Neighbor Embedding XOM for Dimension Reduction and Visualization

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Introduction

Dimension Reduction

- Curse of dimensionality
- Feature extraction
- Reduce redundancies
- Visualization

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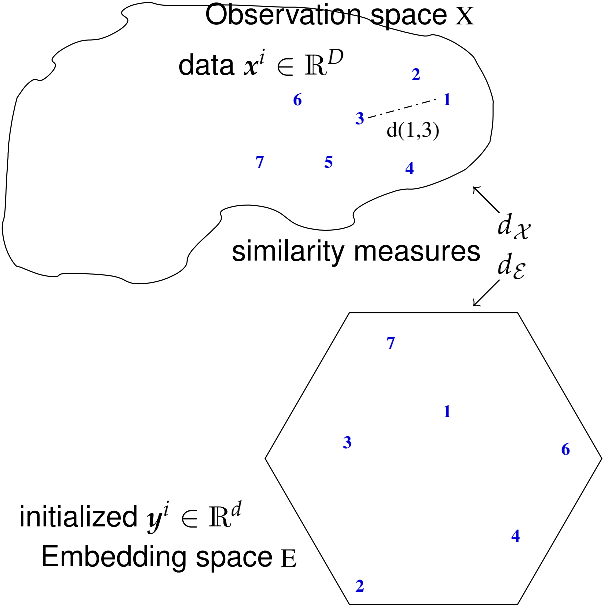
Motivation

- Most methods are quadratic with number of points
- Conceptual links:

fast online learning - direct divergence optimization

Exploratory Observation Morphogenesis (XOM)



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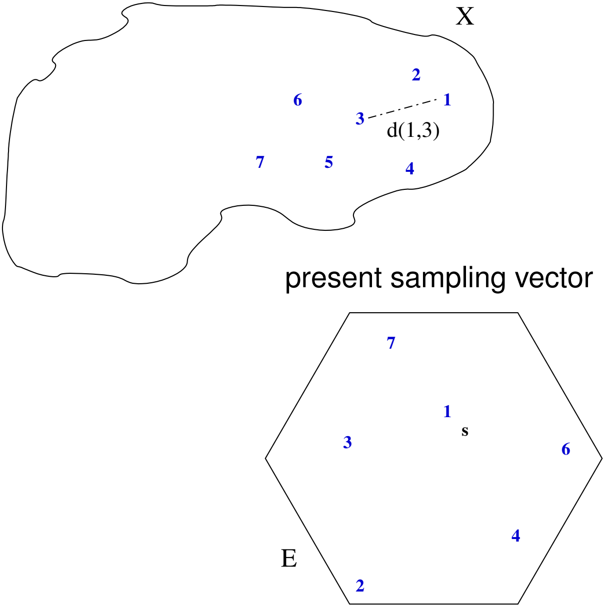

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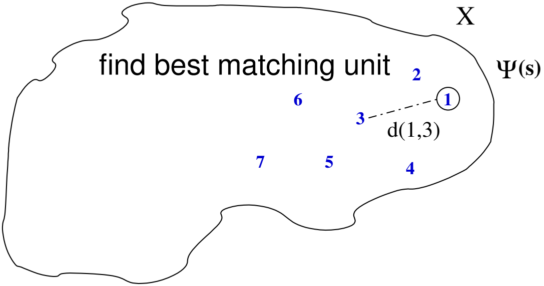
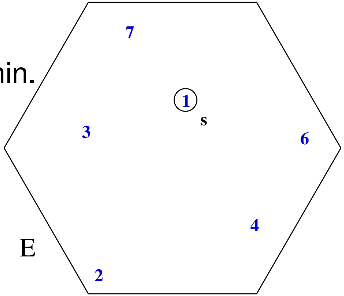


$\Psi(s) = x^i$ where

$d_{\mathcal{E}}(s, y^i)$ is min.



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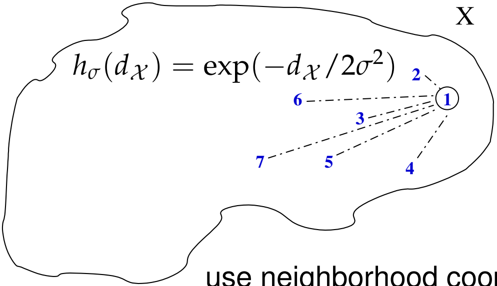
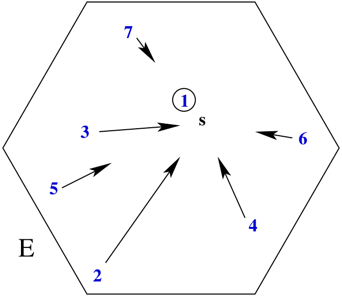


use neighborhood cooperation . . .



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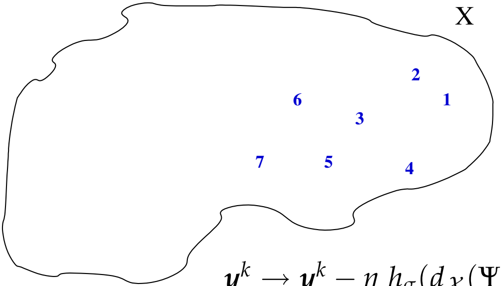
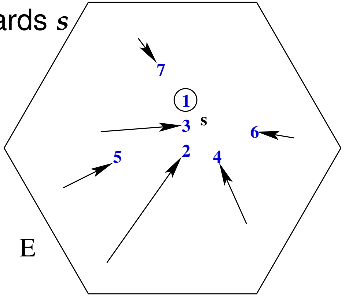


$$\boldsymbol{y}^k \to \boldsymbol{y}^k - \eta\, h_\sigma(d_{\mathcal{X}}(\Psi(\boldsymbol{s}), \boldsymbol{x}^k)) \frac{\partial d_{\mathcal{E}}(\boldsymbol{s}, \boldsymbol{y}^k)}{\partial \boldsymbol{y}^k}$$

… to update $\boldsymbol{y}^k$ towards $\boldsymbol{s}$



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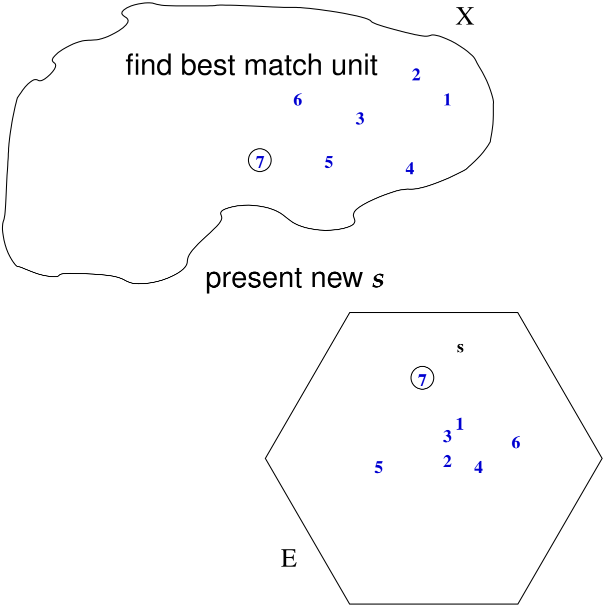

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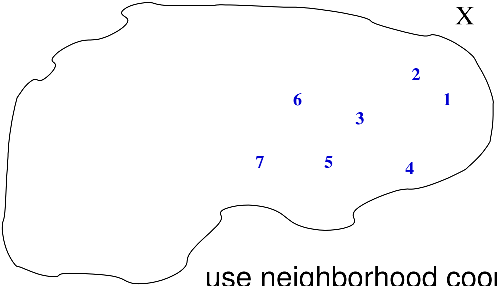
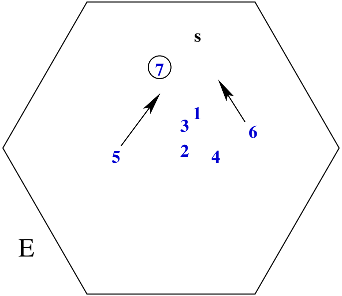


use neighborhood cooperation



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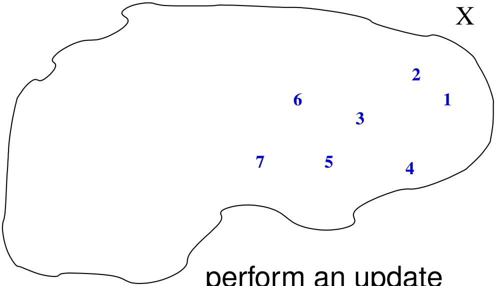
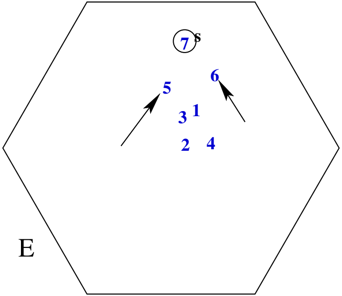


perform an update



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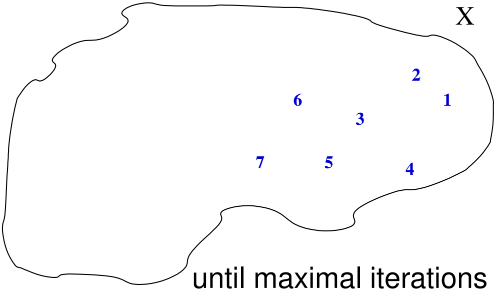
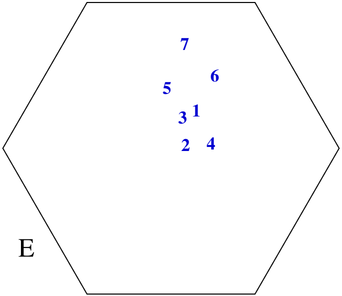


until maximal iterations reached



Cost function

Variation of the winner definition following Heskes:

$$\Psi(\boldsymbol{s}) = \boldsymbol{x}^i \text{ where } \sum_j h_\sigma(d_\mathcal{X}(\boldsymbol{x}^i, \boldsymbol{x}^j)) d_\mathcal{E}(\boldsymbol{s}, \boldsymbol{y}^j) \ ,$$

allows to define a cost function for the XOM:

$$E_{\text{XOM}} \sim \int \sum_i \delta_{\Psi(\boldsymbol{s}),\boldsymbol{x}^i} \sum_{j=1}^N h_\sigma(d_\mathcal{X}(\boldsymbol{x}^i, \boldsymbol{x}^j)) d_\mathcal{E}(\boldsymbol{s}, \boldsymbol{y}^j) p(\boldsymbol{s}) d\boldsymbol{s}$$

δ denotes the Kronecker delta

New XOM inspired cost function

Generalized Kullback Leibler (KL) divergence

$$E_{GKL}(p \,||\, q) = \int \left[p(\boldsymbol{x}) \log \left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} \right) \right] - [p(\boldsymbol{x}) - q(\boldsymbol{x})]\, d\boldsymbol{x}$$

$$0 \leq p(\boldsymbol{x}), q(\boldsymbol{x}) \leq 1$$

Neighborhood functions $h_\sigma(d_{\mathcal{X}}(\boldsymbol{x}^i, \boldsymbol{x}^j))$ and $g_\gamma(d_{\mathcal{E}}(\boldsymbol{s}, \boldsymbol{y}^j))$

$$E_{\text{KLX}} \sim \int \sum_i \delta_{\Psi^{\text{GKL}}(\boldsymbol{s}), \boldsymbol{x}^i} \sum_j \left[h_\sigma^{ij} \ln \left(\frac{h_\sigma^{ij}}{g_\gamma^j} \right) - h_\sigma^{ij} + g_\gamma^j \right] p(\boldsymbol{s}) d\boldsymbol{s}$$

New XOM inspired Learning Rules

Derive the online learning rule from $\frac{\partial E_{\mathrm{KLX}}}{\partial \boldsymbol{y}^k}$ for a given sampling vector $\boldsymbol{s}$:

$$\boldsymbol{y}^k = \boldsymbol{y}^k - \eta \frac{\partial g_\gamma^k}{\partial \boldsymbol{y}_k} \left(1 - \frac{h_\sigma^{ik}}{g_\gamma^k}\right)$$

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In case of Gaussian neighborhood function $g_\gamma^j = \exp\left(\frac{-d_{\mathcal{E}}(\boldsymbol{s}, \boldsymbol{y}^j)}{2\gamma^2}\right)$:

$$\boldsymbol{y}^k = \boldsymbol{y}^k - \frac{\eta}{\gamma^2} \frac{\partial d_{\mathcal{E}}(\boldsymbol{s}, \boldsymbol{y}^k)}{\partial \boldsymbol{y}^k} \left(h_\sigma^{ik} - g_\gamma^k\right)$$

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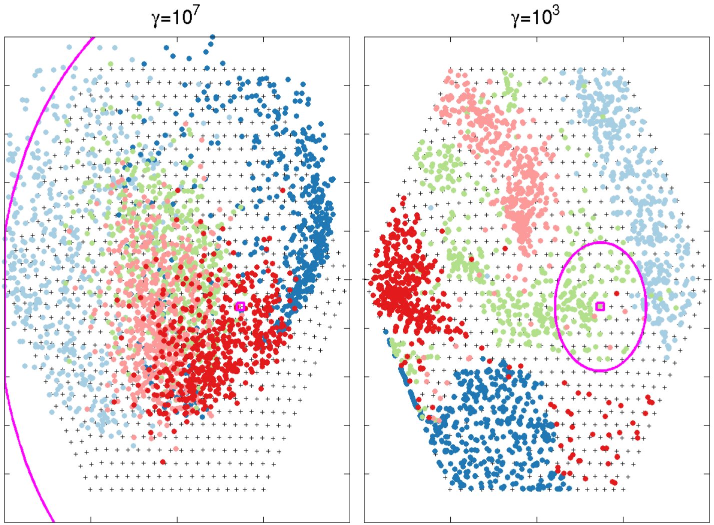
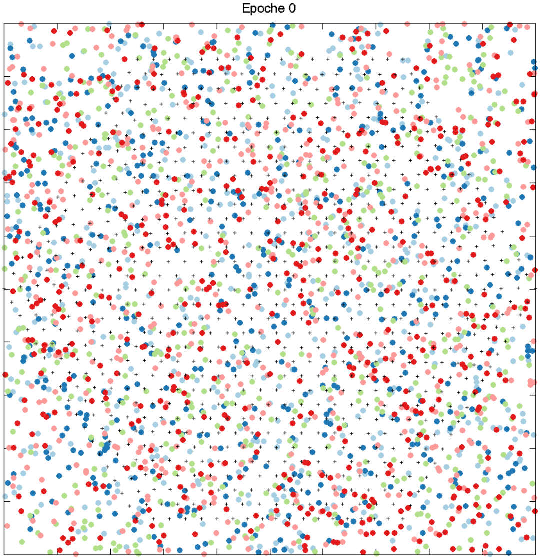
In case of t-distributed $g_\gamma^j = \left(1 + d_{\mathcal{E}}(\boldsymbol{s},\boldsymbol{y}^j)/\gamma\right)^{\left(-\frac{\gamma+1}{2}\right)}$:

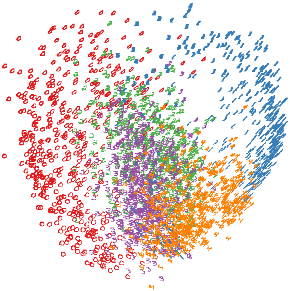
$$\boldsymbol{y}^k = \boldsymbol{y}^k - \frac{\eta}{2}\frac{\partial d_{\mathcal{E}}(\boldsymbol{s},\boldsymbol{y}^k)}{\partial \boldsymbol{y}^k}\alpha\left(h_\sigma^{ik} - g_\gamma^k\right) \rightarrow \alpha = \frac{1}{\left(1 + \frac{d_{\mathcal{E}}(\boldsymbol{s},\boldsymbol{y}^k)}{\gamma}\right)}$$

Influence of γ in t-NEXOM

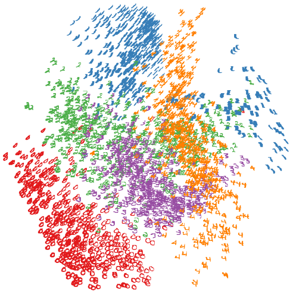


Training video



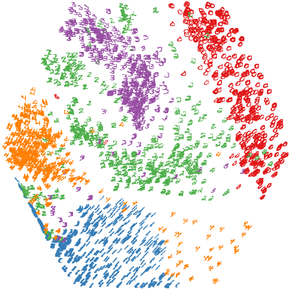


(a) PCA (37.7%)



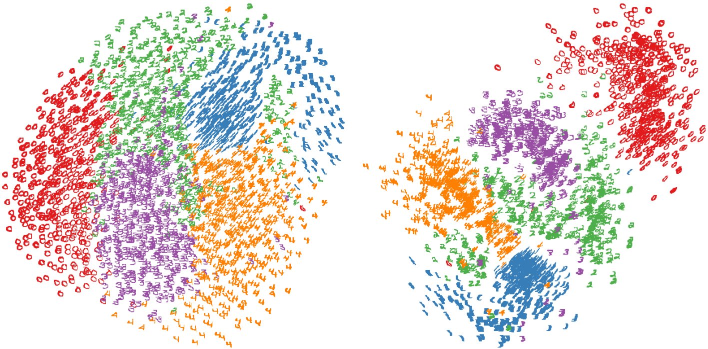
(b) NEXOM (23.8%)

USPS Digits



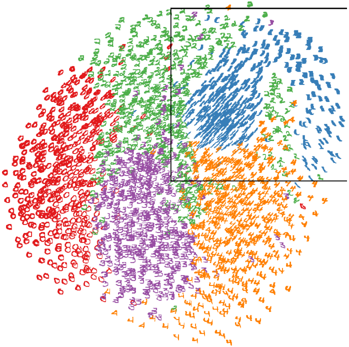
(c) t-NEXOM (4.6%)

Without structure hypothesis

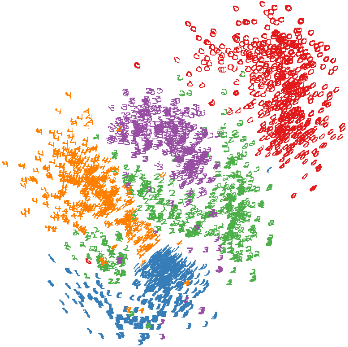


(d) NEXOM (14.4%) (e) t-NEXOM (4.5%)

Without structure hypothesis

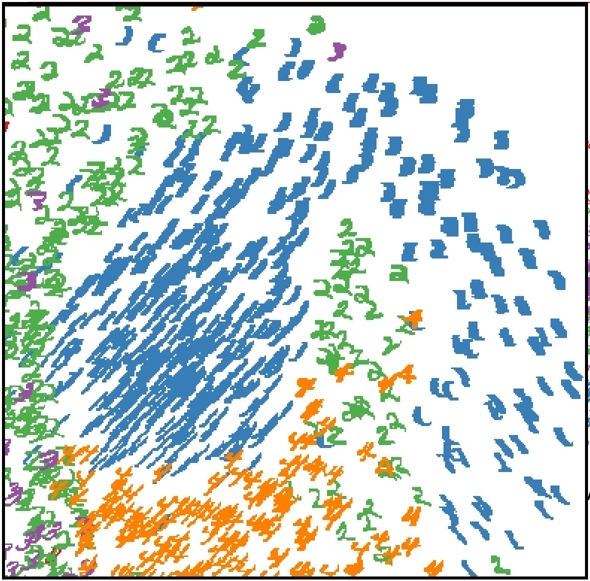


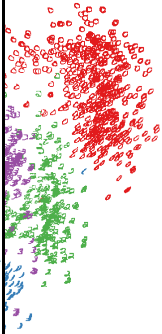
(f) NEXOM (14.4%)



(g) t-NEXOM (4.5%)

Without structure hypothesis





M (4.5%)

Summary

Neighbor Embedding XOM:

- conceptually links between
  - fast sequential online learning
  - direct divergence optimization
- competitive trade-off:
  - high embedding quality
  - low computational expense
- different distributions and learning rules