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

- $\rightarrow$ Model functionality
- $\rightarrow$ Interpretability
- $\rightarrow$ Generalization ability

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

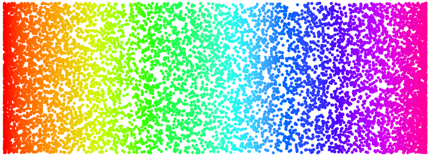
How to find a meaningful, structure-preserving embedding?

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 $d \ll D, d \in \mathbb{N}$
$\Rightarrow \mathcal{X} \sim \mathcal{M} \subset \mathbb{R}^D$

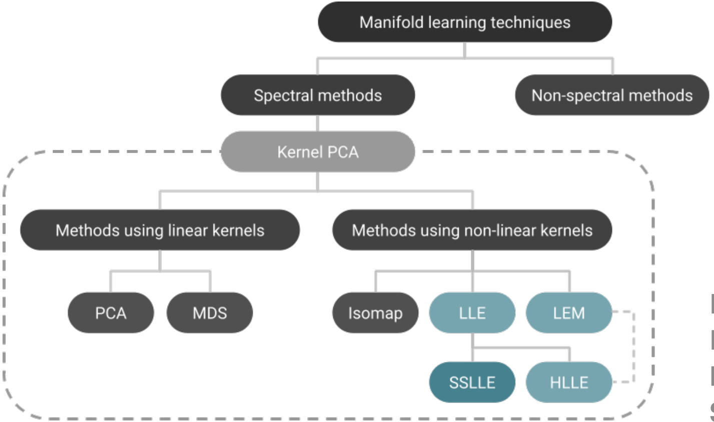
→ **Goal.** Find d-dimensional Euclidean representation
$\Rightarrow \mathcal{Y} = (\boldsymbol{y}_1, \boldsymbol{y}_2, ..., \boldsymbol{y}_N)$, with $\boldsymbol{y}_i = \psi(\boldsymbol{x}_i) \in \mathbb{R}^d \; \forall i \in \{1, 2, ..., N\}$.



2 LGML

TAXONOMY

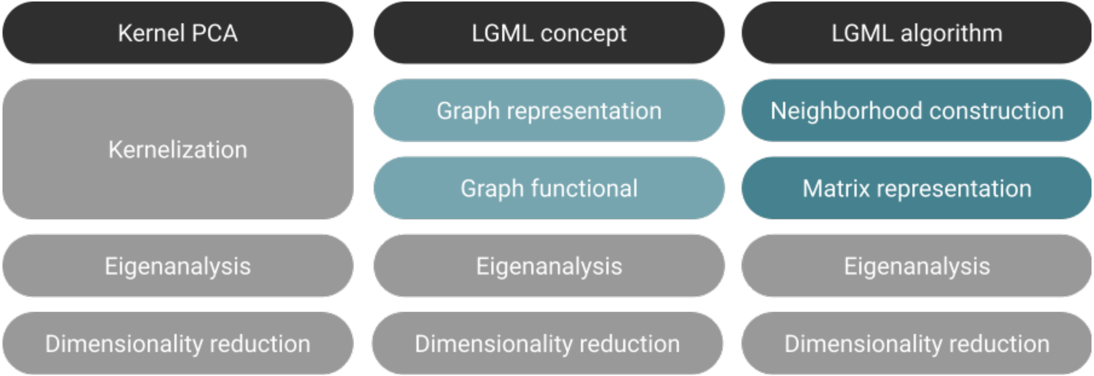
Landscape. Various approaches, many of which may be translated into one another



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

2 LGML CONCEPT

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

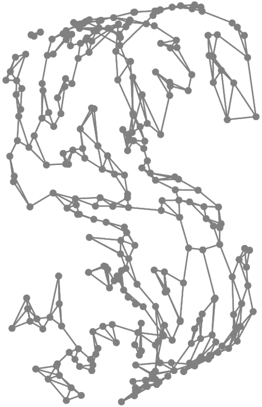


CONCEPT

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
- $\rightarrow$ Curviness HLLE
- $\rightarrow$ ...

Achievements: non-linearity & locality

2 LGML **CONCEPT**

Eigenanalysis. Finding axes of variability in intrinsic manifold structure

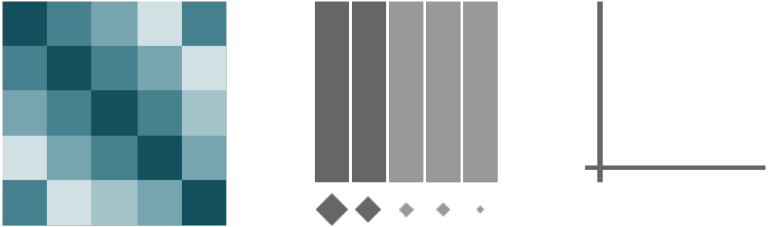
$\rightarrow$ Matrix representation of manifold properties

$\rightarrow$ Assessment through eigenanalysis

  $\rightarrow$ Directions of variability $\Rightarrow$ eigenvectors

  $\rightarrow$ Respective degrees of variability $\Rightarrow$ eigenvalues

Dimensionality reduction. Projection into subspace spanned by d principal eigenvectors



3 TECHNIQUES

3.1 UNSUPERVISED **LEM**

Proposal. Belkin and Niyogi (2001)

Idea. Forcing nearby inputs to be mapped to nearby outputs

$\rightarrow$ Notion of smoothness in mapping function

$\rightarrow$ Second-order penalty on gradient

Graph Laplacian. Discrete approximation of Laplace-Beltrami operator

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

$\rightarrow$ Graph Laplacian. $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{W} \in \mathbb{R}^{N \times N}$, $\boldsymbol{D} = diag(\sum_j w_{ij}) \in \mathbb{R}^{N \times N}$

Generalized eigenvalue problem.

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

Solution: bottom $d + 1$ eigenvectors

3.1 UNSUPERVISED LLE

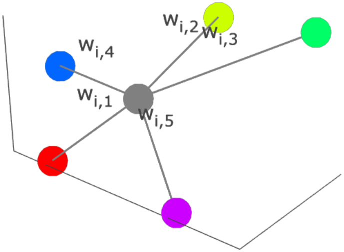
Proposal. Roweis and Saul (2000)

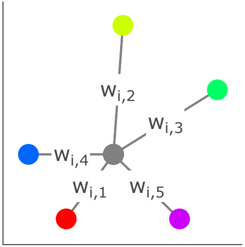
Idea. Preserving locally linear reconstructions

→ Linear reconstruction of points in $\mathbb{R}^D$ by their neighbors

→ Reconstruction weights = topological properties

→ Neighborhood patches invariant to dimensionality reduction





3.1 UNSUPERVISED **LLE**

Reconstruction loss minimization. Finding optimal reconstruction weights

$$\min_{\boldsymbol{W}} \varepsilon(\boldsymbol{W}) = \min_{\boldsymbol{W}} \sum_i \left\| \boldsymbol{x}_i - \sum_j w_{ij} \boldsymbol{x}_j \right\|^2, \quad \text{s.t. } \mathbf{1}^T \boldsymbol{w}_i = 1 \quad \forall i \in \{1, 2, ..., N\} \tag{2}$$

Embedding loss minimization. Finding optimal embedding coordinates

$$\min_{\mathcal{Y}} \Phi(\mathcal{Y}) = \min_{\mathcal{Y}} \sum_i \left\| \boldsymbol{y}_i - \sum_j w_{ij} \boldsymbol{y}_j \right\|^2, \quad \text{s.t. } \frac{1}{N} \sum_i \boldsymbol{y}_i \boldsymbol{y}_i^T = \boldsymbol{I}, \quad \sum_i \boldsymbol{y}_i = \mathbf{0} \quad \forall i \in \{1, 2, ..., N\} \tag{3}$$

Eigenvalue problem. Define $\boldsymbol{E} = (\boldsymbol{I} - \boldsymbol{W})^T (\boldsymbol{I} - \boldsymbol{W})$, such that

$$\min_{\mathcal{Y}} \mathit{trace}(\mathcal{Y}^T \boldsymbol{E} \mathcal{Y}), \quad \text{s.t. } \frac{1}{N} \mathcal{Y}^T \mathcal{Y} = \boldsymbol{I}, \quad \mathcal{Y}^T \mathbf{1} = \mathbf{0}. \tag{4}$$

Solution: bottom $d + 1$ eigenvectors

3.1 UNSUPERVISED **HLLE**

Proposal. Donoho and Grimes (2003)

Idea. Finding a truly locally linear mapping while preserving local isometry

$\rightarrow$ Notion of curviness in mapping function

$\rightarrow$ Second-order penalty on Hessian

$\rightarrow$ Strong convergence guarantees but rather complex computations

Hessian functional. Measuring average curviness over $\mathcal{M}$

$\rightarrow$ Continuous functional. $\mathscr{H}(f) = \int_{\mathcal{M}} \left\| \boldsymbol{H}_f^{\text{loc}}(\boldsymbol{p}) \right\|_F^2 d\boldsymbol{p}$

$\rightarrow$ Hessian estimators $\boldsymbol{H}_\ell$ derived from locally linear neighborhood patches

$\rightarrow$ Empirical approximator. $\mathcal{H}_{ij} = \sum_\ell \sum_m (\boldsymbol{H}_\ell)_{m,i} (\boldsymbol{H}_\ell)_{m,j}$

$\rightarrow$ Finding null space of $\mathcal{H}$

$\boxed{\textbf{Solution: bottom } d + 1 \textbf{ eigenvectors + scaling}}$

SSLLE

Proposal. Yang et al. (2006)

Problem. Embedding found by unsupervised methods not always meaningful

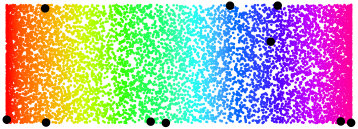
Idea. Improving LLE by use of prior knowledge

Semi-supervision. Anchoring embedding at some prior points with known coordinates

→ More active than semi-supervised learning?

→ Setting. Information available or to be obtained by querying the oracle

→ Goal. Maximum information at little expense ⇒ careful choice of prior points



SSLLE

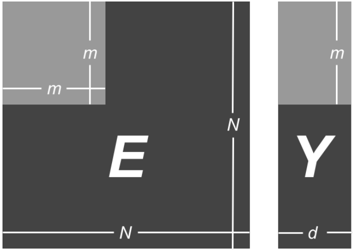
Types of prior information. Exact vs inexact

$\rightarrow$ Level of confidence encoded in parameter β

Algorithmic impact. Recall LLE eigenvalue problem

$$\min_{\mathcal{Y}} \mathit{trace}(\mathcal{Y}^T \boldsymbol{E} \mathcal{Y}), \quad \text{s.t. } \frac{1}{N} \mathcal{Y}^T \mathcal{Y} = \boldsymbol{I}, \quad \mathcal{Y}^T \mathbf{1} = \mathbf{0}.$$

$\Rightarrow$ Partitioning of $\boldsymbol{E}$ and $\mathcal{Y}$



3.2 SEMI-SUPERVISED **SSLLE**

Modified optimization problem. Exact information

$$\min_{\mathcal{Y}_2} \begin{bmatrix} \mathcal{Y}_1 & \mathcal{Y}_2 \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \mathcal{Y}_1^T \\ \mathcal{Y}_2^T \end{bmatrix} \tag{5}$$

$$\Leftrightarrow \mathcal{Y}_2^T = M_{22}^{-1} M_{12} \mathcal{Y}_1^T \tag{6}$$

Modified optimization problem. Inexact information

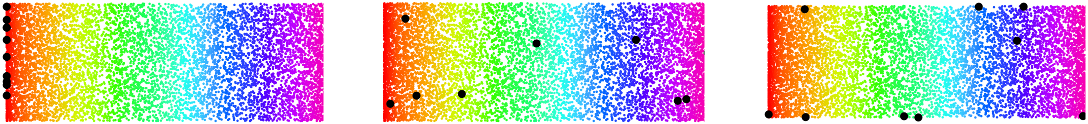
$$\min_{\mathcal{Y}} \begin{bmatrix} \mathcal{Y}_1 & \mathcal{Y}_2 \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \mathcal{Y}_1^T \\ \mathcal{Y}_2^T \end{bmatrix} + \beta \left\| \mathcal{Y}_1^T - \hat{\mathcal{Y}}_1^T \right\|_F^2 \tag{7}$$

$$\Leftrightarrow \begin{bmatrix} M_{11} + \beta \boldsymbol{I} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \mathcal{Y}_1^T \\ \mathcal{Y}_2^T \end{bmatrix} = \begin{bmatrix} \hat{\mathcal{Y}}_1^T \\ \mathbf{0} \end{bmatrix} \tag{8}$$

SSLLE

Choice of prior points. Basically, three options

- $\rightarrow$ Pre-existing prior information $\Rightarrow$ worst case: poor coverage
- $\rightarrow$ Random sampling
- $\rightarrow$ Maximum coverage



Maximum coverage. Points scattered across manifold surface

- $\rightarrow$ Goodness of solution depending on condition number $\kappa(M_{22})$
- $\rightarrow$ $\kappa(M_{22})$ minimal at maximization of minimum pairwise distances between prior points

CRITICAL PARAMETERS

Intrinsic dimensionality. True sources of variability

$\rightarrow$ Considered known with availability of prior information

Neighborhood size. Global vs local structure

$\rightarrow$ Tunable (expensive)

Regularization constant. Singularity for $D < k$

$\rightarrow$ Heuristics

Number & location of prior points. Utility of prior knowledge ANALYSIS

$\rightarrow$ Exploration vs labeling cost

Noise level. Quality of prior knowledge ANALYSIS

$\rightarrow$ How exact must prior information be?

Confidence parameter. Belief in prior knowledge

$\rightarrow$ Rather robust

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

Belkin, M. and Niyogi, P. (2001). Laplacian eigenmaps and spectral technique for embedding and clustering, *Proceedings of the 14th International Conference on Neural Information Processing Systems: Natural and Synthetic*, p. 585–591.

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.

Yang, X., Fu, H., Zha, H. and Barlow, J. (2006). Semi-supervised nonlinear dimensionality reduction, *Proceedings of the 23rd International Conference on Machine Learning*.