Comparisons of nonlinear dimensionality reduction methods

NLDR seminar presentation

Andrey Ermolov
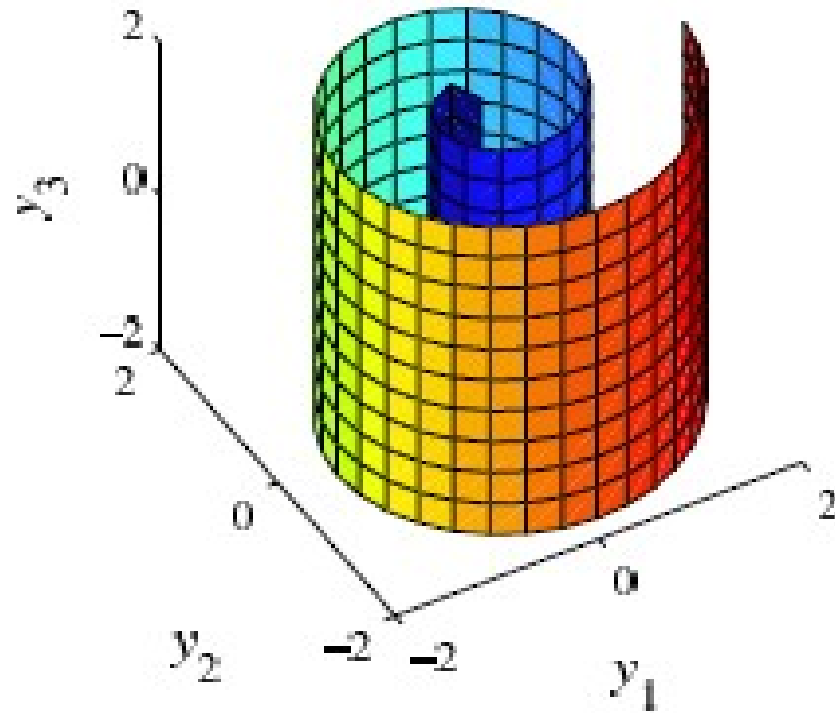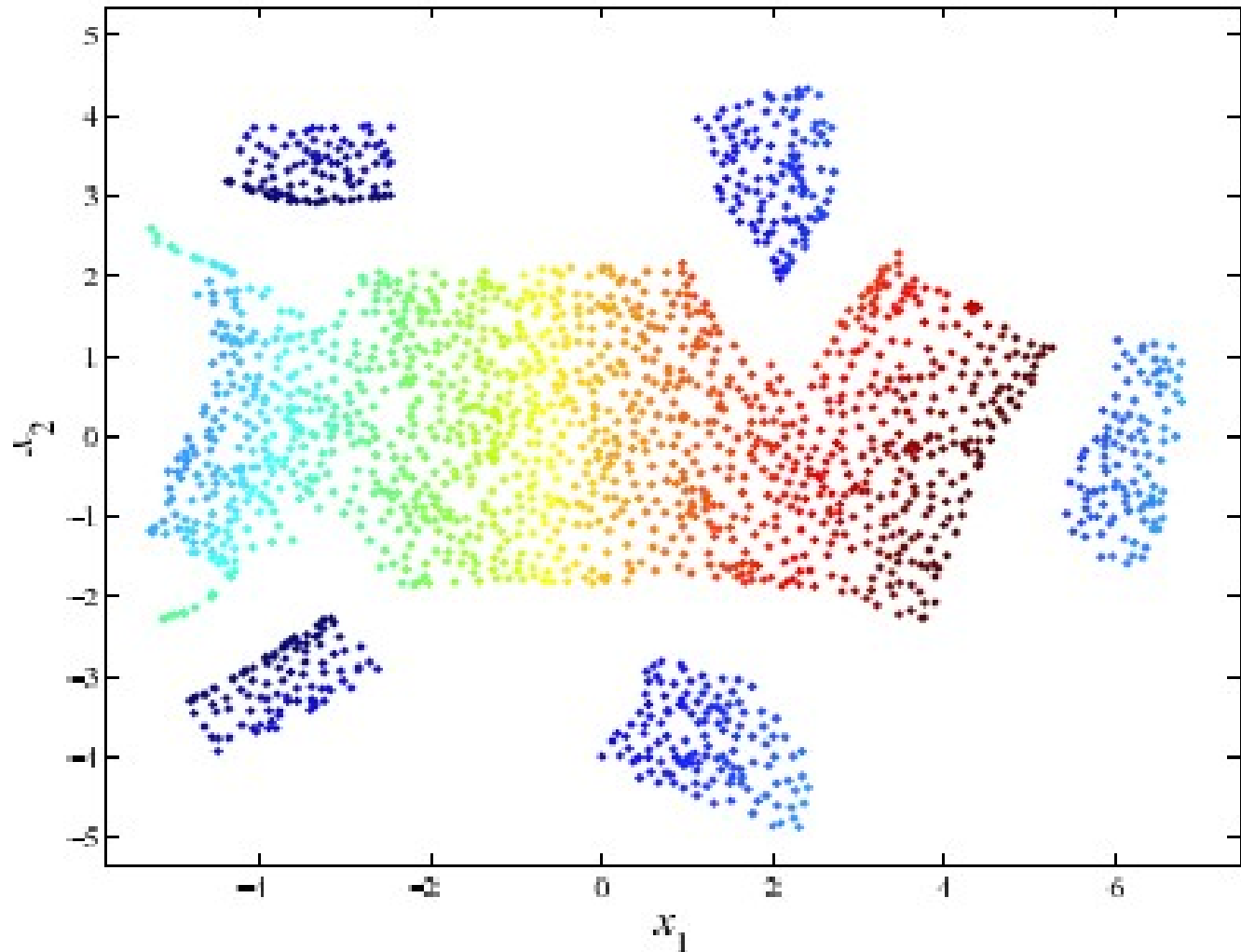
13.11.2007

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- Toy examples: Swiss roll
- Brain shell unfolding
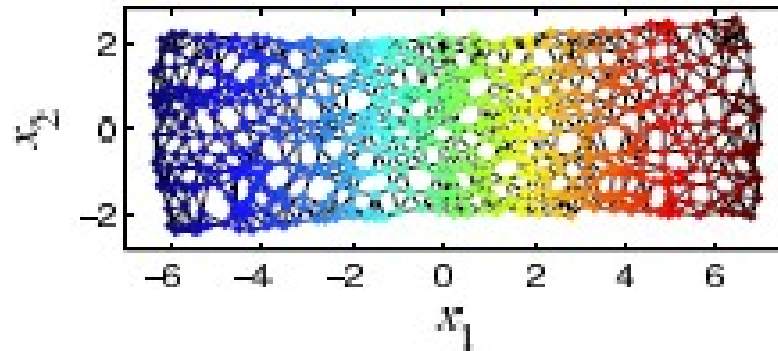- Image processing

Toy examples: Swiss roll

- developable, but heavily crumpled on itself
- demonstrates benefits of using graph distances
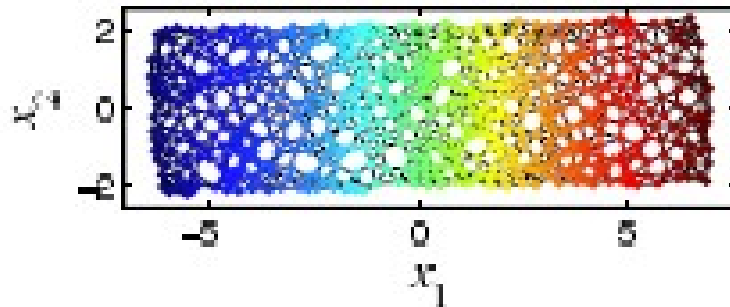
Toy examples: CCA for Swiss roll

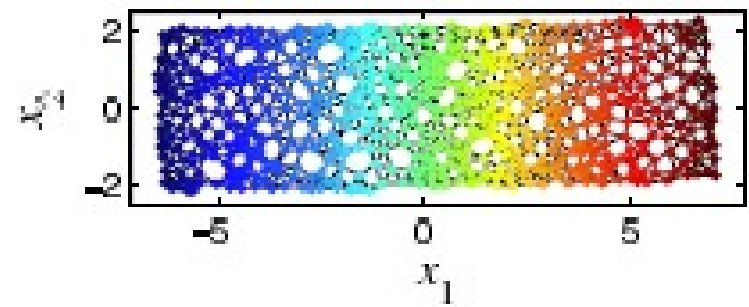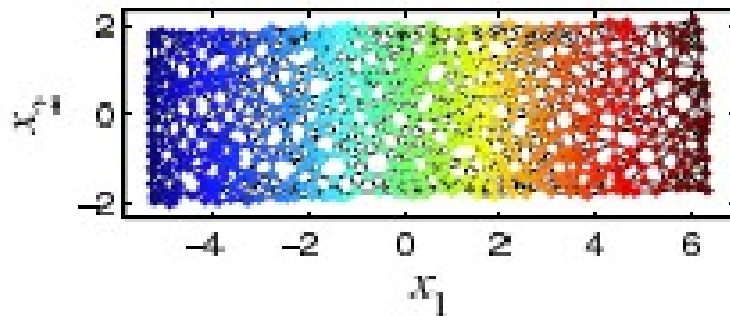# Toy examples: Graph distances methods for Swiss roll
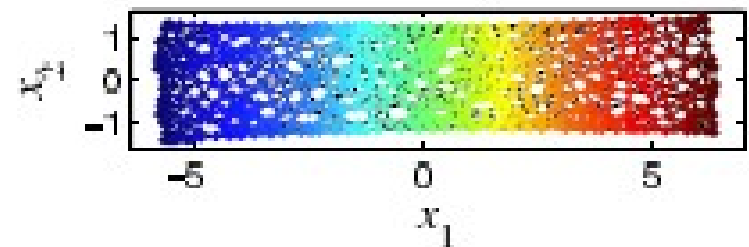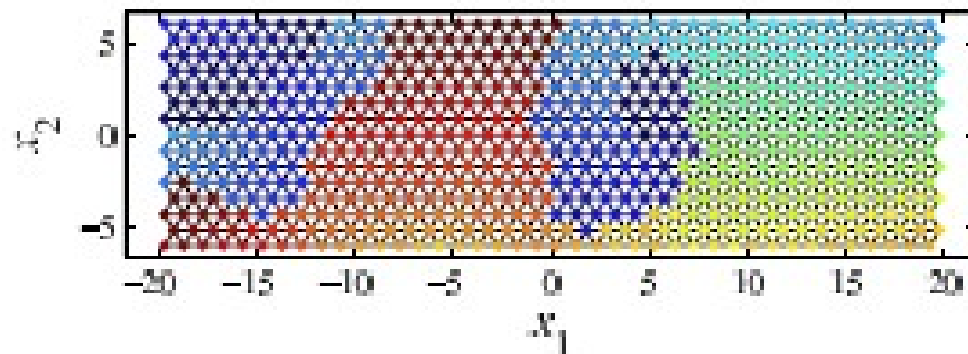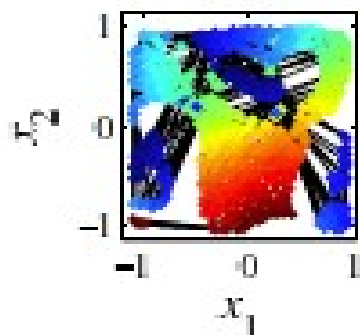
Toy examples: Topology preservation methods for Swiss roll
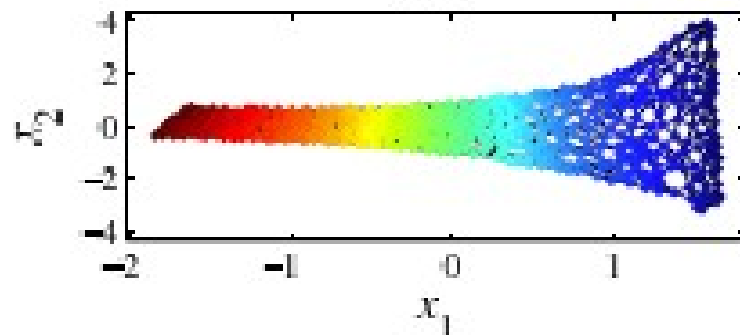
Toy examples: "Heated" Swiss roll

- Nondevelopable!

Toy examples: "Heated" Swiss roll Distance preserving methods
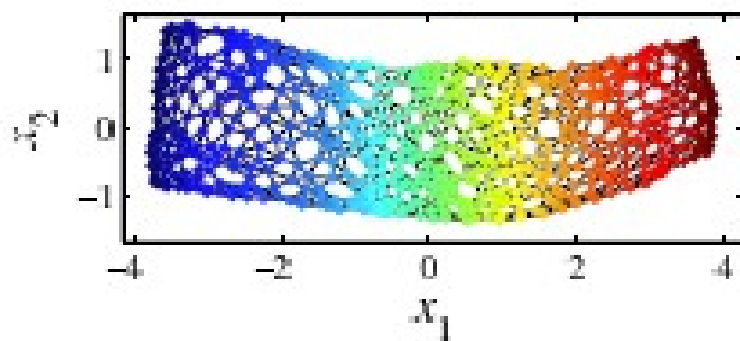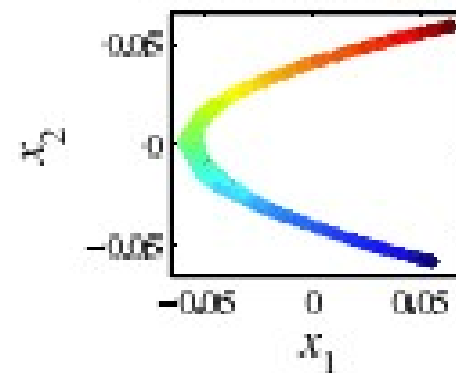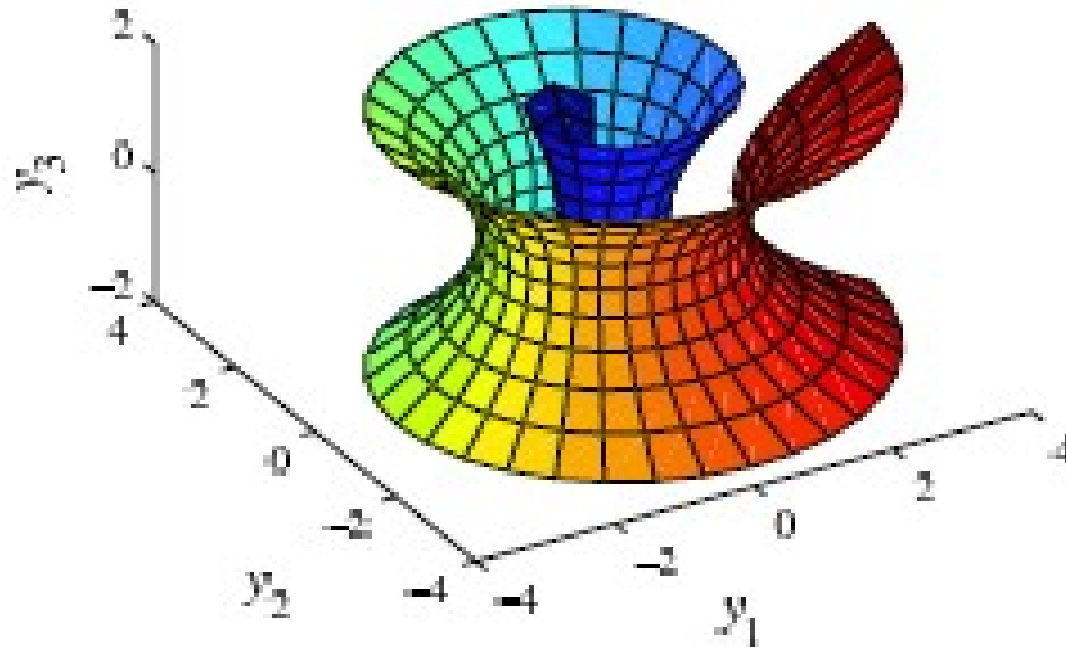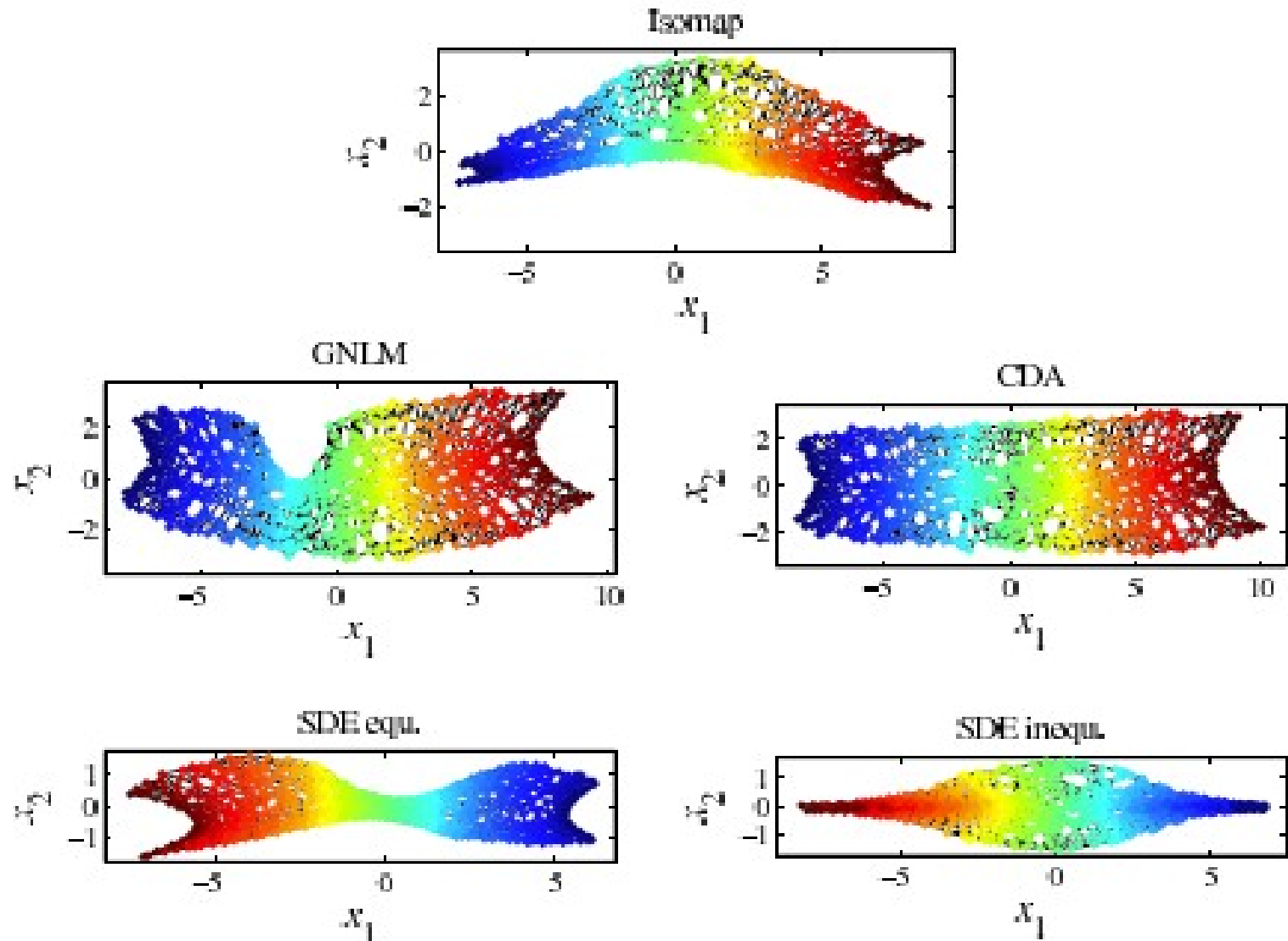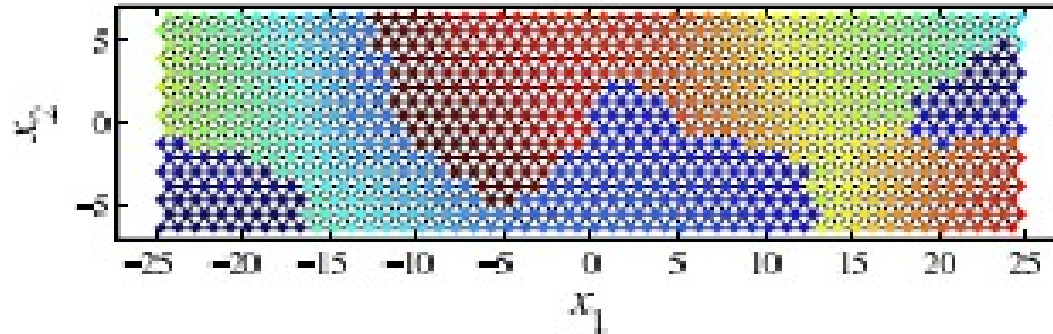

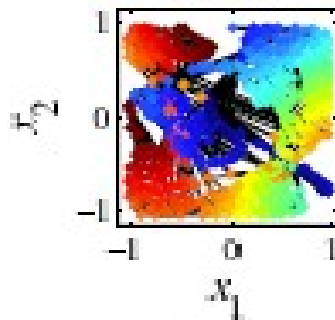- Topology preserving methods are supposed to be better, but...

Toy examples: "Heated" Swiss roll
Topology preserving methods
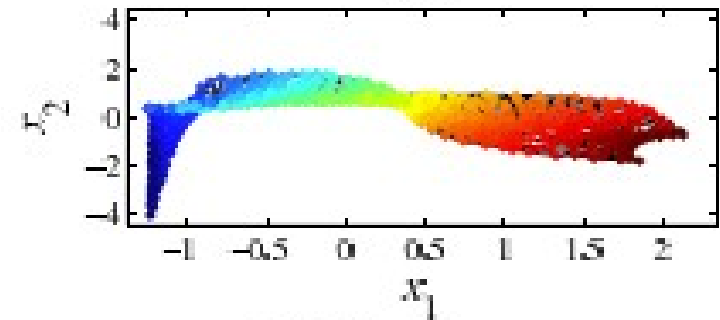
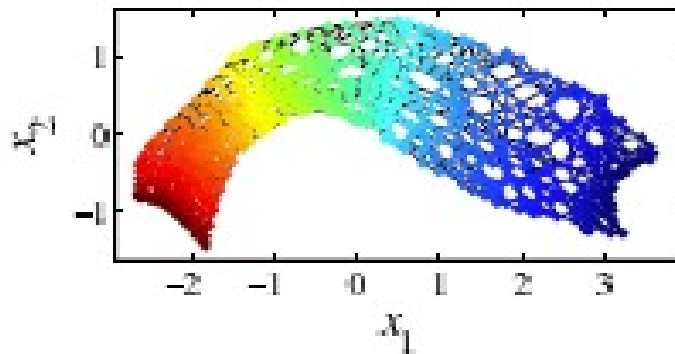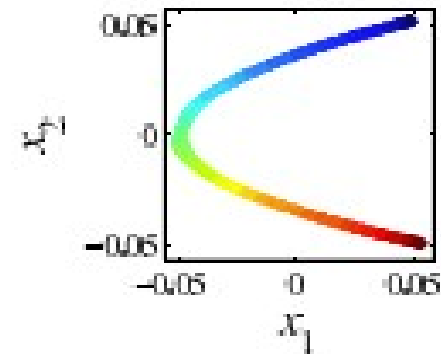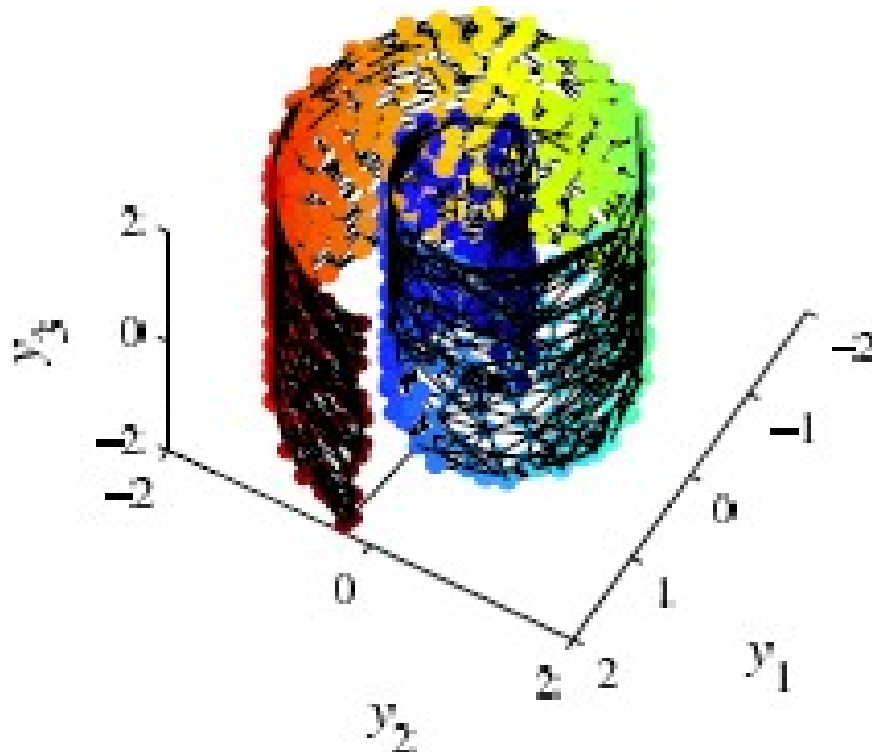# Toy examples: Swiss roll

- Spectral methods:
  - Simple
  - Exact optimization
  - Sensitive to departures from underlying model
- Iterative methods based on gradient descent:
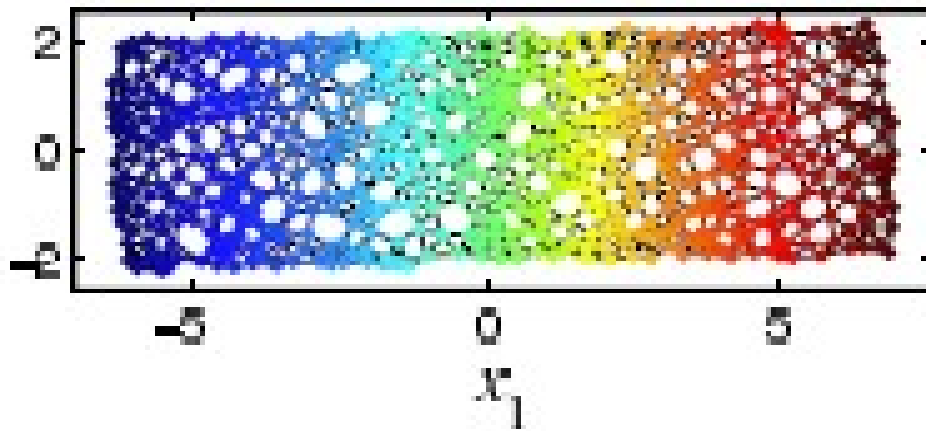 - Complex objective functions
  - Computationally heavy

Toy examples: Inadequate parameter values

○ Suppose using 8 neighbours instead of 5 in vector quantization:
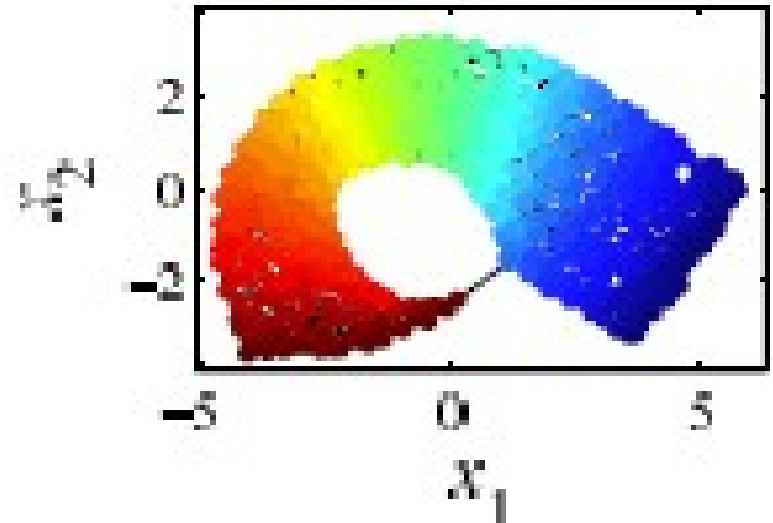
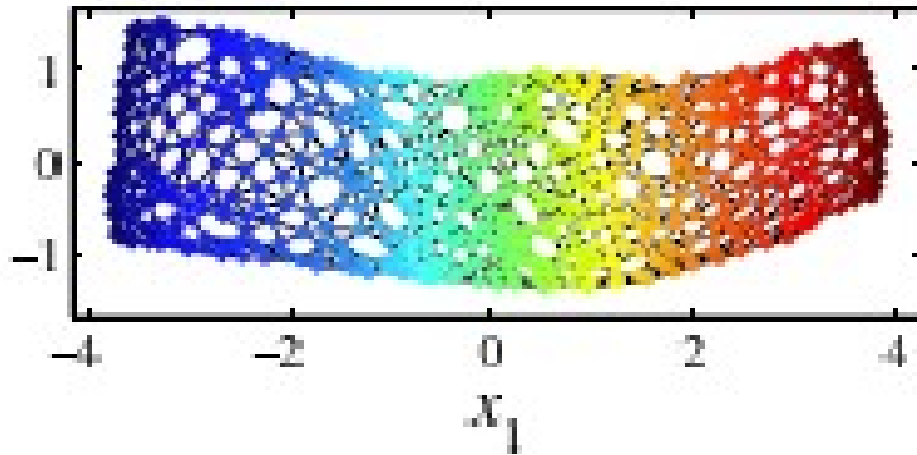# Toy examples: inadequate parameter values for GNLM

"right"   current
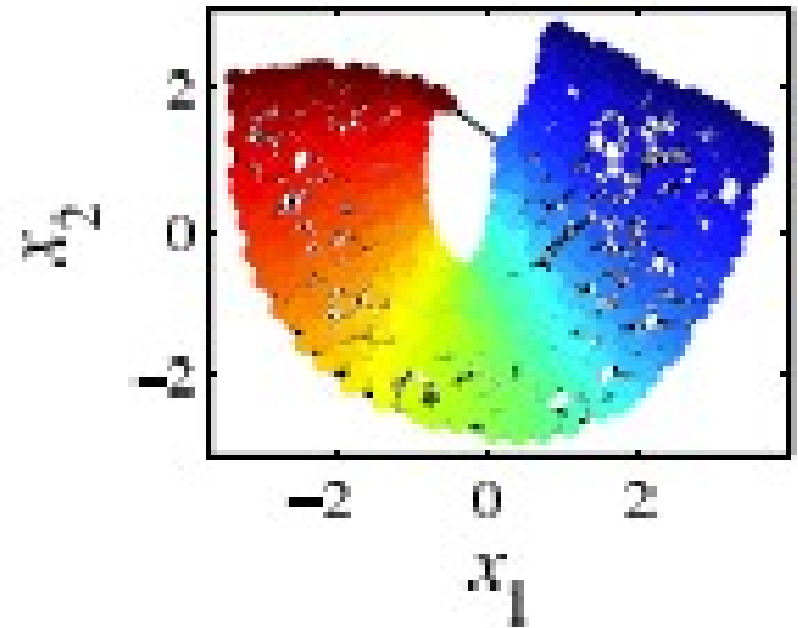
Toy examples: Inadequate parameter values for Isotop
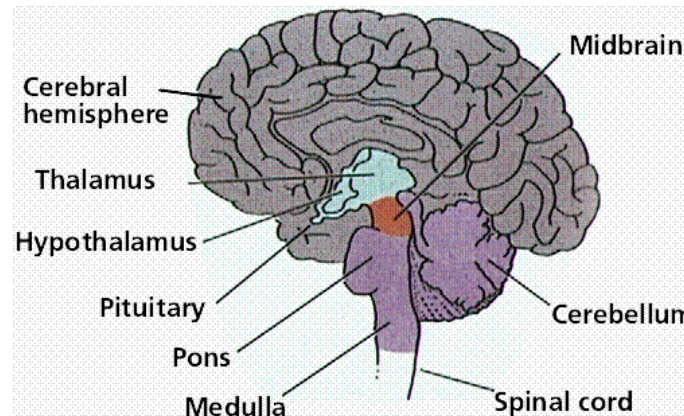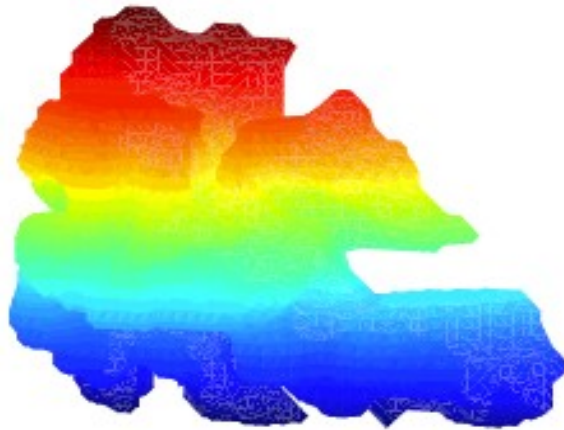
"right"   current

Brain shell (cortex) unfolding

○ Brain is composed of roughly two tissues:

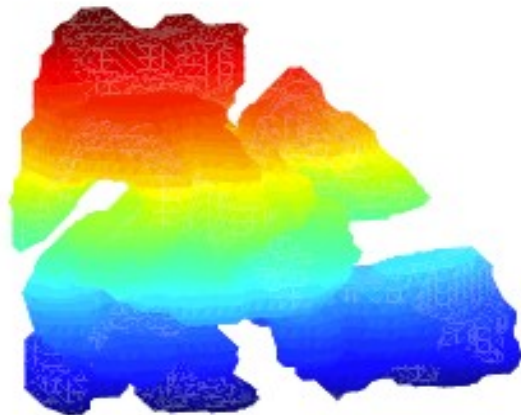- White (inside)
- Gray (thin outside) – cortex

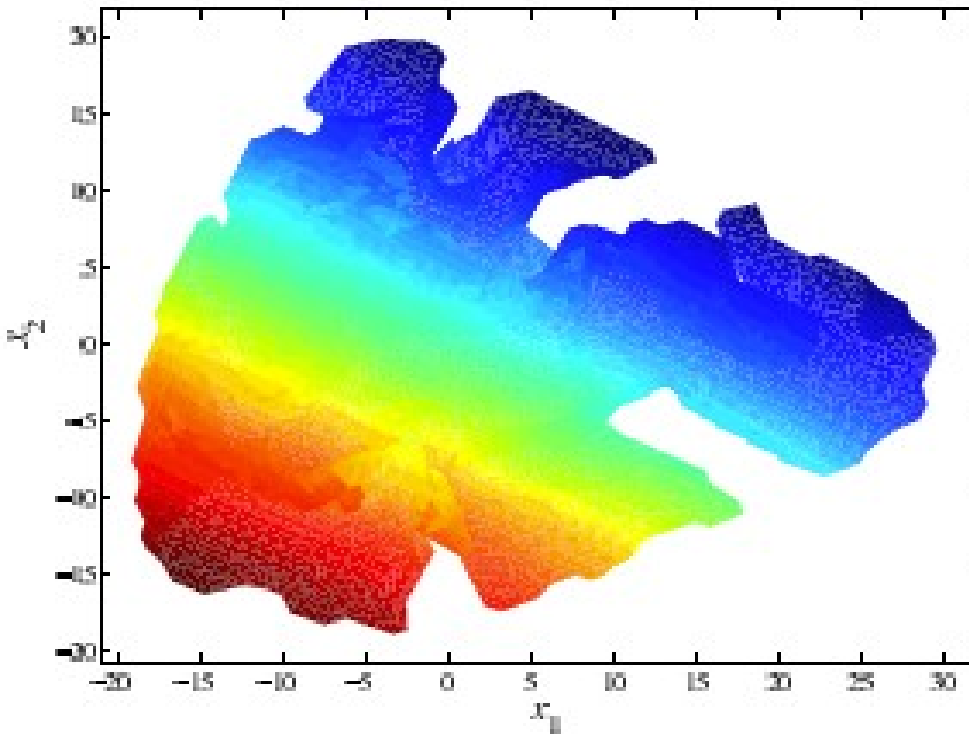○ Usually easier to have 2D-"map" of the cortex

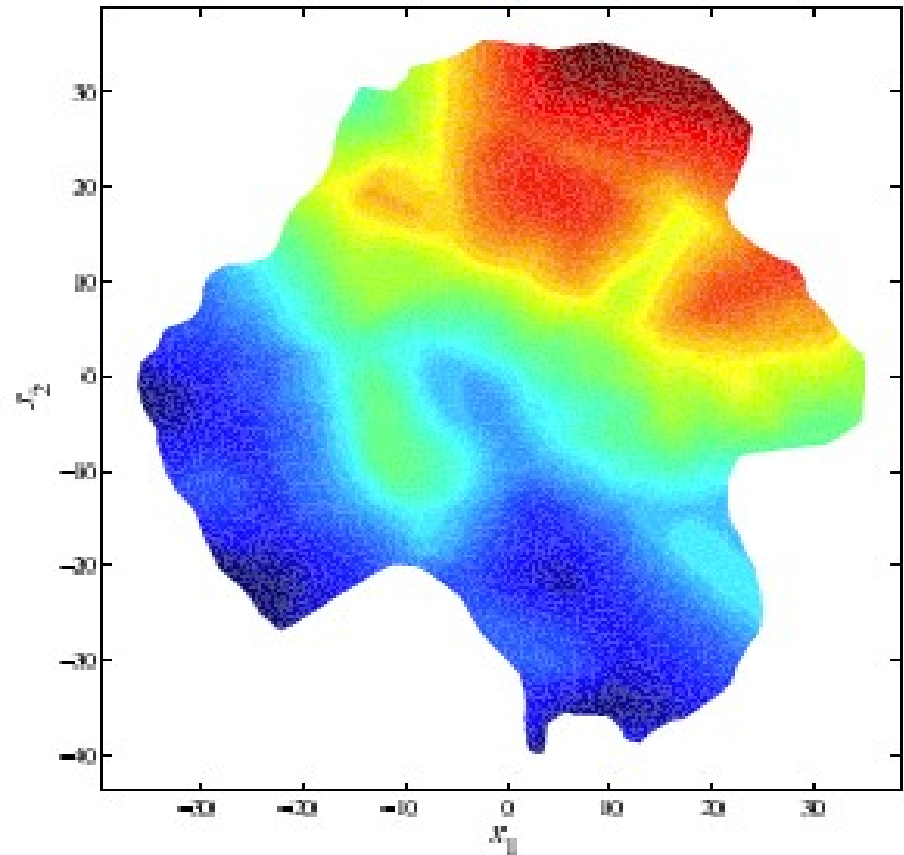# Cortex unfolding: 3D pictures of a small piece

-Methods using EVD fail, because there are too many points and no opportunity for vector quantization!
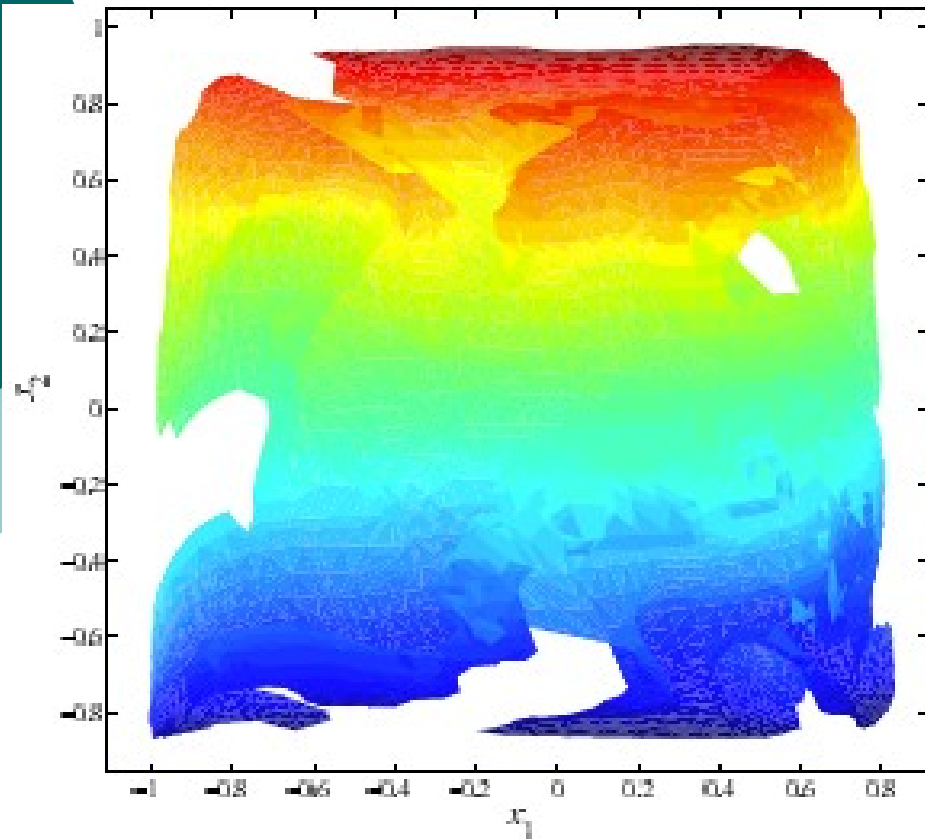
Cortex unfolding: NLM vs GNLM

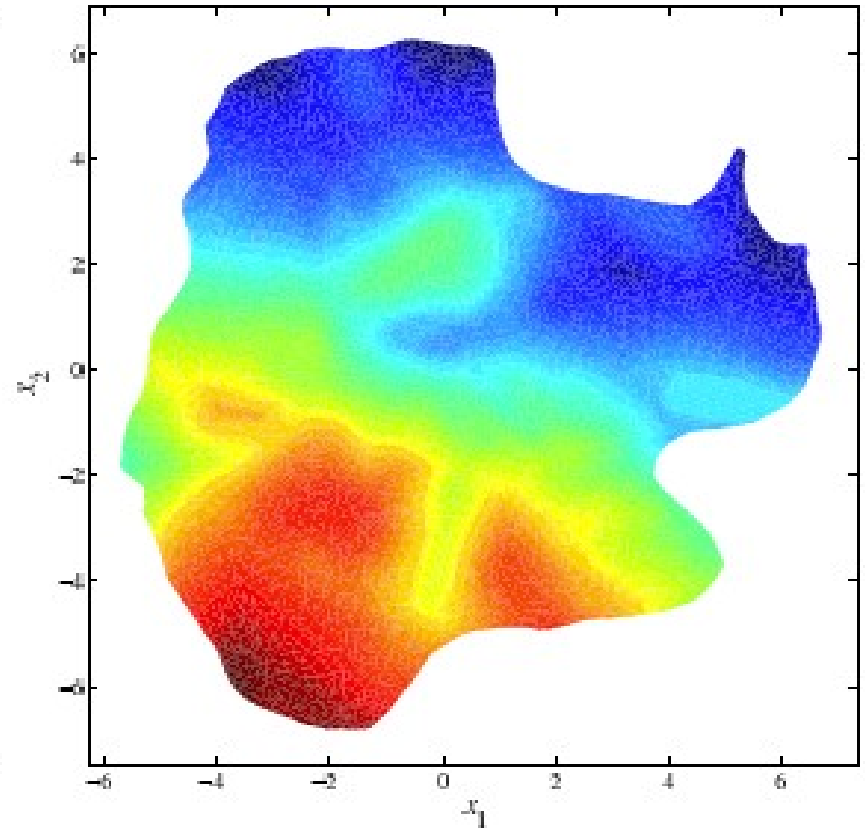$$E_{NLM} = 0.0162$$

$$E_{GNLM} = 0.0038$$

- Graph distances definetely help to unfold

Cortex unfolding: GTM vs Isotop

GTM   Isotop

- Predefined lattice – even if it is able to preserve topology – ofthen distort shape of the data

Image processing: Idea

- Each pixel is dimension in high-dimensional space
- Intrinsic dimensionality often quite low
- Initial dimensionality reduction, for instance, with PCA
- Embeddings with different methods!

Image processing: Artifical faces

- Intrinsic dimension=3:
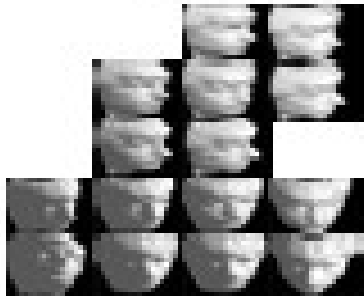 - Pose: left/right
  - Pose: up/down
  - Light: left/right

Image processing: Artifical faces

- 3D-embeddings
- Results are visualised using 6-by-6-by-6 grid
- Image associated with one point in each cell is selected
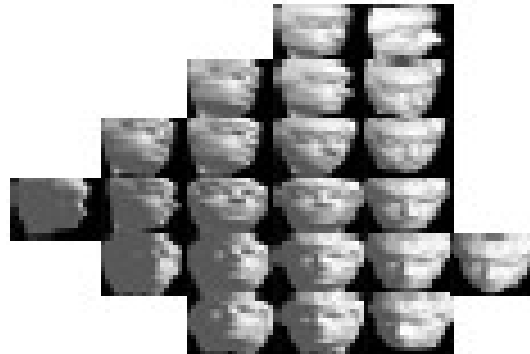- Good result: similar neighbours and smooth changes

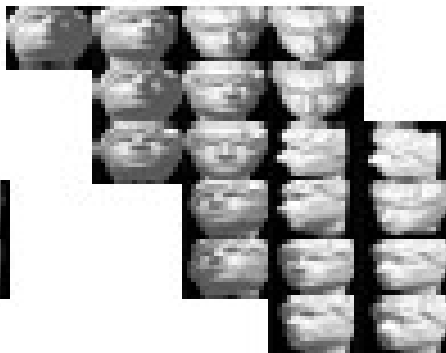# Image processing: Artificial faces
Metric MDS
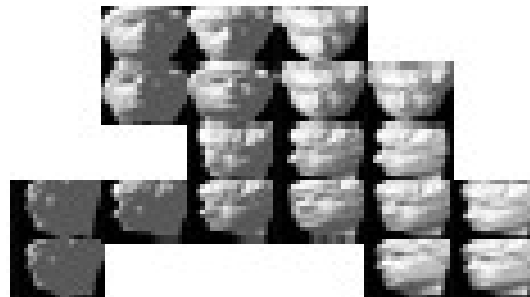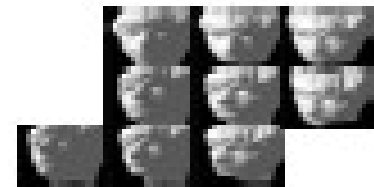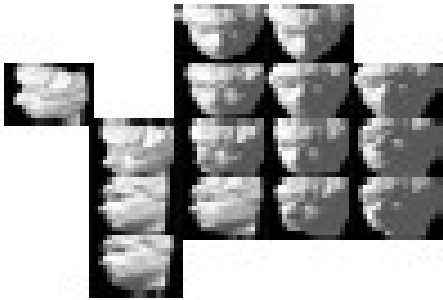

Layer 1   Layer 2   Layer 3

Layer 4   Layer 5   Layer 6

- Quite poor visual performance (explains only 60% percents of variance)

Image processing: Artificial faces
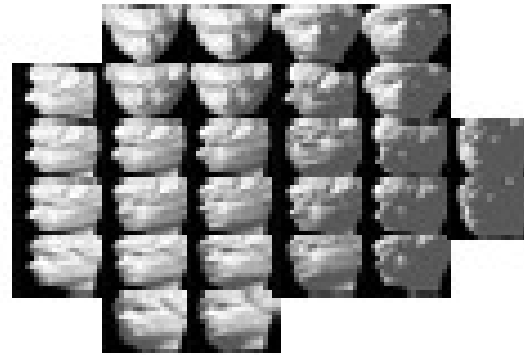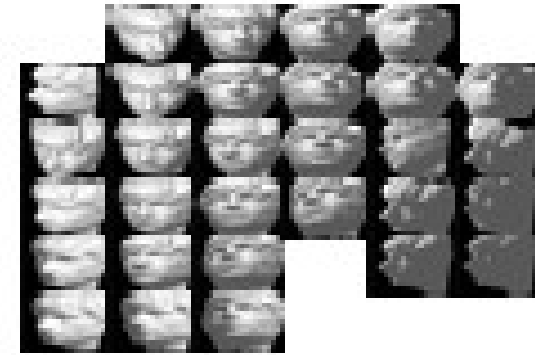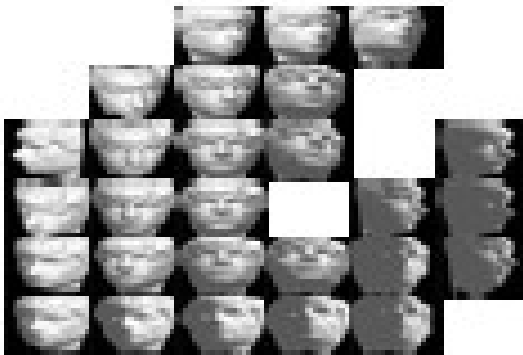# Sammon's NLM

- Smoother than MDS, but still not very impressive

Image processing: Artificial faces Isomap

Layer 1   Layer 2   Layer 3
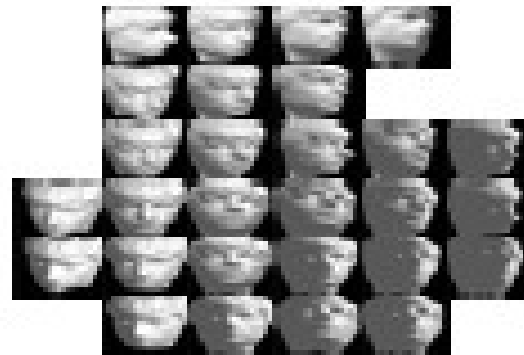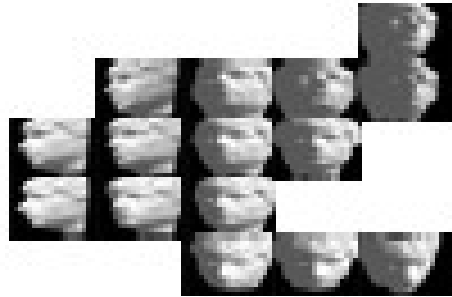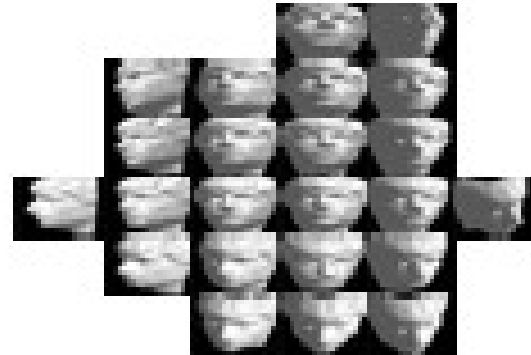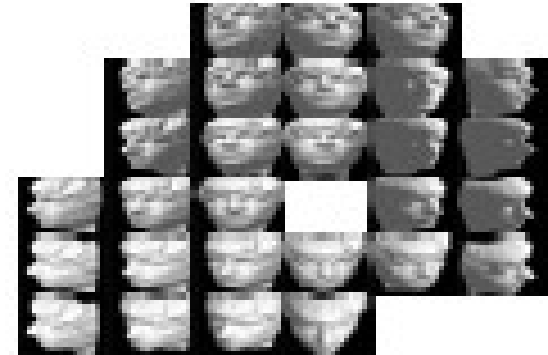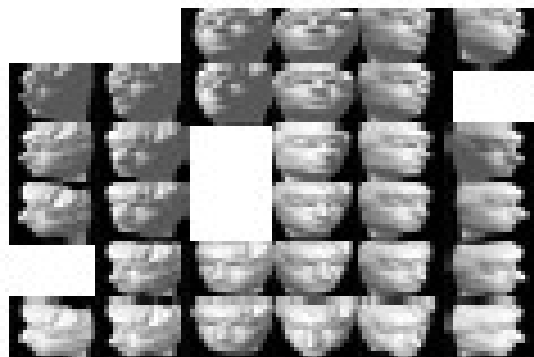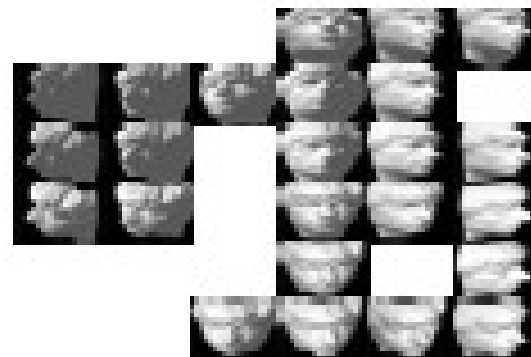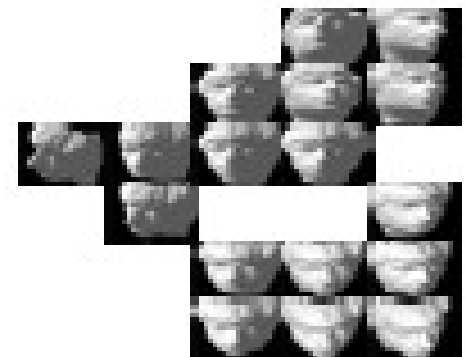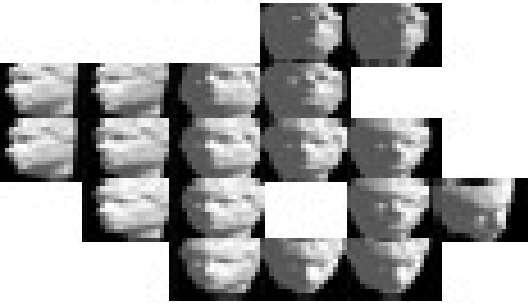
Layer 4   Layer 5   Layer 6

- Very nice: able to catch even light direction!
- Graph-distances – key to success?

Image processing: Artificial faces GNLM

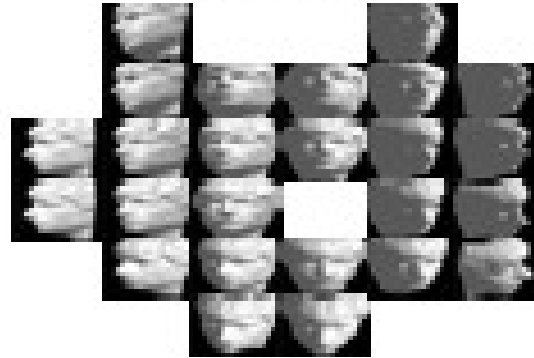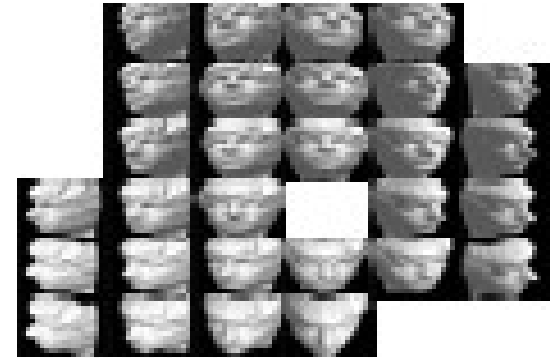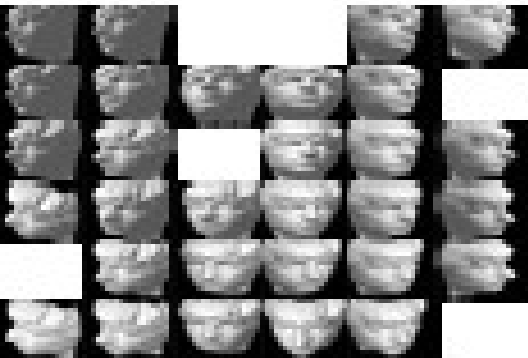- Approximately as good performance as by Isomap
- Graph distances seem working well

Image processing: Artificial faces LLE

Layer 1 Layer 2 Layer 3
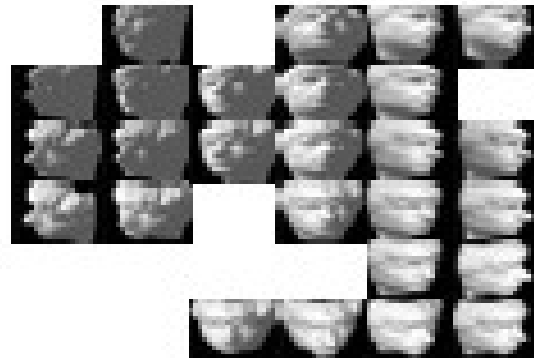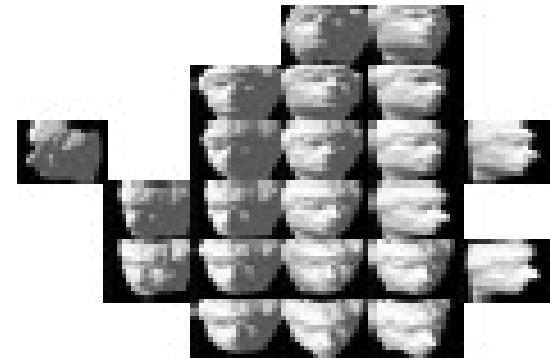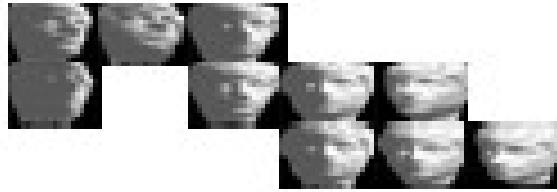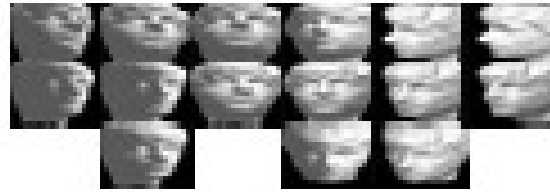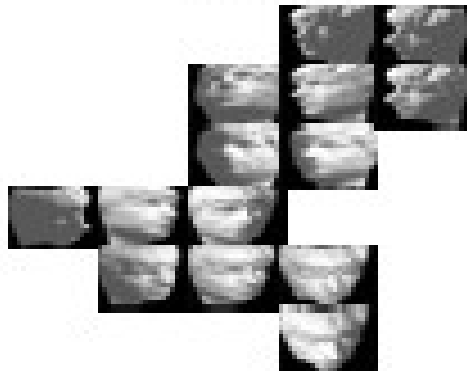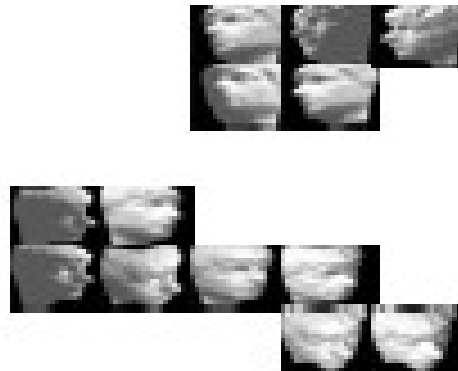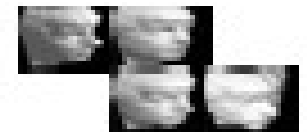
Layer 4 Layer 5 Layer 6

○ Sparse layers
○ Not very smooth

Image processing: Artificial faces Isotop

Layer 1   Layer 2   Layer 3
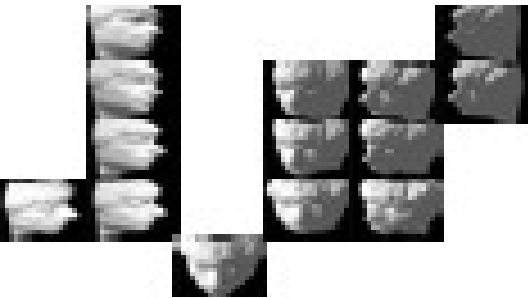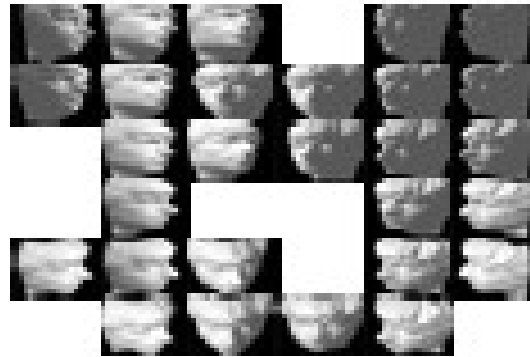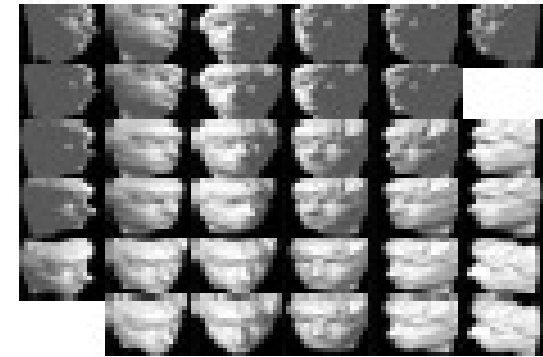
Layer 4   Layer 5   Layer 6

○ Visually better than LLE, but some clear discountinuities

Image processing: Quantitative criterion

- Verification of visual impression
- Order statistics:
  - In vector set *X* taking *i*th vector as reference, compute all Euclidean distances: for other vectors $\| x(k) - x(i) \|$
  - Sort distances in ascending order
  - Output *r* – rank of *x(j)* according to the sorted distance

Image processing: Mean relative rank errors

○ Measure of continuity:

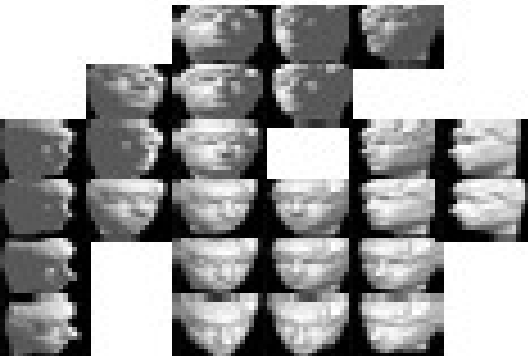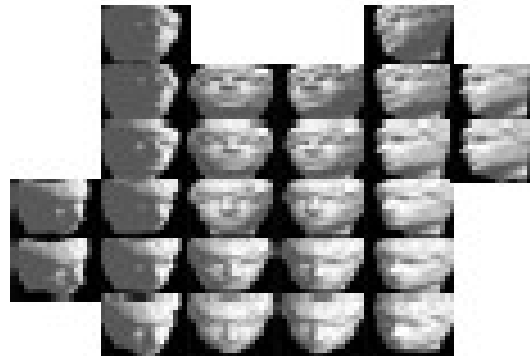$$MRRE_{Y->X}(K) = \frac{1}{C} \sum_{i=1}^{N} \sum_{j \in N(y(i),K)} \frac{|rank(X,i,j) - rank(Y,i,j)|}{rank(Y,i,j)}$$

○ Measure of trustworthiness:

$$MRRE_{X->Y}(K) = \frac{1}{C} \sum_{i=1}^{N} \sum_{j \in N(x(i),K)} \frac{|rank(X,i,j) - rank(Y,i,j)|}{rank(X,i,j)}$$

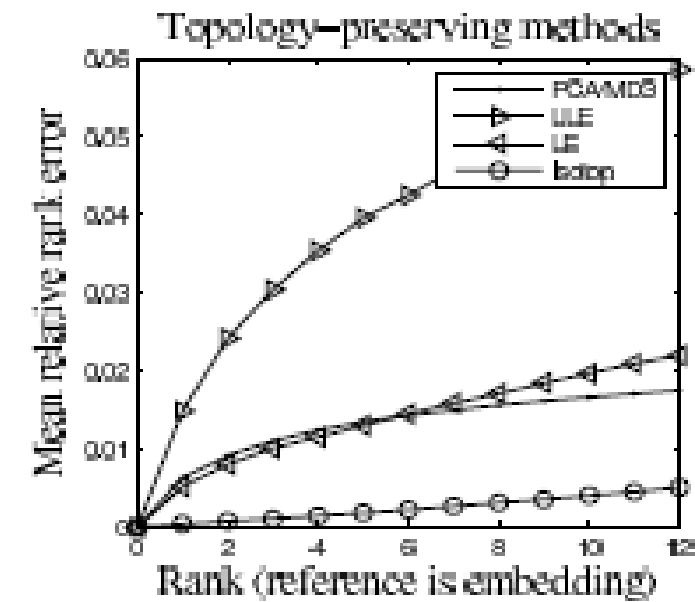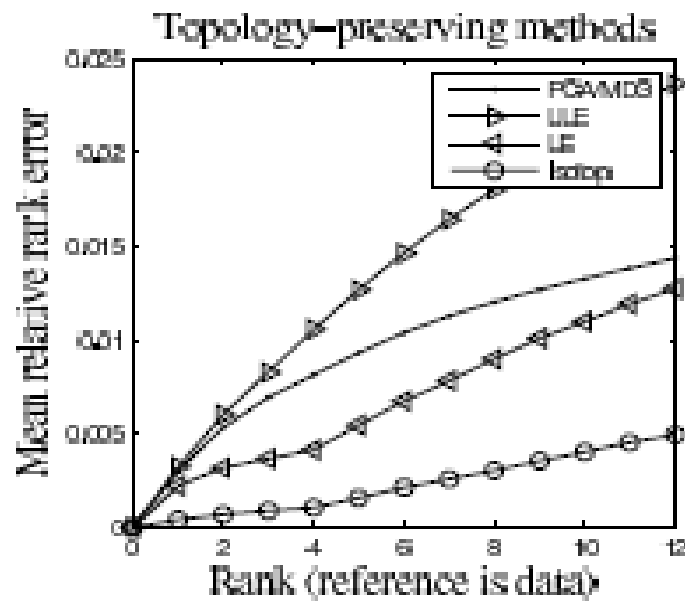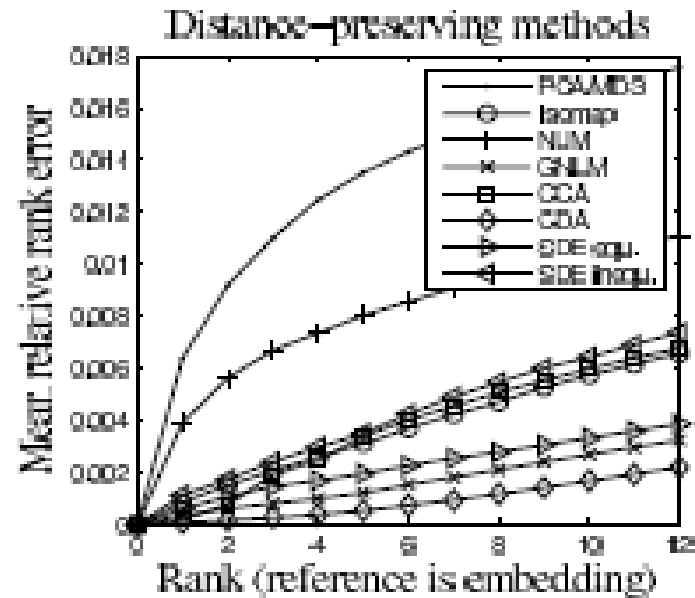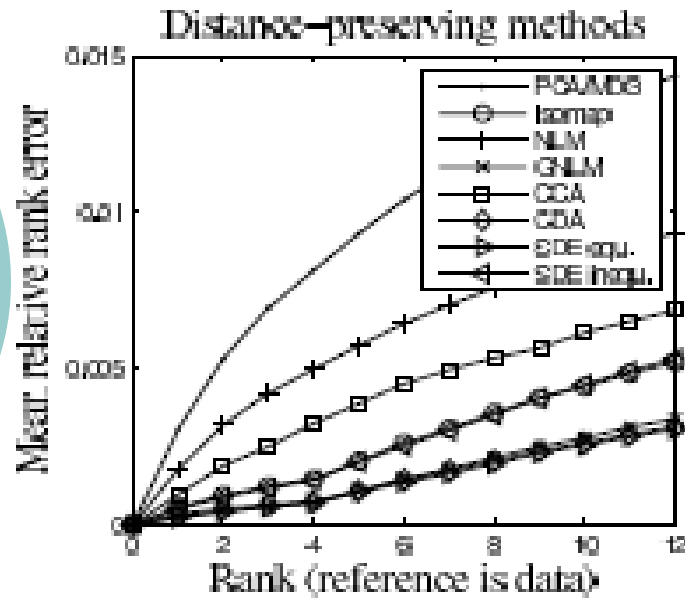# Image processing: Mean relative rank errors

Image processing: Mean relative rank errors

- Poor performance of metric MDS (linear method)
- Graph distances seem working better than Euclidean distances
- Very poor performance by LLE
- Isotop quite impressive (quantitative results better than visual?)

Summary

- **Try different methods!**
- **Parameters selection crucial!**
- Graph distances work usually better than Euclidean distances
- Predefined lattice can distort shape very much