CASH

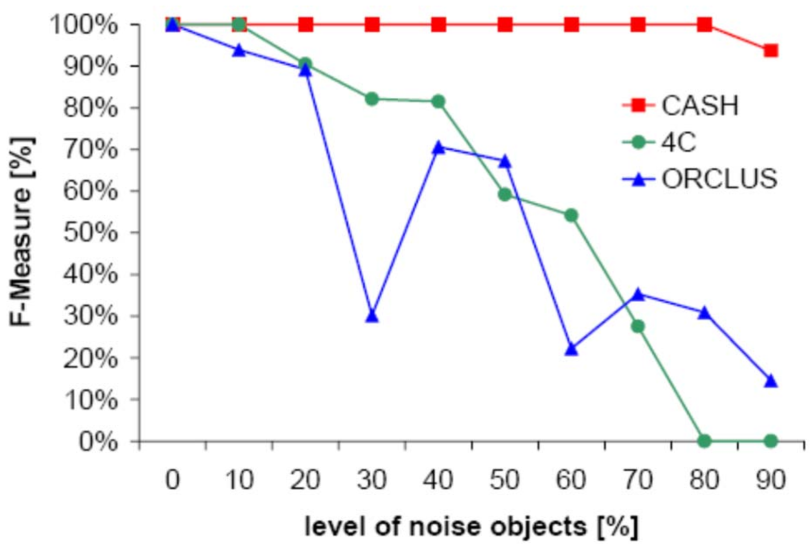
- Complexity (*c* = number of cluster found – not an input parameter!!!)
  - Bisecting search O($s \cdot c$)
  - Determination of curves in a cell O($n \cdot d^3$)
  - Over all O($s \cdot c \cdot n \cdot d^3$)

    (algorithms for PCA are also in O(d^3))

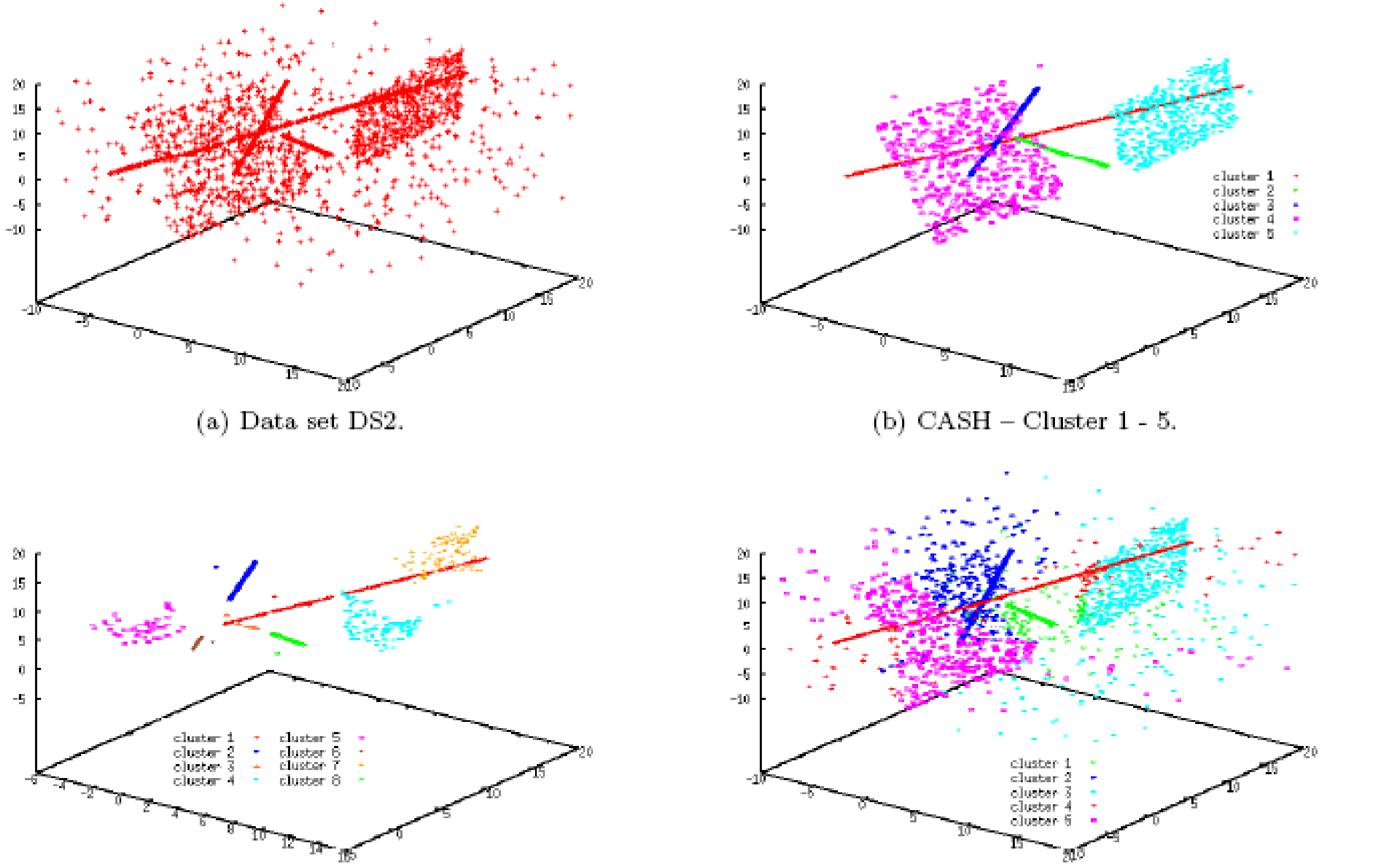




- Robustness against noise



CASH



(a) Data set DS2.

(b) CASH – Cluster 1 - 5.

(c) 4C – Cluster 1 - 8.

(d) ORCLUS – Cluster 1 - 5.

Clustering High Dimensional Data: Discussion 1/2

- Finding clusters in (arbitrarily oriented) subspaces of the original feature space.
- The subspace (where the cluster exists) is part of the cluster definition.
- The challenge is 2-fold: finding the correct subspace for each cluster and the correct cluster in each relevant subspace
  - Integrate subspace search in the clustering process
- Traditional full dimensional clustering paradigms transferred in the high dimensional space.

Clustering High Dimensional Data: Discussion 2/2

- Different types of methods
  - Bottom-Up approaches: Subspace Clustering
    - Find clusters in all subspaces
    - Restrict the search space by downward closure property
    - Axis-parallel subspaces
    - CLIQUE [AGGR98], SUBCLU [KKK04]
  - Top-Down Approaches: Projected Clustering
    - Each point is assigned to one subspace cluster or noise.
    - Subspaces are discovered based on the locality (cluster-based, instance-based)
    - Axis-parallel subspaces
    - PROCLUS [APW+99], PREDECON[BKKK04]
  - Top-Down Approaches: Correlation Clustering
    - Each point is assigned to one subspace cluster or noise.
    - Subspace are discovered based on the locality (cluster-based, instance-based)
    - Arbitrary oriented subspaces
    - ORCLUS[AY00], 4C [BKKZ04], CASH []
  - Pattern based clustering (not covered here)

DATABASE SYSTEMS GROUP

Literature

[AGGR98] R. Agrawal, J. Gehrke, D. Gunopulos, and P. Raghavan.
Automatic subspace clustering of high dimensional data for data mining applications.
In Proceedings of the ACM International Conference on Management of Data (SIGMOD), Seattle, WA, 1998.

[KKK04 K. Kailing, H.-P. Kriegel, and P. Kröger.
Density-connected subspace clustering for highdimensional data.
In Proceedings of the 4th SIAM International Conference on Data Mining (SDM), Orlando, FL, 2004.

[BKKK04] C. Böhm, K. Kailing, H.-P. Kriegel, and P. Kröger.
Density connected clustering with local subspace preferences.
In Proceedings of the 4th International Conference on Data Mining (ICDM), Brighton, U.K., 2004.

[APW+99] C. C. Aggarwal, C. M. Procopiuc, J. L. Wolf, P. S. Yu, and J. S. Park.
Fast algorithms for projected clustering.
In Proceedings of the ACM International Conference on Management of Data (SIGMOD), Philadelphia, PA, 1999.

[AY00] C. C. Aggarwal and P. S. Yu.
Finding generalized projected clusters in high dimensional space.
In Proceedings of the ACM International Conference on Management of Data (SIGMOD), Dallas, TX, 2000.

[BKKZ04] C. Böhm, K. Kailing, P. Kröger, and A. Zimek.
Computing clusters of correlation connected objects.
In Proceedings of the ACM International Conference on Management of Data (SIGMOD), Paris, France, 2004.

[ABKKZ07] Elke Achtert, Christian Böhm, Hans-Peter Kriegel, Peer Kröger, Arthur Zimek:
Robust, Complete, and Efficient Correlation Clustering. SDM 2007: 413-418