Comparisons of nonlinear dimensionality reduction methods

NLDR seminar presentation

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Contents

- 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
Topological 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

\[ E_{NLM} = 0.0162 \quad \text{and} \quad E_{GNLM} = 0.0038 \]

- Graph distances definitely help to unfold
Cortex unfolding: GTM vs Isotop

- Predefined lattice – even if it is able to preserve topology – often 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: Artificial faces

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

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

- Approximately as good performance as by Isomap
- Graph distances seem working well
Image processing: Artificial faces

- Sparse layers
- Not very smooth
Image processing: Artificial faces

Isotop

- Visually better than LLE, but some clear discontinuities
Image processing: Quantitative criterion

- Verification of visual impression
- Order statistics:
  - In vector set \( X \) taking \( i \)th vector as reference, compute all Euclidean distances:
    \[ \| x(k) - x(i) \| \]
  - 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:**

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

- **Measure of trustworthiness:**

\[
MRRE_{X \rightarrow Y}(K) = \frac{1}{C} \sum_{i=1}^{N} \sum_{j \in N(x(i),K)} \frac{|\text{rank}(X,i,j) - \text{rank}(Y,i,j)|}{\text{rank}(X,i,j)}
\]
Image processing: Mean relative rank errors

Distance-preserving methods

Topology-preserving methods
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