Helsinki University of Technology

Topology Preservation - part I

Self-organising maps

Dušan Sovilj

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Outline

- Distance vs Topology
- Topology-preserving methods
- Self-organising map in dimensionality reduction
  - embedding of data set
  - embedding of test set
  - example
  - summary

Distance vs Topology

- Distance
  - simple to understand
  - easy to compute
  - rigid in dimensionality reduction
- Topology
  - can fully describe manifolds
  - hard to represent with few points
  - without a good description of topology, dimensionality reduction is impossible

Topology-preserving methods

- Very ofted they use the discrete mapping model
  - the topology is then also discrete, called *lattice*
- Topology can be discretely represented with a graph
- Classified according to type of topology used in embedding space
  - predefined lattice
  - data-driven lattice

'Predefined lattice' methods

- Methods
  - self-organising map
  - generative topographic mapping
- Application very limited (few manifolds fit predefined shape)
- Good way for visualization of labeled data

SOM in DR

- Can be interpreted as non-linear & discrete PCA
  - fitting of hyperplane inside the data cloud
  - hyperplane is described with discrete points
  - fitting of a 'fishing net' around an object
- SOM uses a mix of vector quantization and topology preservation

Classic VQ & SOM's VQ

- Vector quantization in SOMs are mandatory
- Classic VQ doesn't take into account the relations between the prototypes/representatives
- SOM tries to 'preserve' the lattice in data space by moving prototypes in neighbouring groups

SOM definition

- Set $\boldsymbol{C}$ containing the prototypes in the data space for vector quantization. Prototypes are D-dimensional points $\mathbf{c}(r)$
- Distance function $d_g(r, s)$ between the prototypes in the lattice
- r & s are indices of prototypes

Embedding of data points in SOM

- Lattice plays the role of embedding space
  - $d_g(r, s)$ cannot be any distance function
  - $d_g(r, s)$ is often defined as $d_g(g(r), g(s)),\ \ g(r), g(s) \in G \subset \mathbb{R}^P$
    P is dimensionality of embedding space
- Prototypes have coordinates both in data and embedding space
  - coordinates in embedding space are known (predefined lattice)
  - coordinates in data space are unknown, and SOM has to find them
- Embedding of data points $y(i)$

$$x(i) = g(r) \qquad r = \arg\min_s d(y(i), c(s))$$

where d is Euclidean distance

Prototypes' coordinates

- Iteratively by going through all data points in $\mathbf{Y}$ (epochs)
- For every point $y(i)$

1. Find closest prototype

$$r = \arg\min_s d(y(i), c(s))$$

2. Update coordinates of all prototypes

$$c(s) \leftarrow c(s) + \alpha\ \nu_\lambda(r, s)\ (y(i) - c(s))$$

α learning rate, $0 \leq \alpha \leq 1$ decreases with epochs

ν_λ neighbourhood function

Neighbourhood functions

- 'Bubble'

$$\nu_\lambda(r,s)=\begin{cases}0 & \text{if } d_g(r,s)>\lambda\\ 1 & \text{if } d_g(r,s)\leq\lambda\end{cases}$$

$$d_g(r,s)=L_1, L_2, L_\infty$$

- Gaussian like

$$\nu_\lambda(r,s)=\exp\left(-\frac{d_g^2(r,s)}{2\lambda^2}\right)$$

$$d_g(r,s)=L_2$$

Shape of lattice

- In most implementations the points in the lattice are equally spaced in the plane which forces the embedding space to be two-dimensional
  - square structure (8 neighbours)
  - hexagonal struture (6 neighbours)
- For higher dimension lattices the hyper-cubic neighbourhoods are mostly used

SOM batch algorithm

1. Define the lattice by assigning the low-dimensional coordinates $g(r)$ of the prototypes in the embedding space
2. Initialize the coordinates $c(r)$ of prototypes in the data space
3. Give α and ν their scheduled values for epoch q
4. For all points $y(i)$ in the data set, find it's closest prototype and update coordinates of all prototypes
5. Return the step 3 until convergence is reached (the updates of prototypes become negligible)

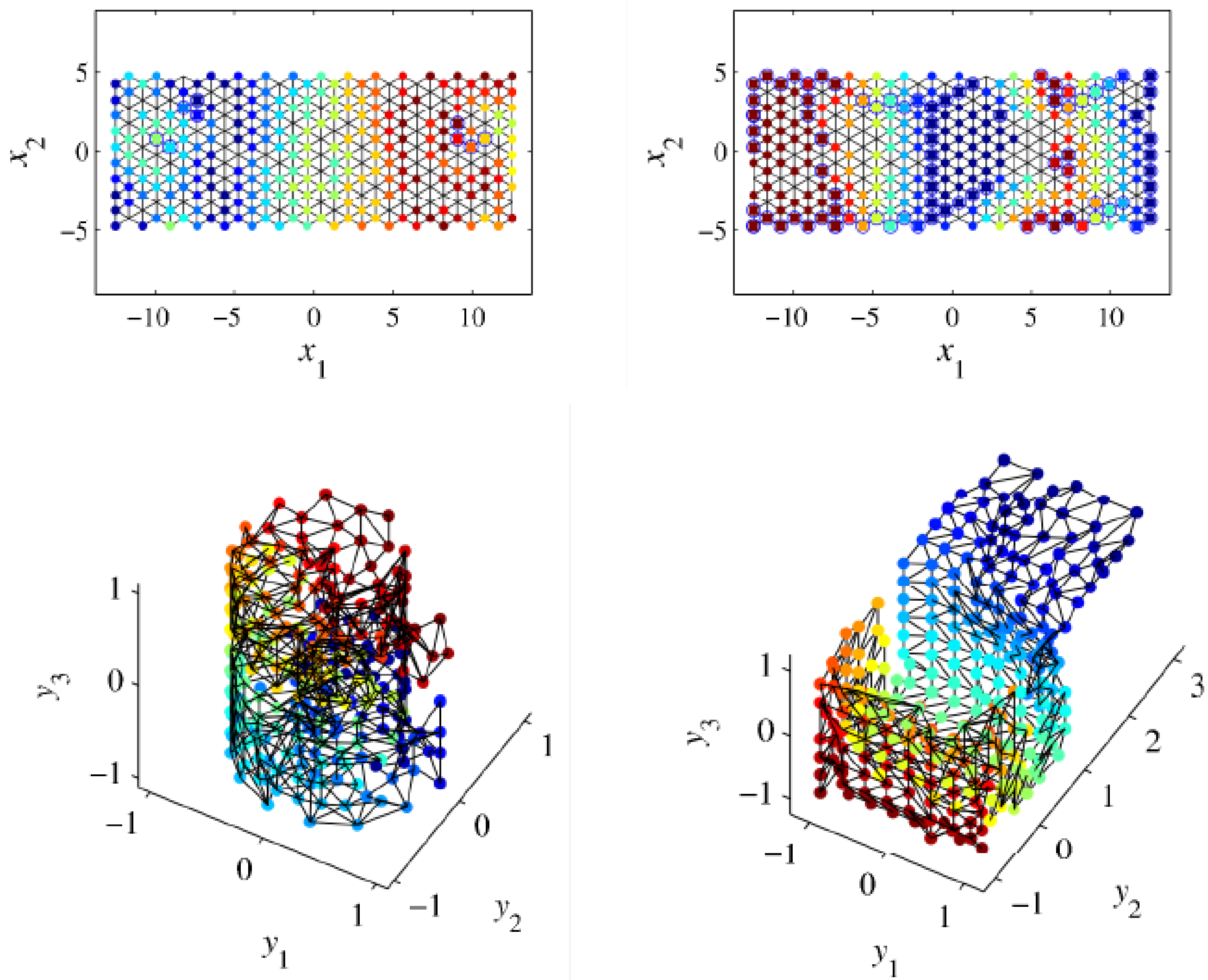
Embedding of test points

- Calculation is done exactly as for data points

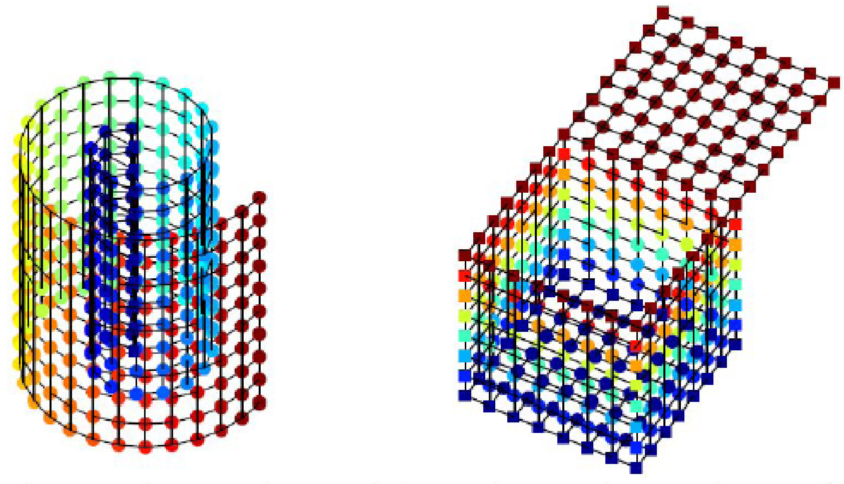
$$c(s) \leftarrow c(s) + \alpha\ \nu_\lambda(r,s)\ (y(i) - c(s))$$

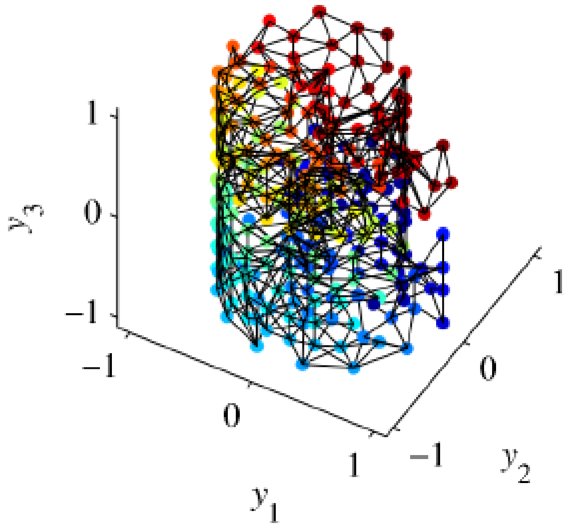
- This gives rough estimate of exact coordinates of test points in embedding space, since there is fixed number of outputs
- There exist precise interpolation methods for finding these coordinates

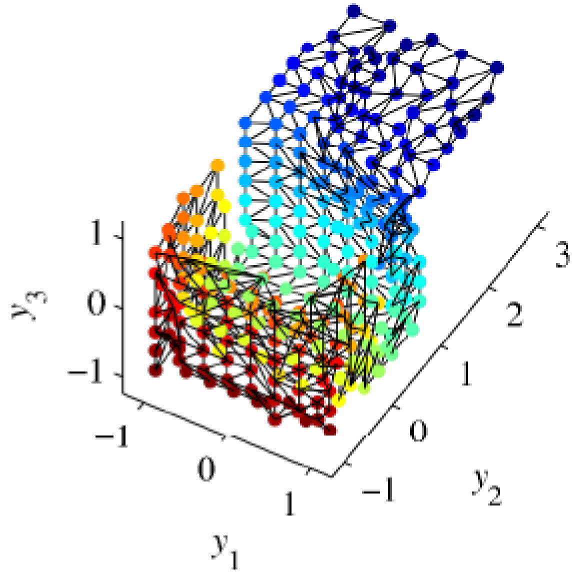
Example



Example (cont.)







SOM summary (1)

- Vector quantization is mandatory
- Models data in nonlinear and discrete way
- Mappings is explicit (prototypes only)

SOM summary (2)

- Advantages
  - Easy to understand
  - Nice visualization method
  - Applicable to various fields
- Drawbacks
  - Low dimensionality of embedding space (usually 1 or 2 dimensions)
  - Vector quantization
  - Shape of lattice predefined (often arbitrary)
  - No objective function or error criterion
  - What are good values for parameters α and ν

SOM variants

- Extend the lattice by adding rows and colums
  - GG (Growing Grid) & GSOM (Growing SOM)
- Change the shape appropriatelly to fit data
  - GCS (Growing Cell Structure)