Semi-Supervised Locally Linear Embedding (SSLLE)

Application & Sensitivity Analysis of Critical Hyperparameters

0 AGENDA

MANIFOLD LEARNING

Situation. Rapidly increasing amount of data thanks to novel applications and data sources

Problem. High data dimensionality detrimental to

- → Model functionality
- → Interpretability
- → Generalization ability

Manifold assumption. Data in high-dimensional observation space truly sampled from low-dimensional manifold

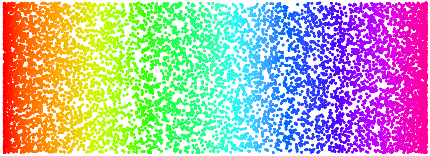
How to find a meaningful, structure-preserving embedding?

MANIFOLD LEARNING

Formal goal of manifold learning.

→ **Given.** Data $\mathcal{X} = (\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N)$, with $\boldsymbol{x}_i \in \mathbb{R}^D \; \forall i \in \{1, 2, ..., N\}$ and $N, D \in \mathbb{N}$, supposedly lying on d-dimensional manifold $\mathcal{M}$
$\Rightarrow \psi : \mathcal{M} \rightarrow \mathbb{R}^d$ with $d \ll D, d \in \mathbb{N}$
$\Rightarrow \mathcal{X} \sim \mathcal{M} \subset \mathbb{R}^D$

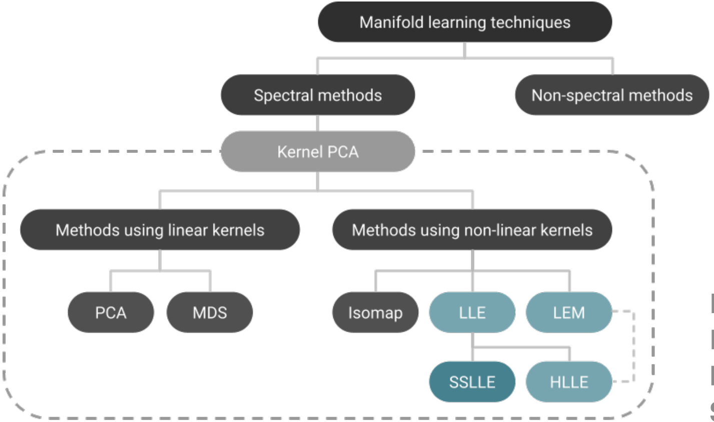
→ **Goal.** Find d-dimensional Euclidean representation
$\Rightarrow \mathcal{Y} = (\boldsymbol{y}_1, \boldsymbol{y}_2, ..., \boldsymbol{y}_N)$, with $\boldsymbol{y}_i = \psi(\boldsymbol{x}_i) \in \mathbb{R}^d \; \forall i \in \{1, 2, ..., N\}$.



2 LGML

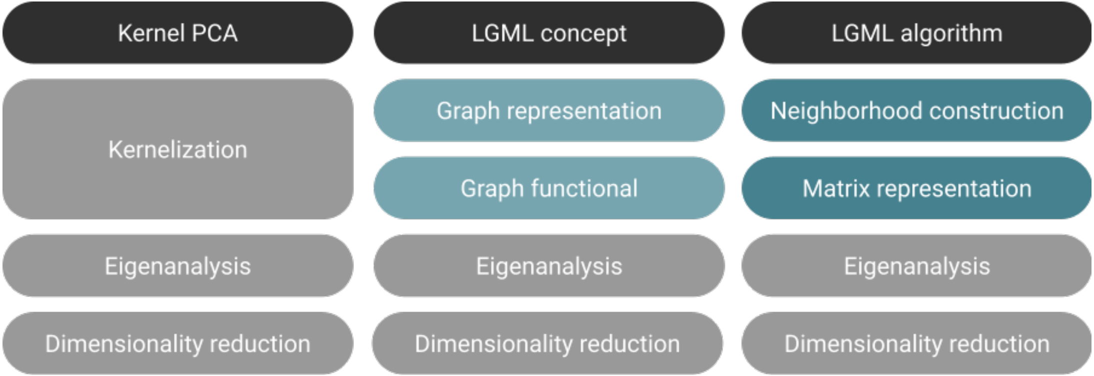
TAXONOMY

Landscape. Various approaches, many of which may be translated into one another



LEM Laplacian eigenmaps
LLE Locally linear embedding
HLLE Hessian LLE
SSLLE Semi-supervised LLE

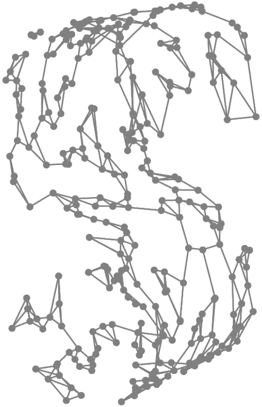
Idea. Capture intrinsic geometry, find principal axes of variability, retain most salient ones



Graph representation. Constructing a skeletal model of the manifold in $\mathbb{R}^D$

Vertices. Given by observations
Edges. Present between neighboring points

- $\rightarrow$ Typically, *k*-neighborhoods
- $\rightarrow$ Edge weights determined by nearness



Graph functional. Belief about intrinsic manifold properties at the heart of each method

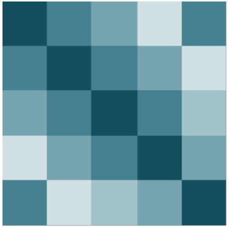
- $\rightarrow$ Smoothness LEM
- $\rightarrow$ Local linearity LLE SSLLE
- $\rightarrow$ Curvature HLLE
- $\rightarrow$ ...

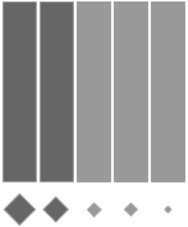
CONCEPT

Eigenanalysis. Finding axes of variability in intrinsic manifold structure

- → Matrix representation of manifold properties
- → Assessment through eigenanalysis
  - → Directions of variability ⇒ eigenvectors
  - → Respective degrees of variability ⇒ eigenvalues

Dimensionality reduction. Projection into subspace spanned by *d* principal eigenvectors





3 TECHNIQUES

LEM

Proposal. Donoho and Grimes (2003)

Idea. Forcing nearby inputs to be mapped to nearby outputs

$\rightarrow$ Notion of smoothness in mapping function

$\rightarrow$ Second-order penalty on large gradients

Graph Laplacian. Coercing neighborhood graph information into a matrix

$\rightarrow$ Weight matrix. $\boldsymbol{W} = (w)_{ij} \in \mathbb{R}^{N \times N}$, where $w_{ij} = w_{ij}(\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2)$

$\rightarrow$ Diagonal matrix of row sums. $\boldsymbol{D} = diag(\sum_j w_{ij}) \in \mathbb{R}^{N \times N}$

$\rightarrow$ Graph Laplacian. $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{W} \in \mathbb{R}^{N \times N}$

Generalized eigenvalue problem.

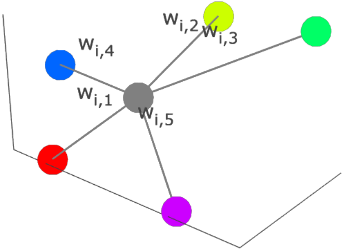
$$\min_{\mathcal{Y}} trace(\mathcal{Y}^T \boldsymbol{L} \mathcal{Y}), \quad \text{s.t. } \mathcal{Y}^T \boldsymbol{D} \mathcal{Y} = \boldsymbol{I} \tag{1}$$

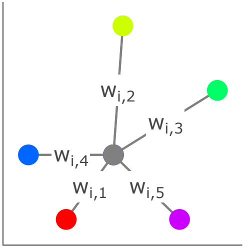
LLE

Proposal. Roweis and Saul (2000)

Idea. Preserving locally linear reconstructions

- → Linear reconstruction of points in $\mathbb{R}^D$ by their neighbors
- → Reconstruction weights = topological properties
- → Neighborhood patches invariant to dimensionality reduction





SSLLE

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NEIGHBORHOOD RELATIONS

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4 SENSITIVITY ANALYSIS

SCENARIOS

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EVALUATION

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4.2 RESULTS **FOO**

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5 DISCUSSION

FOO

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REFERENCES

Donoho, D. L. and Grimes, C. (2003). Hessian eigenmaps: Locally linear embedding techniques for high-dimensional data, *Proceedings of the National Academy of Sciences of the United States of America* **100**(10): 5591–5596.

Roweis, S. T. and Saul, L. K. (2000). Nonlinear dimensionality reduction by locally linear embedding, *Science* **290**(5500): 2323–2326.