Generative Topographic Mapping

Nonlinear Dimensionality Reduction Seminar

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- Nonlinear Dimensionality Reduction
  - Distance-preserving methods
  - Topology-preserving methods
    - Predefined-lattice
      - SOM
      - **Generative Topographic Mapping**
    - Data-driven lattice
      - ...
  - ...

Generative Topographic Mapping

- Generative model
- Probabilistic method based on Bayesian learning
- Introduced by Bishop, Svensén, et. al. in 1996
- http://www.ncrg.aston.ac.uk/GTM/

GTM in a nutshell

- R^D – data space
- R^L – latent space
- D > L
  1. probabilistically pick a point in R^L
  2. map the point to R^D via a nonlinear, smooth function
  3. add noise
- probability distribution in R^L , smooth function, noise can all be learned through EM-algorithm

GTM is “a principled SOM”

- explicit density model over data
- objective function that quantifies how well the map is trained
- sound, provably convergent optimization method (EM-algorithm)

Generative Topographic Mapping

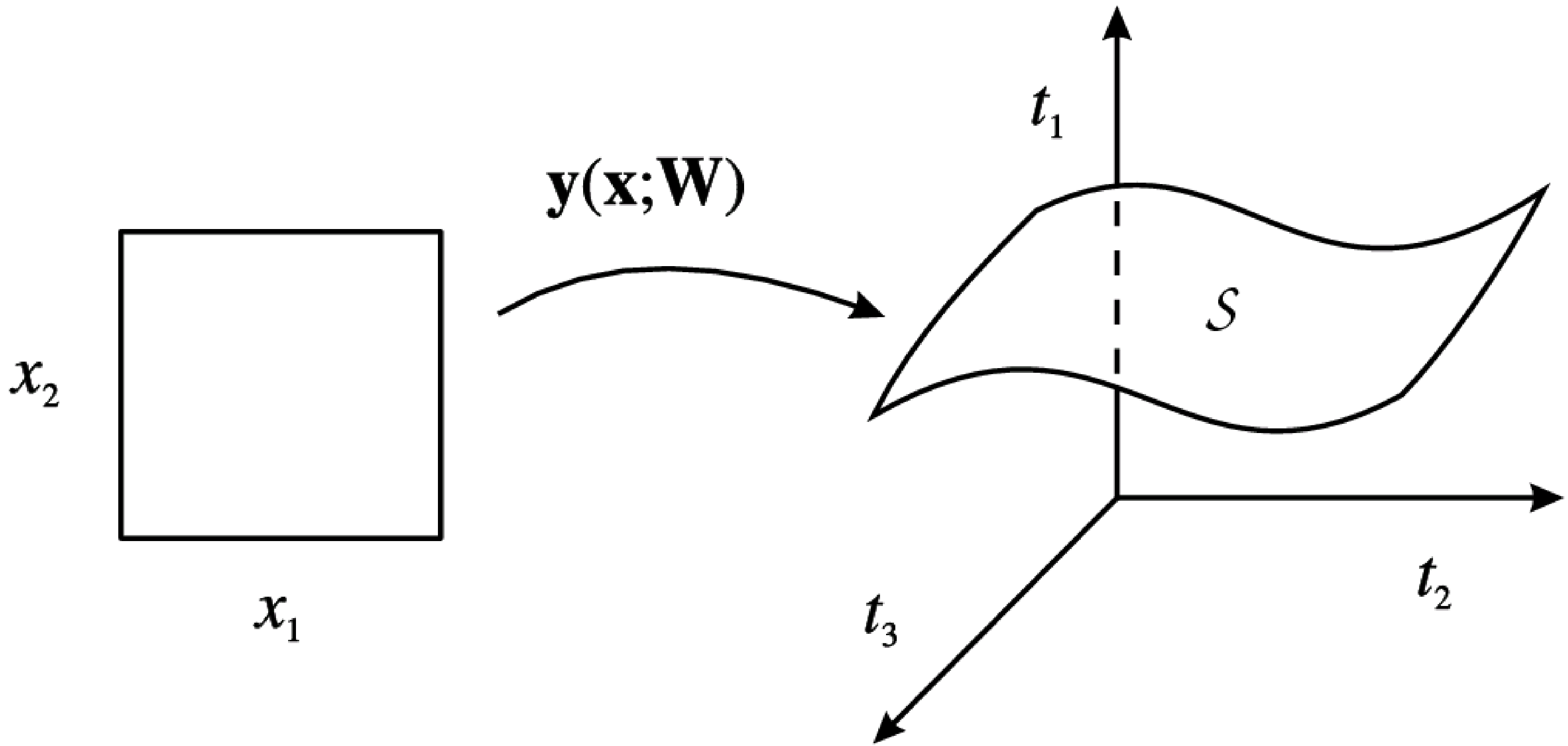
- Data space: R^D
- Latent space: R^L

- Find a nonlinear, smooth function:

$$y(x, W): R^L \to R^D$$

(for example a MLP, where W-weights)

- y maps an L dimensional space into an L-dimensional manifold non-linearly embedded in D-dimensions

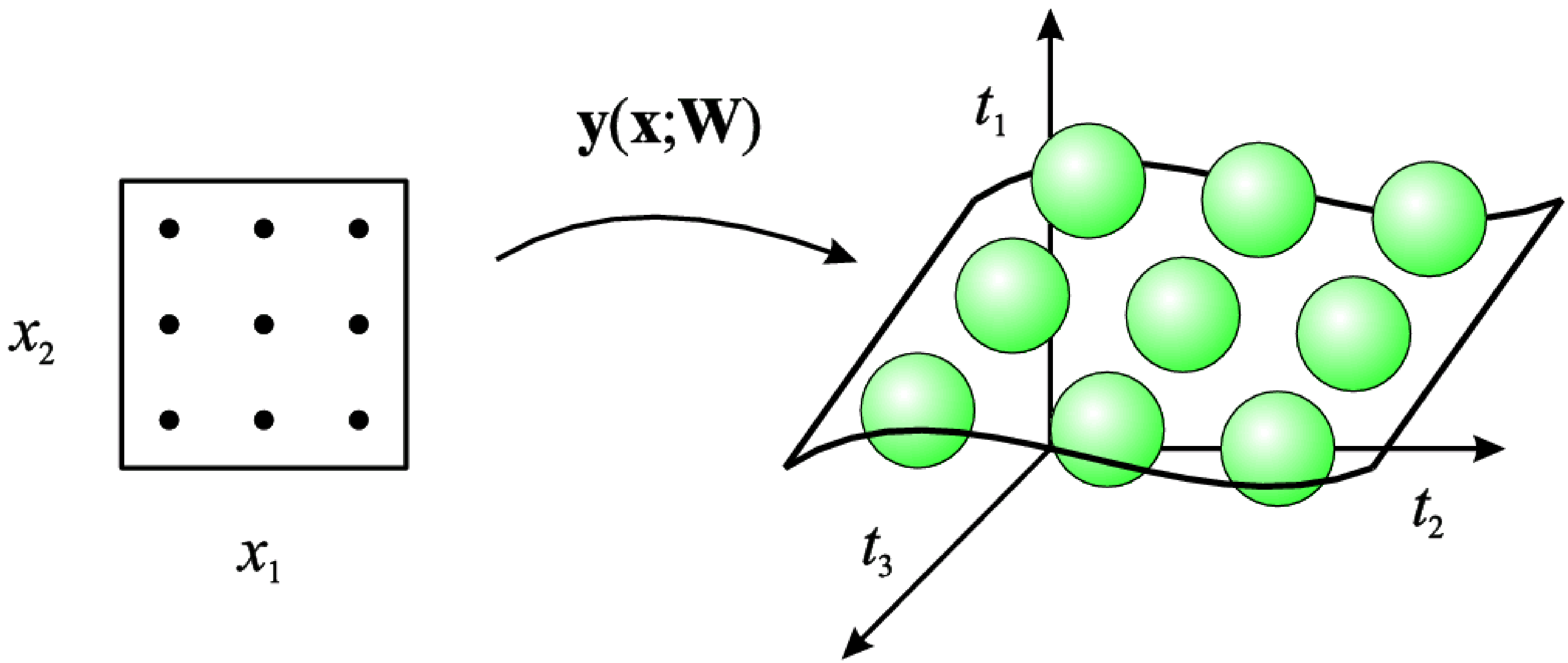


- p(x) – probability distribution in latent space
- induces probability distibution in data space

- Convolve distribution with Gaussian noise:

$$
\begin{aligned}
p(\mathbf{t}|\mathbf{x}, \mathbf{W}, \beta) &= \mathcal{N}(\mathbf{y}(\mathbf{x}, \mathbf{W}), \beta) \\
&= \left(\frac{\beta}{2\pi}\right)^{-D/2} \exp\left\{-\frac{\beta}{2}\sum_{d}^{D}(t_d - y_d(\mathbf{x}, \mathbf{W}))^2\right\}
\end{aligned}
$$

  - β – inverse of variance
  - D – dimension of data space



x_2
x_1
$\mathbf{y}(\mathbf{x};\mathbf{W})$
t_1
t_2
t_3

- Integrate out the latent variables:

$$p(\mathbf{t}|\mathbf{W},\beta) = \int p(\mathbf{t}|\mathbf{x},\mathbf{W},\beta)\, p(\mathbf{x})\, d\mathbf{x}.$$

- generally not solvable analytically
- choose grid points in latent space:

$$p(\mathbf{x}) = \frac{1}{K}\sum_{k}^{K} \delta(\mathbf{x} - \mathbf{x}_k),$$

$$p(\mathbf{t}|\mathbf{W},\beta) = \frac{1}{K}\sum_{k}^{K} p(\mathbf{t}|\mathbf{x}_k,\mathbf{W},\beta).$$

- Likelihood of the model

$$\mathcal{L} = \prod_{n}^{N} p(\mathbf{t}|\mathbf{W}, \beta) = \prod_{n}^{N} \left[\frac{1}{K} \sum_{k}^{K} p(\mathbf{t}_n|\mathbf{x}_k, \mathbf{W}, \beta) \right]$$

- Log-likelihood:

$$\ell = \sum_{n}^{N} \ln \left(\frac{1}{K} \sum_{k}^{K} p(\mathbf{t}_n|\mathbf{x}_k, \mathbf{W}, \beta) \right)$$

- Maximize it with respect to β and W
- For example with gradient descent
- Mixture of Gaussians: use EM-algorithm

EM - algorithm

- E-step:
  - responsibility of latent point x_k for data point t_n

$$r_{kn} = p(\mathbf{x}_k|\mathbf{t}_n, \mathbf{W}, \beta) = \frac{p(\mathbf{t}_n|\mathbf{x}_k, \mathbf{W}, \beta)p(\mathbf{x}_k)}{\sum_{k'} p(\mathbf{t}_n|\mathbf{x}_{k'}, \mathbf{W}, \beta)p(\mathbf{x}_{k'})}$$

  - $p(x_k)$ constant (1/K)
- M-step:
  - r_{kn} used as weights to update β and W
  - "move each component of the mixture towards data points for which it is most responsible"

The nonlinear function y

- choice important if we want to preserve topology
- linear combination of linear and non-linear basis functions

$$y_d(\mathbf{x}, \mathbf{W}) = \sum_{m}^{M} \phi_m(\mathbf{x}) w_{md}$$

- L linear basis functions can be initialized using PCA
- non-linear basis functions typically Gaussian kernels
- nr. of basis functions ~ nr. of grid points

Initialization

- Latent space dimension (1 or 2)
- Prior distribution in latent space (grid points)
- Center and width of Gaussian basis functions
- Weights W:
  - can be chosen randomly, such that variance over y equals variance of test data
  - if y has linear components, they can be initialized with PCA
  - non-linear component-weights can be set to zero or to small random values
- Noise variance: $1/\beta$ (at least the length of (L+1)th PC)

Algorithm

Pick latent space dimension, grid points

Choose basis functions

Initialize W, β

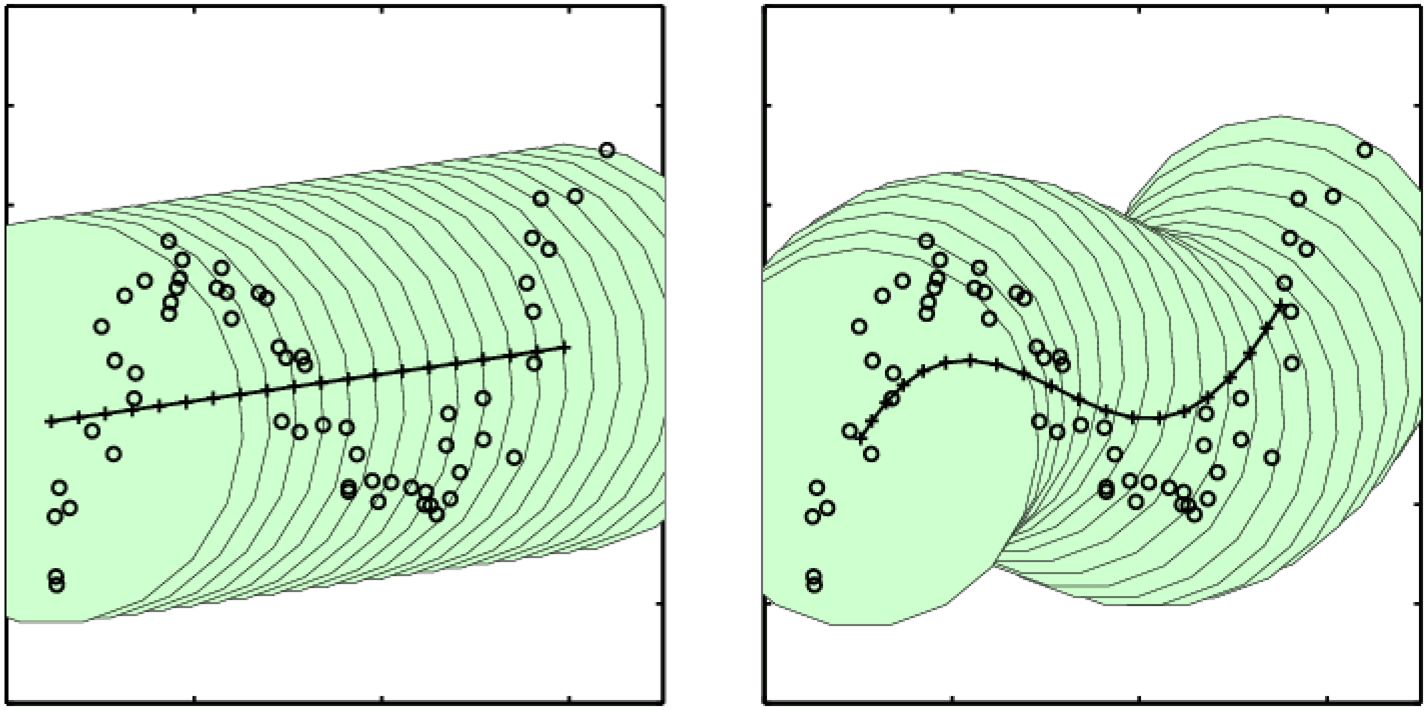
repeat

    E-step

    M-step

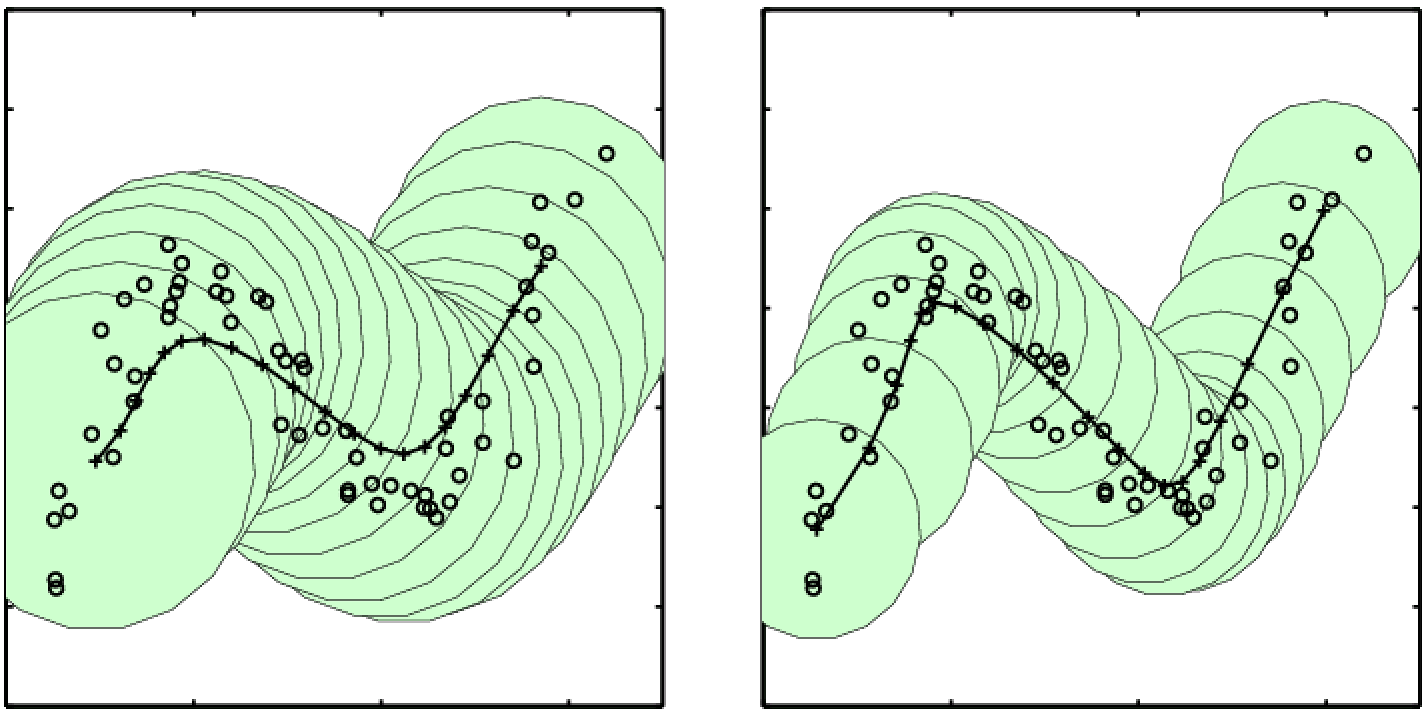
until Convergence

Example...



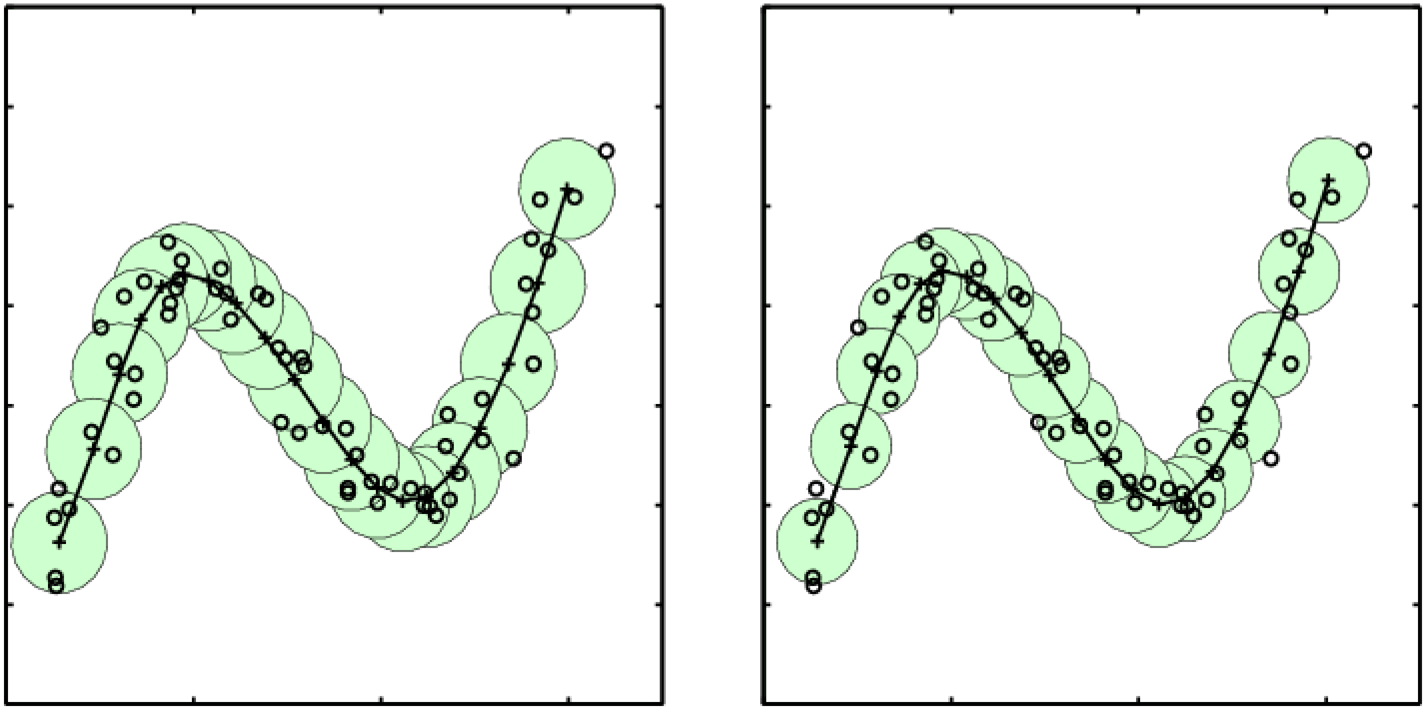
iteration 0,1

Example...



iteration 2,4

Example...



iteration 8,15

Dimension Reduction

- Suppose we found suitable W* and β*
- We have a probability distribution in data space: $p(t|x_k)$ k=1,2,3,...,K
- Prior distribution in latent space: $p(x_k)=1/K$
- Use Bayes-theorem:

$$p(\mathbf{x}_k|\mathbf{t}) = \frac{p(\mathbf{t}|\mathbf{x}_k, \mathbf{W}^*, \beta^*)p(\mathbf{x}_k)}{\sum_{k'} p(\mathbf{t}_n|\mathbf{x}_{k'}, \mathbf{W}^*, \beta^*)p(\mathbf{x}_{k'})}$$

Dimension Reduction

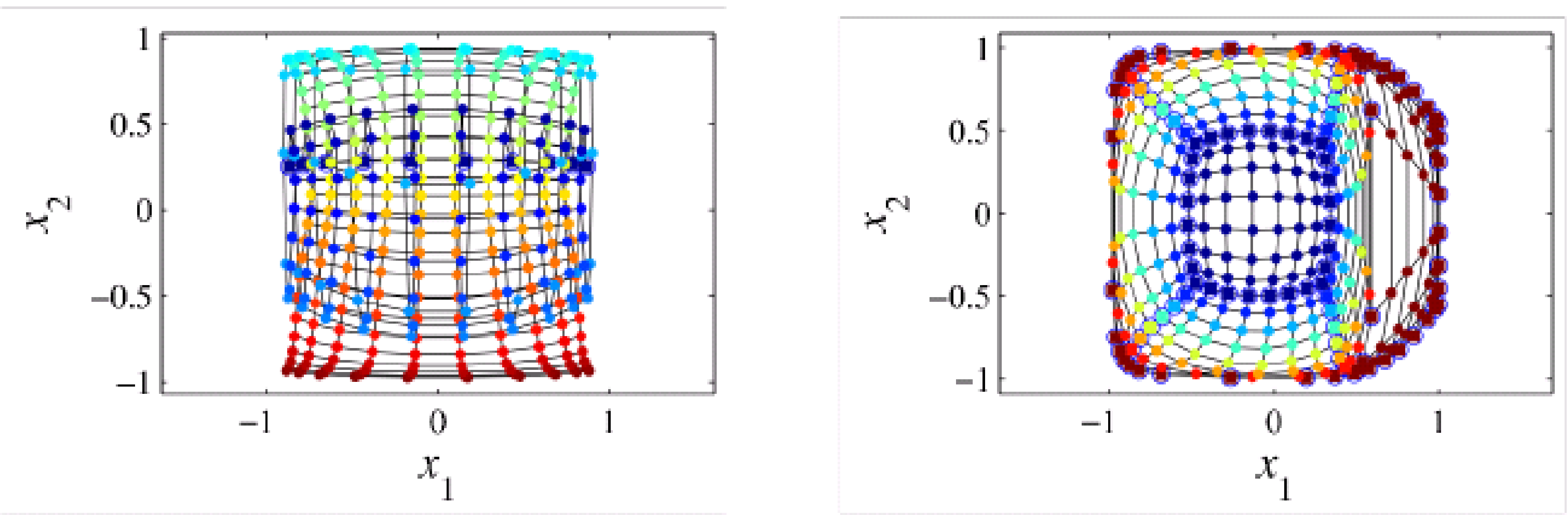
- posterior-mode projection:

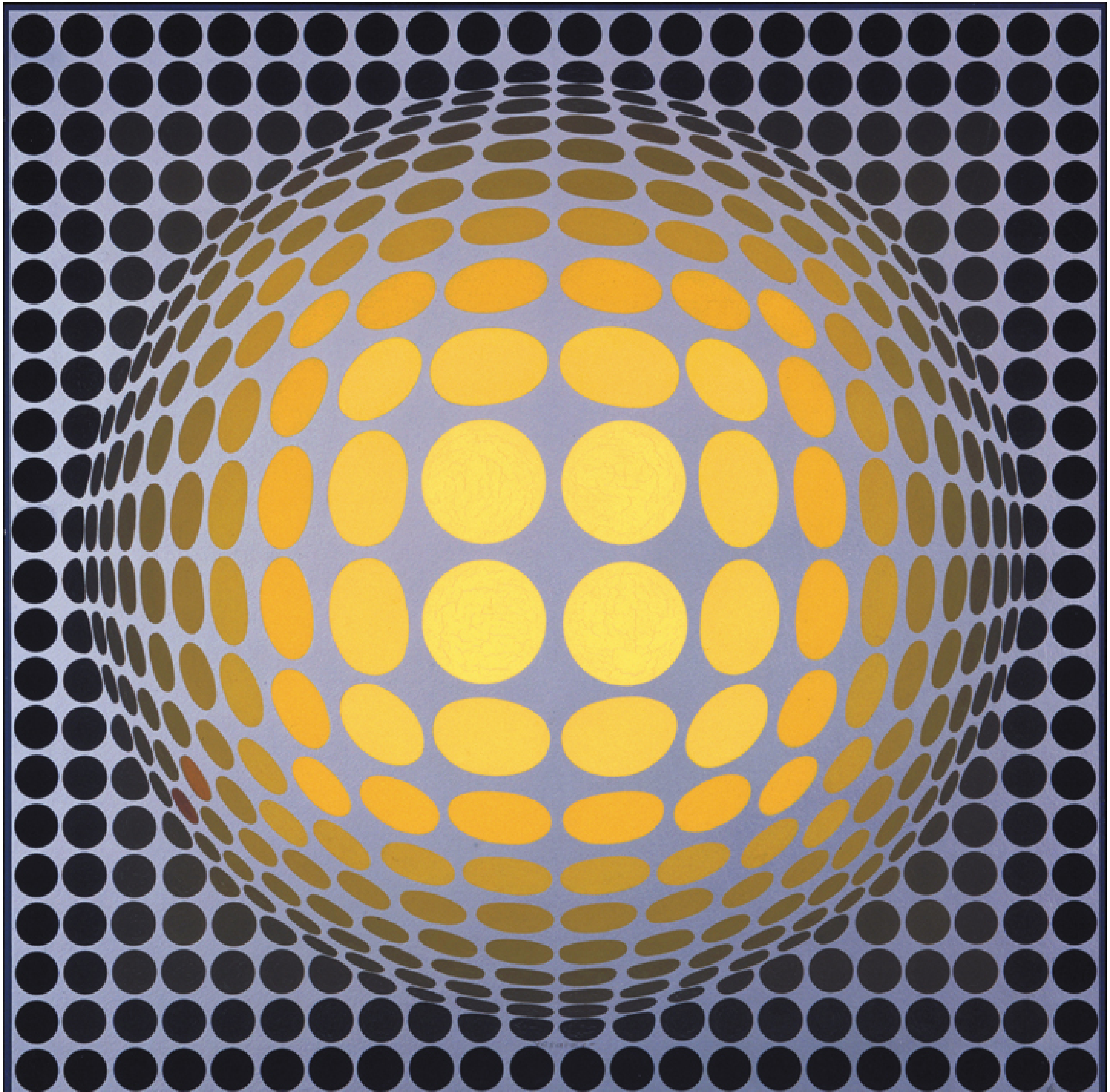
$$\mathbf{x}_n^{\mathrm{mode}} = \underset{\mathbf{x}_k}{\operatorname{argmax}}\, p(\mathbf{x}_k|\mathbf{t}_n)$$

- posterior-mean projection:

$$\mathbf{x}_n^{\mathrm{mean}} = \sum_{k}^{K} \mathbf{x}_k p(\mathbf{x}_k|\mathbf{t}_n)$$

Results





GTM summary

- Advantages:
  - In addition to finding $\hat{x}$ for given y, it can also approximate $\hat{p}(x|y)$
  - Easy to generalize to new points
  - Optimizes well-defined function (log-likelihood)
  - EM maximizes log-likelihood monotonically, converges after few iterations
- Disadvantages:
  - Inefficient for more than 2 latent dimensions
  - Doesn't estimate intrinsic dimension
  - Limited mapping power: kernel centers, variances fixed, only weights adjusted