Vorlesung Knowledge Discovery,
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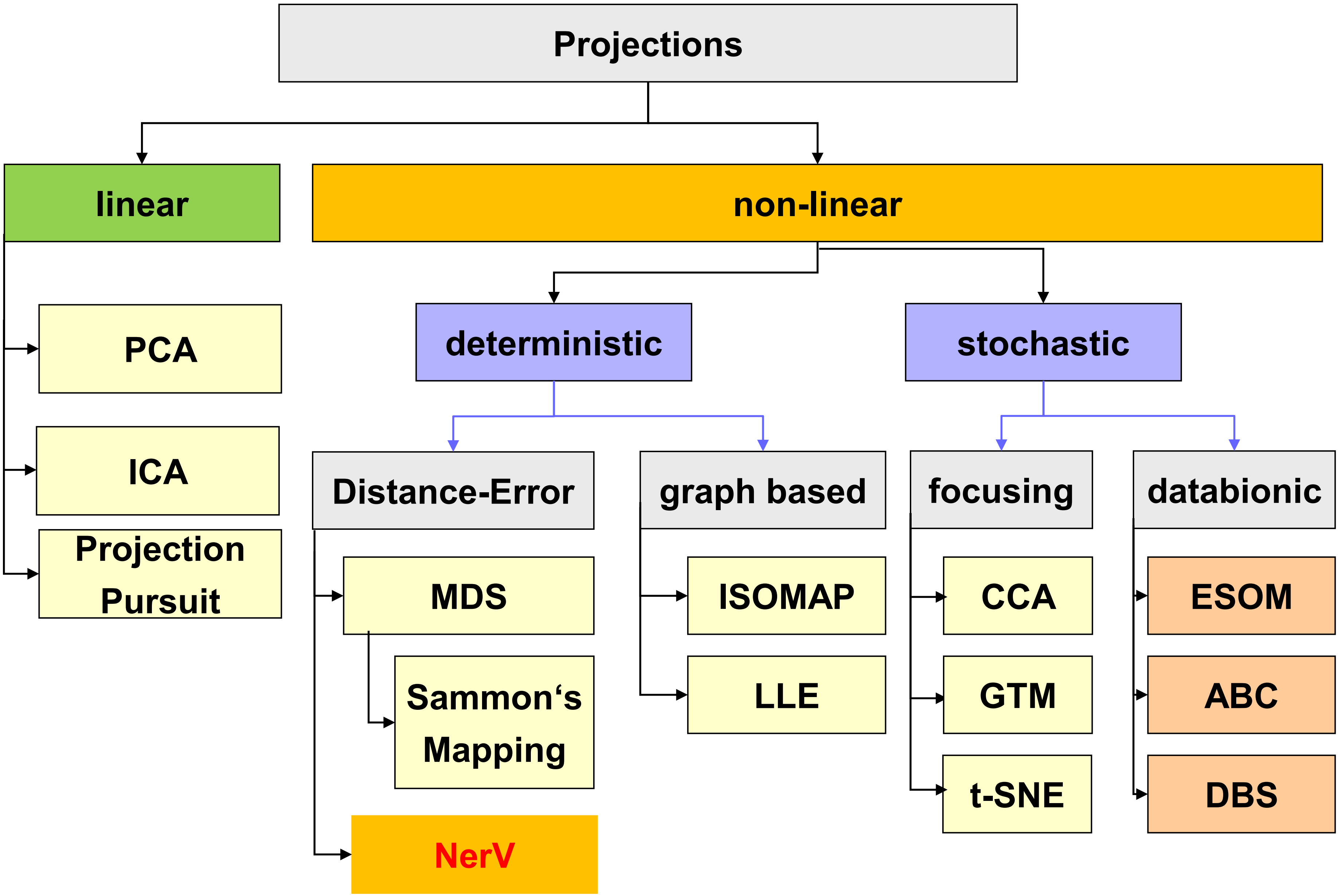
neighbor retrieval visualizer - NeRV

Databionics Research Group

Philipps Universität Marburg


Projections
linear
non-linear
PCA
ICA
Projection Pursuit
deterministic
stochastic
Distance-Error
graph based
focusing
databionic
MDS
Sammon‘s Mapping
NerV
ISOMAP
LLE
CCA
GTM
t-SNE
ESOM
ABC
DBS

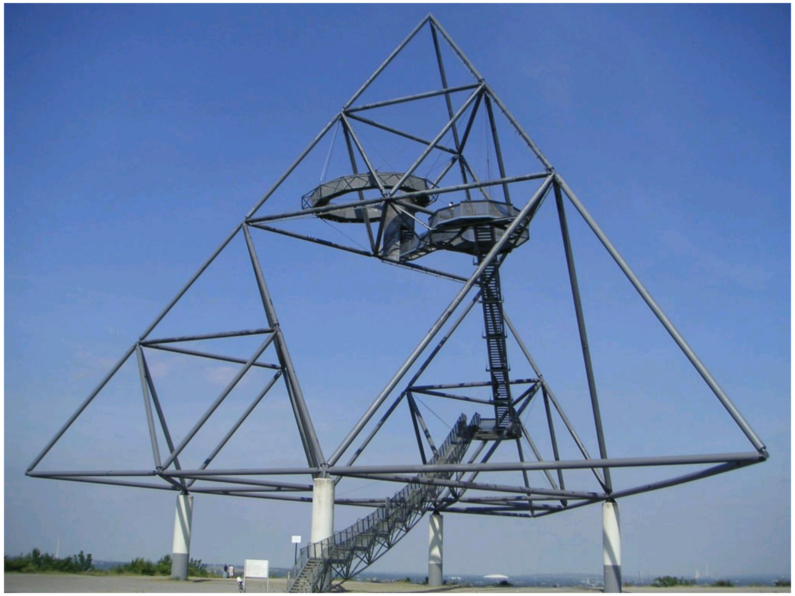
Grundlagen

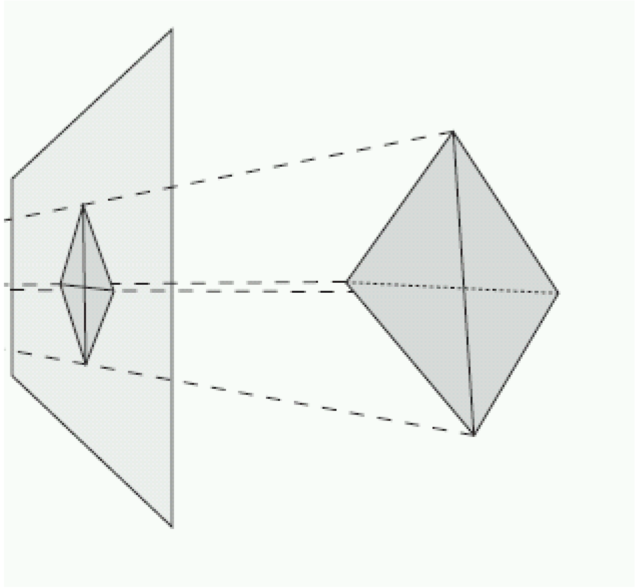
- Input Space $I \subset \mathbb{R}^{\boldsymbol{n}}$, D(l,j) Distanz
- Output Space $O \subset \mathbb{R}^{\mathbf{2}}$, d(l,j) Distanz
- Projektion: $proj\colon\ I \to O,\ D(l,j) \mapsto\ d(l,j)$, *where a l and j are points in the corresponding metric spaces*
- Backward Projection Error (BPE)
- Forward Projection Error (FPE)

Problem

Bei einer Projektion $\mathbb{R}^n$ ->$\mathbb{R}^m$, m<<n können NIE alle Nachbarschaften oder gar Distanzen perfekt erhalten werden

-> ShepardDiagram



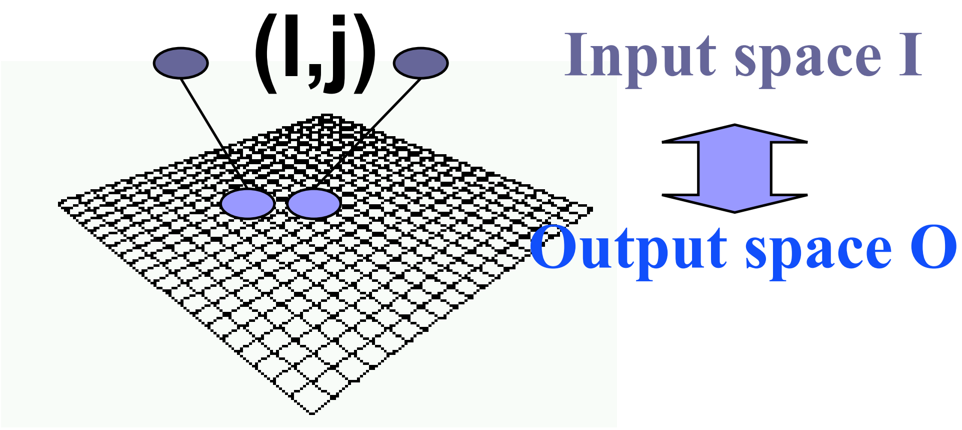


Precision – Quality for BPE

- **Good if:**

  Points that are close in the output space are close in the original space

http://www.uta.fi/sis/mtt/mtts1-dimensionality_reduction/...
2014Peltonen_drv_lecture7



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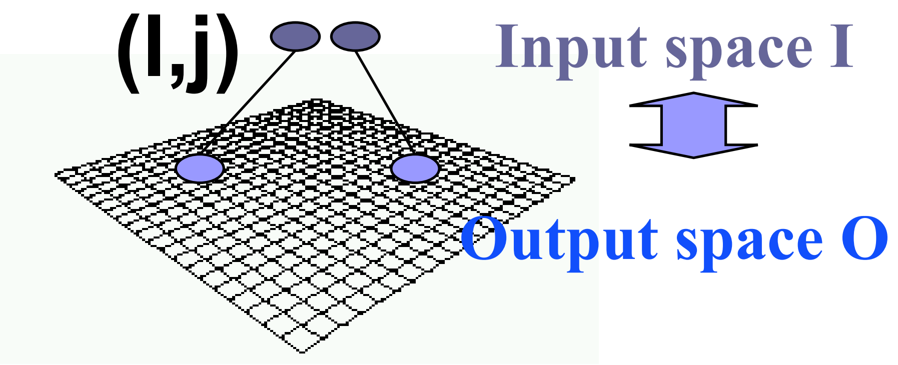
Recall – Quality for FPE

- **Good if**:

  Points that are close in the input space are close in the output space

2014Peltonen_drv_lecture7



Prinzip: NeRV

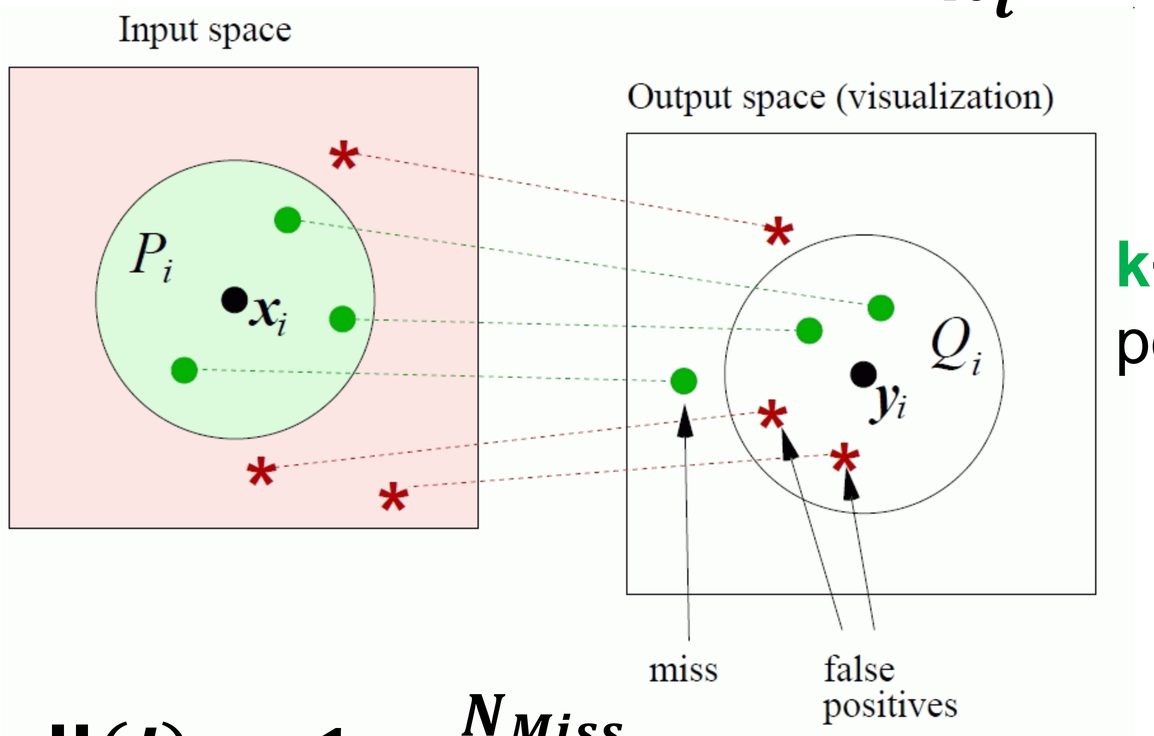
- Lyapunov Funktion E (objective function)
- Idee: SNE mit Precision und Recall und kaum Fokussierung

Zuerst: Nachbahrschaftsdefinition…

"Hard" Neighborhoods

$$Precision(i) = 1 - \frac{N_{False\ positive}}{k_i}$$

r~number of relevant points (green)



k~retrieved points (green)

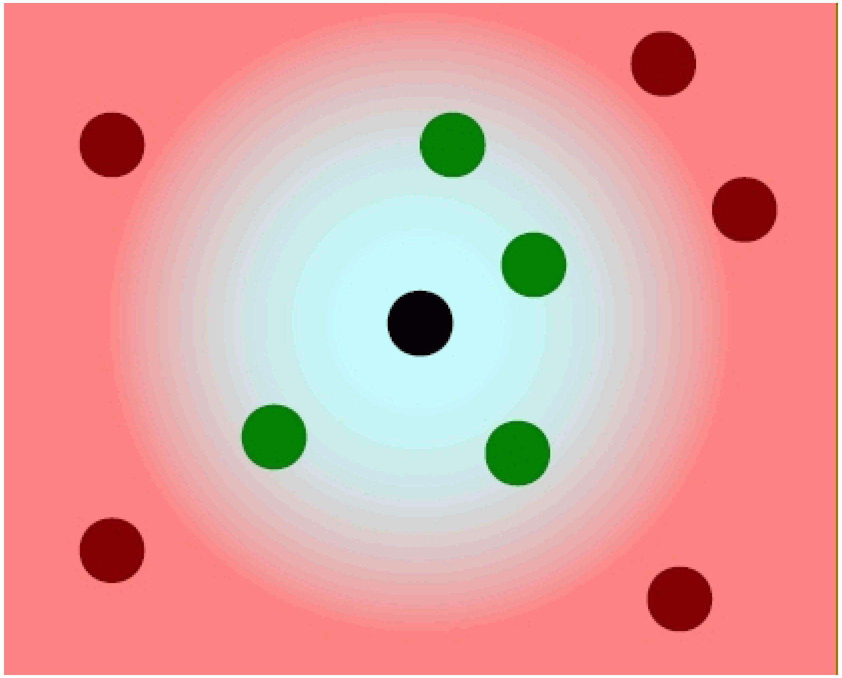
$$\text{Recall}(i) = 1 - \frac{N_{Miss}}{r_i}$$

2010, Venna et al. Information Retrieval Perspective to Nonlinear Dimensionality Reduction for Data Visualization

Motivation: “Soft” Neighborhoods

http://www.uta.fi/sis/mtt/mtts1-dimensionality_reduction/...

2015Peltonen_MTTS_lecture10:



- “In vectorial data, if nothing else is known, it is reasonable that close-by points in some metric can be considered neighbors
- each point is a neighbor with some weight and a non-neighbor with some Weight”

Probabilistic neighborhood

- die Wahrscheinlichkeit, dass Datenpunkt j den Punkt j zum Nachbarn hat

$$p(l,j)=\frac{exp(-\frac{D(l,j)^2}{2}/2\sigma^2)}{\sum_{l\neq j} \; exp(-D(l,j)^2/2\sigma^2)}$$

Output space:

$$q(l,j)=\frac{exp(-d(l,j)^2/2\sigma^2)}{\sum_{l\neq j} \; exp(-d(l,j)^2/2\sigma^2)}$$

⇒ **The same as SNE**

(Stochastic Neighbor Embedding)

SNE

- Two probability distributions over a set of items can be compared by the **Kullback-Leibler (KL) divergence**

= relative entropy

= amount of surprise when encountering items from the 1st distribution when items were expected to come from the 2nd

$$E_{SNE} = \sum_{l} \sum_{j \neq l} p(l,j) \log\left(\frac{p(l,j)}{q(l,j)}\right) := \boldsymbol{KL(p)}$$

http://www.uta.fi/sis/mtt/mtts1-dimensionality_reduction/...

2015Peltonen_MTTS_lecture10:

SNE - Details

- Minimization of Objective function E
- nonnegative, and zero if and only if the distributions are equal
- value of the divergence sum depends on output coordinates, and can be minimized with respect to them
- σ as radius if neighborhood

In NeRV

- "Scale parameter" $\boldsymbol{\sigma}$ fest
  - Peltonen: effective number of neighbors
  - Peltonen: $c(j) = \log(\mathbf{k}(\mathrm{j}))$,

k~retrieved points (green) around point j

http://www.uta.fi/sis/mtt/mtts1-dimensionality_reduction/...

2015Peltonen_MTTS_lecture10:

Äquivalenz Recall R

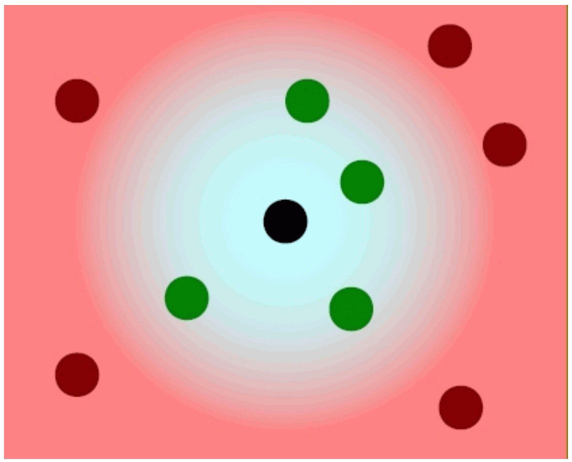
$$\mathbf{R}(\boldsymbol{l}) = \mathbf{1} - \frac{\boldsymbol{N_{Miss}}}{\boldsymbol{r_l}} \Leftrightarrow \sum_l \sum_{j \neq l} p(l,j) \log\left(\frac{p(l,j)}{q(l,j)}\right)$$

Soft neighborhood

Proof: 2010, Venna et al. Information Retrieval Perspective to Nonlinear Dimensionality Reduction for Data Visualization

Peltonen: “assume some probabilities are uniformly-large, some are uniformly-small. Then there are 4 different kinds of terms in the sum. Show that above KL divergence is dominated by a cost that is proportional to a constant times number of misses”

“Soft” Neighborhoods II



$$p(l,j)\log\left(\frac{p(l,j)}{q(l,j)}\right) = p(l,j) * weight$$

=> R ~”sum over **observed center-neighbor pairs,** weighted by their proportional counts pij,
We sum the log-likelihoods of those observations (2015Peltonen_MTTS_lecture10)

Folgerung: Precision Pr

- “SNE focuses on recall (misses) because its cost function is dominated by misses”

$$Pr(l) = 1 - \frac{N_{False\ positive}}{k_l} \Leftrightarrow \sum_l \sum_{j \neq l} q(l,j) \log\left(\frac{q(l,j)}{p(l,j)}\right)$$

- “change the retrieval model so that misses become less dominant, so that the model can also focus on false positives”

Proof: 2010, Venna et al. Information Retrieval Perspective to Nonlinear Dimensionality Reduction for Data Visualization

Peltonen: “assume some probabilities are uniformly-large, some are uniformly-small. Then there are 4 different kinds of terms in the sum. Show that above KL divergence is dominated by a term proportional to a constant times number of false neighbors”

Neighbor Retrieval Visualizer

$$E_{NeRV} = \lambda * Ex\{KL(p)\} + (1 - \lambda) * Ex\{KL(q)\}$$

- Minimize with respect to output space points
- Ex ~ "Expectation" (Mittelwert)
- λ ~ tradoff between Precision and Recall
- User has to choose λ

1.) Initialization "To speed up convergence and avoid local minima"

2.) standard conjugate gradient step (analog MDS)

2010, Venna et al.
Information Retrieval
Perspective to Nonlinear
Dimensionality Reduction
for Data Visualization

Details NeRV

- 20 steps with decreasing σ per two steps
- Linear decreasing

$\sigma_{max} \sim half\ diamater\ of\ input\ data$

$\sigma_{min} = \log(\mathbf{k}(\mathrm{j}))$

After Initialization

- 20 standard conjugate gradient steps with σ_{min}

2010, Venna et al.
Information Retrieval
Perspective to Nonlinear
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λ ~ Tradoff between Pr and R

- A: λ niedrig -> Precison hoch

“minimizes false positives (false retrieved neighbors)”

- b: λ hoch -> Recall hoch

“minimizes misses (neighbors that were not retrieved)”

2010, Venna et al.
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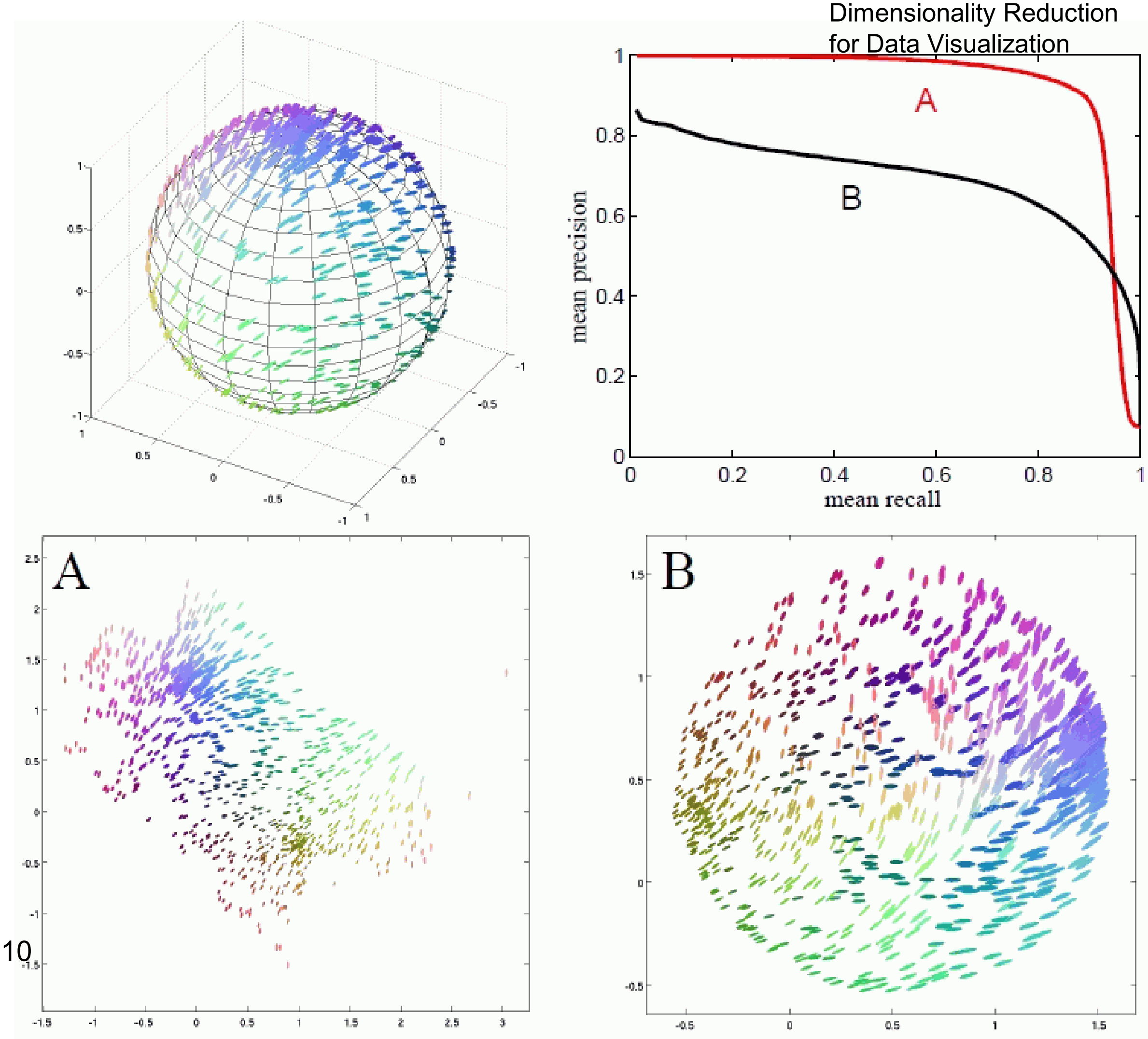

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Venna 2010, Information Retrieval Perspective to Nonlinear Dimensionality Reduction for Data Visualization

- "In unsupervised visualization, NeRV outperformed alternatives for most of the six data sets we tried, for four different pairs of measures, and was overall the best method."
  - verglichen wurde mit PCA, MDS, LLE, Laplacian eigenmap, Hessian-based locally linear embedding, isomap, curvilinear component analysis (CCA), curvilinear distance analysis (CDA), maximum variance unfolding (MVU), landmark maximum variance unfolding (LMVU), and local MDS (LMDS), LE, HLLE
  - Bewiesen wird mit Trustworthiness und Continuity
- „NeRV also performed well in a comparison by unsupervised classification." (Letter, Phoneme, Landsat, TIMIT)
- NeRV for supervised visualization (distance = Riemannian topology preserving metric) für 4 Datensätze

FCPS und echte Daten

- Problem: $\mathbb{R}^2$ -> $\mathbb{R}^2$ ändert sich nichts
- Echter Datensatz von 10000 Zeilen:
  - Bad_alloc Fehler (Speicherproblem)
- Echter Datensatz: 800 Dimension in

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