Ludwig Maximilians Universität München
Institut für Informatik
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Skript zur Vorlesung

Knowledge Discovery in Databases II

im Wintersemester 11/12

Kapitel 3: Clustering in hochdimensionalen Räumen

Skript basiert auf Tutorial von Hans-Peter Kriegel, Peer Kröger und Arthur Zimek, ICDM 2007, PAKDD 2008, KDD 2008, VLDB 2008

http://www.dbs.ifi.lmu.de/Lehre/KDD_II

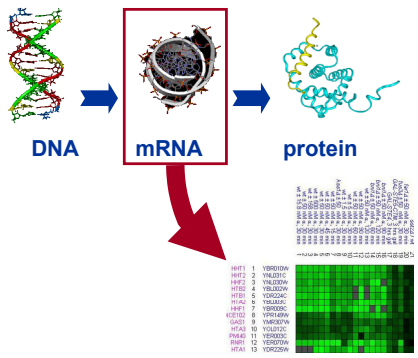
Outline

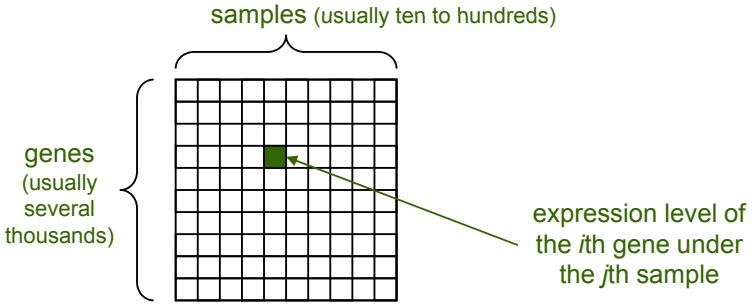
Outline: Introduction

- Sample Applications
- General Problems and Challenges
- A First Taxonomy of Approaches

Sample Applications

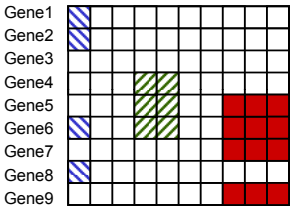
- Gene Expression Analysis
  - Data:
    - Expression level of genes under different samples such as
      - different individuals (patients)
      - different time slots after treatment
      - different tissues
      - different experimental environments
    - Data matrix:





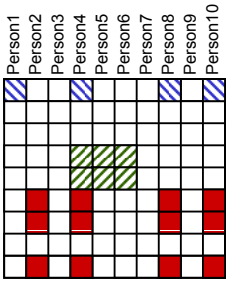
Sample Applications

- Task 1: Cluster the rows (i.e. genes) to find groups of genes with similar expression profiles indicating homogeneous functions
  - *Challenge*:
    genes usually have
    different functions
    under varying
    (combinations of) conditions



Cluster 1: {G1, G2, G6, G8}
Cluster 2: {G4, G5, G6}
Cluster 3: {G5, G6, G7, G9}

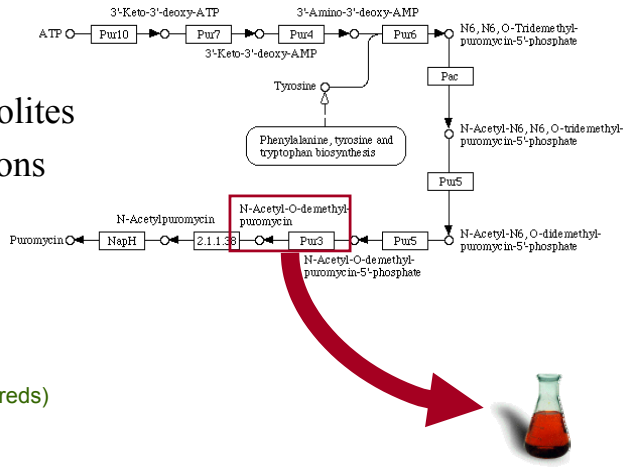
- Task 2: Cluster the columns (e.g. patients) to find groups with similar expression profiles indicating homogeneous phenotypes
  - *Challenge*:
    different phenotypes
    depend on different
    (combinations of)
    subsets of genes

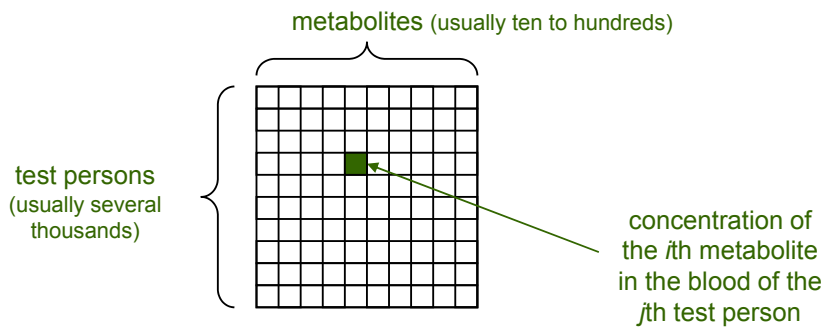


Cluster 1: {P1, P4, P8, P10}
Cluster 2: {P4, P5, P6}
Cluster 3: {P2, P4, P8, P10}

Sample Applications

- Metabolic Screening
  - Data
    - Concentration of different metabolites in the blood of different test persons
    - Example:
      Bavarian Newborn Screening
    - Data matrix:

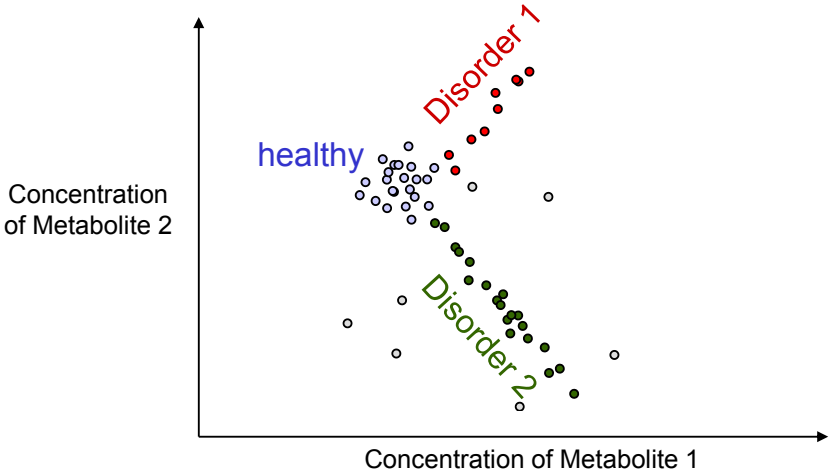




Sample Applications

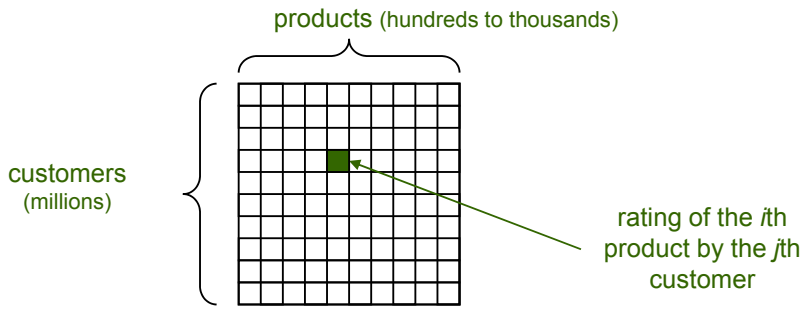
- Task: Cluster test persons to find groups of individuals with similar correlation among the concentrations of metabolites indicating homogeneous metabolic behavior (e.g. disorder)
  - *Challenge*:

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



Sample Applications

- 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

General Problems & Challenges

The *"curse of dimensionality"*: one buzzword for many problems

- First aspect: *Optimization Problem* (Bellman).

  "[The] curse of dimensionality [… is] a malediction that has plagued the scientists from earliest days." [Bel61]

  - The difficulty of any global optimization approach increases exponentially with an increasing number of variables (dimensions).
  - General relation to clustering: fitting of functions (each function explaining one cluster) becomes more difficult with more degrees of freedom.
  - Direct relation to subspace clustering: number of possible subspaces increases dramatically with increasing number of dimensions.

General Problems & Challenges

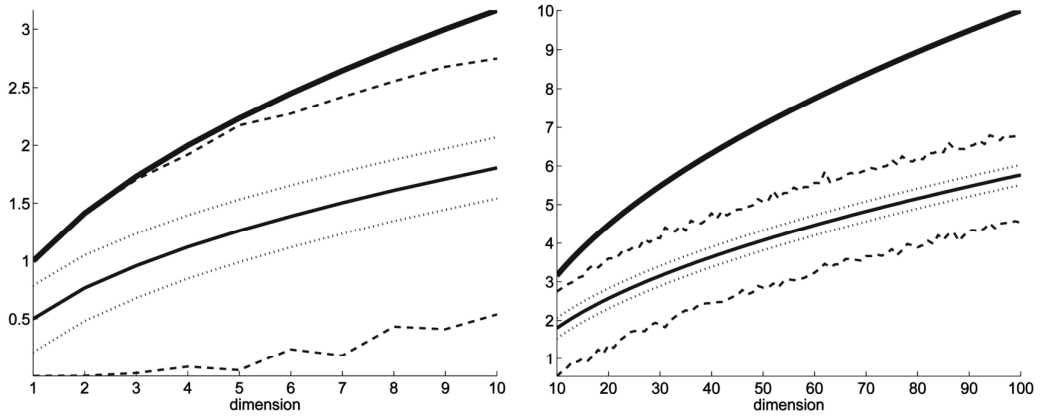
- Second aspect: *Concentration effect of L_p-norms*
  - In [BGRS99,HAK00] it is reported that the ratio of (Dmax_d – Dmin_d) to Dmin_d converges to zero with increasing dimensionality d
    - Dmin_d = distance to the nearest neighbor in d dimensions
    - Dmax_d = distance to the farthest neighbor in d dimensions

    Formally:

$$\forall \varepsilon > 0 : \lim_{d \to \infty} \mathrm{P}\left[dist_d\left(\frac{\text{Dmax}_d - \text{Dmin}_d}{\text{Dmin}_d}, 0 \right) \leq \varepsilon \right] = 1$$

    - This holds true for a wide range of data distributions and distance functions

General Problems & Challenges



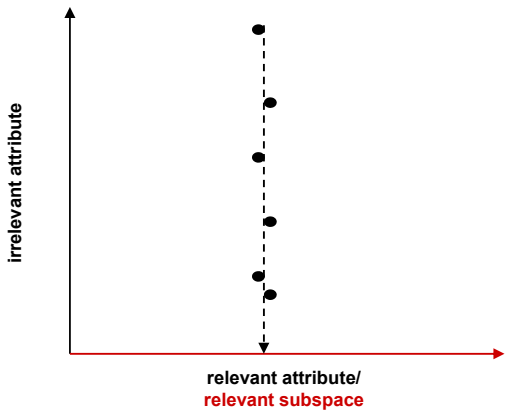
(a) (b)

From bottom to top: minimum observed value, average minus standard deviation, average value, average plus standard deviation, maximum observed value, and maximum possible value of the Euclidean norm of a random vector. The expectation grows, but the variance remains constant. A small subinterval of the domain of the norm is reached in practice. (Figure and caption: [FWV07])

- The observations stated in [BGRS99,HAK00] are valid *within* clusters but *not between different* clusters as long as the clusters are well separated [BFG99,FWV07,HKK+10].
- This is *not* the main problem for subspace clustering, although it should be kept in mind for range queries.

General Problems & Challenges

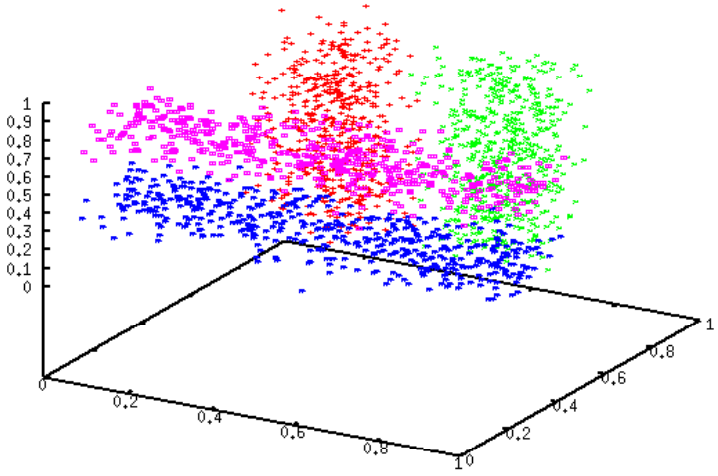
- Third aspect: *Relevant and Irrelevant attributes*
  - A subset of the features may be relevant for clustering
  - Groups of similar ("dense") points may be identified when considering these features only



- Different subsets of attributes may be relevant for different clusters

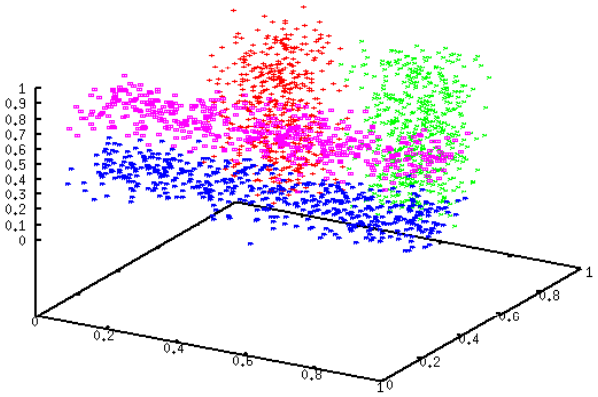
General Problems & Challenges

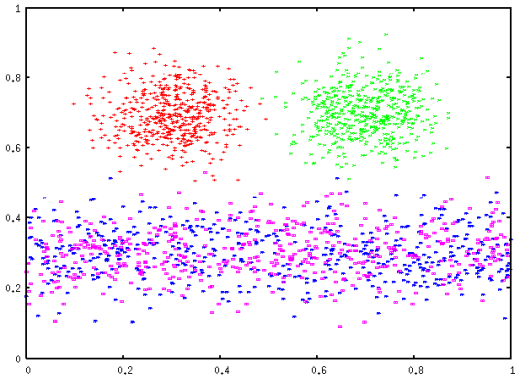
- Effect on clustering:
  - Usually the distance functions used give equal weight to all dimensions
  - However, not all dimensions are of equal importance
  - Adding irrelevant dimensions ruins any clustering based on a distance function that equally weights all dimensions

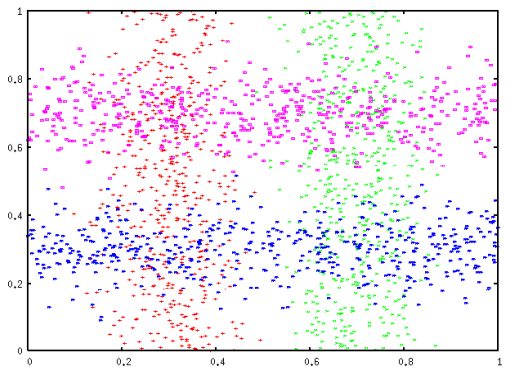


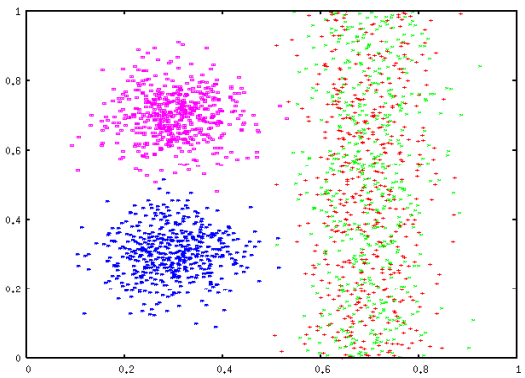
General Problems & Challenges

- again: different attributes are relevant for different clusters



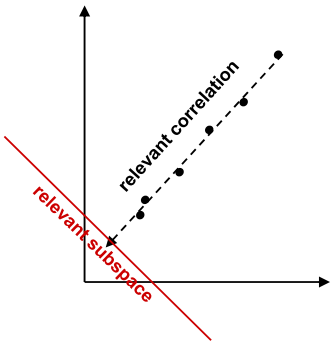






General Problems & Challenges

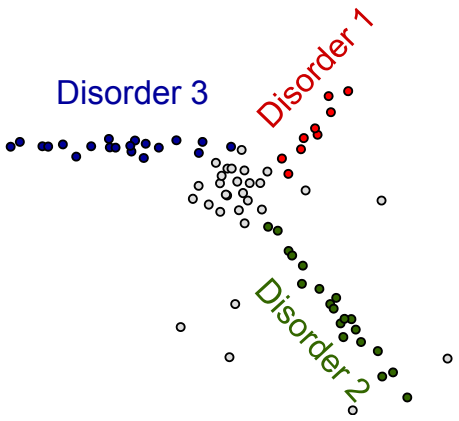
- Fourth aspect: *Correlation among attributes*
  - A subset of features may be correlated
  - Groups of similar ("dense") points may be identified when considering this correlation of features only



  - Different correlations of attributes may be relevant for different clusters

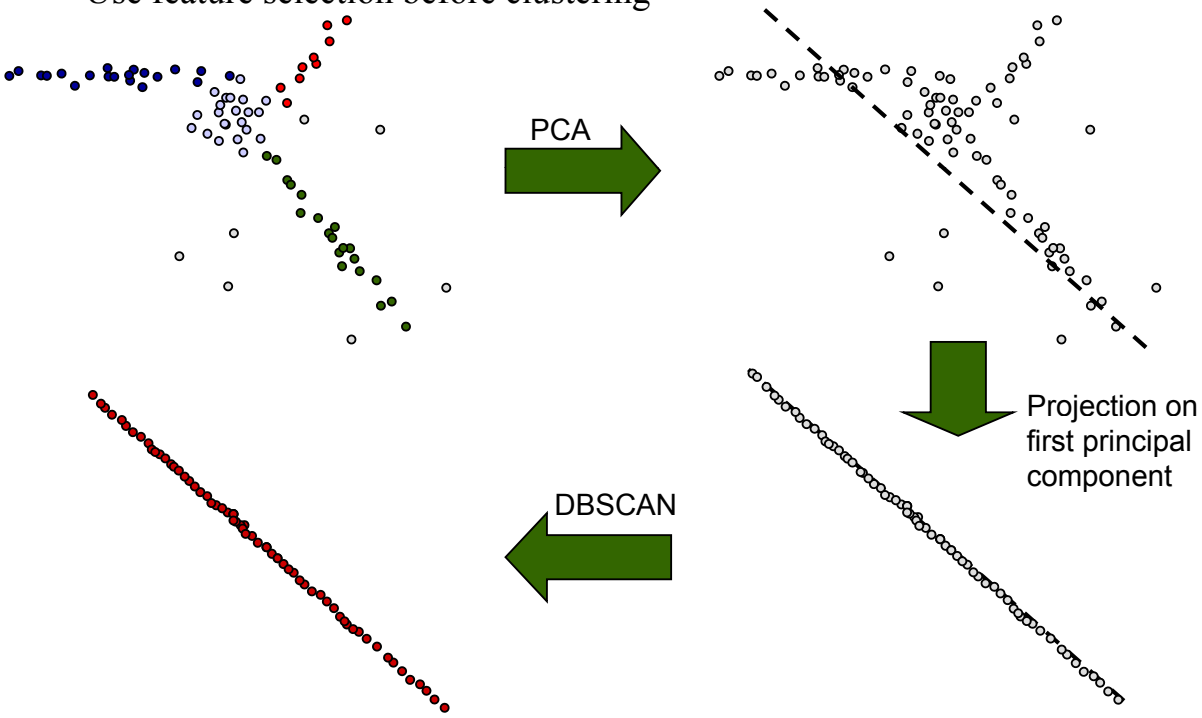
General Problems & Challenges

- Why not feature selection?
  - (Unsupervised) feature selection 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



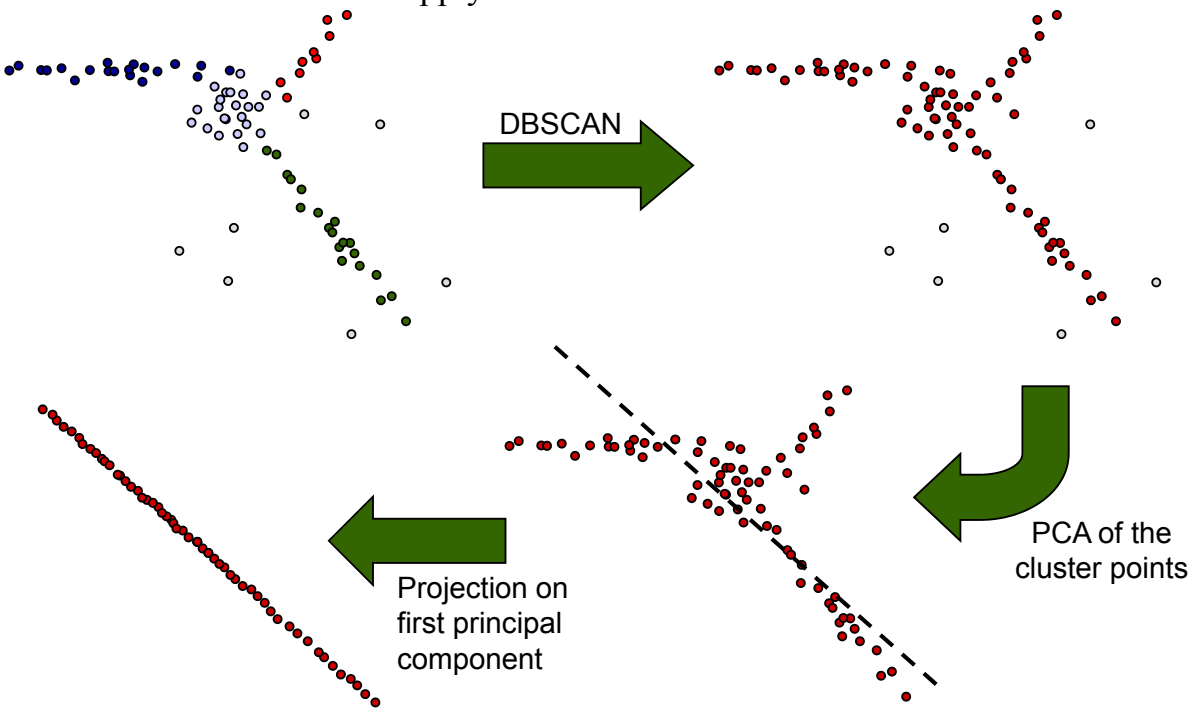
General Problems & Challenges

- Use feature selection before clustering



General Problems & Challenges

- Cluster first and then apply PCA



General Problems & Challenges

- Problem Summary
  - Curse of dimensionality/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

General Problems & Challenges

- 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]

General Problems & Challenges

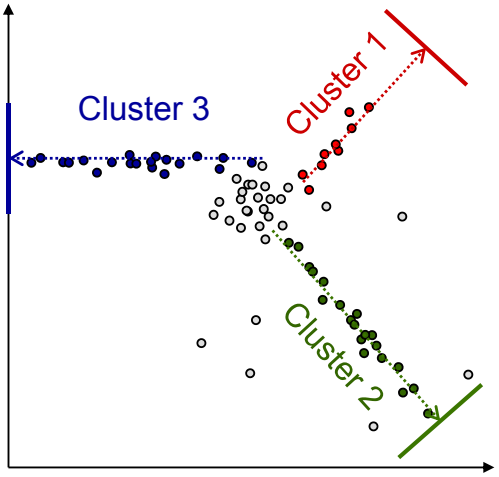
- Even worse: ***Circular Dependency***
  - Both challenges depend on each other
  - In order to determine the correct subspace of a cluster, we need to know (at least some) cluster members
  - In order to determine the correct cluster memberships, we need to know the subspaces of all clusters

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

    simultaneously

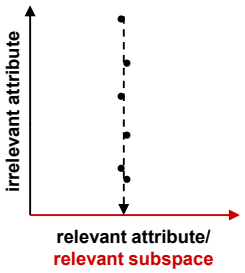
General Problems & Challenges

- Solution: integrate variance / covariance analysis into the clustering process
  - Variance analysis:
    - Find clusters in axis-parallel subspaces
    - Cluster members exhibit low variance along the relevant dimensions
  - Covariance/correlation analysis:
    - Find clusters in arbitrarily oriented subspaces
    - Cluster members exhibit a low covariance w.r.t. a given combination of the relevant dimensions (i.e. a low variance along the dimensions of the arbitrarily oriented subspace corresponding to the given combination of relevant attributes)

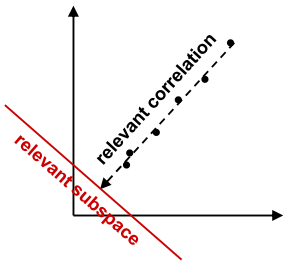


A First Taxonomy of Approaches

- So far, we can distinguish between
  - Clusters in axis-parallel subspaces
    (common assumption to restrict the search space)
    Approaches are usually called
    - "subspace clustering algorithms"
    - "projected clustering algorithms"
    - "bi-clustering or co-clustering algorithms"

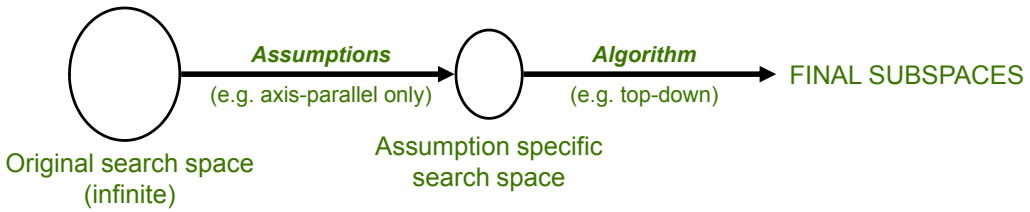


  - Clusters in arbitrarily oriented subspaces
    Approaches are usually called
    - "bi-clustering or co-clustering algorithms"
    - "pattern-based clustering algorithms"
    - "correlation clustering algorithms"

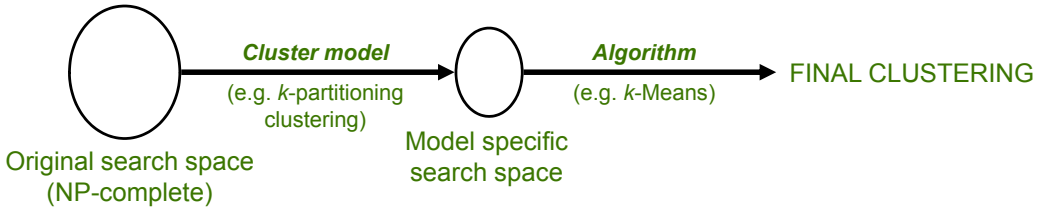


A First Taxonomy of Approaches

- A first big picture
  - We have two problems to solve
  - For both problems we need heuristics that have huge influence on the properties of the algorithms
    - ***Subspace search***



    - ***Cluster search***



A First Taxonomy of Approaches

- Note: this taxonomy considers only the subspace search space
- the clustering search space is equally important
- other important aspects for classifying existing approaches are e.g.
  - The underlying cluster model that usually involves
    - Input parameters
    - Assumptions on number, size, and shape of clusters
    - Noise (outlier) robustness
  - Determinism
  - Independence w.r.t. the order of objects/attributes
  - Assumptions on overlap/non-overlap of clusters/subspaces
  - Efficiency

Extensive survey: [KKZ09]
http://doi.acm.org/10.1145/1497577.1497578

Outline

Outline: Axis-parallel Subspace Clustering

- Challenges and Approaches
- Bottom-up Algorithms
- Top-down Algorithms
- Summary

Challenges

- What are we searching for?
  - Overlapping clusters: points may be grouped differently in different subspaces
    => "***subspace clustering***"
  - Disjoint partitioning: assign points uniquely to clusters (or noise)
    => "***projected clustering***"

Notes:

- The terms **subspace** clustering and **projected** clustering are not used in a unified or consistent way in the literature
- These two problem definitions are products of the presented algorithms:
  - The first "projected clustering algorithm" integrates a distance function accounting for clusters in subspaces into a "flat" clustering algorithm (k-medoid) => DISJOINT PARTITION
  - The first "subspace clustering algorithm" is an application of the APRIORI algorithm => ALL CLUSTERS IN ALL SUBSPACES

Challenges

- The naïve solution:
  - Given a cluster criterion, explore each possible subspace of a *d*-dimensional dataset whether it contains a cluster
  - Runtime complexity: depends on the search space, i.e. the number of all possible subspaces of a *d*-dimensional data set
  - What is the number of all possible subspaces of a *d*-dimensional data set?

Challenges

- What is the number of all possible subspaces of a *d*-dimensional data set?
  - How many *k*-dimensional subspaces ($k \leq d$) do we have?

    The number of all *k*-tupels of a set of *d* elements is

$$\binom{d}{k}$$

  - Overall:

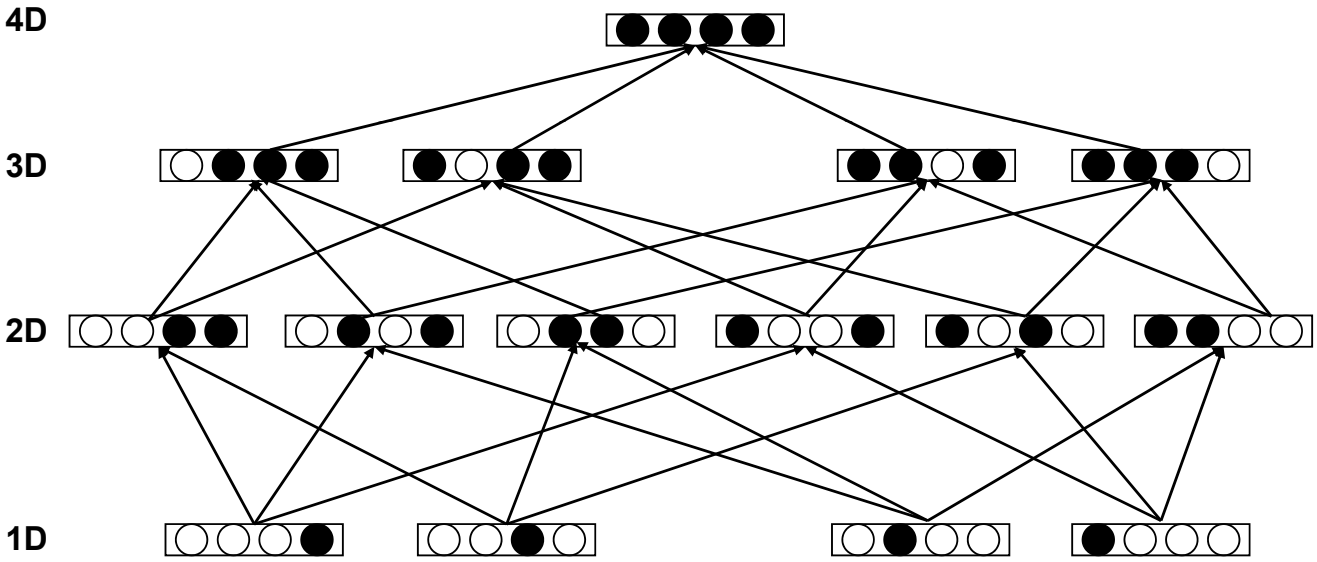
$$\sum_{k=1}^{d} \binom{d}{k} = 2^d - 1$$

  - So the naïve solution is computationally infeasible:

    We face a runtime complexity of $O(2^d)$

Challenges

- Search space for $d = 4$



Wiederholung: Frequent-Itemset-Mining

Gegeben:

- eine Menge von Items I
- eine Transaktionsdatenbank DB über I
- Ein absoluter support-Grenzwert s

- Finde alle frequent Itemsets in DB, d.h.
  $\{X \subseteq I \mid support(X) \geq s\}$

TransaktionsID	Items
2000	A,B,C
1000	A,C
4000	A,D
5000	B,E,F

Support der 1-Itemsets:
(A): 75%, (B), (C): 50%, (D), (E), (F): 25%,
Support der 2-Itemsets:
(A, C): 50%,
(A, B), (A, D), (B, C), (B, E), (B, F), (E, F): 25%

Wiederholung: Frequent-Itemset-Mining

„naiver“ Algorithmus: zähle die Häufigkeit aller k-elementigen Teilmengen von I - ineffizient, da $\binom{|I|}{k}$ solcher Teilmengen

Gesamt-Kosten: $O(2^{|I|})$

=> Apriori-Algorithmus und Varianten, Tiefensuch-Algorithmen

Wiederholung: Frequent-Itemset-Mining

tid	X_T
1	{Bier, Chips, Wein}
2	{Bier, Chips}
3	{Pizza, Wein}
4	{Chips, Pizza}

Transaktionsdatenbank

Itemset	Cover	Sup.	Freq.
{}	{1,2,3,4}	4	100 %
{Bier}	{1,2}	2	50 %
{Chips}	{1,2,4}	3	75 %
{Pizza}	{3,4}	2	50 %
{Wein}	{1,3}	2	50 %
{Bier, Chips}	{1,2}	2	50 %
{Bier, Wein}	{1}	1	25 %
{Chips, Pizza}	{4}	1	25 %
{Chips, Wein}	{1}	1	25 %
{Pizza, Wein}	{3}	1	25 %
{Bier, Chips, Wein}	{1}	1	25 %

Monotonie Eigenschaft von frequent Itemsets

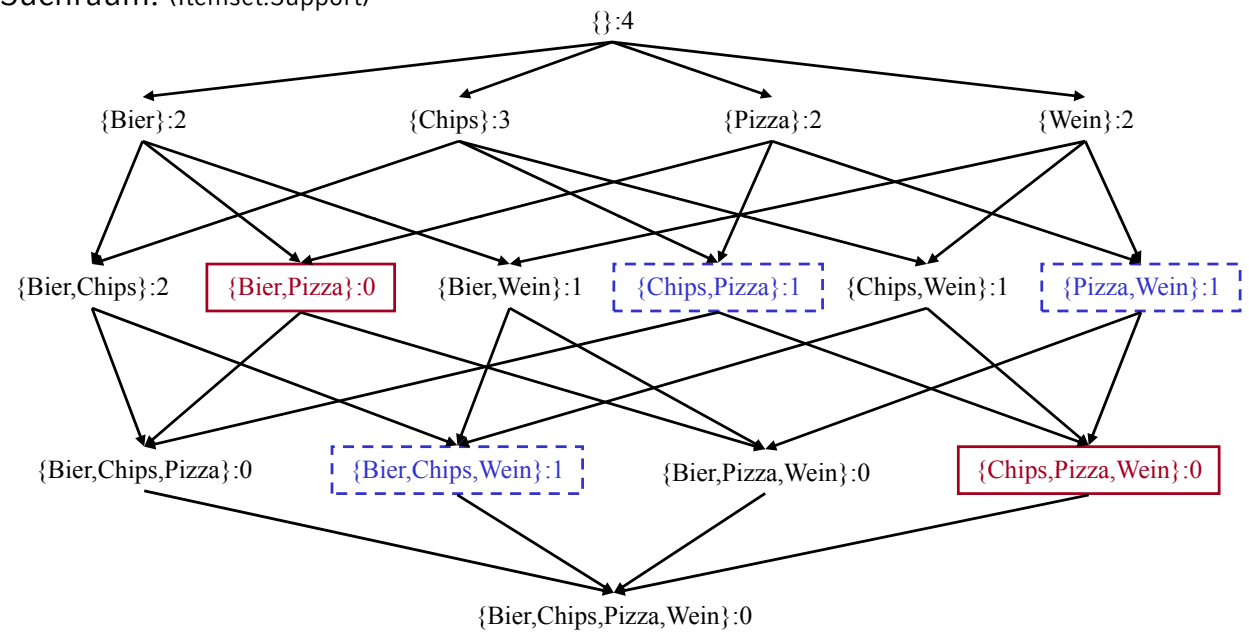
wenn X frequent ist, sind alle Teilmengen $Y \subseteq X$ auch frequent

Umkehrung:

wenn X nicht frequent, können alle Itemsets die X als Teilmenge enthalten auch nicht mehr frequent sein!

Wiederholung: Frequent-Itemset-Mining

Suchraum: (Itemset:Support)

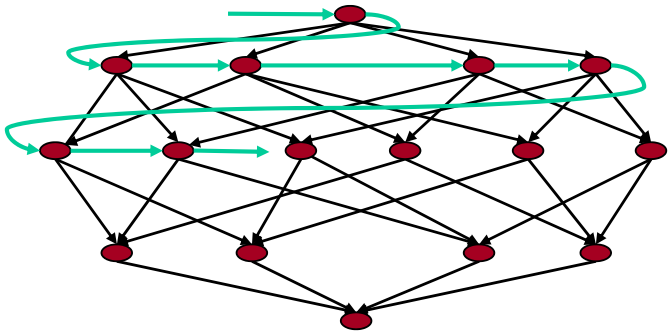


Positive Rand-Itemsets | Minimaler Support $s = 1$ | Negative Rand-Itemsets

Wiederholung: Frequent-Itemset-Mining:

Apriori Algorithmus [AS94]

- zuerst die ein-elementigen Frequent Itemsets bestimmen, dann die zwei-elementigen und so weiter (Breitensuche)



Finden von k+1-elementigen Frequent Itemsets:

- nur solche k+1-elementigen Itemsets betrachten, für die alle k-elementigen Teilmengen häufig auftreten
- Bestimmung des Supports durch Zählen auf der Datenbank (ein Scan)

Approaches

- Basically, there are two different ways to efficiently navigate through the search space of possible subspaces
  - Bottom-up:
    - If the cluster criterion implements the downward closure, one can use any bottom-up frequent itemset mining algorithm (e.g. APRIORI [AS94])
    - *Key*: downward-closure property OR merging-procedure
  - Top-down:
    - The search starts in the full *d*-dimensional space and iteratively learns for each point or each cluster the correct subspace
    - *Key*: procedure to learn the correct subspace

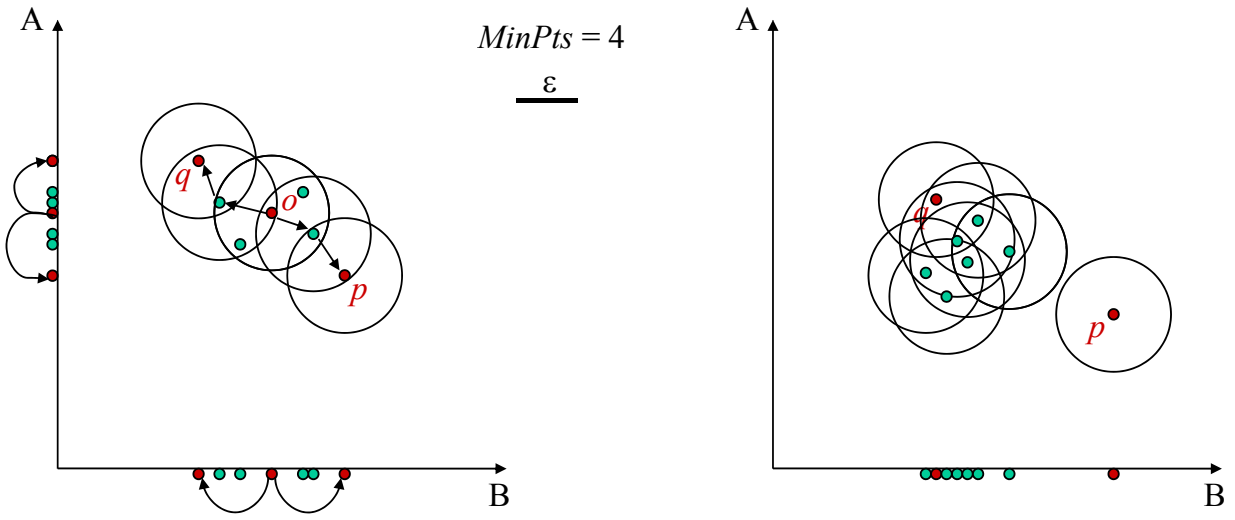
Bottom-up Algorithms

- Rational:
  - Start with 1-dimensional subspaces and merge them to compute higher dimensional ones
  - Most approaches transfer the problem of subspace search into frequent item set mining
    - The cluster criterion must implement the downward closure property
      - If the criterion holds for any *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*
    - Apply any frequent itemset mining algorithm (e.g. APRIORI)
  - Some approaches use other search heuristics 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

if C is a dense set of points in subspace S,
then C is also a dense set of points in any subspace $T \subset S$



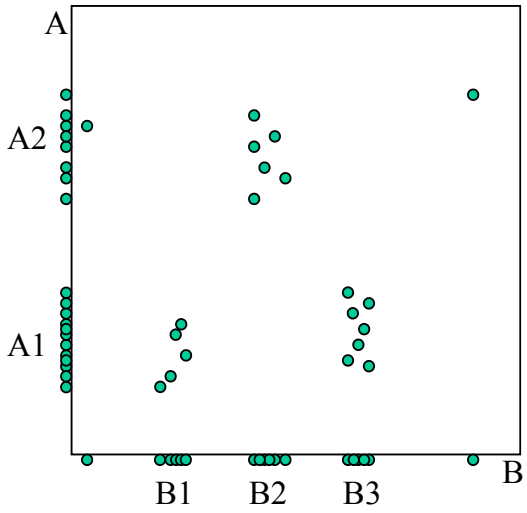
p and q density-connected in {A,B}, {A} and {B}

p and q not density-connected in {B} and {A,B}

Bottom-up Algorithms

- Downward-closure property

the reverse implication does not hold necessarily



Bottom-up Algorithms

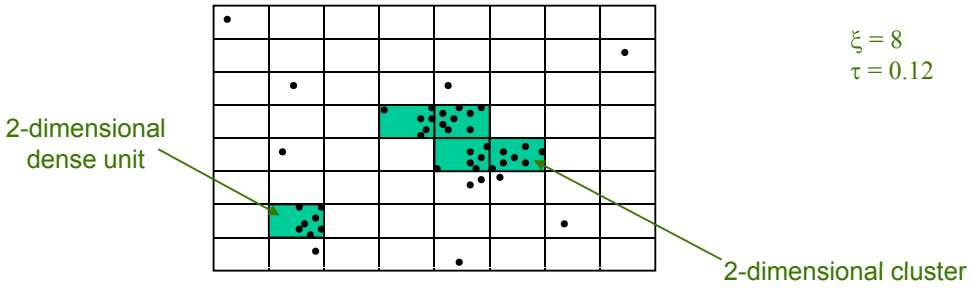
- The key limitation: ***global density thresholds***
  - Usually, the cluster criterion relies on density
  - In order to ensure the downward closure property, the density threshold must be fixed
  - Consequence: the points in a 20-dimensional subspace cluster must be as dense as in a 2-dimensional cluster
  - This is a rather optimistic assumption since the data space grows exponentially with increasing dimensionality
  - 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

Bottom-up Algorithms

- Properties (APRIORI-style algorithms):
  - Generation of all clusters in all subspaces => overlapping clusters
  - Subspace clustering algorithms usually rely on bottom-up subspace search
  - Worst-case: complete enumeration of all subspaces, i.e. $O(2^d)$ time
  - Complete results

Bottom-up Algorithms

- CLIQUE [AGGR98]
  - Cluster model
    - Each dimension is partitioned into ξ equi-sized intervals called units
    - A *k*-dimensional unit is the intersection of *k* 1-dimensional units (from different dimensions)
    - A unit *u* is considered dense if the fraction of all data points in *u* exceeds the threshold τ
    - A cluster is a maximal set of connected dense units



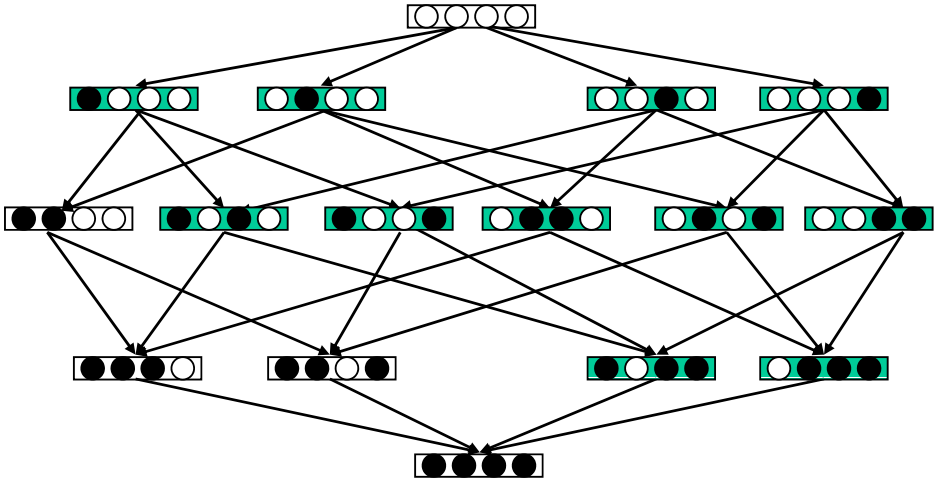
Bottom-up Algorithms

- Downward-closure property holds for dense units
- Algorithm
  - All dense cells are computed using APRIORI-style search
  - A heuristic based on the coverage of a subspace is used to further prune units that are dense but are in less interesting subspaces

    (coverage of subspace *S* = fraction of data points covered by the dense units of *S*)
  - All connected dense units in a common subspace are merged to generate the subspace clusters

Bottom-up Algorithms

- Discussion
  - Input: ξ and τ specifying the density threshold
  - Output: *all* clusters in *all* subspaces, clusters may overlap
  - Uses a fixed density threshold for all subspaces (in order to ensure the downward closure property)
  - Simple but efficient cluster model



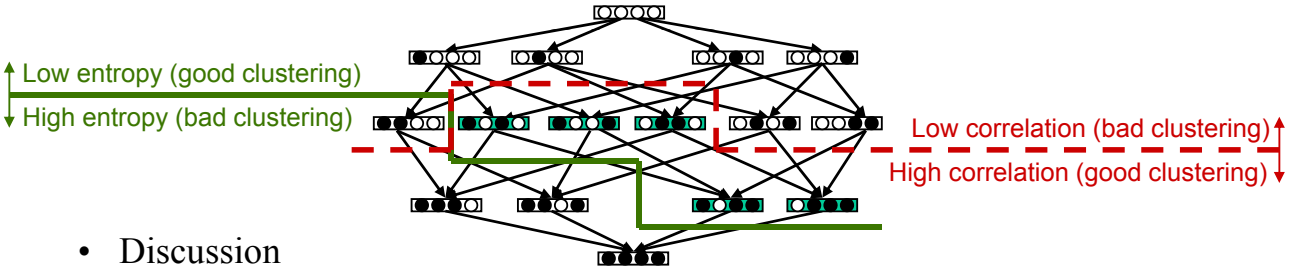
Bottom-up Algorithms

- ENCLUS [CFZ99]
  - Cluster model uses a fixed grid similar to CLIQUE
  - Algorithm first searches for subspaces rather than for dense units
  - Subspaces are evaluated following three criteria
    - Coverage (see CLIQUE)
    - Entropy
      - Indicates how densely the points are packed in the corresponding subspace (the higher the density, the lower the entropy)
      - Implements the downward closure property
    - Correlation
      - Indicates how the attributes of the corresponding subspace are correlated to each other
      - Implements an upward closure property

Bottom-up Algorithms

- Subspace search algorithm is bottom-up similar to CLIQUE but determines subspaces having

$$\textit{Entropy} < \omega \quad \text{and} \quad \textit{Correlation} > \varepsilon$$

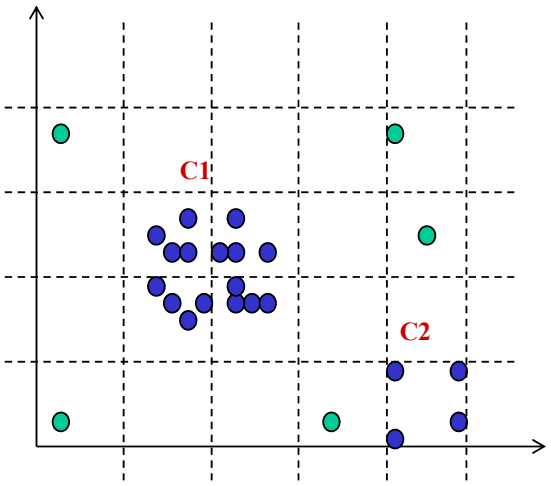


- Discussion
  - Input: thresholds ω and ε
  - Output: all subspaces that meet the above criteria (far less than CLIQUE), clusters may overlap
  - Uses fixed thresholds for entropy and correlation for all subspaces
  - Simple but efficient cluster model

Bottom-up Algorithms

- drawback of grid-based approaches:
  choice of ξ and τ

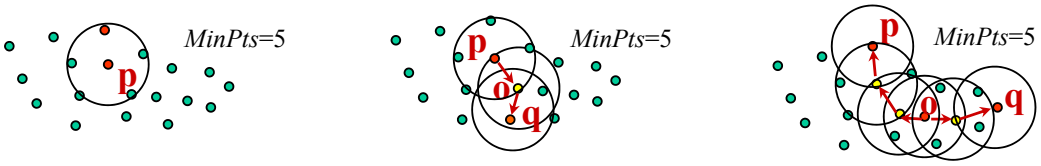
  cluster for τ = 4
  (is C2 a cluster?)
  for τ > 4: no cluster found
  (esp. C1 is lost)



- motivation for density-based approaches

Bottom-up Algorithms

- SUBCLU [KKK04]
  - Cluster model:
    - Density-based cluster model of DBSCAN [EKSX96]
    - 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



    - Detects clusters of arbitrary size and shape (in the corresponding subspaces)
  - Downward-closure property holds for sets of density-connected points

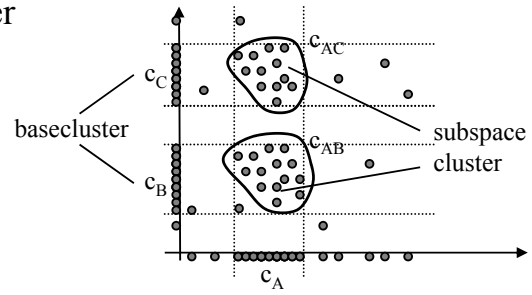
Bottom-up Algorithms

- Algorithm
  - All subspaces that contain any density-connected set are computed using the bottom-up approach
  - 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

- FIRES[KKRW05]
  - Proposes a bottom-up approach that uses different heuristic for subspace search
  - 3-Step algorithm
    - Starts with 1-dimensional clusters called *base clusters* (generated by applying any traditional clustering algorithm to each 1-dimensional subspace)
    - Merges these clusters to generate subspace cluster approximations by applying a clustering of the base clusters using a variant of DBSCAN (similarity between two clusters $C1$ and $C2$ is defined by $|C1 \cap C2|$)
    - Refines the resulting subspace cluster approximations
      - Apply any traditional clustering algorithm on the points within the approximations
      - Prune lower dimensional projections

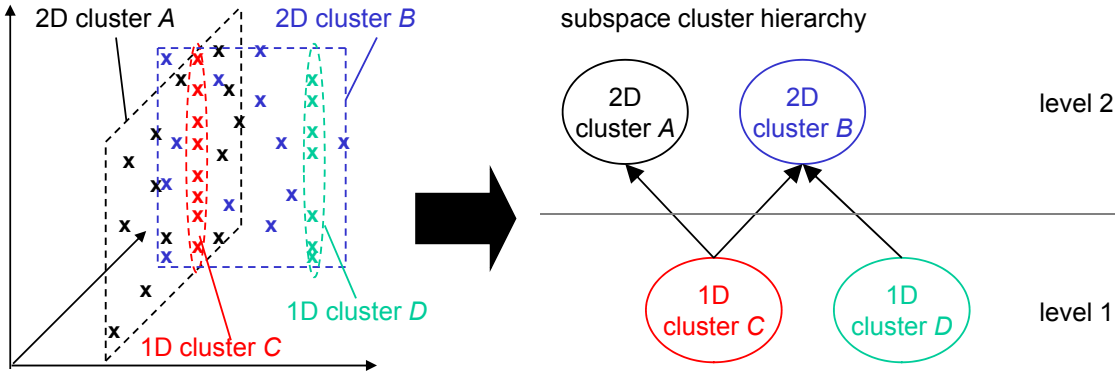


Bottom-up Algorithms

- Discussion
  - Input:
    - Three parameters for the merging procedure of base clusters
    - Parameters for the clustering algorithm to create base clusters and for refinement
  - Output: clusters in maximal dimensional subspaces, clusters may overlap
  - Allows overlapping clusters (subspace clustering) but avoids complete enumeration; runtime of the merge step is O(d)
  - Output heavily depends on the accuracy of the merge step which is a rather simple heuristic and relies on three sensitive parameters
  - Cluster model can be chosen by the user

Bottom-up Algorithms

- DiSH [ABK+07a]
  - Idea:
    - Not considered so far: lower dimensional clusters embedded in higher dimensional ones



    - Now: find hierarchies of subspace clusters
    - Integrate a proper distance function into hierarchical clustering

Bottom-up Algorithms

- Distance measure that captures subspace hierarchies assigns
  - 1 if both points share a common 1D subspace cluster
  - 2 if both points share a common 2D subspace cluster
  - …
- Sharing a common k-dimensional subspace cluster means
  - Both points are associated to the same k-dimensional subspace cluster
  - Both points are associated to different (k-1)-dimensional subspace clusters that intersect or are parallel (but not skew)
- This distance is based on the subspace dimensionality of each point *p* representing the (highest dimensional) subspace in which *p* fits best
  - Analyze the local ε-neighborhood of *p* along each attribute *a*
    => if it contains more than μ points: *a* is interesting for *p*
  - Combine all interesting attributes such that the ε-neighborhood of *p* in the subspace spanned by this combination still contains at least μ points (e.g. use APRIORI algorithm or best-first search)

Bottom-up Algorithms

- Discussion
  - Input: ε and μ specify the density threshold for computing the relevant subspaces of a point
  - Output: a hierarchy of subspace clusters displayed as a graph, clusters may overlap (but only w.r.t. the hierarchical structure!)
  - Does not rely on a global density threshold
  - Complex but costly cluster model

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
  - 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

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 each 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***

Top-down Algorithms

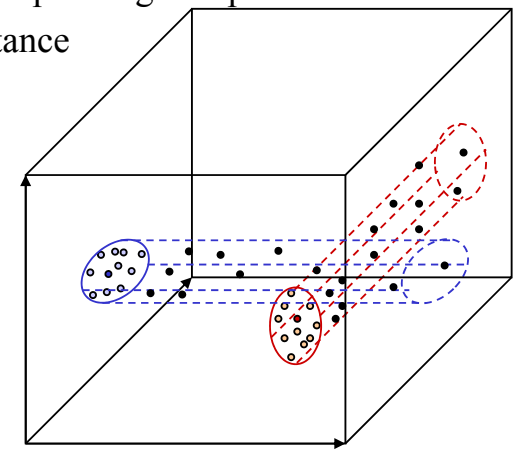
- Discussion:
  - Locality assumption
    - Recall the effects of the curse of dimensionality on concepts like "local neighborhood"
    - The neighborhood will most likely contain a lot of noise points
  - Random sampling
    - The larger the number of total points compared to the number of cluster points is, the lower the probability that cluster members are sampled
  - Consequence for both approaches
    - The learning procedure is often misled by these noise points

Top-down Algorithms

- Properties:
  - Simultaneous search for the "best" partitioning of the data points and the "best" subspace for each partition => disjoint partitioning
  - Projected clustering algorithms usually rely on top-down subspace search
  - Worst-case:
    - Usually complete enumeration of all subspaces is avoided
    - Worst-case costs are typically in $O(d^2)$

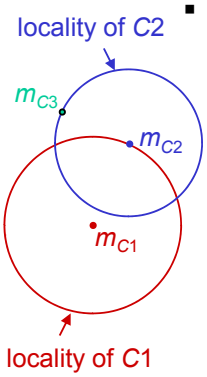
Top-down Algorithms

- PROCLUS [APW+99]
  - *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 subspaces of the medoids)
    - Points that have a large distance to its nearest medoid are classified as noise



Top-down Algorithms

- 3-Phase Algorithm
  - Initialization of cluster medoids
    - A superset M of $b \cdot k$ medoids is computed from a sample of $a \cdot k$ data points such that these medoids are well separated
    - k randomly chosen medoids from M are the initial cluster representatives
    - Input parameters a and b are introduced for performance reasons
  - Iterative phase works similar to any k-medoid clustering
    - Approximate subspaces for each cluster C
      - » The locality of C includes all points that have a distance to the medoid of C less than the distance between the medoid of C and the medoid of the neighboring cluster
      - » Compute standard deviation of distances from the medoid of C to the points in the locality of C along each dimension
      - » Add the dimensions with the smallest standard deviation to the relevant dimensions of cluster C such that
        - in summary $k \cdot l$ dimensions are assigned to all clusters
        - each cluster has at least 2 dimensions assigned



Top-down Algorithms

- Reassign points to clusters
  - » Compute for each point the distance to each medoid taking only the relevant dimensions into account
  - » Assign points to a medoid minimizing these distances
- Termination (criterion not really clearly specified in [APW+99])
  - » 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)

- Refinement
  - Reassign subspaces to medoids as above (but use only the points assigned to each cluster rather than the locality of each cluster)
  - Reassign points to medoids; points that are not in the locality of their corresponding medoids are classified as noise

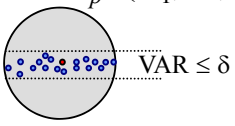
Top-down Algorithms

- Discussion
  - Input:
    - Number of clusters k
    - Average dimensionality of clusters l
    - Factor a to determine the size of the sample in the initialization step
    - Factor b to determine the size of the candidate set for the medoids
  - Output: partitioning of points into k disjoint clusters and noise, each cluster has a set of relevant attributes specifying its subspace
  - Relies on cluster-based locality assumption: subspace of each cluster is learned from local neighborhood of its medoid
  - Biased to find l-dimensional subspace clusters
  - Simple but efficient cluster model

Top-down Algorithms

- PreDeCon [BKKK04]
  - Cluster model:
    - Density-based cluster model of DBSCAN [EKSX96] adapted to projected clustering
      - For each point p a subspace preference indicating the subspace in which p clusters best is computed
      - ε-neighborhood of a point p is constrained by the subspace preference of p
      - Core points have at least *MinPts* other points in their ε-neighborhood
      - Density connectivity is defined based on core points
      - Clusters are maximal sets of density connected points
    - Subspace preference of a point p is d-dimensional vector $w_p=(w_1,\ldots,w_d)$, entry w_{pi} represents dimension i with

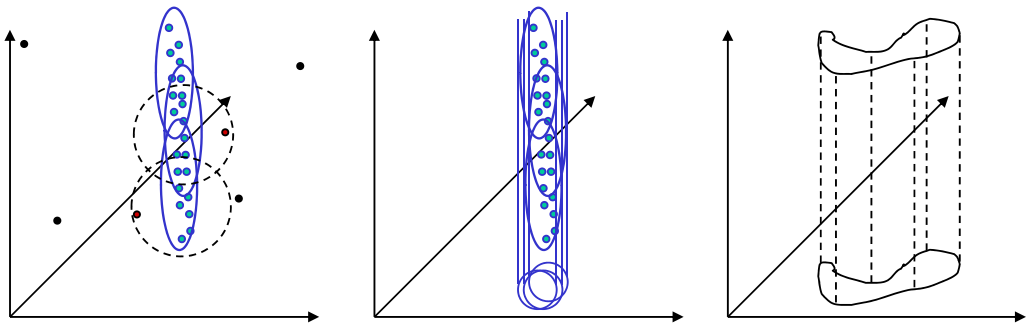
$$w_{pi} = \begin{cases} 1 & if \quad \text{VAR}_i > \delta \\ \kappa & if \quad \text{VAR}_i \leq \delta \end{cases}$$



VAR_i is the variance of the ε-neighborhood of p in the entire d-dimensional space, δ and κ >> 1 are input parameters

Top-down Algorithms

- Algorithm
  - PreDeCon applies DBSCAN with a weighted Euclidean distance function
    $dist_p(p,q) = \sqrt{\sum_i w_{pi} \cdot (p_i - q_i)^2}$
    $dist(p,q) = max\{dist_p(p,q), dist_q(q,p)\}$
  - Instead of shifting spheres (full-dimensional Euclidean ε-neighborhoods), clusters are expanded by shifting axis-parallel ellipsoids (weighted Euclidean ε-neighborhoods)
  - Note: In the subspace of the cluster (defined by the preference of its members), we shift spheres (but this intuition may be misleading)



Top-down Algorithms

- Discussion
  - Input:
    - δ and κ to determine the subspace preference
    - λ specifies the maximal dimensionality of a subspace cluster
    - ε and *MinPts* specify the density threshold
  - Output: a disjoint partitioning of data into clusters and noise
  - Relies on instance-based locality assumption: subspace preference of each point is learned from its local neighborhood
  - Advanced but costly cluster model

Summary

- The big picture
  - Basic assumption:
    "subspace search space is limited to axis-parallel subspaces"
  - Algorithmic view:
    - Bottom-up subspace search
    - Top-down subspace search
  - Problem-oriented view:
    - Subspace clustering (overlapping clusters)
    - Projected clustering (disjoint partitioning)

Summary

- How do both views relate?
  - Subspace clustering algorithms compute overlapping clusters
    - Many approaches compute all clusters in all subspaces
      - These methods usually implement a bottom-up search strategy á la itemset mining
      - These methods usually rely on global density thresholds to ensure the downward closure property
      - These methods usually do not rely on the locality assumption
      - These methods usually have a worst case complexity of $O(2^d)$
    - Other focus on maximal dimensional subspace clusters
      - These methods usually implement a bottom-up search strategy based on simple but efficient heuristics
      - These methods usually do not rely on the locality assumption
      - These methods usually have a worst case complexity of at most $O(d^2)$

Summary

- The big picture
  - Projected clustering algorithms compute a disjoint partitioning of the data
    - They usually implement a top-down search strategy
    - They usually rely on the locality assumption
    - They usually do not rely on global density thresholds
    - They usually scale at most quadratic in the number of dimensions

Outline

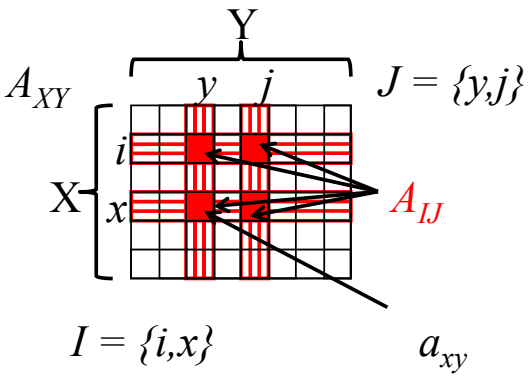
Outline: Pattern-based Clustering

- Challenges and Approaches, Basic Models for
  - Constant Biclusters
  - Biclusters with Constant Values in Rows or Columns
  - Pattern-based Clustering: Biclusters with Coherent Values
  - Biclusters with Coherent Evolutions
- Algorithms for
  - Constant Biclusters
  - Pattern-based Clustering: Biclusters with Coherent Values
- Summary

Challenges and Approaches, Basic Models

Pattern-based clustering relies on patterns in the data matrix.

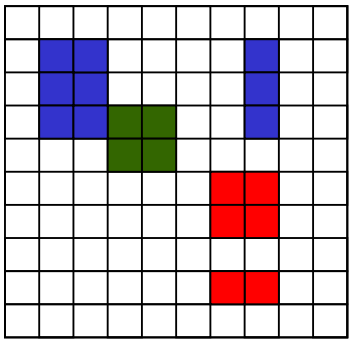
- Simultaneous clustering of rows and columns of the data matrix (hence *bi*clustering).
  - Data matrix $\boldsymbol{A}$ = (X,Y) with set of rows X and set of columns Y
  - a_{xy} is the element in row x and column y.
  - submatrix A_{IJ} = (I,J) with subset of rows I ⊆ X and subset of columns J ⊆ Y contains those elements a_{ij} with $i \in$ I und $j \in$ J



Challenges and Approaches, Basic Models

General aim of biclustering approaches:

Find a set of submatrices $\{(I_1,J_1),(I_2,J_2),...,(I_k,J_k)\}$ of the matrix $\boldsymbol{A}=(X,Y)$ (with $I_i \subseteq X$ and $J_i \subseteq Y$ for $i = 1,...,k$) where each submatrix (= bicluster) meets a given homogeneity criterion.



Challenges and Approaches, Basic Models

- Some values often used by bicluster models:
  - mean of row i:

$$a_{iJ} = \frac{1}{|J|}\sum_{j\in J} a_{ij}$$

  - mean of column j:

$$a_{Ij} = \frac{1}{|I|}\sum_{i\in I} a_{ij}$$

  - mean of all elements:

$$a_{IJ} = \frac{1}{|I||J|}\sum_{i\in I, j\in J} a_{ij}$$

$$= \frac{1}{|J|}\sum_{j\in J} a_{Ij}$$

$$= \frac{1}{|I|}\sum_{i\in I} a_{iJ}$$

Challenges and Approaches, Basic Models

Different types of biclusters (cf. [MO04]):

- constant biclusters
- biclusters with
  - constant values on columns
  - constant values on rows
- biclusters with coherent values (aka. pattern-based clustering)
- biclusters with coherent evolutions

Challenges and Approaches, Basic Models

Constant biclusters

- all points share identical value in selected attributes.
- The constant value μ is a typical value for the cluster.
- Cluster model:

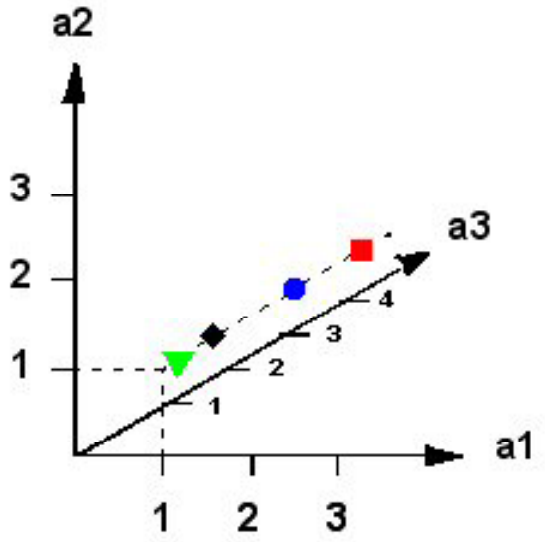
$$a_{ij} = \mu$$

- Obviously a special case of an axis-parallel subspace cluster.

Challenges and Approaches, Basic Models

- example – embedding 3-dimensional space:

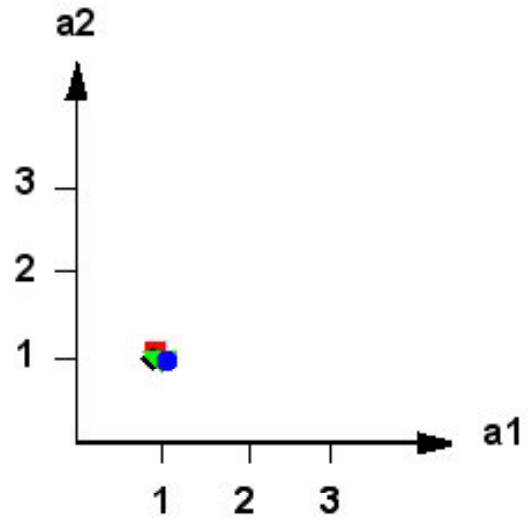
	a1	a2	a3
P1	1	1	3.5
P2	1	1	2.3
P3	1	1	0.2
P4	1	1	0.7



Challenges and Approaches, Basic Models

- example – 2-dimensional subspace:

	a1	a2
P1	1	1
P2	1	1
P3	1	1
P4	1	1

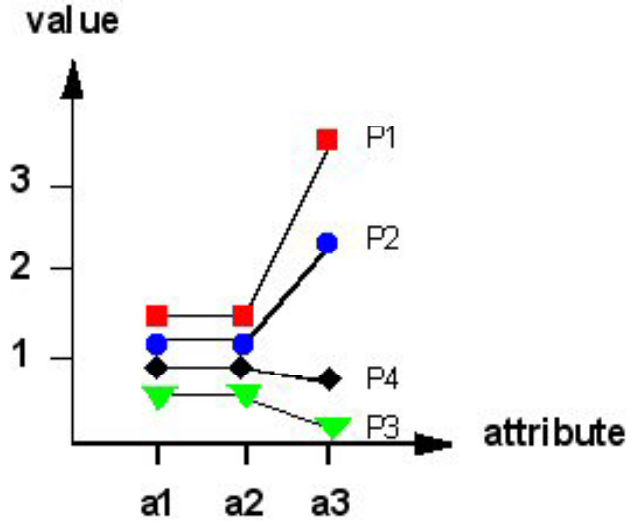


- points located on the bisecting line of participating attributes

Challenges and Approaches, Basic Models

- example – transposed view of attributes:

	a1	a2	a3
P1	1	1	3.5
P2	1	1	2.3
P3	1	1	0.2
P4	1	1	0.7



- pattern: identical constant lines

Challenges and Approaches, Basic Models

- real-world constant biclusters will not be perfect
- cluster model relaxes to:

$$a_{ij} \approx \mu$$

- Optimization on matrix $A = (X,Y)$ may lead to $|X| \cdot |Y|$ singularity-biclusters each containing one entry.
- Challenge: Avoid this kind of overfitting.

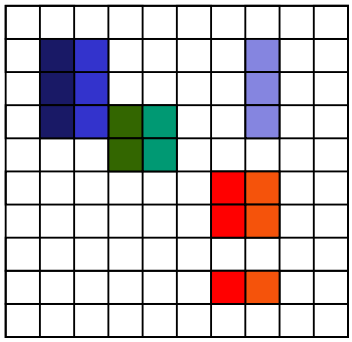
Challenges and Approaches, Basic Models

Biclusters with constant values on columns

- Cluster model for $\boldsymbol{A}_{IJ} = (I,J)$:

$$a_{ij} = \mu + c_j$$

$$\forall i \in I, j \in J$$

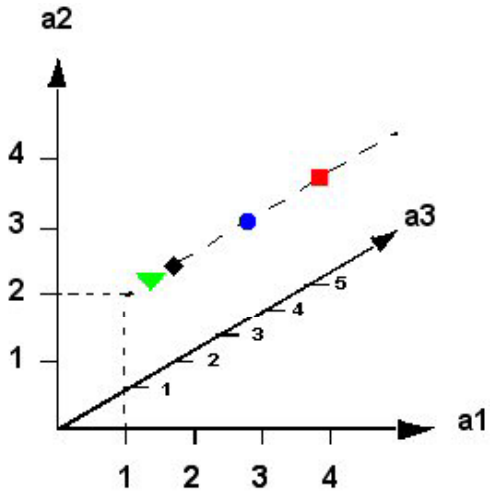


- adjustment value c_j for column $j \in J$
- results in axis-parallel subspace clusters

Challenges and Approaches, Basic Models

- example – 3-dimensional embedding space:

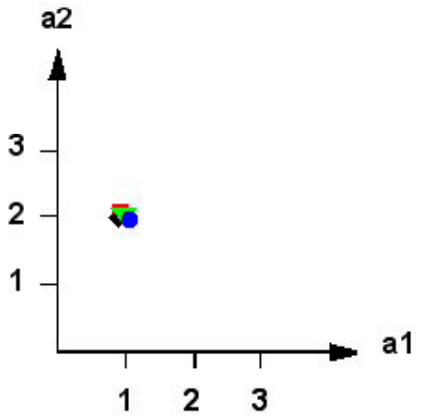
	a1	a2	a3
P1	1	2	3.5
P2	1	2	2.3
P3	1	2	0.2
P4	1	2	0.7



Challenges and Approaches, Basic Models

- example – 2-dimensional subspace:

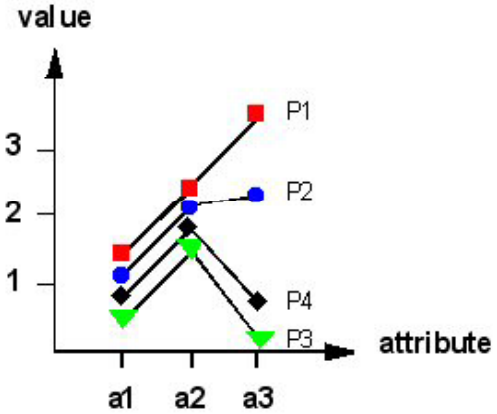
	a1	a2
P1	1	2
P2	1	2
P3	1	2
P4	1	2



Challenges and Approaches, Basic Models

- example – transposed view of attributes:

	a1	a2	a3
P1	1	2	3.5
P2	1	2	2.3
P3	1	2	0.2
P4	1	2	0.7



- pattern: identical lines

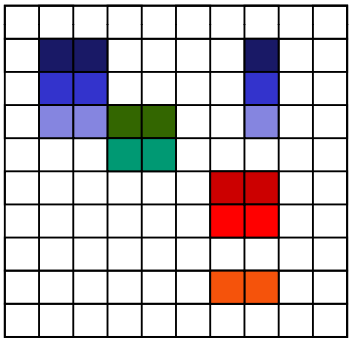
Challenges and Approaches, Basic Models

Biclusters with constant values on rows

- Cluster model for A_{IJ} = (I,J):

$$a_{ij} = \mu + r_i$$

$$\forall i \in I, j \in J$$

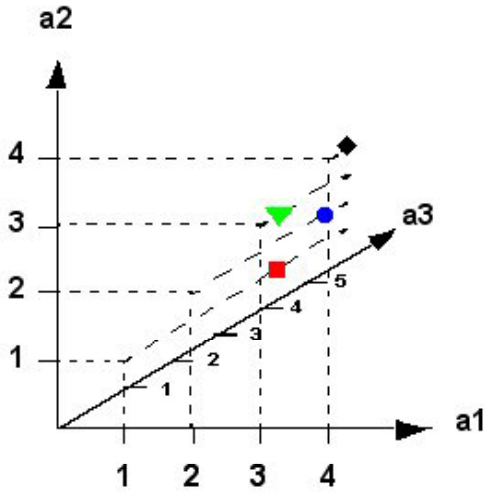


- adjustment value r_i for row $i \in I$

Challenges and Approaches, Basic Models

- example – 3-dimensional embedding space:

	a1	a2	a3
P1	1	1	3.5
P2	2	2	2.3
P3	3	3	0.2
P4	4	4	0.7

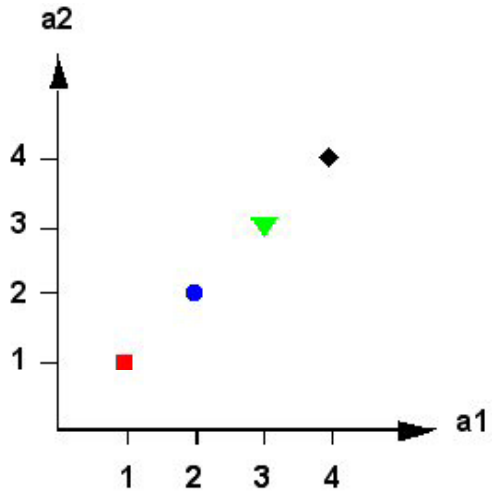


- in the embedding space, points build a sparse hyperplane parallel to irrelevant axes

Challenges and Approaches, Basic Models

- example – 2-dimensional subspace:

	a1	a2
P1	1	1
P2	2	2
P3	3	3
P4	4	4

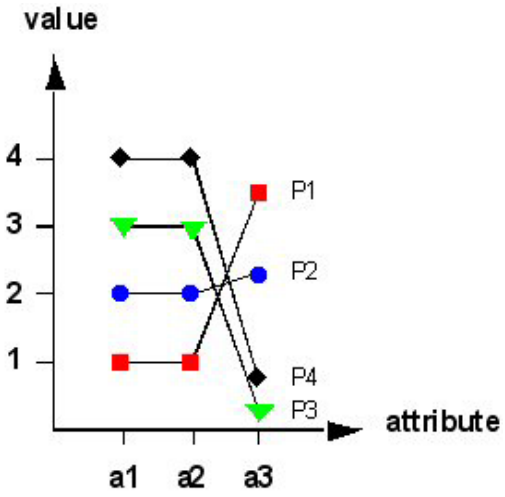


- points are accommodated on the bisecting line of participating attributes

Challenges and Approaches, Basic Models

- example – transposed view of attributes:

	a1	a2	a3
P1	1	1	3.5
P2	2	2	2.3
P3	3	3	0.2
P4	4	4	0.7



- pattern: parallel constant lines

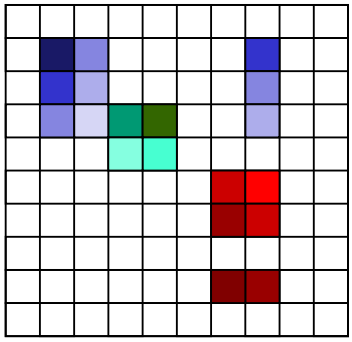
Challenges and Approaches, Basic Models

Biclusters with coherent values

- based on a particular form of covariance between rows and columns

$$a_{ij} = \mu + r_i + c_j$$

$$\forall i \in I, j \in J$$

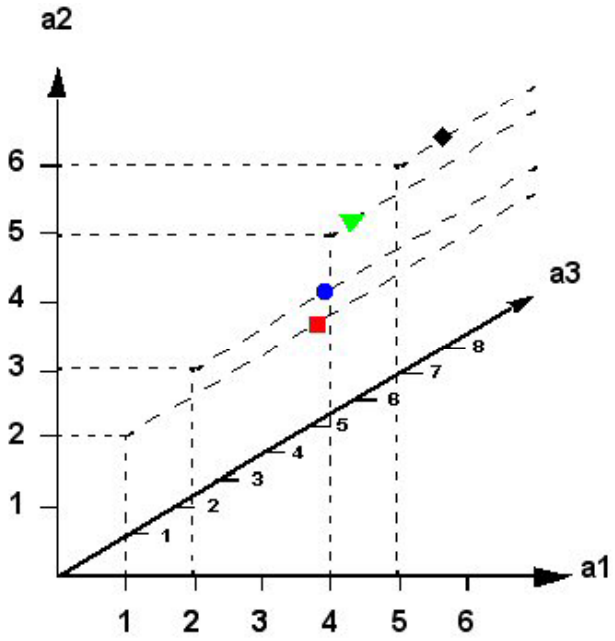


- special cases:
  - $c_j = 0$ for all j → constant values on rows
  - $r_i = 0$ for all i → constant values on columns

Challenges and Approaches, Basic Models

- embedding space: sparse hyperplane parallel to axes of irrelevant attributes

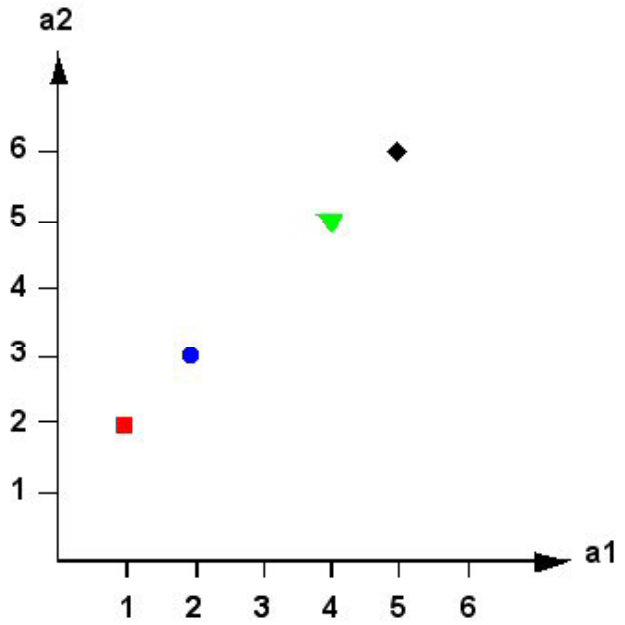
	a1	a2	a3
P1	1	2	3.5
P2	2	3	2.3
P3	4	5	0.2
P4	5	6	0.7



Challenges and Approaches, Basic Models

- subspace: increasing one-dimensional line

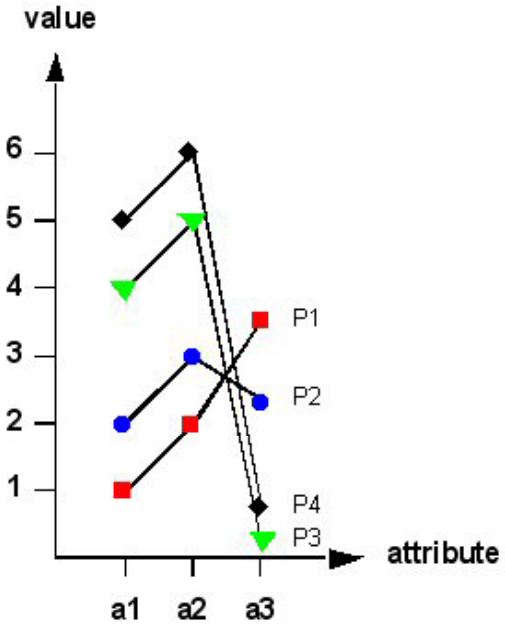
	a1	a2
P1	1	2
P2	2	3
P3	4	5
P4	5	6



Challenges and Approaches, Basic Models

- transposed view of attributes:

	a1	a2	a3
P1	1	2	3.5
P2	2	3	2.3
P3	4	5	0.2
P4	5	6	0.7

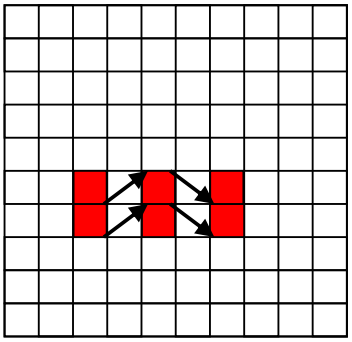


- pattern: parallel lines

Challenges and Approaches, Basic Models

Biclusters with coherent evolutions

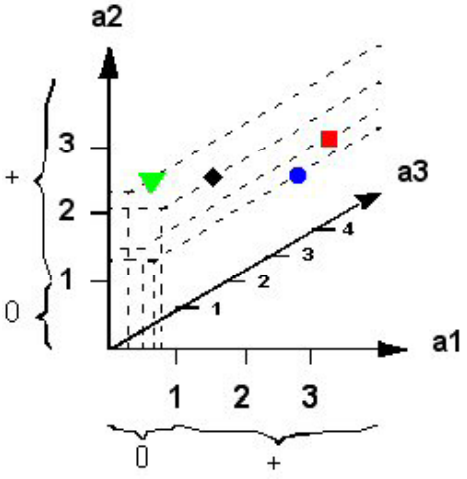
- for all rows, all pairs of attributes change simultaneously
  - discretized attribute space: coherent state-transitions
  - change in same direction irrespective of the quantity



Challenges and Approaches, Basic Models

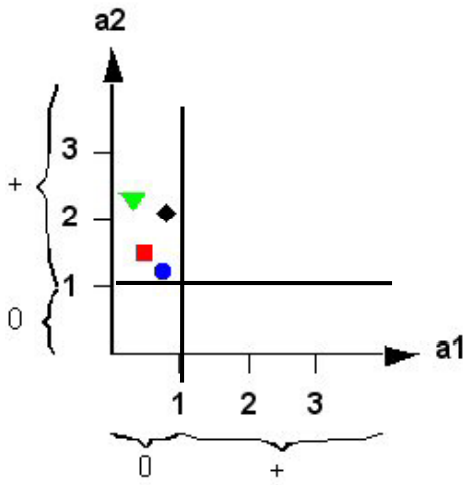
- Approaches with coherent state-transitions: [TSS02,MK03]
- reduces the problem to grid-based axis-parallel approach:

	a1	a2	a3
P1	0.5	1.5	3.5
P2	0.7	1.3	2.3
P3	0.3	2.3	0.2
P4	0.8	2.1	0.7

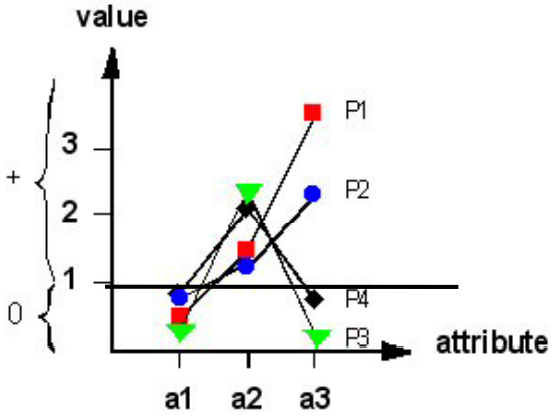


Challenges and Approaches, Basic Models

	a1	a2
P1	0	+
P2	0	+
P3	0	+
P4	0	+



	a1	a2	a3
P1	0.5	1.5	3.5
P2	0.7	1.3	2.3
P3	0.3	2.3	0.2
P4	0.8	2.1	0.7



pattern: all lines cross border between states (in the same direction)

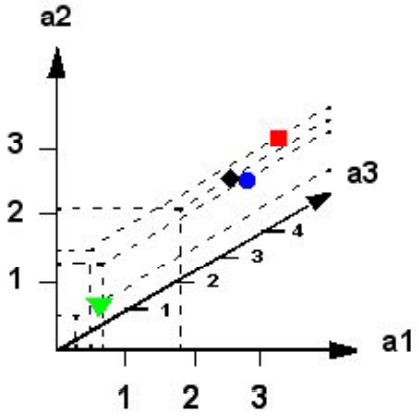
Challenges and Approaches, Basic Models

- change in same direction – general idea: find a subset of rows and columns, where a permutation of the set of columns exists such that the values in every row are increasing
- clusters do not form a subspace but rather half-spaces
- related approaches:
  - quantitative association rule mining [Web01,RRK04,GRRK05]
  - adaptation of formal concept analysis [GW99] to numeric data [Pfa07]

Challenges and Approaches, Basic Models

- example – 3-dimensional embedding space

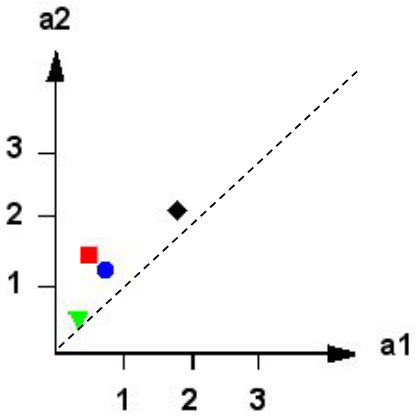
	a1	a2	a3
P1	0.5	1.5	3.5
P2	0.7	1.3	2.3
P3	0.3	0.5	0.2
P4	1.8	2.1	0.7



Challenges and Approaches, Basic Models

- example – 2-dimensional subspace

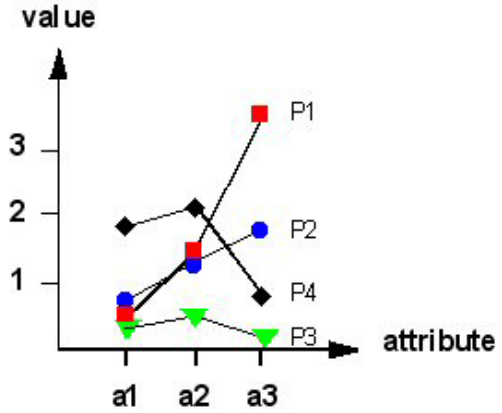
	a1	a2
P1	0.5	1.5
P2	0.7	1.3
P3	0.3	0.5
P4	1.8	2.1



Challenges and Approaches, Basic Models

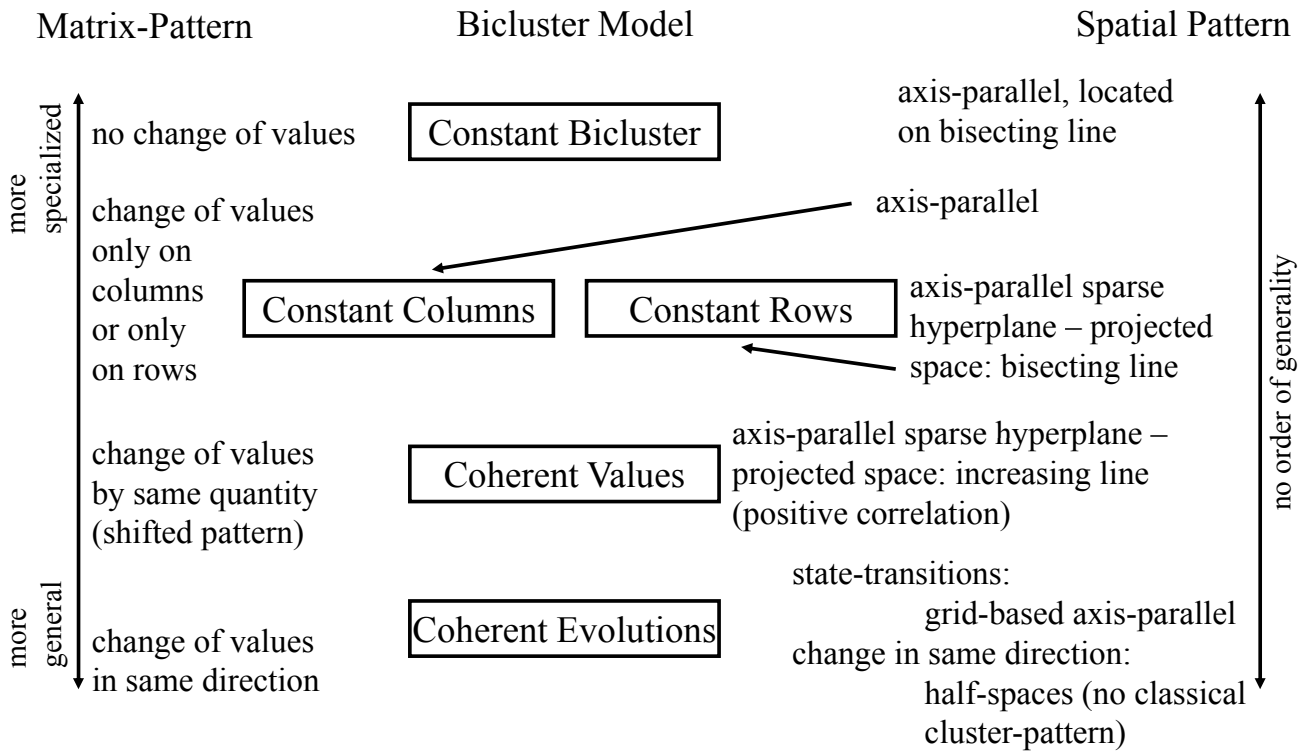
- example – transposed view of attributes

	a1	a2	a3
P1	0.5	1.5	3.5
P2	0.7	1.3	2.3
P3	0.3	0.5	0.2
P4	1.8	2.1	0.7



- pattern: all lines increasing

Challenges and Approaches, Basic Models



Algorithms for Constant Biclusters

- classical problem statement by Hartigan [Har72]
- quality measure for a bicluster: variance of the submatrix $\boldsymbol{A}_{IJ}$:

$$VAR\left(A_{IJ}\right) = \sum_{i \in I,\, j \in J} \left(a_{ij} - a_{IJ}\right)^2$$

- avoids partitioning into |X|·|Y| singularity-biclusters (optimizing the sum of squares) by comparing the reduction with the reduction expected by chance
- recursive split of data matrix into two partitions
- each split chooses the maximal reduction in the overall sum of squares for all biclusters

Biclusters with Constant Values in Rows or Columns

- simple approach: normalization to transform the biclusters into constant biclusters and follow the first approach (e.g. [GLD00])
- some application-driven approaches with special assumptions in the bioinformatics community (e.g. [CST00,SMD03,STG+01])
- constant values on columns: general axis-parallel subspace/projected clustering
- constant values on rows: special case of general correlation clustering
- both cases special case of approaches to biclusters with coherent values

Algorithms for Biclusters with Coherent Values

classical approach: Cheng&Church [CC00]

- introduced the term biclustering to analysis of gene expression data
- quality of a bicluster: *mean squared residue* value *H*

$$H(I,J) = \frac{1}{|I||J|} \sum_{i \in I, j \in J} \left(a_{ij} - a_{iJ} - a_{Ij} + a_{IJ}\right)^2$$

- submatrix (I,J) is considered a bicluster, if H(I,J) < δ

Algorithms for Biclusters with Coherent Values

- δ =0 → *perfect* bicluster:
  - each row and column exhibits absolutely consistent bias
  - bias of row *i* w.r.t. other rows:

$$a_{iJ} - a_{IJ}$$

- the model for a perfect bicluster predicts value a_{ij} by a row-constant, a column-constant, and an overall cluster-constant:

$$a_{ij} = a_{iJ} + a_{Ij} - a_{IJ}$$

$$\Updownarrow \mu = a_{IJ}, r_i = a_{iJ} - a_{IJ}, c_j = a_{Ij} - a_{IJ}$$

$$a_{ij} = \mu + r_i + c_j$$

Algorithms for Biclusters with Coherent Values

- for a non-perfect bicluster, the prediction of the model deviates from the true value by a residue:

$$a_{ij} = \text{res}(a_{ij}) + a_{iJ} + a_{Ij} - a_{IJ}$$

$$\Updownarrow$$

$$\text{res}(a_{ij}) = a_{ij} - a_{iJ} - a_{Ij} + a_{IJ}$$

- This residue is the optimization criterion:

$$H(I,J) = \frac{1}{|I||J|} \sum_{i \in I, j \in J} \left(a_{ij} - a_{iJ} - a_{Ij} + a_{IJ}\right)^2$$

Algorithms for Biclusters with Coherent Values

- The optimization is also possible for the row-residue of row *i* or the column-residue of column *j*.
- Algorithm:
  1. find a δ -bicluster: greedy search by removing the row or column (or the set of rows/columns) with maximal mean squared residue until the remaining submatrix (I,J) satisfies H(I,J)< δ.
  2. find a maximal δ -bicluster by adding rows and columns to (I,J) unless this would increase *H*.
  3. replace the values of the found bicluster by random numbers and repeat the procedure until *k* δ -biclusters are found.

Algorithms for Biclusters with Coherent Values

Weak points in the approach of Cheng&Church:

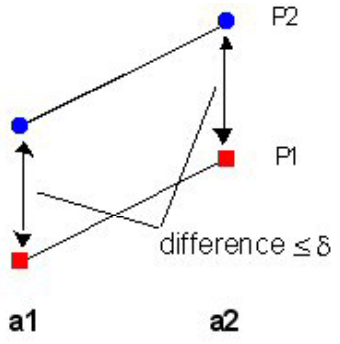
1. One cluster at a time is found, the cluster needs to be masked in order to find a second cluster.
2. This procedure bears an inefficient performance.
3. The masking may lead to less accurate results.
4. The masking inhibits simultaneous overlapping of rows and columns.
5. Missing values cannot be dealt with.
6. The user must specify the number of clusters beforehand.

Algorithms for Biclusters with Coherent Values

p-cluster model [WWYY02]

- p-cluster model: deterministic approach
- specializes δ -bicluster-property to a pairwise property of two objects in two attributes:

$$\left|\left(a_{i_1 j_1} - a_{i_1 j_2}\right) - \left(a_{i_2 j_1} - a_{i_2 j_2}\right)\right| \leq \delta$$



- submatrix (I,J) is a δ -p-cluster if this property is fulfilled for any 2x2 submatrix ($\{i_1, i_2\}$, $\{j_1, j_2\}$) where $\{i_1, i_2\} \in$ I and $\{j_1, j_2\} \in$J.

Algorithms for Biclusters with Coherent Values

Algorithm:

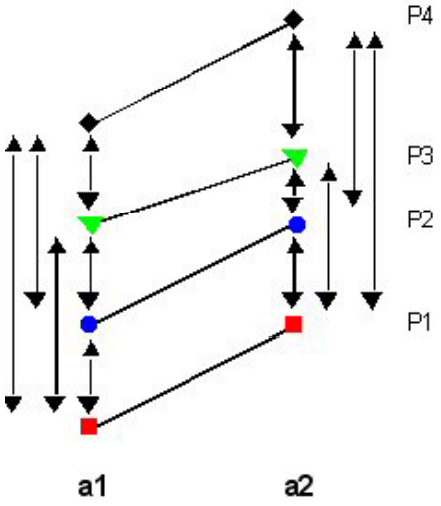
1. create maximal set of attributes for each pair of objects forming a δ -p-cluster
2. create maximal set of objects for each pair of attributes forming a δ -p-cluster
3. pruning-step
4. search in the set of submatrices

Problem: complete enumeration approach

Addressed issues:

1. multiple clusters simultaneously
4. allows for overlapping rows and columns
6. allows for arbitrary number of clusters

Related approaches: FLOC [YWWY02], MaPle [PZC+03]



Summary

- Biclustering models do not fit exactly into the spatial intuition behind subspace, projected, or correlation clustering.
- Models make sense in view of a data matrix.
- Strong point: the models generally do not rely on the locality assumption.
- Models differ substantially → fair comparison is a non-trivial task.
- Comparison of five methods: [PBZ+06]
- Rather specialized task – comparison in a broad context (subspace/projected/correlation clustering) is desirable.
- Biclustering performs generally well on microarray data – for a wealth of approaches see [MO04].

Outline

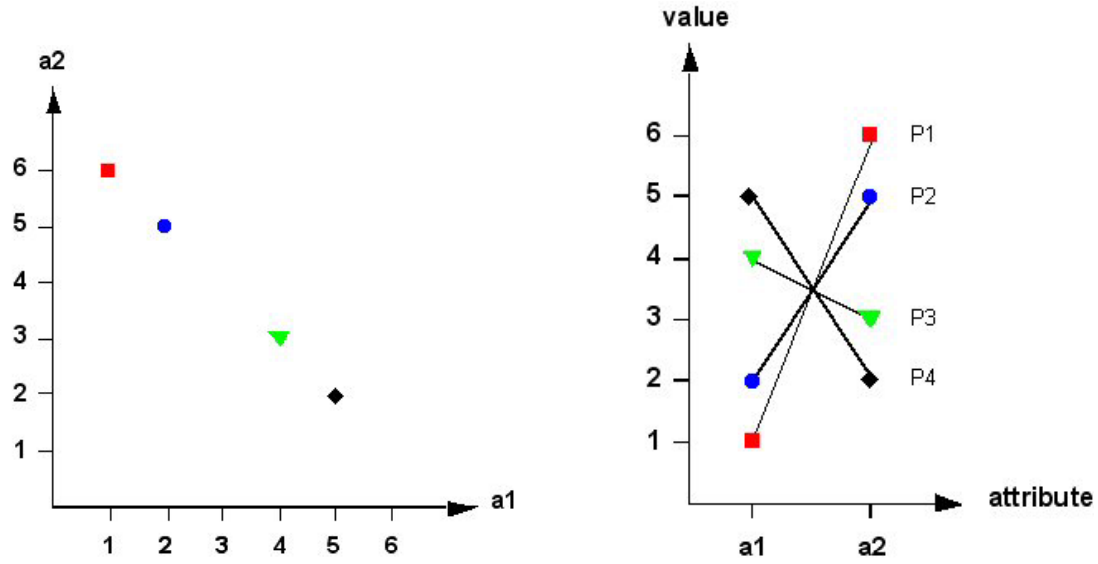
1. Introduction
2. Axis-parallel Subspace Clustering
3. Pattern-based Clustering
4. Arbitrarily-oriented Subspace Clustering
5. Summary

Outline: Arbitrarily-oriented Subspace Clustering

- Challenges and Approaches
- Correlation Clustering Algorithms
- Summary and Perspectives

Challenges and Approaches

- Pattern-based approaches find simple positive correlations
- negative correlations: no additive pattern

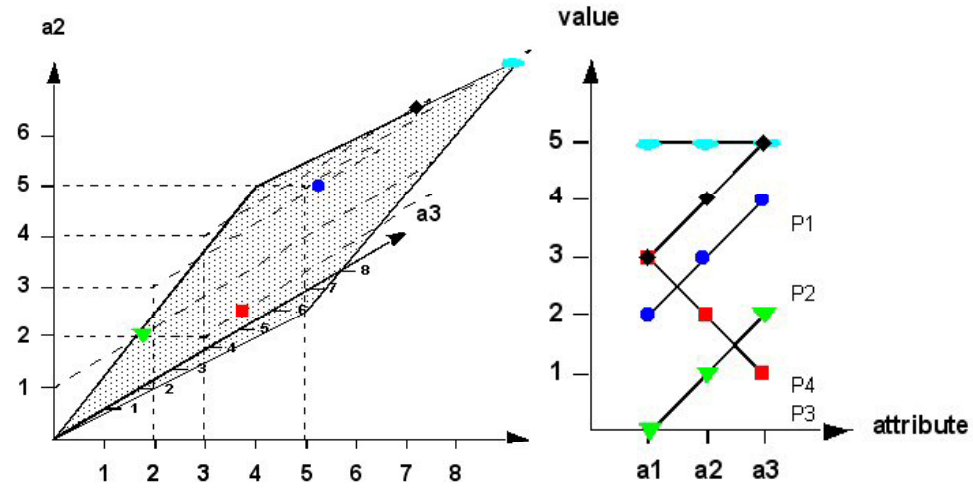


Challenges and Approaches

- more complex correlations: out of scope of pattern-based approaches

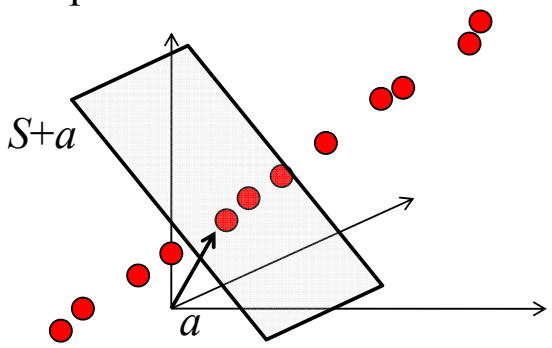
$$a1 - 2 \cdot a2 + a3 = 0$$

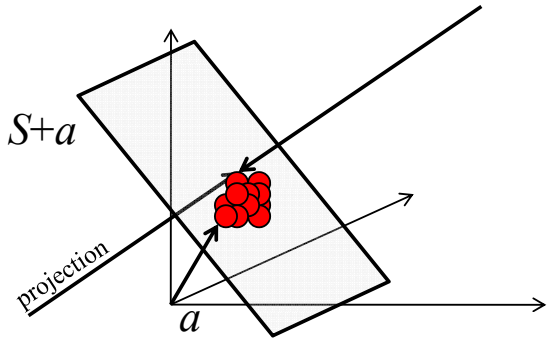
	a1	a2	a3
P1	3	2	1
P2	2	3	4
P3	0	1	2
P4	3	4	5
P5	5	5	6



Challenges and Approaches

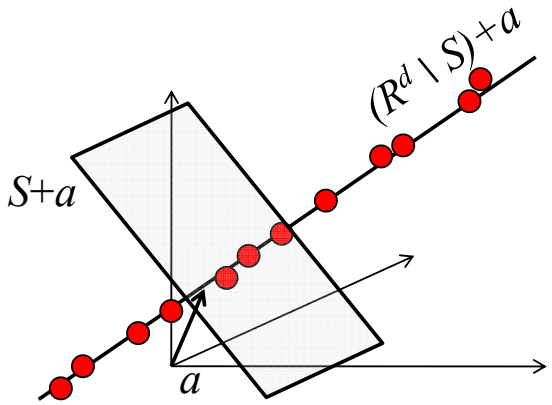
- Pattern-based approaches find simple positive correlations
- More general approach: oriented clustering aka. generalized subspace/projected clustering aka. correlation clustering
  - Note: different notion of "Correlation Clustering" in machine learning community, e.g. cf. [BBC04]
- Assumption: any cluster is located in an arbitrarily oriented affine subspace $S+a$ of R^d

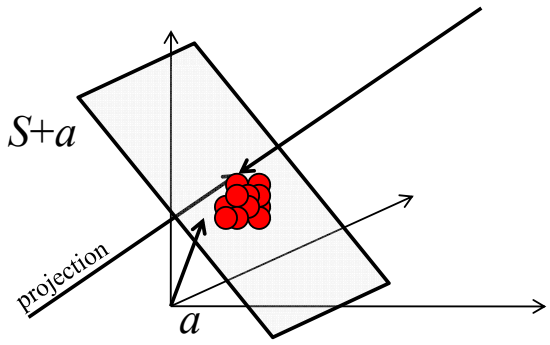




Challenges and Approaches

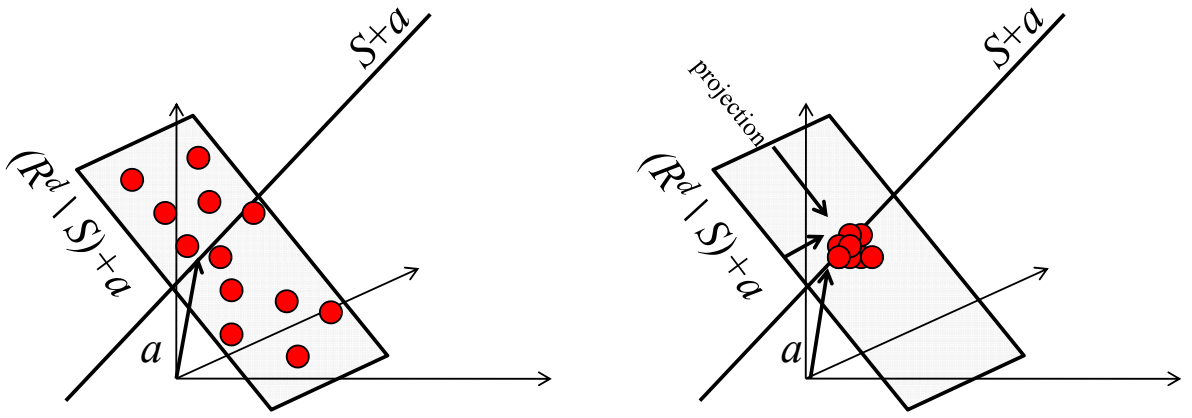
- Affine subspace $S+a$, $S \subset R^d$, *affinity* $a \in R^d$ is interesting if a set of points clusters within this subspace
- Points may exhibit high variance in perpendicular subspace $(R^d \setminus S)+a$





Challenges and Approaches

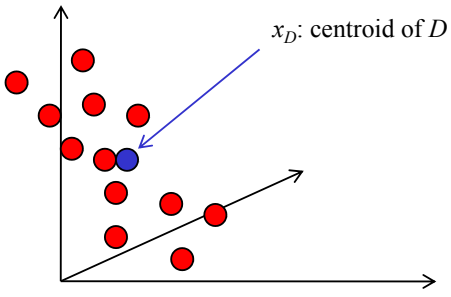
- high variance in perpendicular subspace $(R^d \setminus S)+a$ → points form a hyperplane within R^d located in this subspace $(R^d \setminus S)+a$
- Points on a hyperplane appear to follow linear dependencies among the attributes participating in the description of the hyperplane



Challenges and Approaches

- Directions of high/low variance: PCA (local application)
- locality assumption: local selection of points sufficiently reflects the hyperplane accommodating the points
- general approach: build covariance matrix Σ_D for a selection D of points (e.g. k nearest neighbors of a point)

$$\Sigma_D = \frac{1}{|D|}\sum_{x \in D}(x - x_D)(x - x_D)^T$$



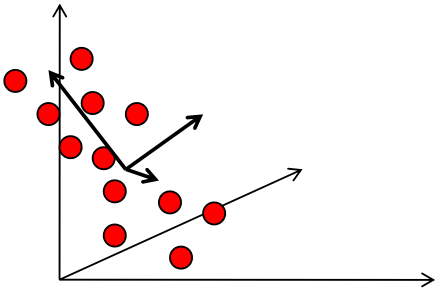
properties of Σ_D:
- d x d
- symmetric
- positive semidefinite
- $\sigma_{D_{ij}}$ (value at row i, column j) = covariance between dimensions i and j
- $\sigma_{D_{ii}}$ = variance in ith dimension

Challenges and Approaches

- decomposition of Σ_D to eigenvalue matrix E_D and eigenvector matrix V_D:

$$\Sigma_D = V_D E_D V_D^{\mathrm{T}}$$

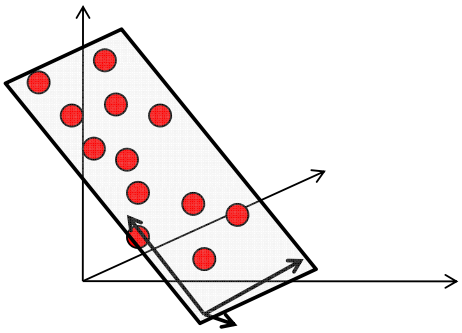
- E_D: diagonal matrix, holding eigenvalues of Σ_D in decreasing order in its diagonal elements
- V_D: orthonormal matrix with eigenvectors of Σ_D ordered correspondingly to the eigenvalues in E_D



- V_D: new basis, first eigenvector = direction of highest variance
- E_D: covariance matrix of D when represented in new axis system V_D

Challenges and Approaches

- points forming λ-dimensional hyperplane → hyperplane is spanned by the first λ eigenvectors (called "strong" eigenvectors – notation: $\breve{V}_D$)
- subspace where the points cluster densely is spanned by the remaining d-λ eigenvectors (called "weak" eigenvectors – notation: $\hat{V}_D$)



for the eigensystem, the sum of the smallest d-λ eigenvalues $\sum_{i=\lambda+1}^{d} e_{D_{ii}}$ is minimal under all possible transformations → points cluster optimally dense in this subspace

Challenges and Approaches

model for correlation clusters [ABK+06]:

- λ-dimensional hyperplane accommodating the points of a correlation cluster $C \subset R^d$ is defined by an equation system of d-λ equations for d variables and the affinity (e.g. the mean point x_C of all cluster members):

$$\hat{V}_C^T x = \hat{V}_C^T x_C$$

- equation system approximately fulfilled for all points $x \in C$
- quantitative model for the cluster allowing for probabilistic prediction (classification)
- Note: correlations are observable, linear dependencies are merely an assumption to explain the observations – predictive model allows for evaluation of assumptions and experimental refinements

Correlation Clustering Algorithms

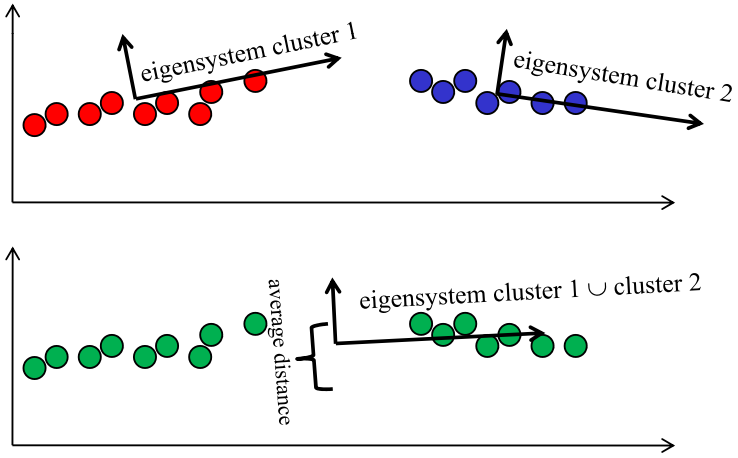
ORCLUS [AY00]:

first approach to *generalized projected clustering*

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

Correlation Clustering Algorithms

- best fitting pair of clusters: least average distance in the projected space spanned by weak eigenvectors of the merged clusters



- assess average distance in all merged pairs of clusters and finally merge the best fitting pair

Correlation Clustering Algorithms

- adapt eigensystem to the updated cluster
- new iteration: assign points according to updated eigensystems (distance along weak eigenvectors)
- dimensionality gradually reduced to a user-specified value *l*
- initially exclude only eigenvectors with very high variance

Correlation Clustering Algorithms

properties:

- finds k correlation clusters (user-specified)
- higher initial k_c → higher runtime, probably better results
- biased to average dimensionality l of correlation clusters (user specified)
- cluster-based locality assumption: subspace of each cluster is learned from its current members (starting in the full dimensional space)

Correlation Clustering Algorithms

4C [BKKZ04]

- density-based cluster-paradigm (cf. DBSCAN [EKSX96])
- extend a cluster from a seed as long as a density-criterion is fulfilled – otherwise pick another seed unless all data base objects are assigned to a cluster or noise
- density criterion: minimal required number of points in the neighborhood of a point
- neighborhood: distance between two points ascertained based on the eigensystems of both compared points

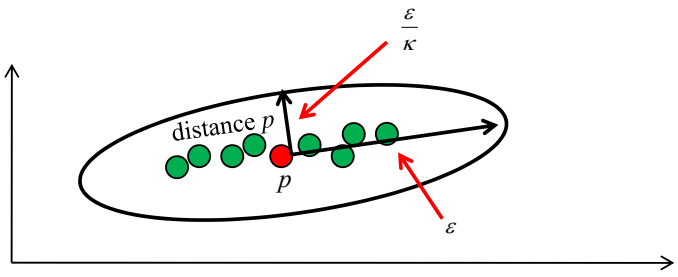
Correlation Clustering Algorithms

- eigensystem of a point p based on its ε-neighborhood in Euclidean space
- threshold δ discerns large from small eigenvalues
- in eigenvalue matrix E_p replace large eigenvalues by 1, small eigenvalues by κ>>1
- adapted eigenvalue matrix yields a correlation similarity matrix for point p:

$$V_p E'_p V_p^{\mathrm{T}}$$

Correlation Clustering Algorithms

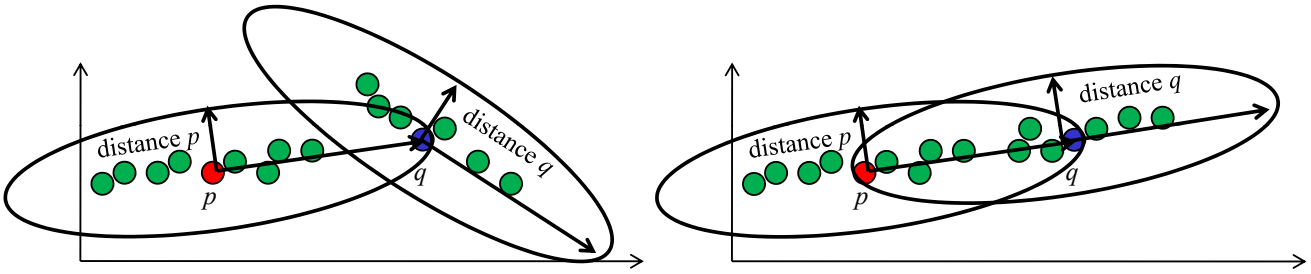
- effect on distance measure:



- 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: $\sqrt{(q-p)\cdot V_q \cdot E'_q \cdot V_q^{\mathrm{T}} \cdot (q-p)^{\mathrm{T}}}$

Correlation Clustering Algorithms

- symmetry of distance measure by choosing the maximum:



- p and q are correlation-neighbors if

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

Correlation Clustering Algorithms

properties:

- 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

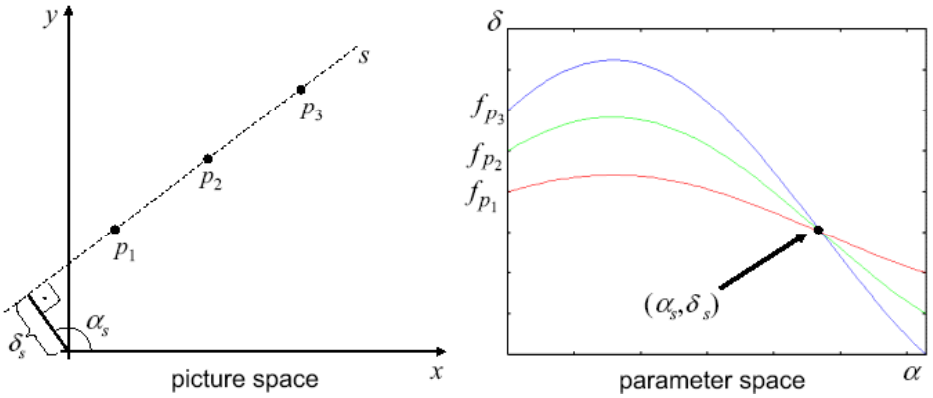
enhancements also based on PCA:

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

Correlation Clustering Algorithms

different correlation primitive: Hough-transform

- points in data space are mapped to functions in the parameter space

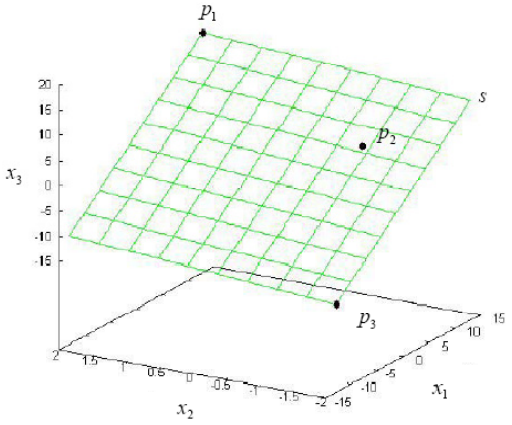


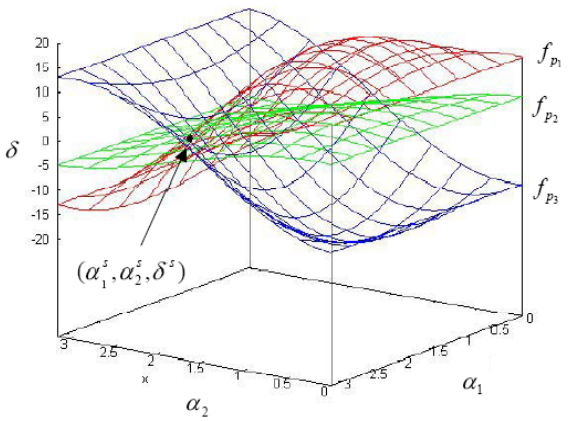
$$f_p(\alpha_1,\ldots,\alpha_{d-1}) = \langle p,n \rangle = \sum_{i=1}^{d} p_i \cdot \left(\prod_{j=1}^{i-1} \sin(\alpha_j) \right) \cdot \cos(\alpha_i)$$

- functions in the parameter space define all lines possibly crossing the point in the data space

Correlation Clustering Algorithms

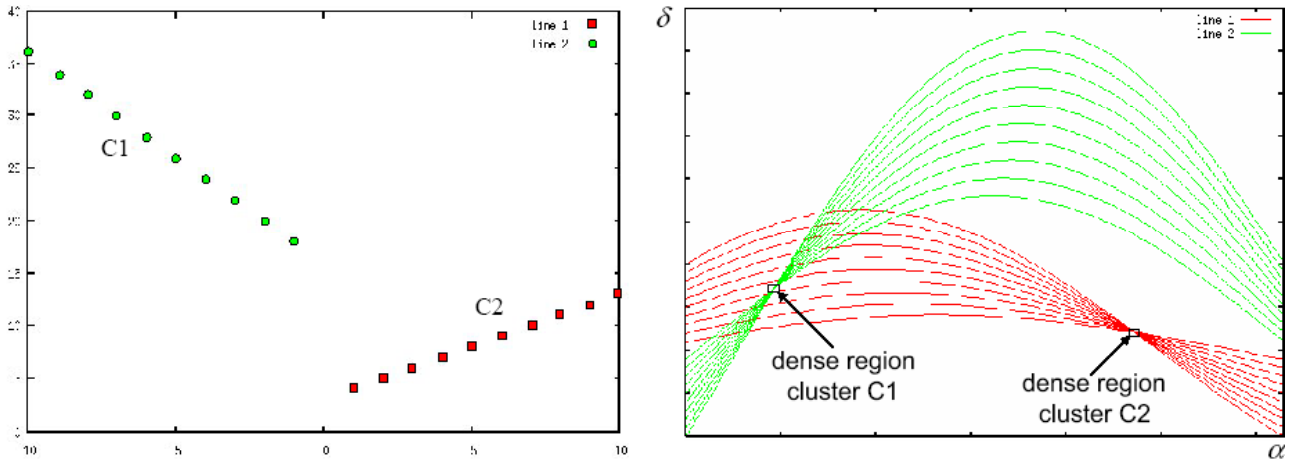
- Properties of the transformation
  - Point in the data space = sinusoidal curve in parameter space
  - Point in parameter space = hyper-plane in data space
  - Points on a common hyper-plane in data space = sinusoidal curves through a common point in parameter space
  - Intersections of sinusoidal curves in parameter space = hyper-plane through the corresponding points in data space





Correlation Clustering Algorithms

Algorithm based on the Hough-transform: CASH [ABD+08]



dense regions in parameter space correspond to linear structures in data space

Correlation Clustering Algorithms

Idea: find dense regions in parameter space

- construct a grid by recursively splitting the parameter space (best-first-search)
- identify dense grid cells as intersected by many parametrization functions
- dense grid represents (*d-1*)-dimensional linear structure
- transform corresponding data objects in corresponding (*d-1*)-dimensional space and repeat the search recursively

Correlation Clustering Algorithms

properties:

- finds arbitrary number of clusters
- requires specification of depth of search (number of splits per axis)
- requires minimum density threshold for a grid cell
- Note: this minimum density does not relate to the locality assumption: CASH is a global approach to correlation clustering
- search heuristic: linear in number of points, but $\sim d^4$
- But: complete enumeration in worst case (exponential in d)

Summary and Perspectives

- 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
- new approach based on Hough-transform:
  - does not rely on locality assumption
  - but worst case again complete enumeration

Summary and Perspectives

- some preliminary approaches base on concept of self-similarity (intrinsic dimensionality, fractal dimension): [BC00,PTTF02,GHPT05]
- interesting idea, provides quite a different basis to grasp correlations in addition to PCA
- drawback: self-similarity assumes locality of patterns even by definition

Summary and Perspectives

comparison: correlation clustering – biclustering:

- model for correlation clusters more general and meaningful
- models for biclusters rather specialized
- in general, biclustering approaches do not rely on locality assumption
- non-local approach and specialization of models may make biclustering successful in many applications
- correlation clustering is the more general approach but the approaches proposed so far are rather a first draft to tackle the complex problem

Outline

1. Introduction
2. Axis-parallel Subspace Clustering
3. Pattern-based Clustering
4. Arbitrarily-oriented Subspace Clustering
5. Summary

Summary

- Let's take a global view:
  - Traditional clustering in high dimensional spaces is most likely meaningless with increasing dimensionality (curse of dimensionality)
  - Clusters may be found in (generally arbitrarily oriented) subspaces of the data space
  - So the general problem of clustering high dimensional data is:

    "find a partitioning of the data where each cluster may exist in its own subspace"
    - The partitioning need not be unique (clusters may overlap)
    - The subspaces may be axis-parallel or arbitrarily oriented
  - Analysis of this general problem:
    - A naïve solution would examine all possible subspaces to look for clusters
    - The search space of all possible arbitrarily oriented subspaces is infinite
    - We need assumptions and heuristics to develop a feasible solution

Summary

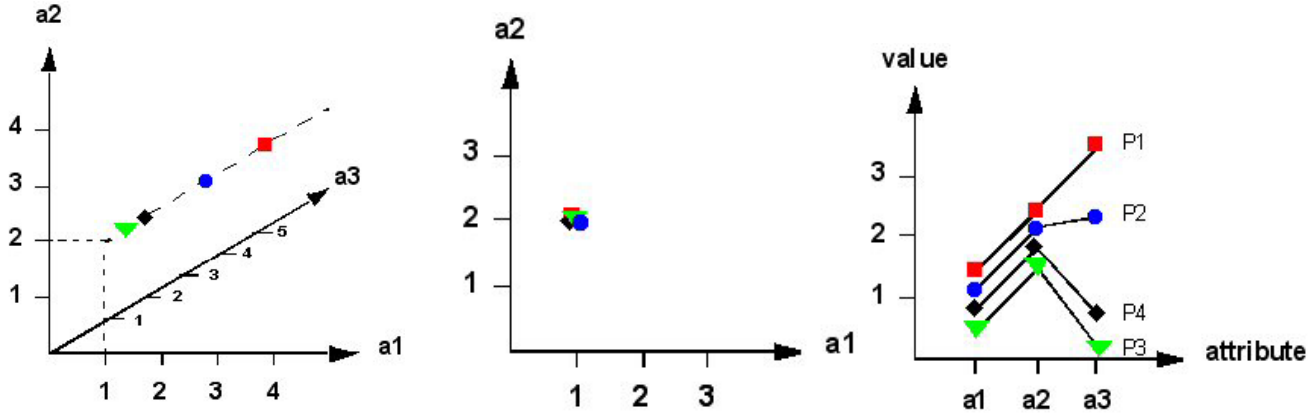
- What assumptions did we get to know here?
  - The search space is restricted to certain subspaces
  - A clustering criterion that implements the downward closure property enables efficient search heuristics
  - The locality assumption enables efficient search heuristics
  - Assuming simple additive models ("patterns") enables efficient search heuristics
  - …
- Remember: also the clustering model may rely on further assumptions that have nothing to do with the infinite search space
  - Number of clusters need to be specified
  - Results are not deterministic e.g. due to randomized procedures
  - …
- We can classify the existing approaches according to the assumptions they made to conquer the infinite search space

Summary

- The global view
  - Subspace clustering/projected clustering:
    - The search space is restricted to axis-parallel subspaces
    - A clustering criterion that implements the downward closure property is defined (usually based on a global density threshold)
    - The locality assumption enables efficient search heuristics
  - Bi-clustering/pattern-based clustering:
    - The search space is restricted to special forms and locations of subspaces or half-spaces
    - Over-optimization (e.g. singularity clusters) is avoided by assuming a predefined number of clusters
  - Correlation clustering:
    - The locality assumption enables efficient search heuristics
- Any of the proposed methods is based on at least one assumption because otherwise, it would not be applicable

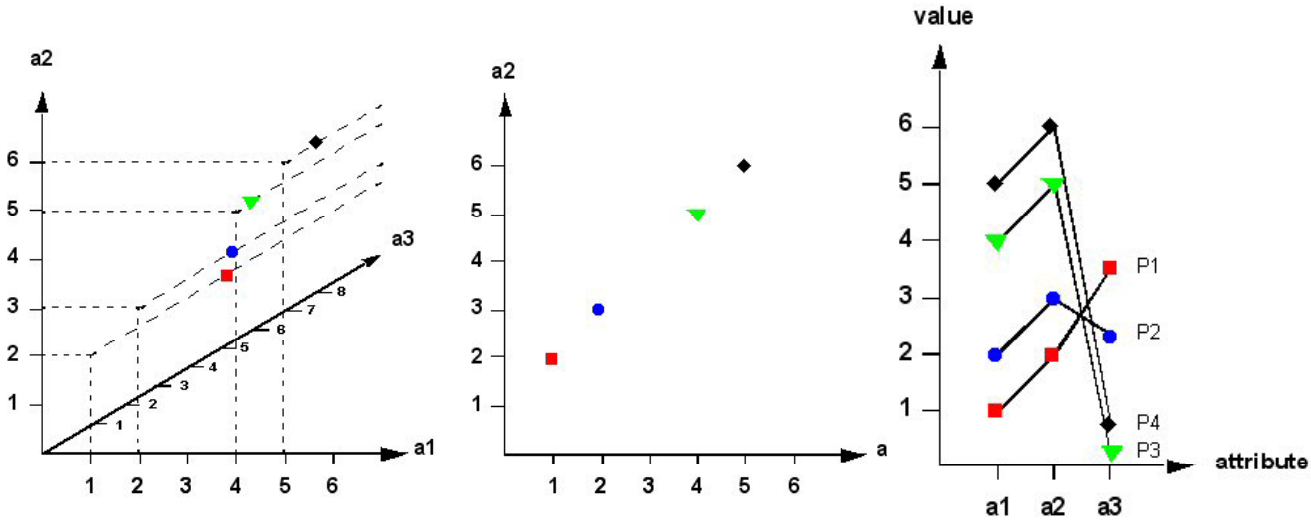
Summary

- The global view
  - Subspace clustering/projected clustering:
    - Search space restricted to axis-parallel subspaces
    - Clustering criterion implementing the downward closure property (usually based on a global density threshold)
    - Locality assumption
    - …



Summary

- The global view
  - Bi-clustering/pattern-based clustering:
    - Search space restricted to special forms and locations of subspaces or half-spaces
    - Greedy-search heuristics based on statistical assumptions

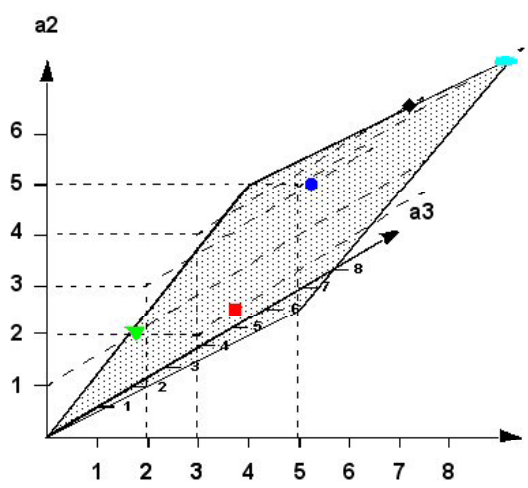


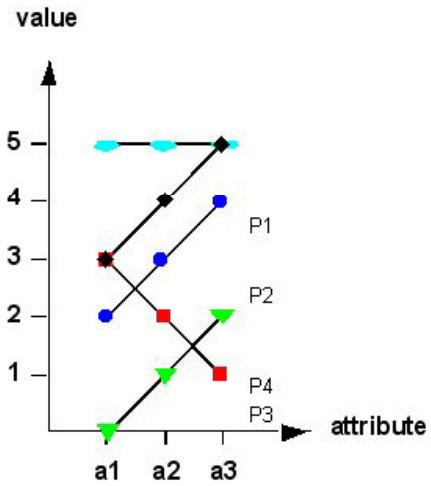
Summary

- The global view
  - Correlation clustering:
    - Locality assumption
    - Greedy-search heuristics

$a1 - 2 \cdot a2 + a3 = 0$

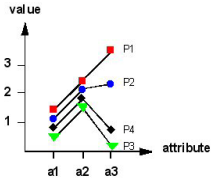
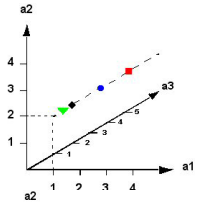
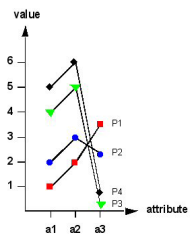
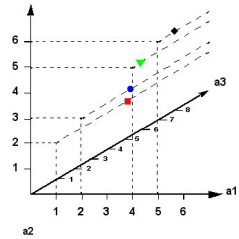
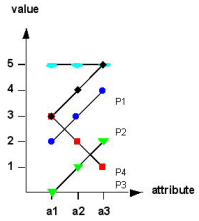
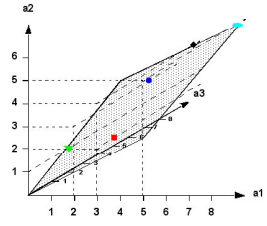
	a1	a2	a3
P1	3	2	1
P2	2	3	4
P3	0	1	2
P4	3	4	5
P5	5	5	6





Summary

- The global view

Matrix-Pattern		Problem	Spatial Pattern	
	Constant values in columns, change of values only on rows	Subspace / Projected Clustering	Axis-parallel hyperplanes	
	From constant values in rows and columns (no change of values) to arbitrary change of values in common direction	Pattern-based / Bi-Clustering	Special cases of axis-parallel to special cases of arbitrarily oriented hyperplanes	
	No particular pattern	Correlation Clustering	Arbitrarily oriented hyperplanes	

Summary

Algorithm	complex correlations	simple positive correlation	simple negative correlation	axis parallel	not relying on locality assumption	adaptive density threshold	independent w.r.t. order of attributes	independent w.r.t. order of objects	deterministic	arbitrary number of clusters	overlapping clusters	overlapping subspaces	simultaneously overlapping clusters and subspaces	arbitrary subspace dimensionality	hierarchical structure	avoiding complete enumeration	noise robust
CLIQUE [AGGR98]				√	√		√	√	√	√	√	√	√	√			√
ENCLUS [CFZ99]				√	√		√	√	√	√	√	√	√	√			√
MAFIA [NGC01]				√	√		√	√	√	√	√	√	√	√			√
SUBCLU [KKK04]				√	√		√	√	√	√	√	√	√	√			√
PROCLUS [APW+99]				√		√						√				√	
PreDeCon [BKKK04]				√			√	√	√	√		√				√	√
P3C [MSE06]				√	√	√	√	√	√	√	√	√	√	√			√
COSA [FM04]				√			√	√	√			√		√		√	√
DOC [PJAM02]				√	√		√	√		√	√	√	√	√			
DiSH [ABK+07a]				√	√	√		√	√	√		√		√	√	√	√
FIRES [KKRW05]				√	√	√		√	√	√	√	√	√	√		√	√

Summary

Algorithm	complex correlations	simple positive correlation	simple negative correlation	axis parallel	not relying on locality assumption	adaptive density threshold	independent w.r.t. order of attributes	independent w.r.t. order of objects	deterministic	arbitrary number of clusters	overlapping clusters	overlapping subspaces	simultaneously overlapping clusters and subspaces	arbitrary subspace dimensionality	hierarchical structure	avoiding complete enumeration	noise robust
Block clustering [Har72]					√	*n a*	√	√	√					√	√		√
δ-bicluster [CC00]		√	√	√	√	*n a*	√	√	√		√	√		√		√	√
FLOC [YWWY02]		√		√	√	*n a*					√	√	√	√		√	√
p-Cluster [WWYY02]		√		√	√	*n a*	√	√	√	√	√	√	√	√			√
MaPle [PZC+03]		√		√	√	*n a*	√	√	√	√	√	√	√	√			√
CoClus [CDGS04]		√		√	√	*n a*								√		√	
OP-Cluster [LW03]					√	*n a*	√	√	√	√	√	*n a*	*n a*	*n a*			√

Summary

Algorithm	complex correlations	simple positive correlation	simple negative correlation	axis parallel	not relying on locality assumption	adaptive density threshold	independent w.r.t. order of attributes	independent w.r.t. order of objects	deterministic	arbitrary number of clusters	overlapping clusters	overlapping subspaces	simultaneously overlapping clusters and subspaces	arbitrary subspace dimensionality	hierarchical structure	avoiding complete enumeration	noise robust
ORCLUS [AY00]	√	√	√	√			√					√				√	
4C [BKKZ04]	√	√	√	√			√	√	√	√		√				√	√
COPAC [ABK+07c]	√	√	√	√			√	√	√	√		√		√		√	√
ERiC [ABK+07b]	√	√	√	√			√	√	√	√		√		√	√	√	√
CASH [ABD+08]	√	√	√	√	√	*n a*		√	√	√		√		√	√		√

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