LUDWIG-MAXIMILIANS-UNIVERSITY MUNICH | DEPARTMENT INSTITUTE FOR INFORMATICS | DATABASE SYSTEMS GROUP

Data Mining and the 'Curse of Dimensionality'

iDB Workshop 2011

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Outline

1. The Curse of Dimensionality
2. Shared-Neighbor Distances
3. Subspace Outlier Detection
4. Subspace Clustering
5. Conclusions

The Curse of Dimensionality

The *"curse of dimensionality"*: one buzzword for many problems [KKZ09]

- 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.

The Curse of Dimensionality

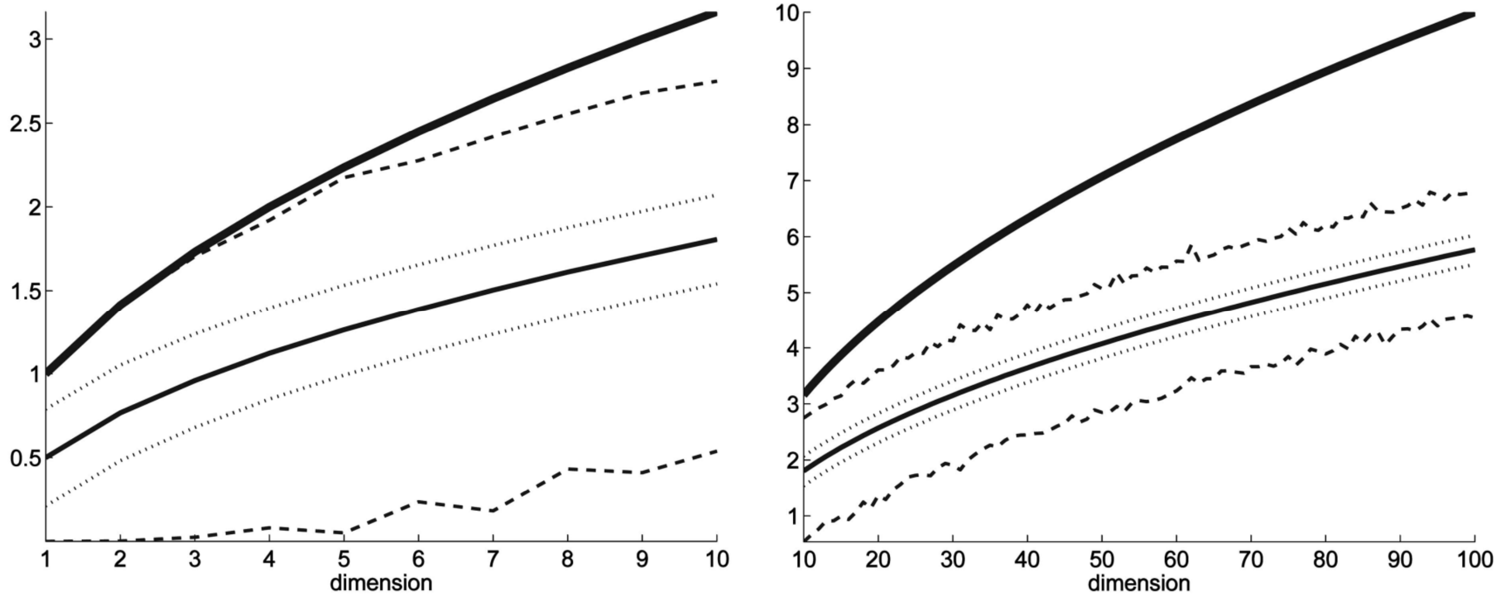
- Second aspect: *Concentration effect of L_p-norms*
  - In [BGRS99,HAK00] it is reported that the ratio of ($Dmax_d$ – $Dmin_d$) to $Dmin_d$ converges to zero with increasing dimensionality *d*
    - $Dmin_d$ = distance to the nearest neighbor in *d* dimensions
    - $Dmax_d$ = distance to the farthest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

    Formally:

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

    - Distances to near and to far neighbors become more and more similar with increasing data dimensionality (loss of *relative contrast* or *concentration effect* of distances).
    - This holds true for a wide range of data distributions and distance functions, but…

The Curse of Dimensionality



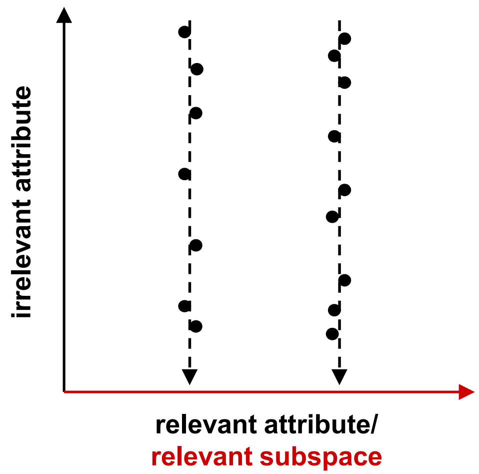
(a) (b)

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, AHK01] 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.

The Curse of Dimensionality

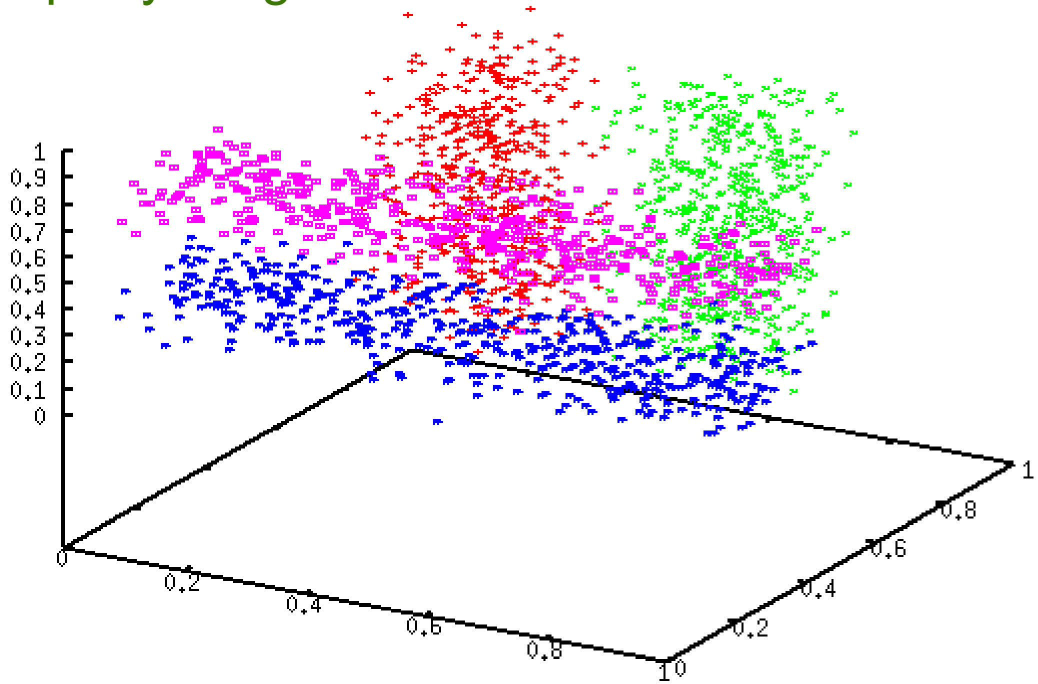
- Third aspect: *Relevant and Irrelevant attributes*
  - A subset of the features may be relevant for clustering
  - Groups of similar ("dense") points may be identified when considering these features only



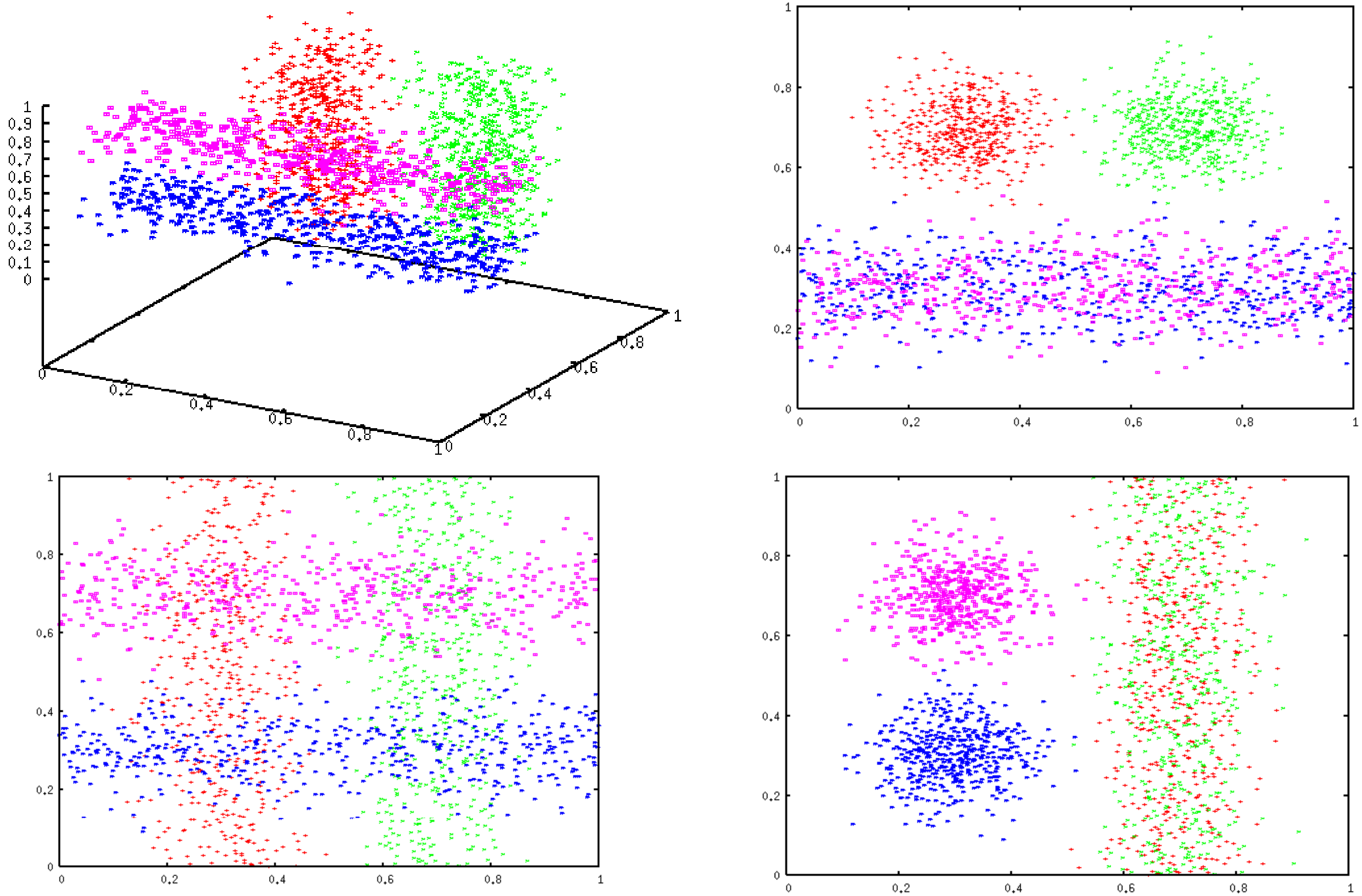
  - Different subsets of attributes may be relevant for different clusters
  - Separation of clusters relates to *relevant attributes* (helpful to discern between clusters) as opposed to *irrelevant attributes* (indistinguishable distribution of attribute values for different clusters).

The Curse of Dimensionality

– 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

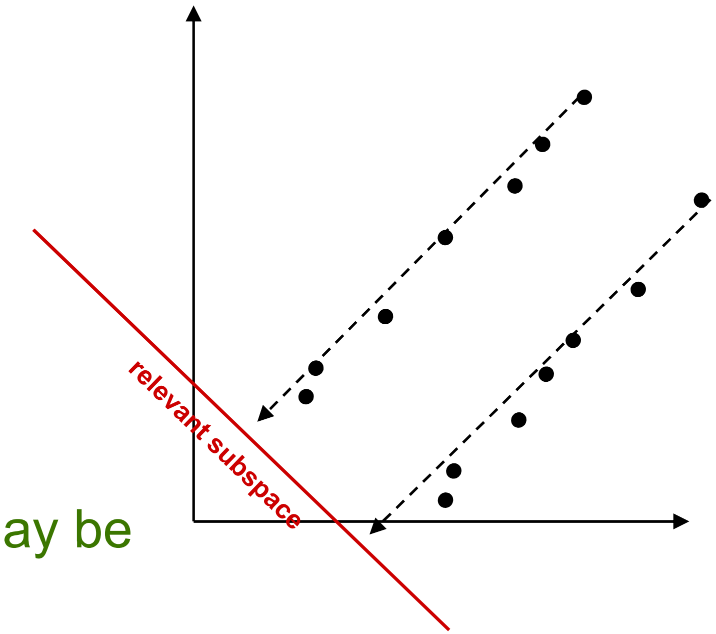


The Curse of Dimensionality



The Curse of Dimensionality

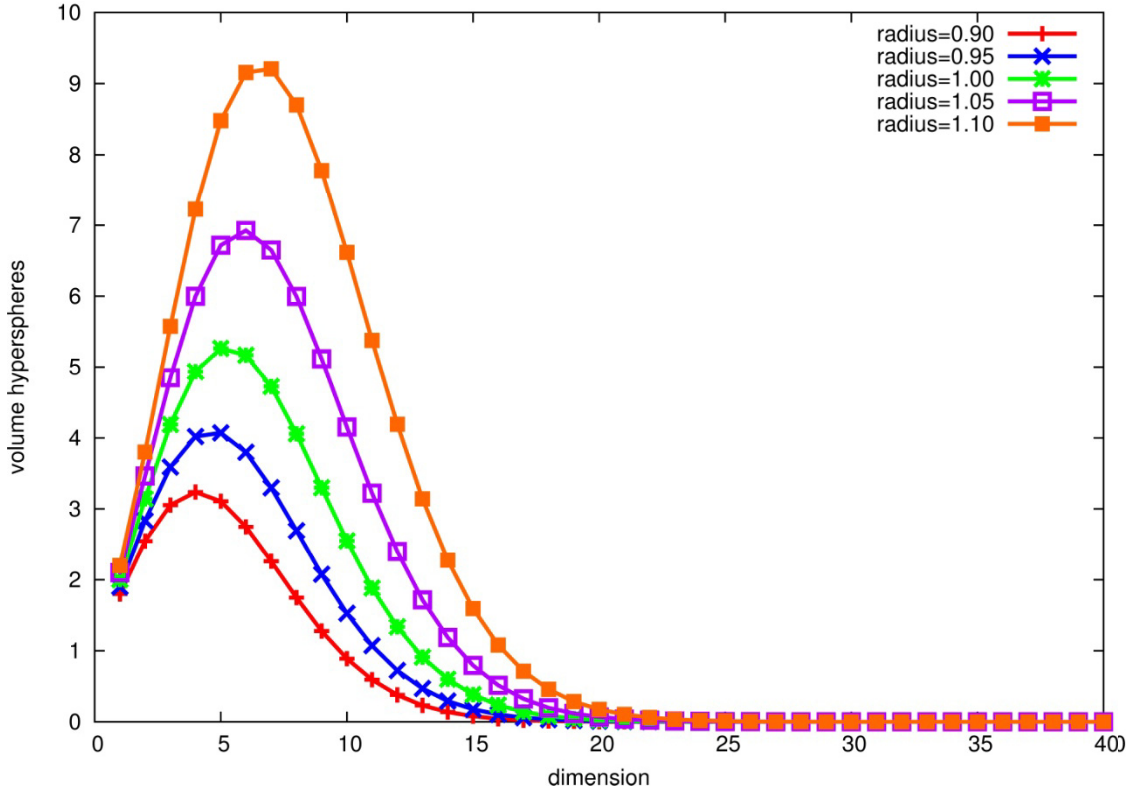
- Fourth aspect: *Correlation among attributes (redundancy?)*
  - A subset of features may be correlated
  - Groups of similar ("dense") points may be identified when considering this correlation of features only



  - different correlations of attributes may be relevant for different clusters
  - can result in lower intrinsic dimensionality of a data set
  - bad discrimination of distances can still be a problem

The Curse of Dimensionality

- there are other effects of the "curse of dimensionality"
- just another strange fact: the volume of hyperspheres shrinks with increasing dimensionality!



$$V_n(r) = \frac{\pi^{\frac{n}{2}} r^n}{\Gamma\left(\frac{n}{2}+1\right)}$$

Shared-Neighbor Distances

[HKK+10]: *Can Shared-Neighbor Distances Defeat the Curse of Dimensionality?* (SSDBM 2010)

- we mainly aim at distinguishing these effects of the 'curse':
  - concentration effect within distributions
  - impediment of similarity search by irrelevant attributes
  - partly: impact of redundant/correlated attributes
- as a remedy for similarity assessment in high dimensional data, to use shared nearest neighbor (SNN) information has been proposed but never evaluated systematically
- [HKK+10]: evaluation of the effects on primary distances (Manhattan, Euclidean, fractional L_p ($L_{0.6}$ and $L_{0.8}$), cosine) and secondary distances (SNN)

Shared-Neighbor Distances

- secondary distances are defined on top of primary distances
- shared nearest neighbor (SNN) information:
  - assess the set of *s* nearest neighbors for two objects *x* and *y* in terms of some primary distance (Euclidean, Manhattan, cosine…)
  - derive overlap of neighbors (common objects in the NN of *x* and *y*)

$$\mathrm{SNN}_s(x,y) = \left|\mathrm{NN}_s(x) \cap \mathrm{NN}_s(y)\right|$$

  - similarity measure

$$\mathrm{simcos}_s(x,y) = \frac{\mathrm{SNN}_s(x,y)}{s}$$

cosine of the angle between membership vectors for NN(*x*) and NN(*y*)

- SNN has been used before in mining high-dimensional data, but alleged quality improvement has never been evaluated

Shared-Neighbor Distances

- distance measures based on SNN:

$$\mathrm{dinv}_{\mathrm{s}}(x,y) = 1 - \mathrm{simcos}_{\mathrm{s}}(x,y)$$

$$\mathrm{dacos}_{\mathrm{s}}(x,y) = \arccos(\mathrm{simcos}_{\mathrm{s}}(x,y))$$

$$\mathrm{dln}_{\mathrm{s}}(x,y) = -\ln(\mathrm{simcos}_{\mathrm{s}}(x,y))$$

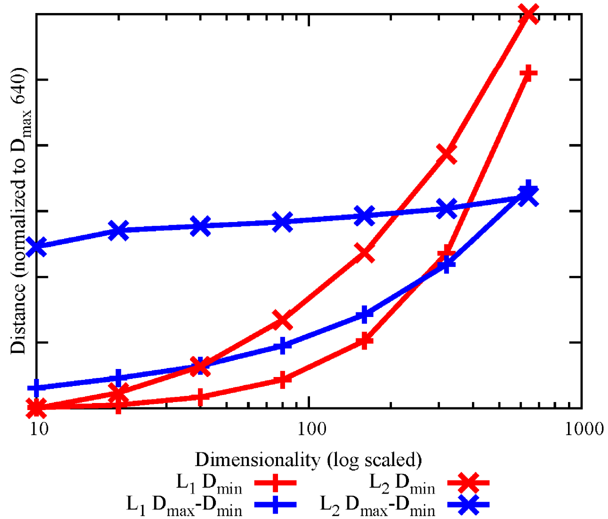
  – dinv: linear inversion
  – dacos penalizes slightly suboptimal similarities more strongly
  – dln more tolerant for relatively high similarity values but approaches infinity for very low similarity values
- for assessment of ranking quality, these formulations are equivalent as the ranking is unaffected
- only dacos is a metric (if the underlying primary distance is a metric)

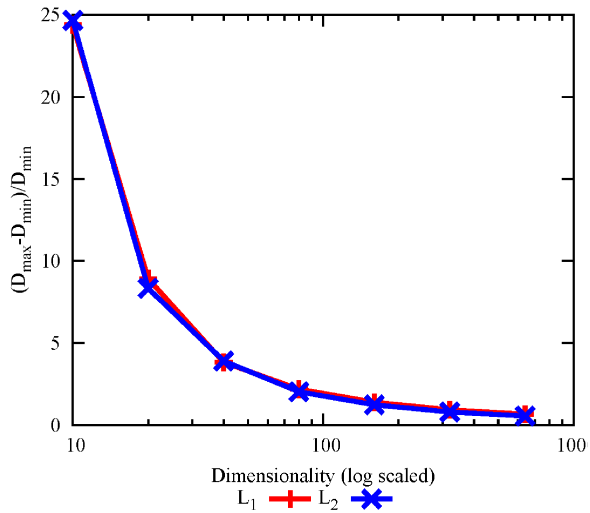
Shared-Neighbor Distances

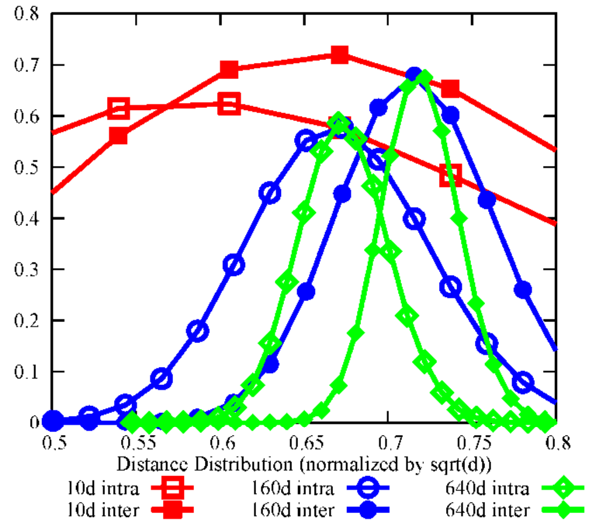
- Artificial data sets: *n = 10.000* items, *c = 100* clusters, up to *d = 640* dimensions, cluster sizes randomly determined.
- Relevant attribute values normally distributed, irrelevant attribute values uniformly distributed.
- Data sets:
  - *All-Relevant:* all dimensions relevant for all clusters
  - *10-Relevant:* first *10* dimensions are relevant for all clusters, the remaining dimensions are irrelevant
  - *Cyc-Relevant: i*th attribute is relevant for the *j*th cluster when *i mod c = j*, otherwise irrelevant (here: *c = 10, n = 1000*)
  - *Half-Relevant:* for each cluster, an attribute is chosen to be relevant with probability *0.5*, and irrelevant otherwise
  - *All-Dependent:* derived from *All-Relevant* introducing correlations among attributes
    $X \in$ *AllDependent*, $Y \in$ *AllRelevant*: $X_i = Y_i$ $(1 \leq i \leq 10)$, $X_i = ½\,(X_{i-10}+Y_i)$ $(i > 10)$
  - *10-Dependent:* derived from *10-Relevant* introducing correlations among attributes

Shared-Neighbor Distances

Data sets show properties of the “curse of dimensionality”





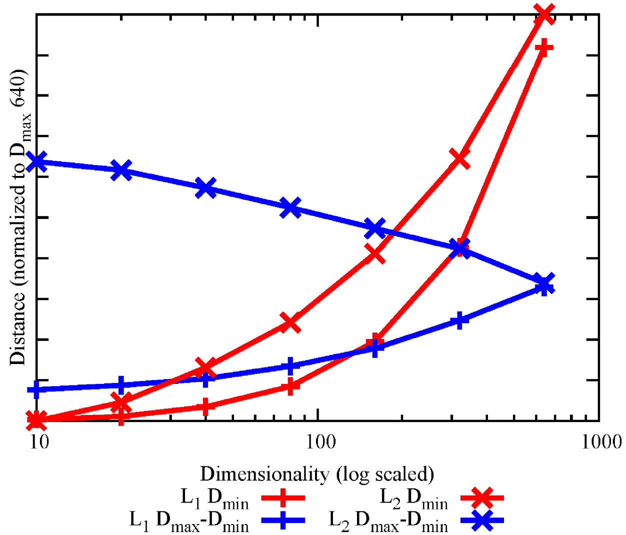


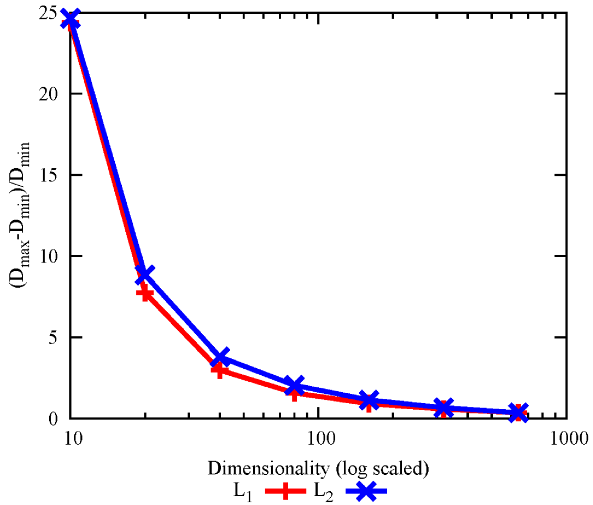
All-Relevant

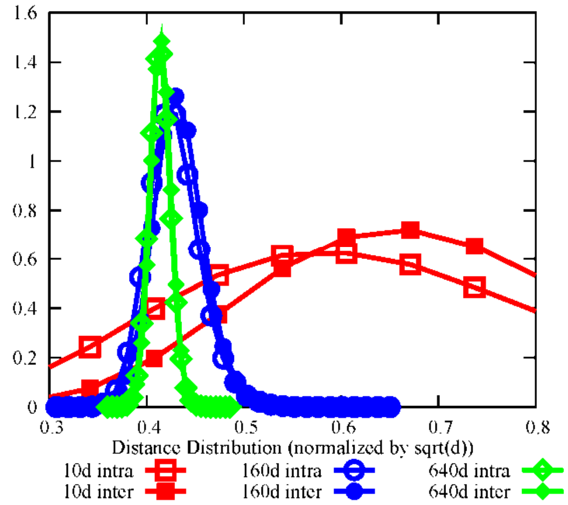
$$\lim_{d\to\infty} \mathrm{var}\left(\frac{\|X_d\|}{E[\|X_d\|]}\right) = 0 \quad \Rightarrow \quad \frac{D_{\max} - D_{\min}}{D_{\min}} \to 0$$

Shared-Neighbor Distances

Data sets show properties of the "curse of dimensionality"





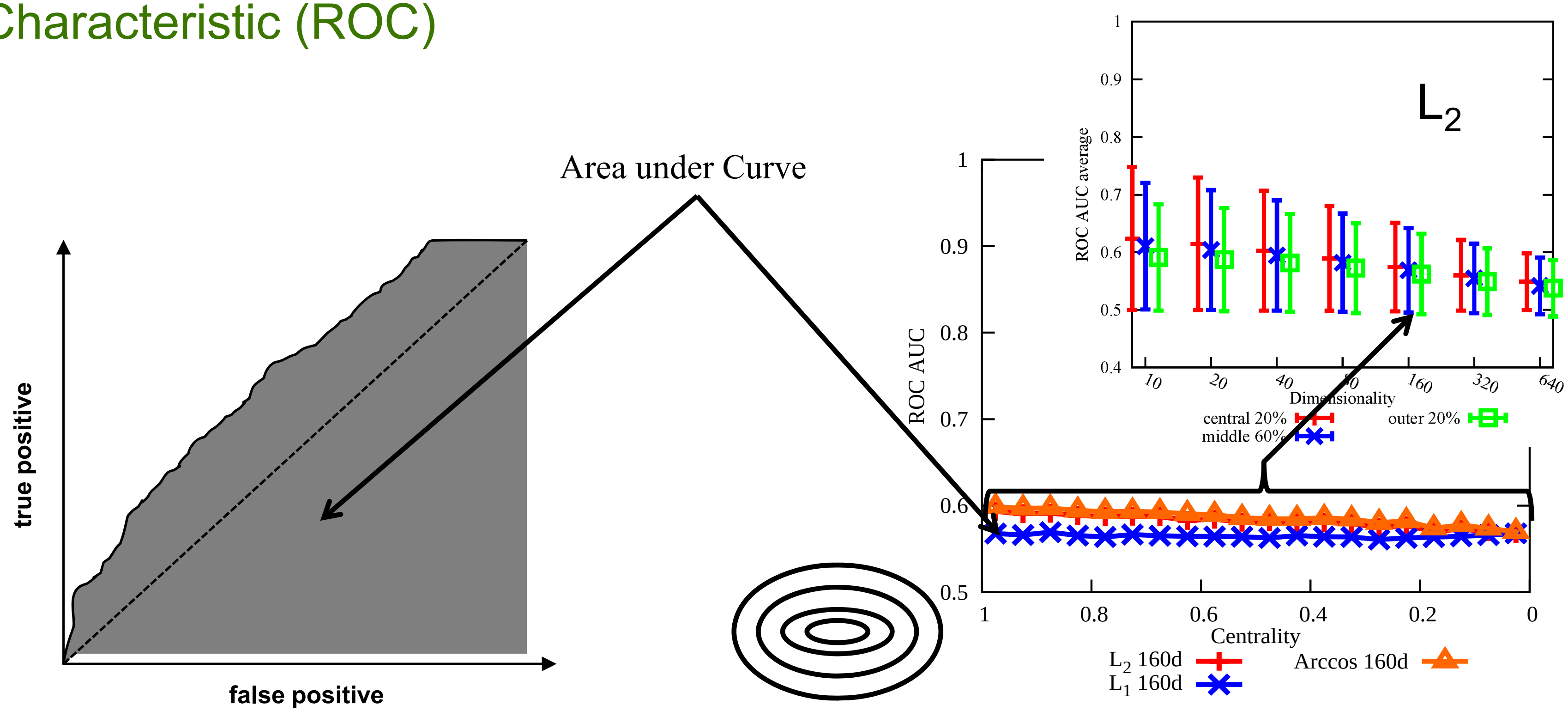


10-Relevant

$$\lim_{d\to\infty} \mathrm{var}\left(\frac{\|X_d\|}{E\left[\|X_d\|\right]}\right)=0 \quad\Rightarrow\quad \frac{D_{\max}-D_{\min}}{D_{\min}}\to 0$$

Shared-Neighbor Distances

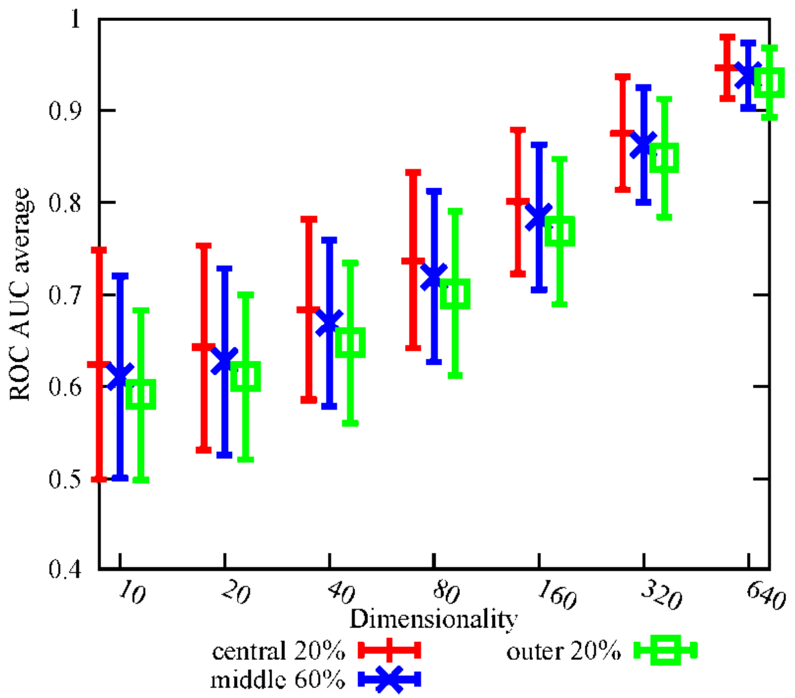
- Using each item in turn as a query, neighborhood ranking reported in terms of the Area under curve (AUC) of the Receiver Operating Characteristic (ROC)



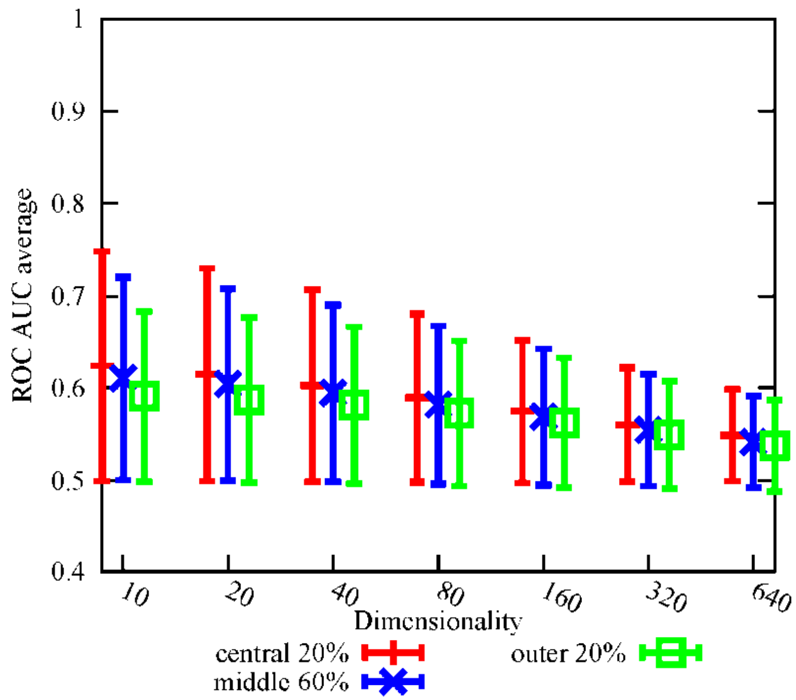
one query (neighbors same/different cluster) average over all items as a query

Shared-Neighbor Distances

Euclidean distance



All-Relevant

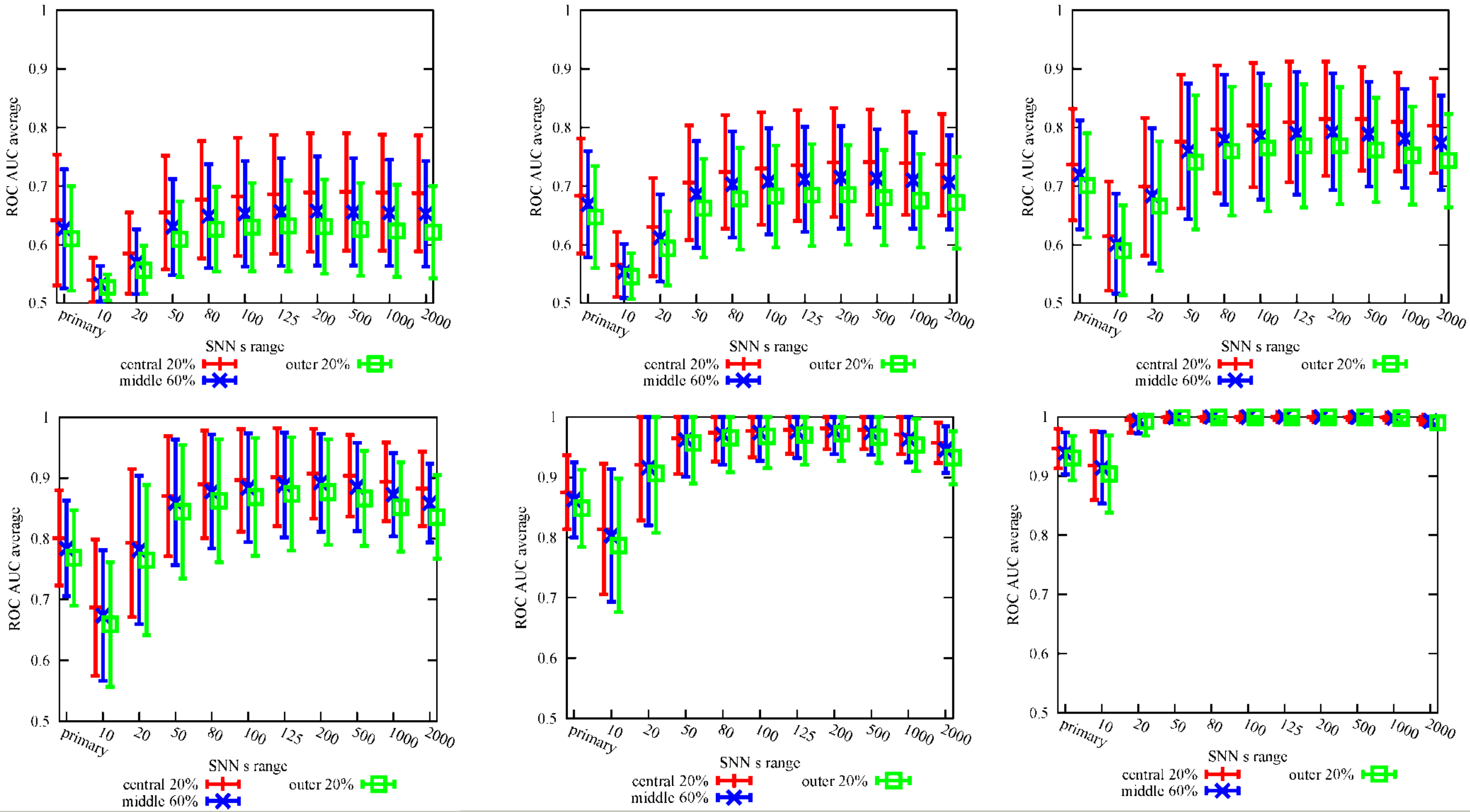


10-Relevant

Shared-Neighbor Distances

SNN based on Euclidean

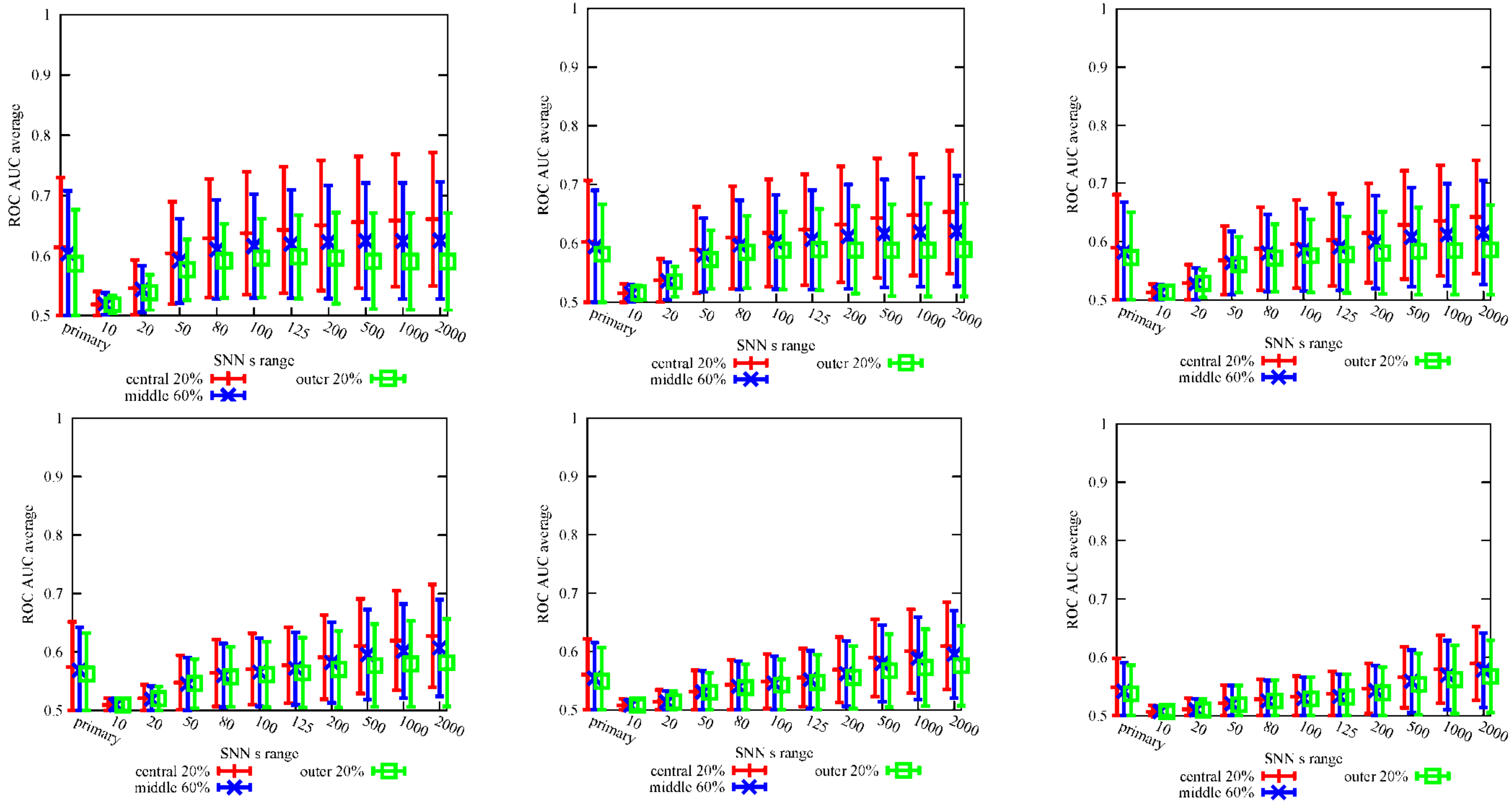
All-Relevant
20/40/80/160/320/640 dimensions



Shared-Neighbor Distances

SNN based on Euclidean

10-Relevant
20/40/80/160/320/640 dimensions



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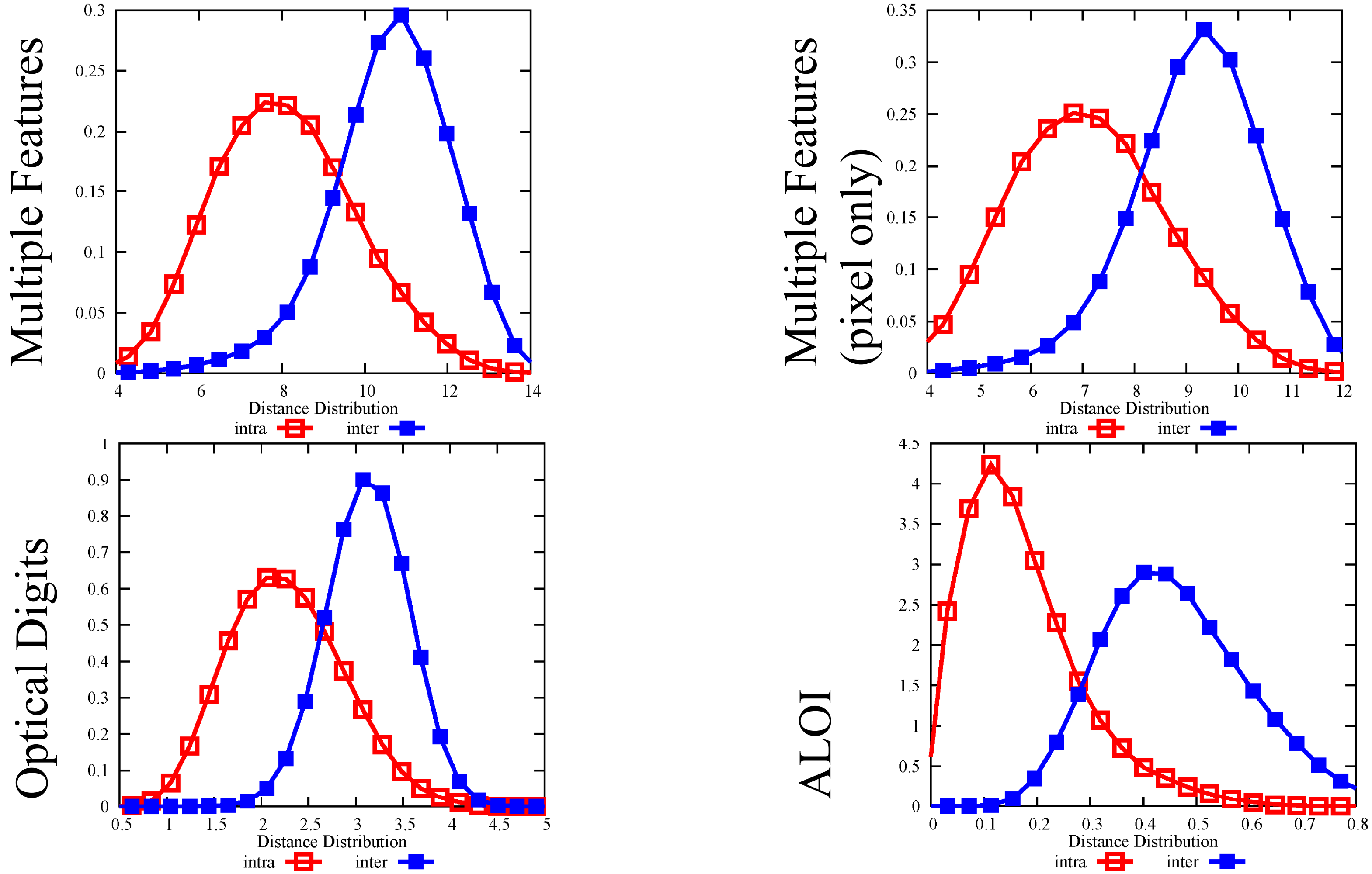
Shared-Neighbor Distances

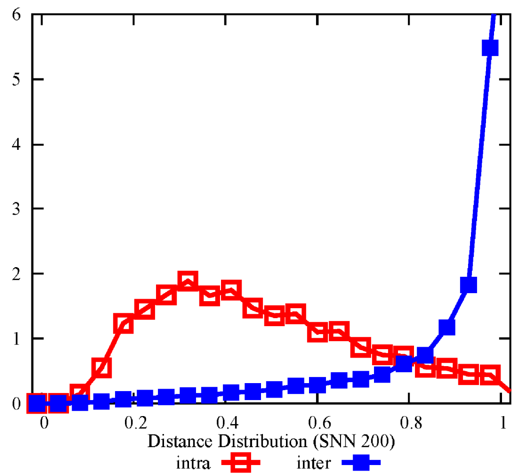
some real data sets: distributions of Euclidean distances



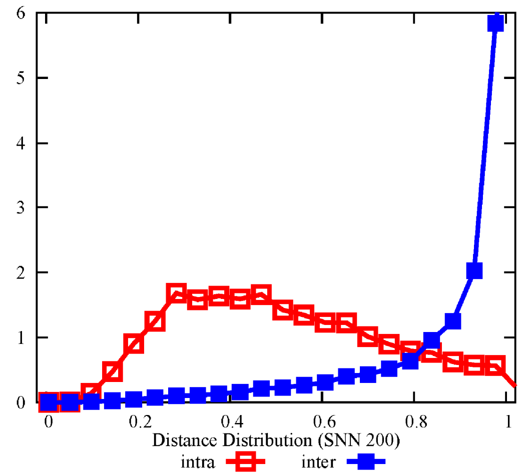
Shared-Neighbor Distances

some real data sets: distributions of SNN distances (Euclidean)

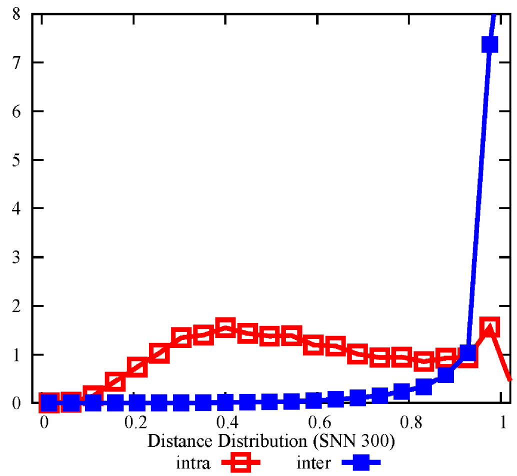
Multiple Features



Multiple Features (pixel only)



Optical Digits



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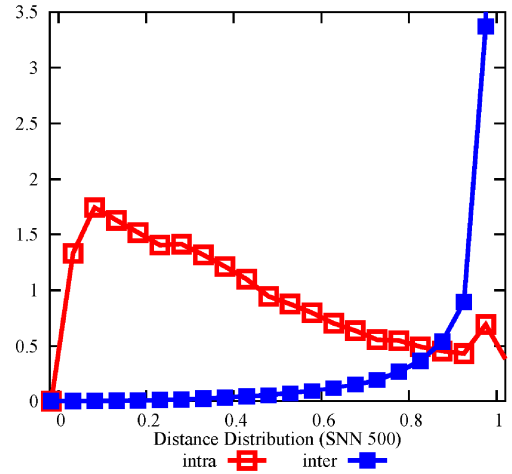
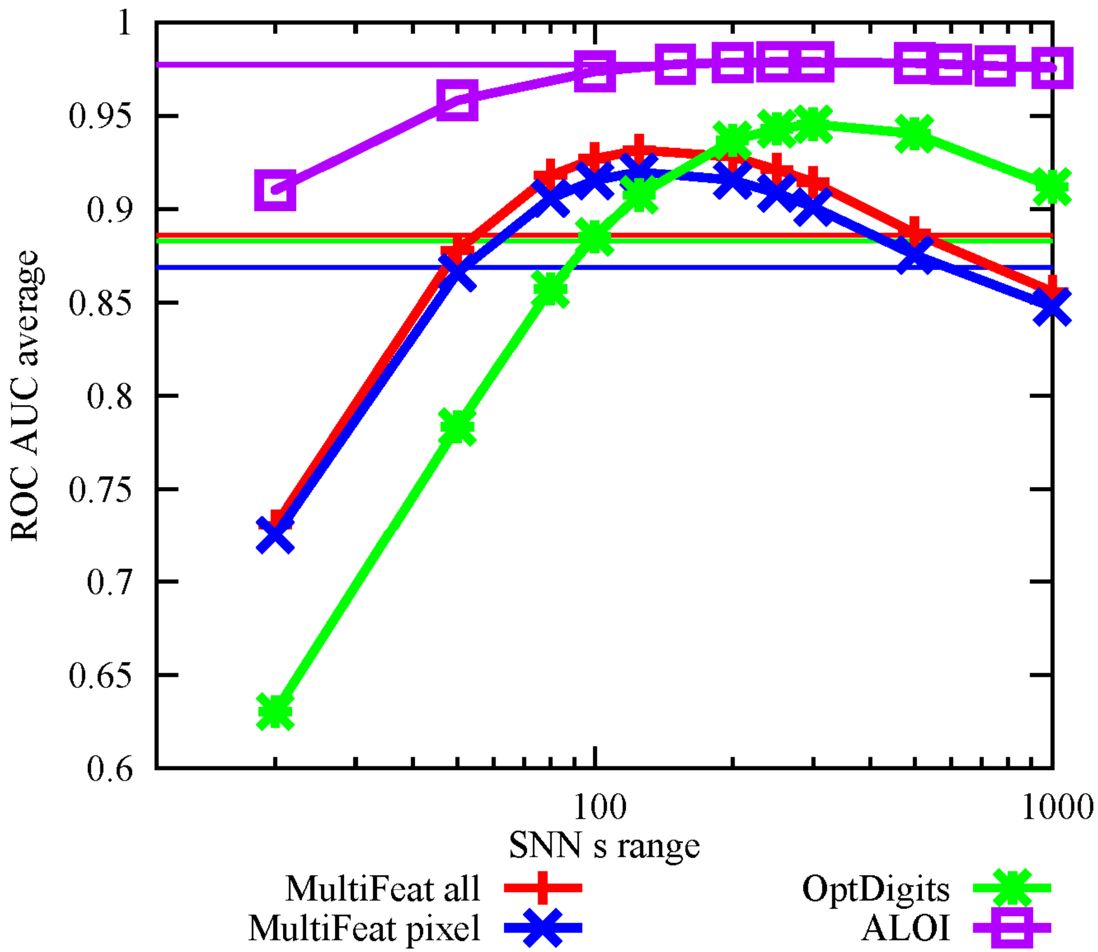


Shared-Neighbor Distances

some real data sets: ranking quality



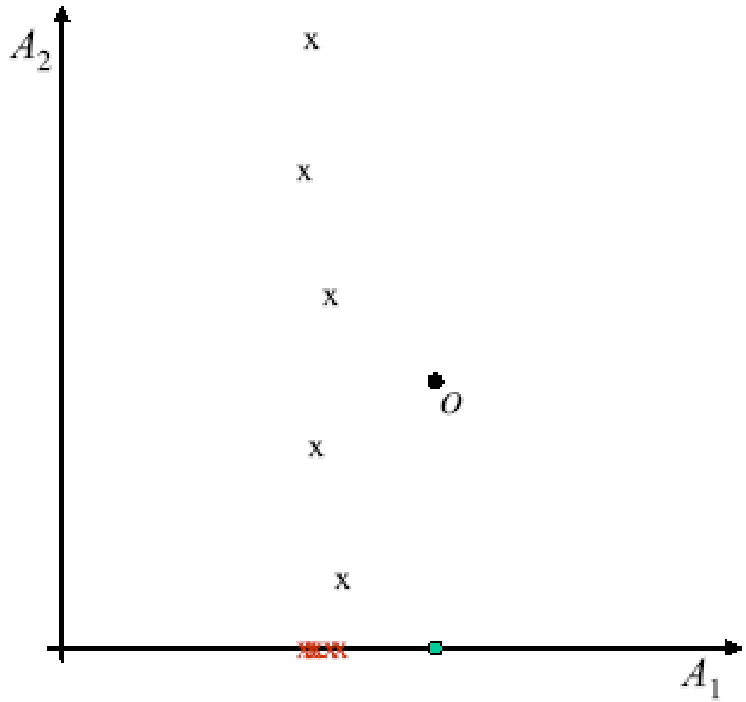
Subspace Outlier Detection

[KKSZ09]: *Outlier Detection in Axis-Parallel Subspaces of High Dimensional Data* (PAKDD 2009)

general idea:

- assign a set of reference points to a point *o*

  (e.g., *k*-nearest neighbors – but keep in mind the "curse of dimensionality": local feature relevance vs. meaningful distances)
- find the subspace spanned by these reference points (allowing some jitter)
- analyze for the point *o* how well it fits to this subspace

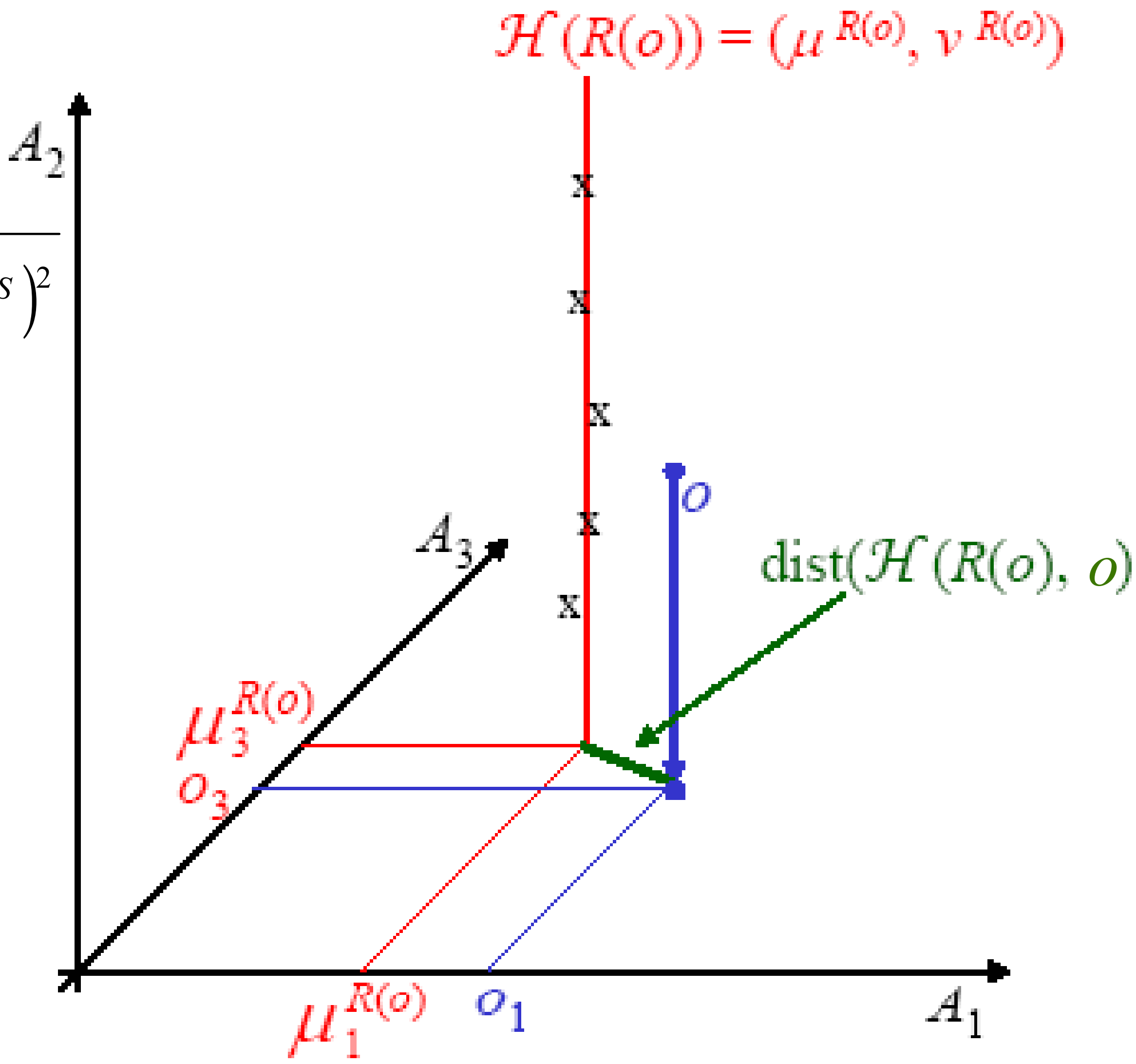


Subspace Outlier Detection

- distance of *o* to the reference hyperplane:

$$dist(o, H(S)) = \sqrt{\sum_{i=1}^{d} v_i^S \cdot (o_i - \mu_i^S)^2}$$

- the higher this distance, the more deviates the point *o* from the behavior of the reference set, the more likely it is an outlier



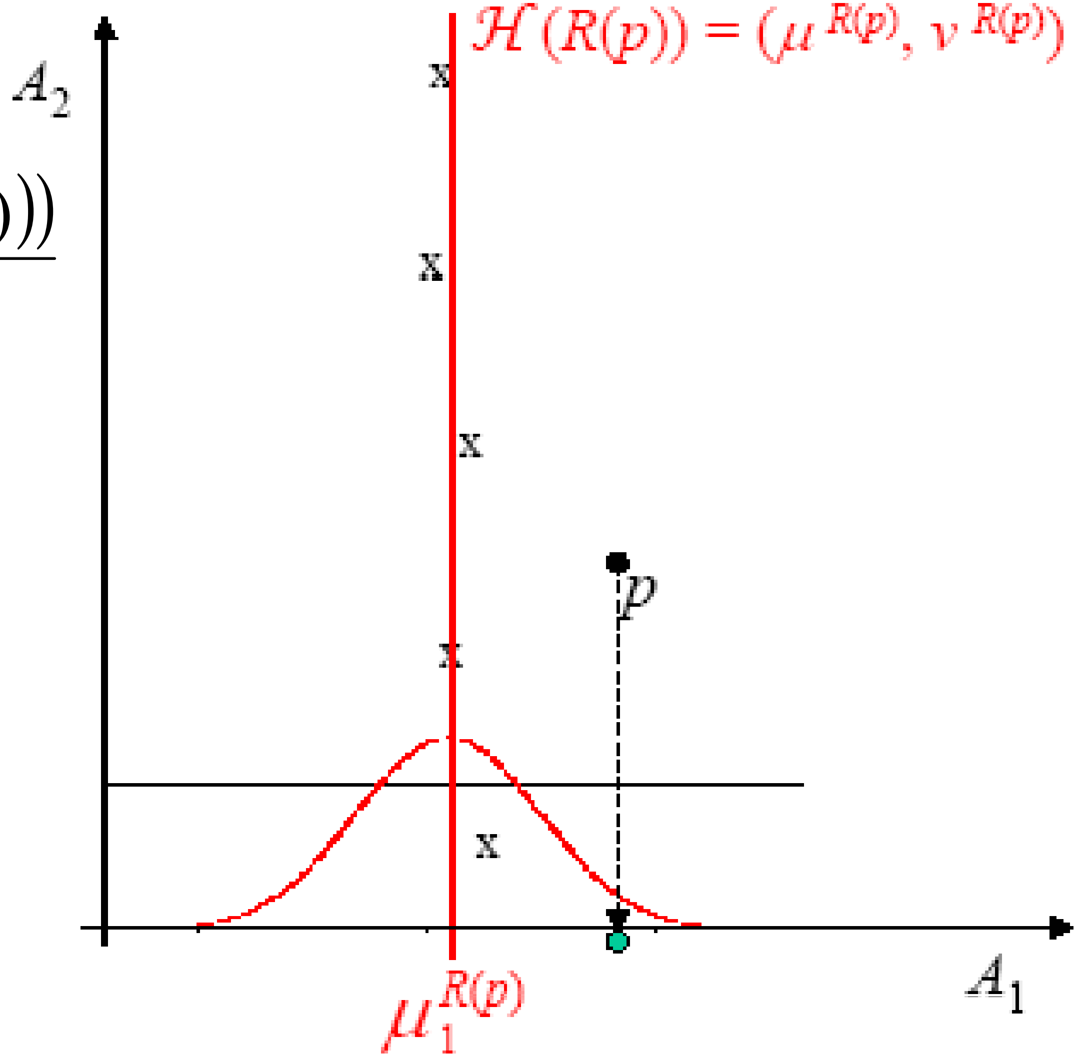
Subspace Outlier Detection

subspace outlier degree (SOD) of a point p:

$$SOD_{R(p)}(p) = \frac{dist\left(o, H\left(R(p)\right)\right)}{\left|v^{R(p)}\right|}$$

i.e., the distance normalized by the number of contributing attributes

possible normalization to a probability-value [0,1] in relation to the distribution of distances of all points in S



Subspace Outlier Detection

Choice of a reference set for outliers?

- recall “curse of dimensionality”
  - local feature relevance → need for a local reference set
  - distances loose expressiveness → how to choose a meaningful local reference set?
- consider k nearest neighbors in terms of the shared nearest neighbor similarity
  - given a primary distance function *dist* (e.g. Euclidean distance)
  - $N_k(p)$: k-nearest neighbors in terms of *dist*
  - SNN similarity for two points p and q:

$$sim_{SNN}(p,q) = \left| N_k(p) \cap N_k(q) \right|$$

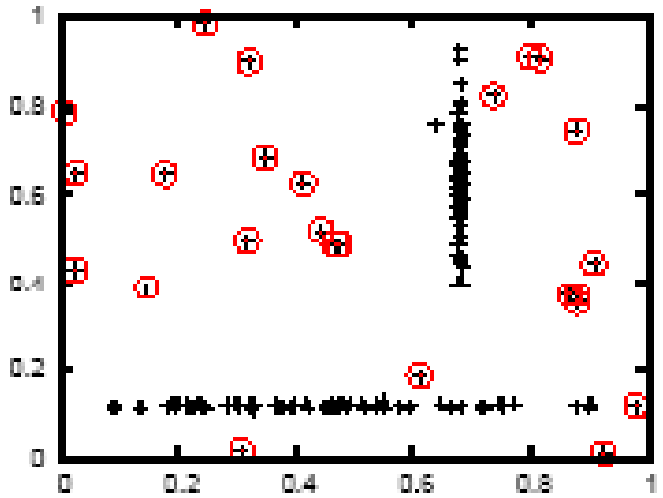
  - reference set $R(p)$: l-nearest neighbors of p using sim_{SNN}

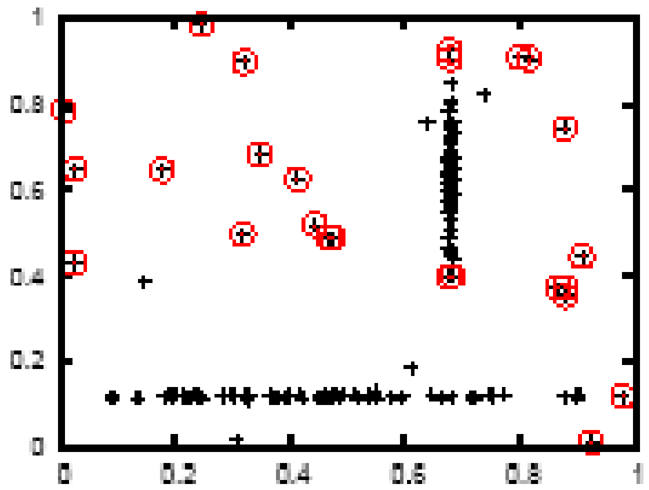
Subspace Outlier Detection

2-d sample data,
comparison to

- LOF [BKNS00]
- ABOD [KSZ08]

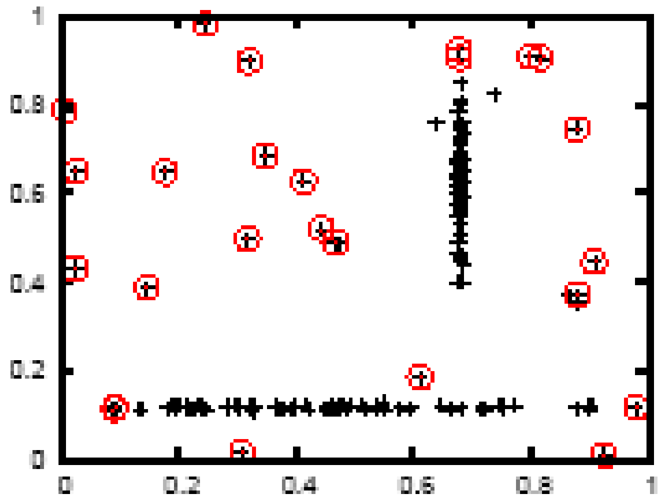
SOD





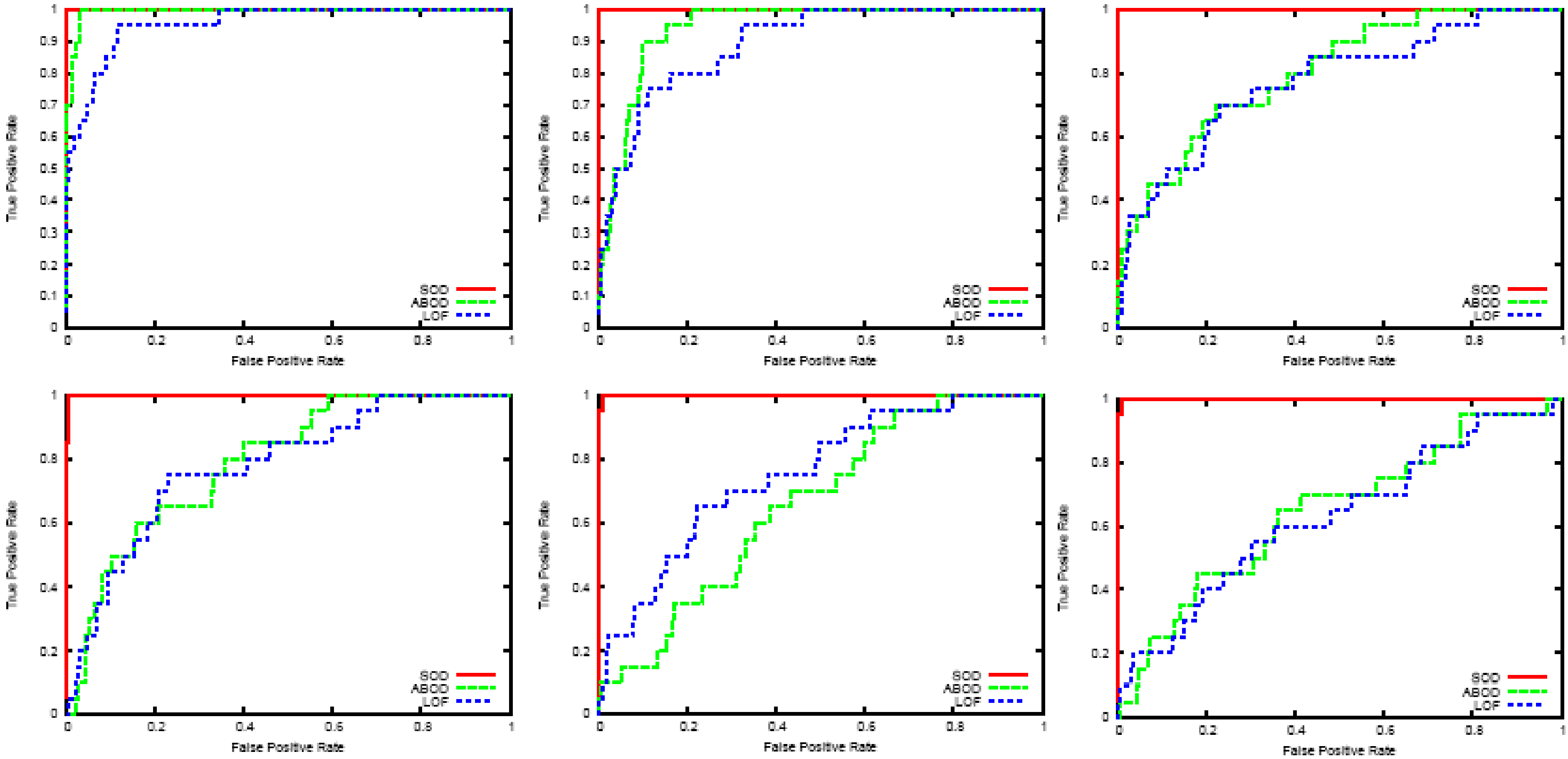
LOF

ABOD



Subspace Outlier Detection

- Gaussian distribution in 3 dimensions, 20 outliers
- adding 7, 17, 27, 47, 67, 97 irrelevant attributes



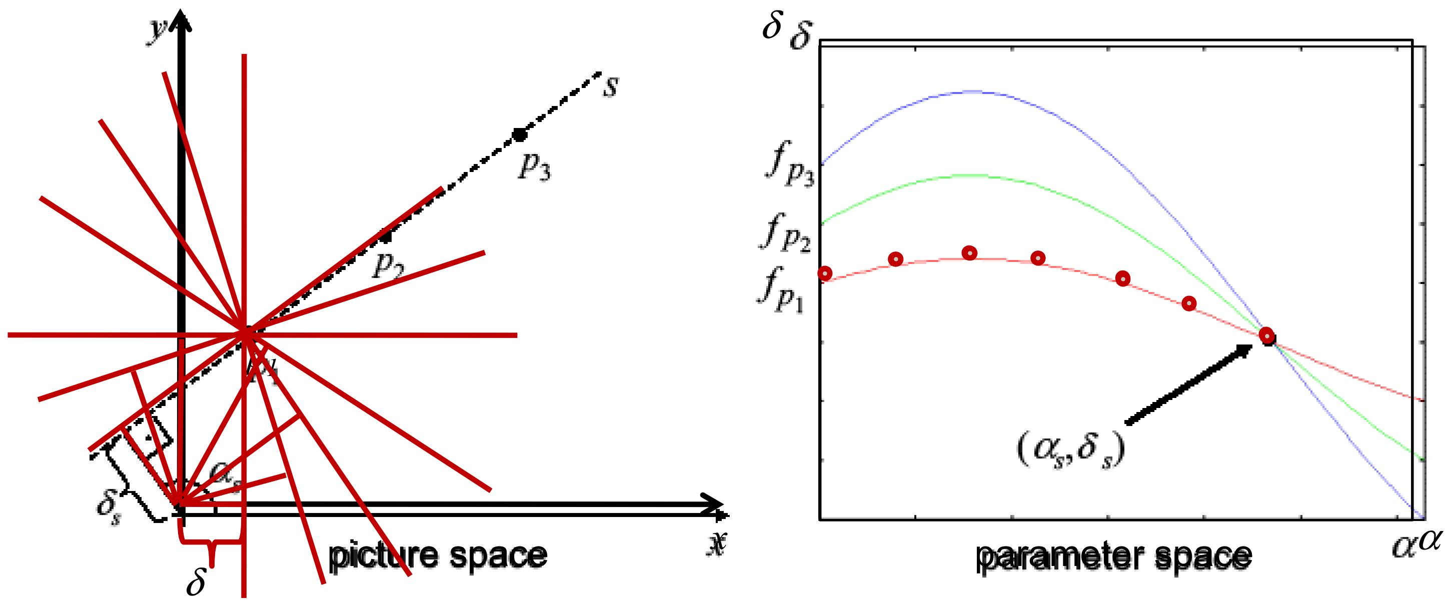
Subspace Clustering

[ABD+08]: *Robust clustering in arbitrarily oriented subspaces* (SDM 2008) (extended version: [ABD+08a])

- Algorithm CASH: Clustering in Arbitrary Subspaces based on the Hough-Transform
- Hough-transform:
  - developed in computer-graphics
  - 2-dimensional (image procesing)
- CASH:
  - generalization to *d*-dimensional spaces
  - transfer of the clustering to a new space (“Parameter-space” of the Hough-transform)
  - restriction of the search space (from innumerable infinite to $O(n!)$)
  - common search heuristic for Hough-transform: $O(2^d)$
    $\rightarrow$ efficient search heuristic

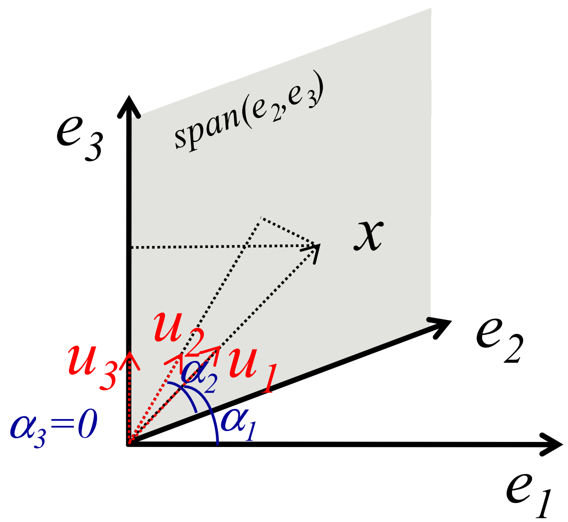
Subspace Clustering

- given: $D \subseteq \Re^d$
- find linear subspaces accommodating many points
- Idea: map points from data space (picture space) onto functions in parameter space



Subspace Clustering

- e_i, $1 \leq i \leq d$: orthonormal-basis
- $x = (x_1,\ldots,x_d)^T$: d-dimensional vector onto hypersphere around the origin with radius r
- u_i: unit-vector in direction of projection of x onto subspace $span(e_i,\ldots,e_d)$
- $\alpha_1,\ldots,\alpha_{d-1}$: α_i angle between u_i and e_i

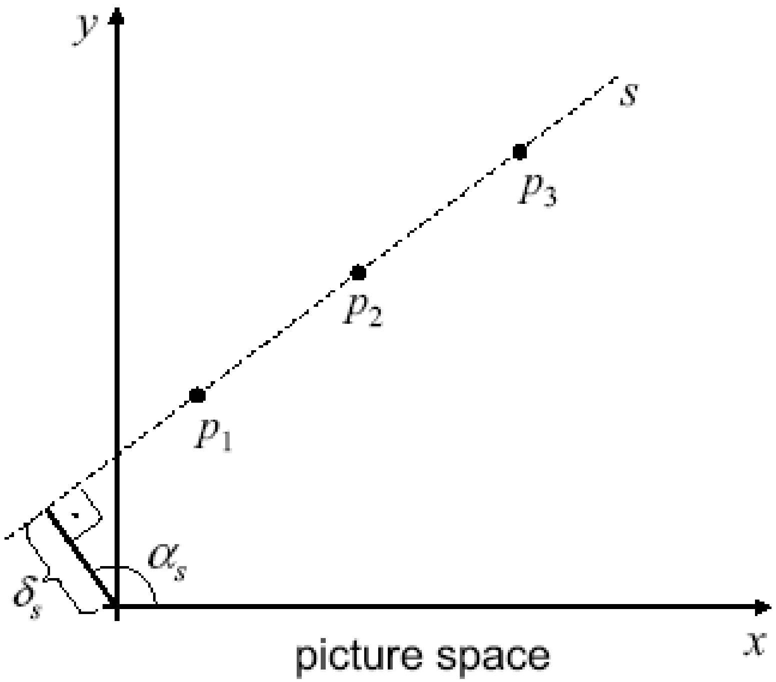


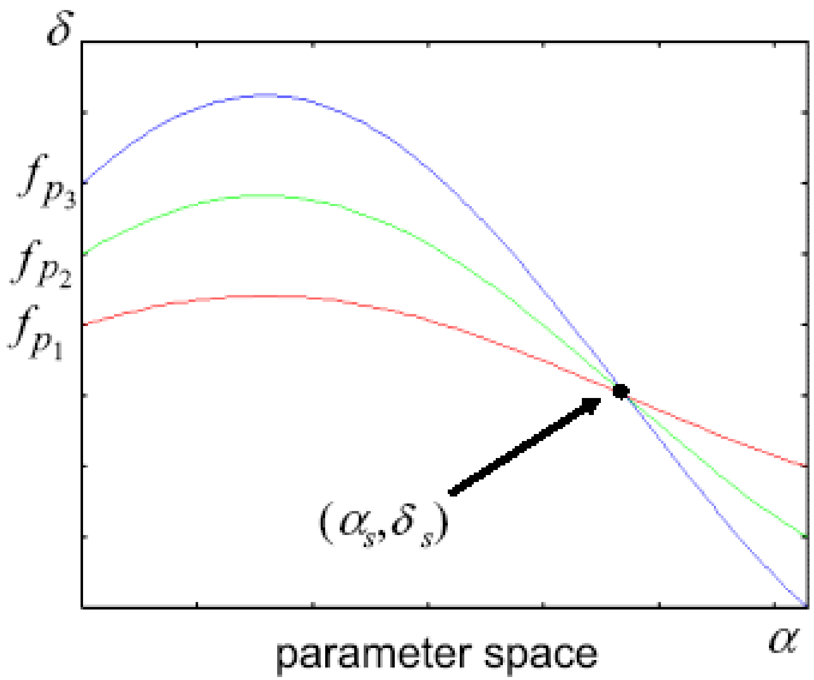
$$x_i = r \cdot \left(\prod_{j=1}^{i-1} \sin(\alpha_j) \right) \cdot \cos(\alpha_i)$$

Subspace Clustering

Length δ of the normal vector $\delta \cdot \vec{n}$ with $\|\vec{n}\| = 1$ and angles $\alpha_1, \ldots, \alpha_{d-1}$ for the line through point *p*:

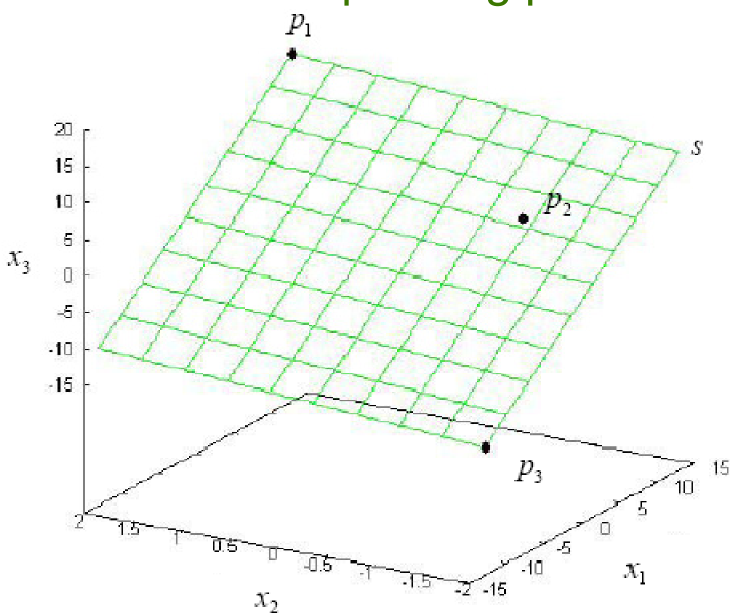
$$f_p(\alpha_1, \ldots, \alpha_{d-1}) = \langle p, n \rangle = \sum_{i=1}^{d} p_i \cdot \left(\prod_{j=1}^{i-1} \sin(\alpha_j) \right) \cdot \cos(\alpha_i)$$

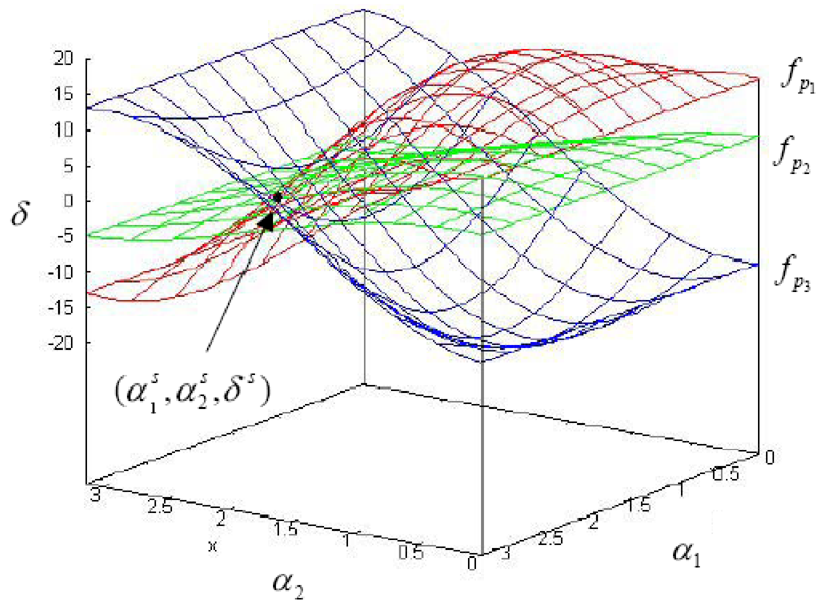




Subspace Clustering

- 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

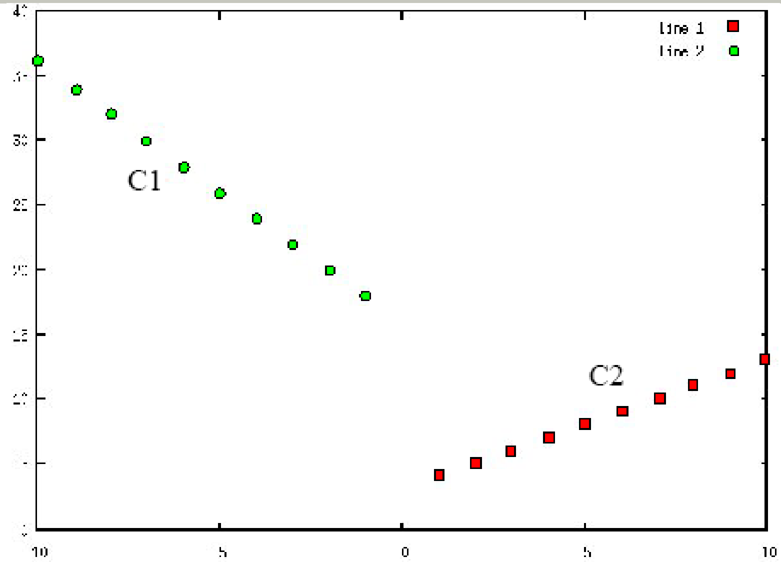


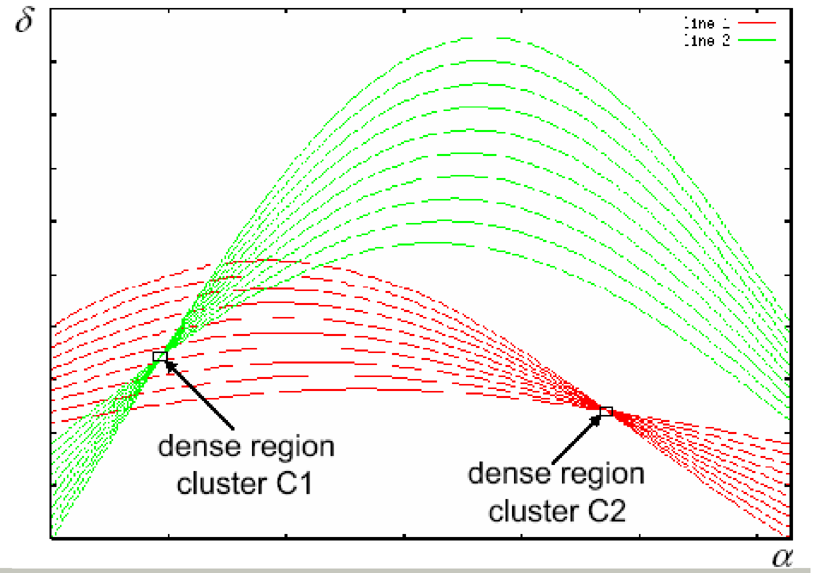


Subspace Clustering

- dense regions in parameter space $\Leftrightarrow$ linear structures in data space (hyperplanes with $\lambda \leq d\text{-}1$)
- exact solution: find all intersection points
  - infeasible
  - too exact
- approximative solution: grid-based clustering in parameter space

  $\rightarrow$ find grid cells intersected by at least *m* sinusoids
  - search space bounded but in $O(r^d)$
  - pure clusters require large value for *r* (grid solution)

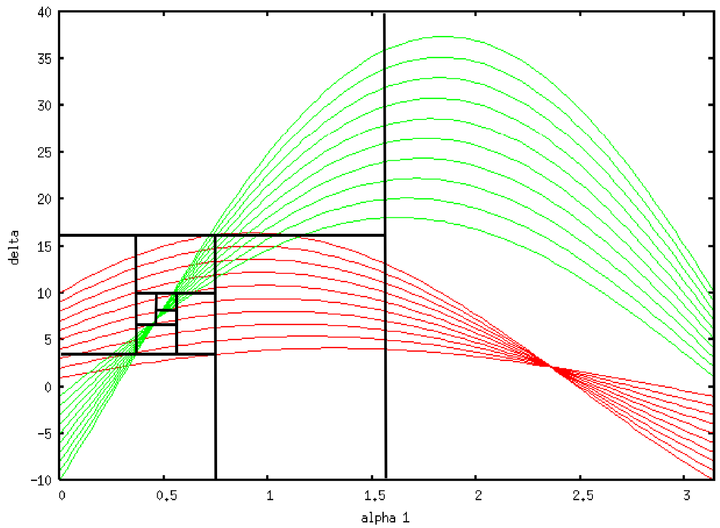




Subspace Clustering

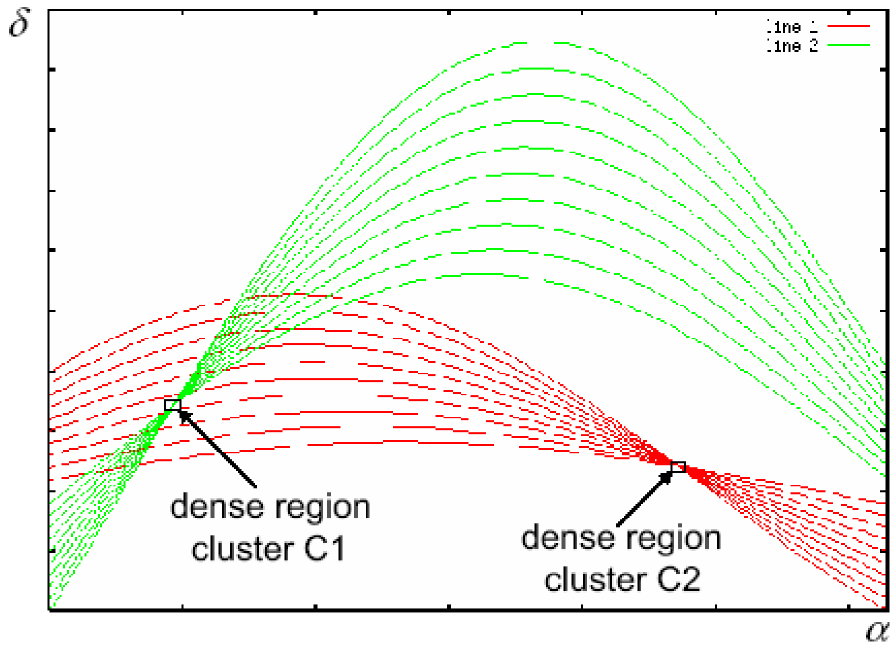
efficient search heuristic for dense regions in parameter space

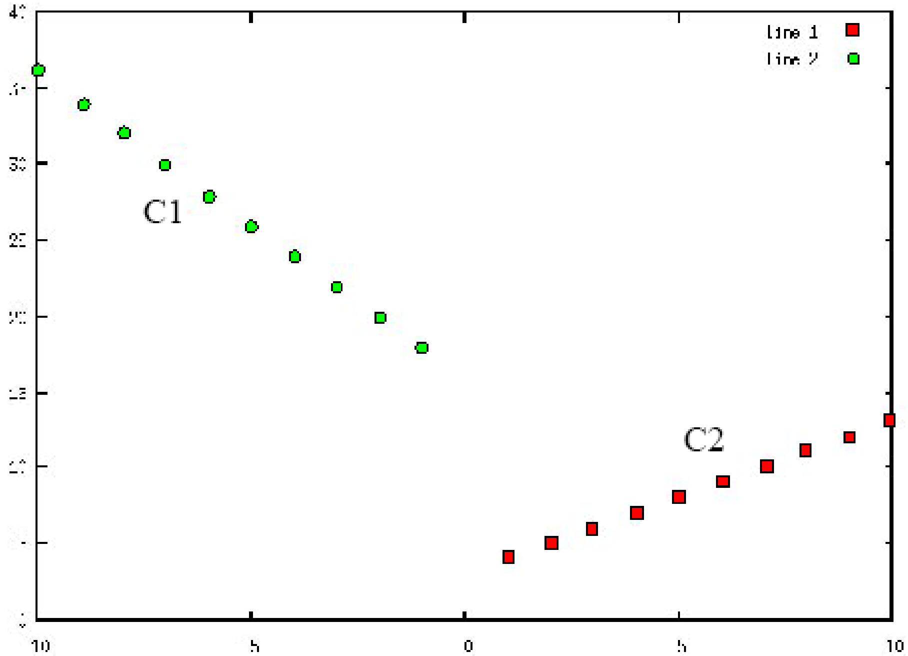
- construct a grid by recursively splitting the parameter space (best-first-search)
- identify dense grid cells as intersected by many parametrization functions
- dense grid cell represents (*d-1*)-dimensional linear structure
- transform corresponding data objects in corresponding (*d-1*)-dimensional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



Subspace Clustering

- grid cell representing less than *m* points can be excluded
  $\rightarrow$ early pruning of a search path
- grid cell intersected by at least *m* sinusoids after *s* recursive splits represents a correlation cluster (with $\lambda \leq d\text{-}1$)
  - remove points of the cluster (and corr. sinusoids) from remaining cells





Subspace Clustering

- search heuristic: linear in number of points, but ~ $O(d^3)$

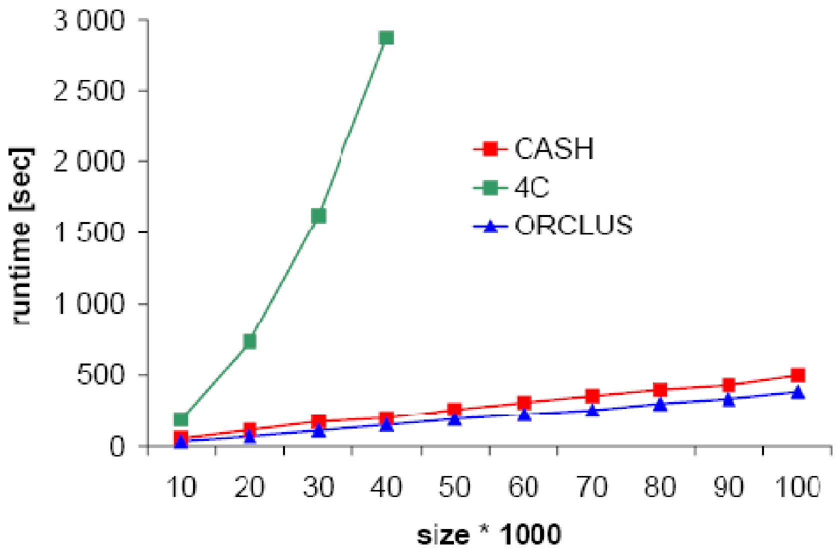
  depth of search s, number c of pursued paths (ideally: c cluster):

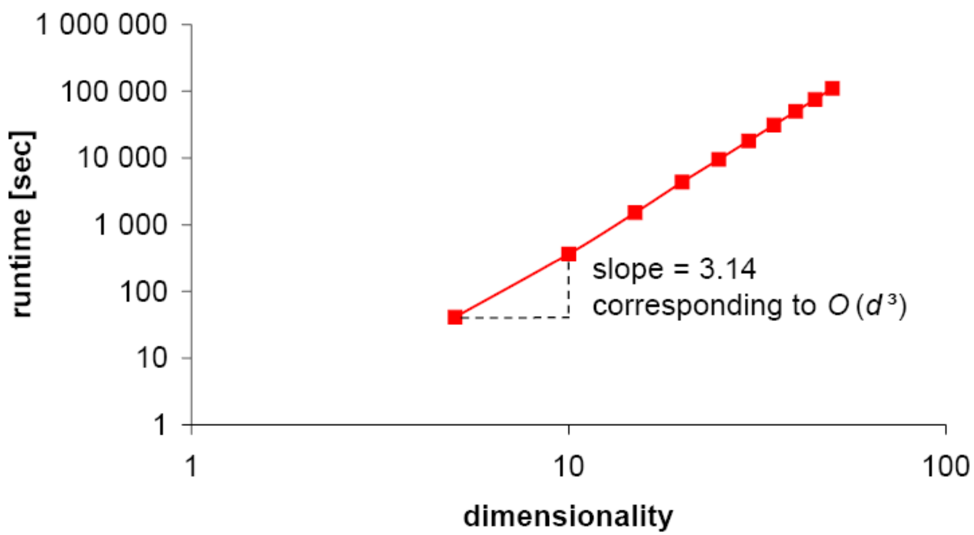
  – priority search: $O(s \cdot c)$

  – determination of curves intersecting a cell: $O(n \cdot d^3)$

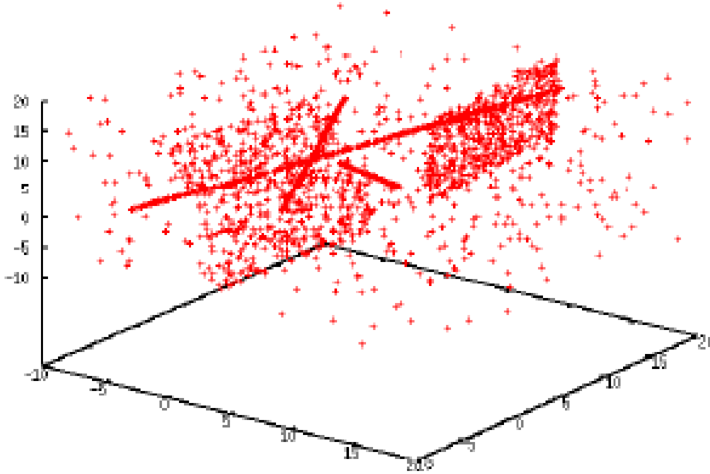
  – overall: $O(s \cdot c \cdot n \cdot d^3)$

    (note: PCA generally in $O(d^3)$)

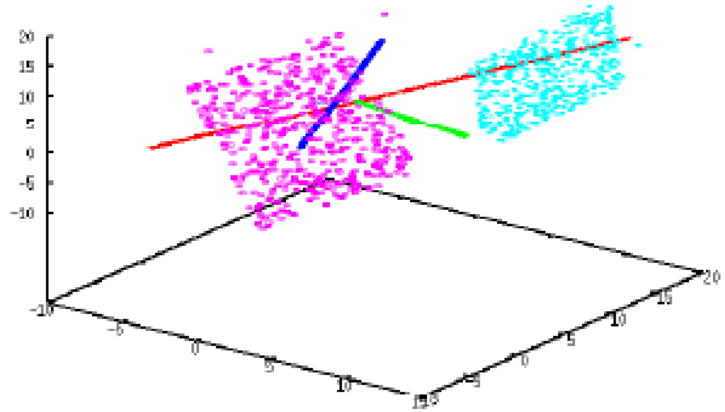




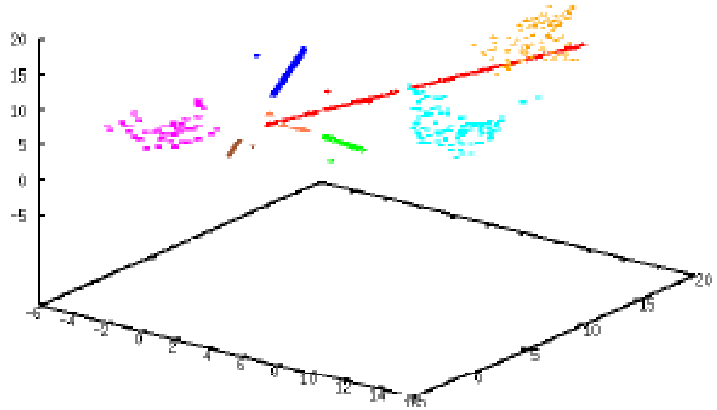
Subspace Clustering



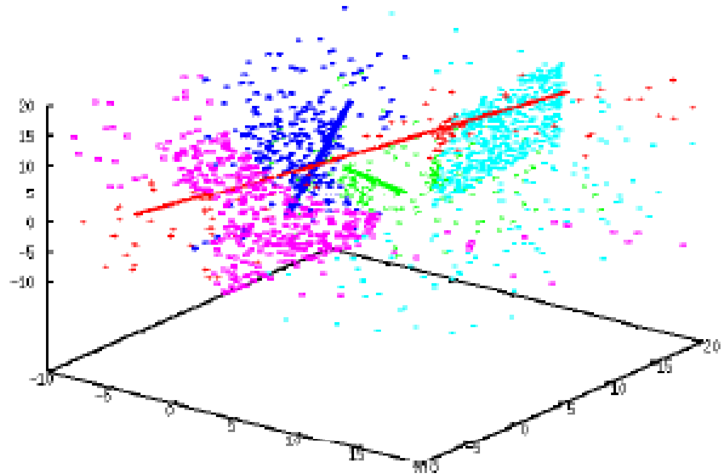
(a) Data set



(b) CASH: Cluster 1-5



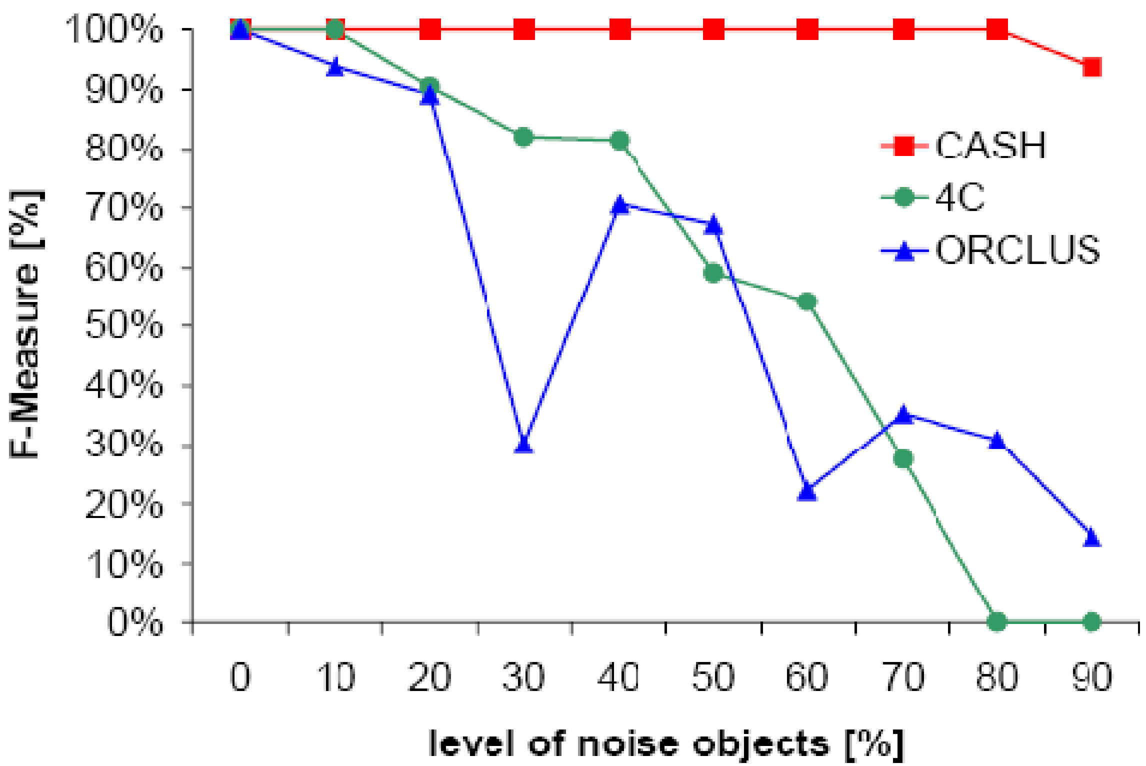
(c) 4C: Cluster 1-8



(d) ORCLUS: Cluster 1-5

Subspace Clustering

- stability with increasing number of noise objects



Conclusions

- The *curse of dimensionality* does not count in general as an excuse for everything – depends on the number and nature of distributions in a data set
- the nature of each particular problem needs to be studied in its own
- part of the curse: it’s always different than expected
- if you ever think, you have solved the problems of the curse: watch out for the curse striking back!

Some Advice

- do not take everything for granted which is stated in the literature
- consider claims in the literature:
  - is there enough evidence to support the claims?
  - is the interpretation of the claims clear?
  - challenge them or support them
- papers report the strengths – you should try to find out the weaknesses and to improve
- have fun!

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