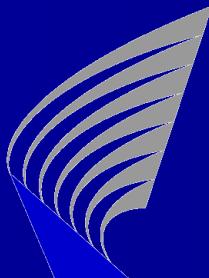


# Nonlinear Dimensionality Reduction

Chapter 5.3 + Appendixes D and E

Antti Sorjamaa and Yoan Miche



Time Series Prediction and ChemoInformatics Group  
Adaptive Informatics Research Centre  
Helsinki University of Technology

# Outline

- Vector Quantization
- Graph Building

## Chapter 5.3

- Locally Linear Embedding (LLE)
- Laplacian Eigenmaps (LE)
- Isotop



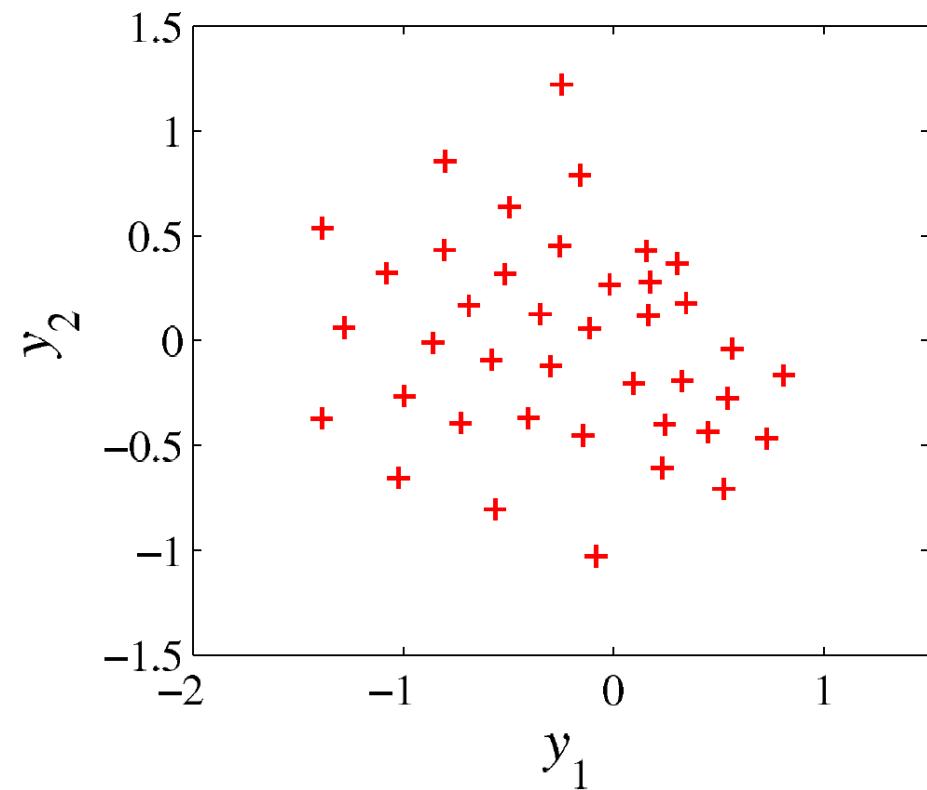
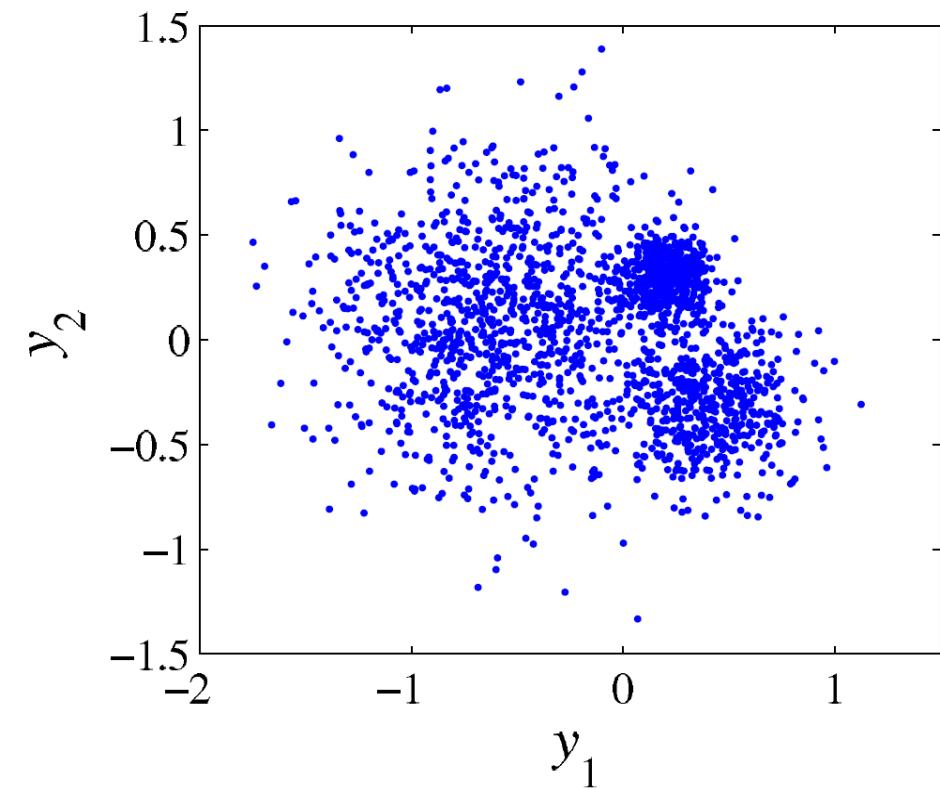
# Vector Quantization

- Aim is to decrease the amount of data
- Many methods use VQ as preprocessing method
- Used in many fields
  - Data analysis and compression
  - Clustering and classification
  - Telecommunications



# Vector Quantization

- Aim is to decrease the amount of data



# Vector Quantization (2)

Quantization distortion

$$E_{\text{VQ}} = \frac{1}{N} \sum_{i=1}^N \|\mathbf{y}(i) - \text{dec}(\text{cod}(\mathbf{y}(i)))\|^2$$

- coding denotes a function for finding the Best Matching Unit (BMU) of the data point
- decoding denotes a function for replacing the data point with the BMU



# Vector Quantization (3)

- $K$ -means

$$\mathbf{c}(j) \leftarrow \frac{1}{|V_j|} \sum_{\mathbf{y}(i) \in V_j} \mathbf{y}(i)$$

- Stochastic Gradient Descent

$$\mathbf{c}(j) \leftarrow \mathbf{c}(j) - \alpha(\mathbf{c}(j) - \mathbf{x}_i)$$



# Vector Quantization (4)

- Static → fixed number of prototypes
  - Classical techniques
    - K-means, LBG
  - Competitive Learning
    - Winner takes all (Stochastic Gradient Descent)
    - Winner takes most (SOM and Neural Gas)
- Incremental → increasing
- Dynamic → increasing and decreasing



# Graph Building

Yoan presents...



# Isotop

Close to SOM algorithm except

- Vector Quantization optional
- No predefined latent space
- Data points are not used in the learning phase, but instead a graph of them
- No online version
- More "data-driven" methodology



# Isotop Algorithm

- n Optional Vector Quantization
- n Build graph with pairwise distances
- n Initialize all nodes to zero
- n Calculate parameters with respect to  $q$
- n For each node
  - I. Generate random point around the node
  - II. Select closest node
  - III. Update coordinates of all nodes according to neighborhood
- n Increase  $q$  and goto step 4 unless converged



# Isotop Algorithm (2)

- 1) Initialize all nodes to zero
  - Place Gaussian kernel of unit variance on each node,  $N(\mathbf{x}(i), \mathbf{I})$
- n Calculate parameters with respect to  $q$ 
  - Learning rate  $\alpha$
  - Neighborhood width  $\lambda$



# For each node from 1 to $N$

- n Generate random point  $\mathbf{r}$  from the distribution of the node  $N(\mathbf{x}(i), \mathbf{I}) \rightarrow \mathbf{r}$
- n Calculate the nearest node
- n Update all nodes

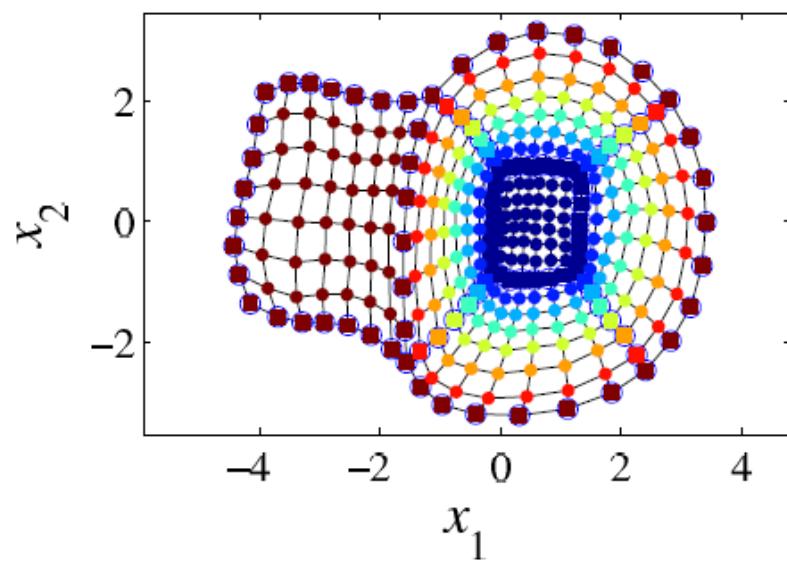
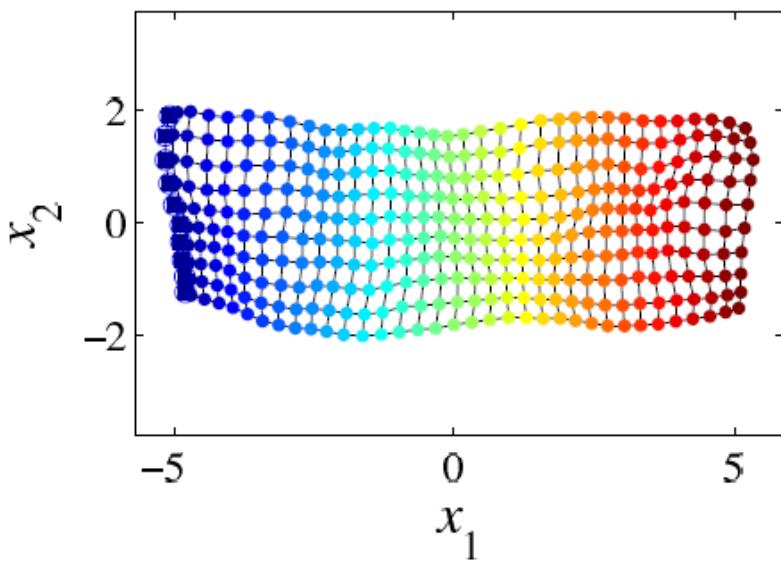
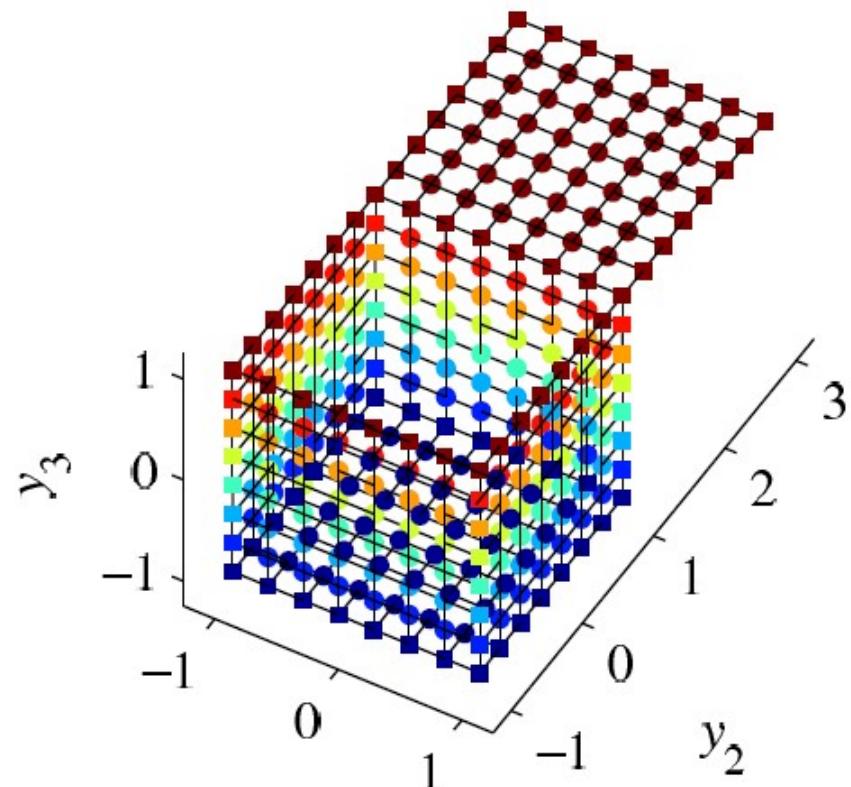
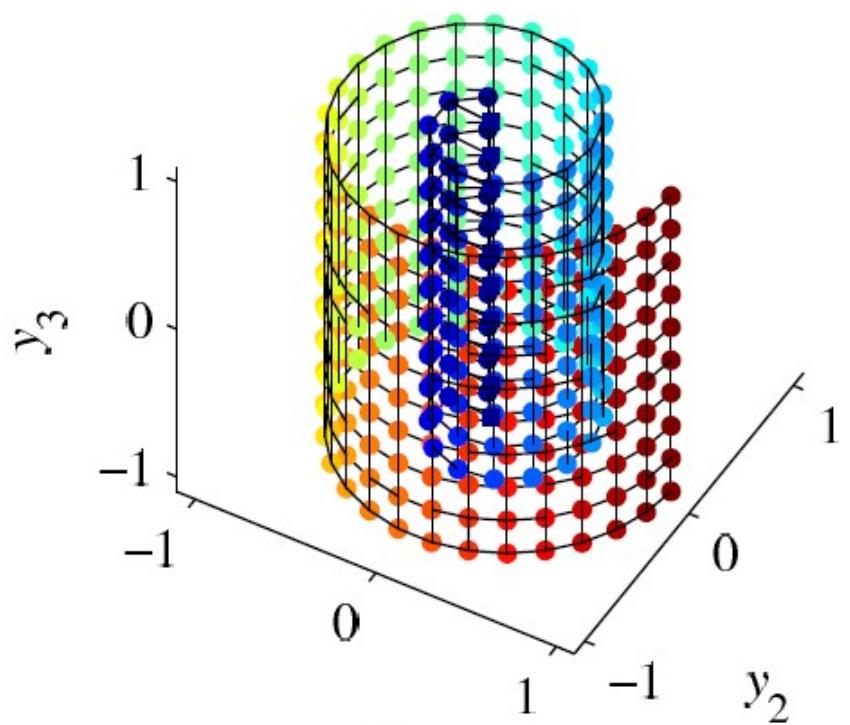
$$\mathbf{x}(i) \leftarrow \mathbf{x}(i) - \alpha v_\lambda(i, j)(\mathbf{r} - \mathbf{x}(i))$$
$$v_\lambda(i, j) = \exp\left(-\frac{1}{2} \frac{\delta_y^2(i, j)}{\lambda^2 \mu_{(v_h, v_j) \in E}(\delta_y(h, j))}\right)$$



# Notes of Convergence

- "Nodes won't collapse"
  - Gaussian centers make boundary nodes expand the graph
  - Neighborhood size must be kept reasonable
- "Nodes won't disperse infinitely"
  - Update rule generates an attractive force
  - Neighborhood size larger than zero





# Questions?

[Antti.Sorjamaa@hut.fi](mailto:Antti.Sorjamaa@hut.fi)

<http://www.cis.hut.fi/projects/tsp>

